Glauber $e^- + \text{He}$ Elastic Scattering Amplitude: A Useful Integral Representation*

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New analytic methods for reducing the Glauber amplitude for charged particle–neutral atom collisions to a one-dimensional integral representation involving modified Lommel functions are proposed. To illustrate these new methods, the reduction of the Glauber amplitude for $e^- + \text{He}$ elastic scattering, using a simple Hylleraas wave function for the He ground state, is described in detail, and the resulting integral for the amplitude is evaluated numerically. The Glauber-approximation-predicted elastic scattering amplitude previously calculated by Franco from a three-dimensional integral representation, with a more complex Hartree-Fock wave function for the ground state, is also recalculated using these new procedures; these results are in good agreement with those obtained by Franco. Thus, the utility and practicality of these new techniques are demonstrated. The application of these procedures to more general charged particle–neutral atom collisions is discussed.

I. INTRODUCTION

Recent applications of the Glauber approximation[1] (GA) to charged particle–neutral atom collisions have been restricted to atoms and model atoms having one or two bound electrons. The GA-predicted differential and total (integrated over scattering angle) cross sections for electron[2] and proton[3] collisions with atomic hydrogen, without rearrangement or ionization, have been calculated from one-dimensional integral representations of the amplitude; moreover, these amplitudes and integrated cross sections can be obtained in closed form.[4,5] Glauber calculations of elastic[6] and inelastic[7] scattering of electrons by ground-state helium atoms have been performed using three- and two-dimensional integral representations, respectively, for the amplitudes. However, electron–lithium atom collisions have been considered in the Glauber approximation only after making a frozen-core approximation,[8] thereby reducing the lithium atom to an effective one-electron system.

Although Franco[9] has proposed a method for obtaining a one-dimensional integral representation for the elastic and inelastic scattering of charged particles by arbitrary neutral atoms—excluding rearrangement (i.e., exchange or charge transfer) and ionization—there are no reported calculations actually using Franco's expressions. Moreover, Franco's final integral representation for these Glauber amplitudes appears to present several *seemingly* serious numerical problems, which generally include the calculation and integration of the differences between strongly (exponentially) divergent functions, as well as the numerical calculation of δ functions whenever elastic scattering is considered. We have, therefore, reexamined the GA-predicted amplitude for structureless charged-particle collisions with arbitrary neutral atoms. In this paper we propose certain new analytic procedures for evaluating the Glauber amplitude; these procedures again lead to a one-dimensional integral representation for the amplitude, which can be computed numerically with relative ease and without the sort of difficulties seemingly inherent in Franco's procedure. To illustrate these procedures we consider only the case of elastic scattering of electrons by helium atoms, using the simplest possible Hylleraas wave function for the ground state. We are able to establish a rather loose criterion for the easy and convenient use of Franco's procedures in this simple case, at least—provided the aforementioned δ function first is removed. The generalization of these procedures to inelastic collisions with He, or to collisions with more complex atoms is, aside from the application of our new analytic techniques, very much along the lines which Franco[9] suggests in general. We shall discuss in some detail how to apply our new analytic methods in the more general case.

The contents of this paper now can be summarized as follows. In Sec. II we describe the reduction of the $e^- + \text{He}$ elastic Glauber amplitude to a one-dimensional integral involving a Bessel function of the first kind and functions $\mathcal{L}_{\mu,\nu}$, which we shall call "modified Lommel functions." In Sec. III we present the results of our numerical calculation of the amplitude obtained in Sec. II. We also describe the rough limits within which we feel Franco's procedures may be conveniently used to evaluate this amplitude. Moreover, we have also recalculated, via our new procedures, the e^- +He elastic Glauber amplitude previously obtained by Franco[6] using a more complex Hartree-Fock wave function for the He ground state. Our new results for this amplitude are in good agreement with those obtained by Franco. Thus we demonstrate that our new procedures are valid and useful for performing actual calculations. The generalization of these procedures to more complicated applications is also discussed in this section.

We have deferred to an Appendix our discussion of the functions $\mathcal{L}_{\mu,\nu}$. Since these functions are the foundation of our new procedures, we describe their properties in much greater detail than is required for the application of Sec. II. In this Appendix we define the functions $\mathcal{L}_{\mu,\nu}(ix)$; we also discuss the recurrence relations which these functions satisfy, together with their differential properties. The asymptotic properties of these functions $\mathcal{L}_{\mu,\nu}(ix)$ are derived both for large and small values of the argument x.

II. REDUCTION OF THE GLAUBER AMPLITUDE FOR He ELASTIC SCATTERING

In this section we describe our new procedures for the reduction of the Glauber amplitude for the scattering of a charged structureless particle by neutral atoms. To illustrate our techniques specifically, we consider the elastic scattering of a particle with charge Z_i by ground-state He. Let $\hbar\vec{K}_i$, $\hbar\vec{K}_f \equiv \mu\vec{v}_i, \mu\vec{v}_f$ define the incident and final momenta of the incident particle in the center-of-mass system; μ is the reduced mass of the incident particle He atom pair and $\vec{v}_i$ and $\vec{v}_f$ are the initial and final relative velocities of the incident particle. Define the momentum transfer vector $\vec{q}$ by

$$\vec{q} = \vec{K}_i - \vec{K}_f .$$

Then, neglecting exchange and spin effects, the Glauber amplitude for elastic scattering by ground-state He atoms with wave function $\phi_i(\vec{r}_1, \vec{r}_2)$ is given by[1,9]

$$F(\vec{q}) = \frac{iK_i}{2\pi} \int \phi_i^*(\vec{r}_1, \vec{r}_2)\, \Gamma(\vec{b}; \vec{r}_1, \vec{r}_2)\, \phi_i(\vec{r}_1, \vec{r}_2) \times e^{i\vec{q}\cdot\vec{b}} d^2b\, d\vec{r}_1 d\vec{r}_2, \tag{1}$$

where

$$\Gamma(\vec{b}; \vec{r}_1\vec{r}_2) = 1 - \left(\frac{|\vec{b} - \vec{s}_1|}{b}\right)^{2i\eta} \left(\frac{|\vec{b} - \vec{s}_2|}{b}\right)^{2i\eta} \tag{2}$$

and $\eta \equiv -Z_i e^2/\hbar v_i$. In Eqs. (1) and (2), $\vec{b}$, $\vec{s}_1$, and $\vec{s}_2$ are the respective projections of the position vectors of the incident particle and bound electrons ($\vec{r}_1$ and $\vec{r}_2$) onto the plane perpendicular to the direction of the Glauber path integration[4]: $\vec{q}$, $\vec{b}$, $\vec{s}_1$, and $\vec{s}_2$ are all coplanar. For our present purposes it is sufficient to take $\phi_i(\vec{r}_1, \vec{r}_2)$ to be the simplest Hylleraas wave function for the helium ground state, namely,[10]

$$\phi_i(\vec{r}_1, \vec{r}_2) = (1/\pi)\,(\alpha/a_0)^3 e^{-\alpha(r_1 + r_2)/a_0}, \tag{3}$$

with $\alpha \equiv 1.69$. Thus

$$F(\vec{q}) = \frac{iK_i}{2\pi^3}\left(\frac{\alpha}{a_0}\right)^6 \int e^{-(2\alpha/a_0)(r_1 + r_2)} \times\left[1 - \left(\frac{|\vec{b} - \vec{s}_1|}{b}\right)^{2i\eta} \left(\frac{|\vec{b} - \vec{s}_2|}{b}\right)^{2i\eta}\right] \times e^{i\vec{q}\cdot\vec{b}} d^2b\, d\vec{r}_1 d\vec{r}_2. \tag{4}$$

Before proceeding further with the reduction of Eq. (4), we remark that the first term (independent of η) under the integral in Eq. (4) leads to a δ function in $\vec{q}$, which Franco[9] drops. We shall retain this term explicitly since, as we shall ultimately show, it is exactly cancelled by a similar factor stemming from the second term (dependent on η) in the amplitude integral. We next note that the amplitude $F(\vec{q})$ of Eq. (4) can be written in terms of a generating function; in particular,

$$F(\vec{q}) = \frac{iK_i}{2}\left(\frac{\alpha}{a_0}\right)^6 \left(\frac{\partial^2}{\partial\lambda_1\partial\lambda_2}\, \mathcal{F}(\lambda_1, \lambda_2; q)\right)\Bigg|_{\lambda_1 = \lambda_2 = 2\alpha/a_0}, \tag{5}$$

where we define

$$\mathcal{F}(\lambda_1, \lambda_2; q) \equiv \frac{1}{\pi^3} \int e^{-\lambda_1 r_1} e^{-\lambda_2 r_2} \frac{1}{r_1 r_2} \times\left[1 - \left(\frac{|\vec{b} - \vec{s}_1|}{b}\right)^{2i\eta} \left(\frac{|\vec{b} - \vec{s}_2|}{b}\right)^{2i\eta}\right] \times e^{i\vec{q}\cdot\vec{b}} d^2b\, d\vec{r}_1 d\vec{r}_2. \tag{5a}$$

We next introduce cylindrical coordinates for $\vec{r}_1$ and $\vec{r}_2$; then the azimuthal angle integrations in the plane containing $\vec{b}$, $\vec{s}_1$ and $\vec{s}_2$ may be separated. The preliminary reduction of $\mathcal{F}$ follows the methods of Franco[9] (among others[2-4]). We find that $\mathcal{F}(\lambda_1, \lambda_2; q)$ can be written as

$$\mathcal{F}(\lambda_1, \lambda_2; q) = 2^5 \int_0^\infty b\,db\, J_0(qb) \int_0^\infty s_1 ds_1 \int_0^\infty s_2 ds_2\, K_0(\lambda_1 s_1) K_0(\lambda_2 s_2) \times\left[1 - \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi_1 \int_0^{2\pi} d\varphi_2 \left(1 + \frac{s_1^2}{b^2} - 2\frac{s_1}{b}\cos\varphi_1\right)^{i\eta} \left(1 + \frac{s_2^2}{b^2} - 2\frac{s_2}{b}\cos\varphi_2\right)^{i\eta}\right]. \tag{6}$$

In Eq. (6) we now change variables so that $s_1 \to s_1 b_1$ and $s_2 \to s_2 b$; furthermore we utilize the result[11] that

$$\int_0^\infty s ds K_0(\lambda b s) = (\lambda b)^{-2}.$$

We obtain

$$\mathfrak{F}(\lambda_1, \lambda_2; q) = 2^5 \int_0^\infty b^5 J_0(qb)[(\lambda_1 b)^{-2}(\lambda_2 b)^{-2} - M(\lambda_1 b) M(\lambda_2 b)], \quad (7)$$

where we define $M(x)$ via

$$M(x) \equiv \frac{1}{2\pi} \int_0^\infty s ds K_0(xs) \times \int_0^{2\pi} d\varphi (1 + s^2 - 2s\cos\varphi)^{i\eta}. \quad (7a)$$

We now introduce the integral representation of Thomas and Gerjuoy[4] to replace the integral over φ in (7a) by an equivalent integral involving Bessel functions; thus

$$M(x) = -2^{2i\eta} \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} \int_0^\infty s ds K_0(xs) \times \int_0^\infty dt\, t^{-2i\eta} \frac{d}{dt}[J_0(t) J_0(st)]. \quad (8)$$

We note that Eq. (8) cannot be simplified by integrating once by parts (see Ref. 4); however, we can interchange the orders of integration and differentiation with respect to t with the integration over s. The integral over s may be done immediately via[12]

$$\int_0^\infty s ds K_0(xs) J_0(st) = (t^2 + x^2)^{-1}.$$

Hence

$$M(x) = -2^{2i\eta} \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} \int_0^\infty dt\, t^{-2i\eta} \frac{d}{dt} \frac{J_0(t)}{t^2 + x^2}. \quad (9)$$

Now, however,

$$\frac{d}{dt}(t^2 + x^2)^{-1} J_0(t) = -(t^2 + x^2)^{-1} J_1(t) - 2t(t^2 + x^2)^{-2} J_0(t) = -(t^2 + x^2)^{-1} J_1(t) + x^{-1} \frac{\partial}{\partial x} t(t^2 + x^2)^{-1} J_0(t), \quad (10)$$

so that

$$M(x) = 2^{2i\eta} \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} \left(\int_0^\infty dt\, t^{-2i\eta} (t^2 + x^2)^{-1} J_1(t) - x^{-1} \frac{\partial}{\partial x} \int_0^\infty dt\, t^{-2i\eta+1} (t^2 + x^2)^{-1} J_0(t) \right). \quad (11)$$

Each of the integrals in Eq. (11) is of the kind $\mathcal{J}_{\mu,m}$ discussed in the first part of the Appendix. Applying Eq. (A7) of the Appendix leads directly to the result

$$M(x) = -(ix)^{-2i\eta-1} \mathcal{L}_{2i\eta,1}(ix) + x^{-1} 2i\eta \frac{\partial}{\partial x} [(ix)^{-2i\eta} \mathcal{L}_{2i\eta-1,0}(ix)]. \quad (12)$$

The modified Lommel functions $\mathcal{L}_{\mu,\nu}(ix)$ are defined in terms of the Lommel function $s_{\mu,\nu}(ix)$ and modified Bessel functions $I_\nu(x)$; we refer the reader to Eq. (A6) of the Appendix. Equation (12) may be reduced and simplified via the recurrence relations for $\mathcal{L}_{\mu,\nu}$ which we derive in the second part of the Appendix. The indicated differentiation may be carried out via Eq. (A10); thus

$$M(x) = (ix)^{-2i\eta-1}\{-\mathcal{L}_{2i\eta,1}(ix) + (2i\eta)^2 (ix)^{-1} \mathcal{L}_{2i\eta-1,0}(ix) - (2i\eta)(2i\eta - 2)\mathcal{L}_{2i\eta-2,1}(ix)\}. \quad (13)$$

However, the functions $\mathcal{L}_{2i\eta,1}$ and $\mathcal{L}_{2i\eta-2,1}$ are related via Eq. (A11):

$$\mathcal{L}_{2i\eta,1}(ix) + (2i\eta)(2i\eta - 2)\mathcal{L}_{2i\eta-2,1}(ix) = (ix)^{2i\eta-1}.$$

Thus

$$M(x) = -(ix)^{-2i\eta-2}\{(ix)^{2i\eta} - (2i\eta)^2 \mathcal{L}_{2i\eta-1,0}(ix)\} \quad (14a)$$

$$= x^{-2} + (2i\eta)^2 (ix)^{-2i\eta-2} \mathcal{L}_{2i\eta-1,0}(ix). \quad (14b)$$

In fact Eq. (14a) may be simplified further; we could apply Eq. (A11) again, to obtain

$$M(x) = -(ix)^{-2i\eta-2} \mathcal{L}_{2i\eta+1,0}(ix). \quad (15)$$

If in Eq. (15), we were to write $\mathcal{L}_{2i\eta+1,0}(ix)$ as the sum of two hypergeometric functions [via Eqs. (A3), (A4), and (A6)] we would have precisely the same result for $M(x)$ that we would have obtained via Franco's methods.[9] However, we do not use Eq. (15) in Eq. (7) to compute $\mathfrak{F}(\lambda_1, \lambda_2; q)$; we use Eq. (14b), which explicitly displays the x^{-2} dependence of $M(x)$. We find then that

$$\mathfrak{F}(\lambda_1, \lambda_2; q) = 2^5 \int_0^\infty b^5 db\, J_0(qb)\{(\lambda_1 b)^{-2}(\lambda_2 b)^{-2} - [(\lambda_1 b)^{-2} + (2i\eta)^2 (i\lambda_1 b)^{-2i\eta-2} \mathcal{L}_{2i\eta-1,0}(i\lambda_1 b)] \times [(\lambda_2 b)^{-2} + (2i\eta)^2 (i\lambda_2 b)^{-2i\eta-1} \mathcal{L}_{2i\eta-1,0}(i\lambda_2 b)]\}, \quad (16)$$

which leads directly to

$$\mathfrak{F}(\lambda_1, \lambda_2; q) = 2^5 \int_0^\infty b^5 db\, J_0(qb)\{(\lambda_1 b)^{-2}(\lambda_2 b)^{-2}(2i\eta)^2 \times [(i\lambda_2 b)^{-2i\eta} \mathcal{L}_{2i\eta-1,0}(i\lambda_2 b) + (i\lambda_1 b)^{-2i\eta} \times \mathcal{L}_{2i\eta-1,0}(i\lambda_1 b)] - (2i\eta)^4 (i\lambda_1 b)^{-2i\eta-2} \times (i\lambda_2 b)^{-2i\eta-2} \mathcal{L}_{2i\eta-1,0}(i\lambda_1 b)\, \mathcal{L}_{2i\eta-1,0}(i\lambda_2 b)\}. \quad (17)$$

Note that in obtaining Eq. (17) we have explicitly removed the aforementioned $\delta(\vec{q})$ stemming from the first term in Eqs. (4) or (16). If, on the other hand, we had dropped the δ function in Eq. (4) and used Eq. (15) (or the equivalent thereof) for $M(x)$ as Franco suggests,[9] then we would have found ourselves in the rather uncomfortable position of having to compute $F(q)$ numerically from an integral representation which includes the integral representation of a δ function. [Note that differentiating $\mathfrak{F}(\lambda_1, \lambda_2; q)$ with respect to λ_1 and λ_2 does not affect the b dependence of the integral; thus, the conclusions drawn from Eqs. (16) or (17) remain valid for $F(q)$.] It is straightforward to show from the results in the third part of the Appendix that the integral representation (17) for $\mathfrak{F}(\lambda_1, \lambda_2; q)$ is well defined and convergent. Therefore, the integral representation for $F(q)$ which we obtain from Eq. (17) via Eq. (5) will be well defined.

Equation (17) may be reduced further without much effort: the integrals in (17) which involve only one modified Lommel function $\mathfrak{L}_{\mu,\nu}$ may be evaluated in closed form. We reintroduce the integral representation, Eq. (A7), for $\mathfrak{L}_{2i\eta-1,0}(i\lambda b)$. The resulting double integrals may be evaluated following the procedures of Appendix B in Thomas and Gerjuoy.[4] We find that

$$\int_0^\infty b\,db\,J_0(qb)(i\lambda b)^{-2i\eta}\,\mathfrak{L}_{2i\eta-1,0}(i\lambda b) = -\tfrac{1}{2}\Gamma(i\eta)\,\Gamma(1-i\eta)\,q^{2i\eta-2}\lambda^{-2i\eta} \times {}_2F_1(1-i\eta, 1-i\eta;\, 1;\, -\lambda^2 q^{-2}), \qquad (18)$$

where the ${}_2F_1$ is the usual hypergeometric function. Hence

$$\mathfrak{F}(\lambda_1, \lambda_2; q) = -2^4(\lambda_1\lambda_2)^{-2}(2i\eta)^2\,\Gamma(i\eta)\,\Gamma(1-i\eta)\,q^{2i\eta-2}\left[\lambda_1^{-2i\eta}\,{}_2F_1(1-i\eta, 1-i\eta;\, 1;\, -\lambda_1^2 q^{-2}) + \lambda_2^{-2i\eta}\,{}_2F_1(1-i\eta, 1-i\eta;\, 1;\, -\lambda_2^2 q^{-2})\right]$$
$$- 2^5(2i\eta)^4\int_0^\infty b^5\,db\,J_0(qb)(i\lambda_1 b)^{-2i\eta-2}\,(i\lambda_2 b)^{-2i\eta-2}\,\mathfrak{L}_{2i\eta-1,0}(i\lambda_1 b)\,\mathfrak{L}_{2i\eta-1,0}(i\lambda_2 b). \qquad (19)$$

To obtain the scattering amplitude from Eq. (19) we need to differentiate Eq. (19) with respect to λ_1 and λ_2 as indicated in Eq. (5). The differentiation of the hypergeometric functions is carried out via[13]

$$\frac{d}{dx}\,{}_2F_1(a, b;\, c;\, x) = abc^{-1}\,{}_2F_1(a+1, b+1;\, c+1;\, x),$$

whereas the modified Lommel functions are differentiated by applying Eq. (A10). We ultimately find that the GA-predicted amplitude for elastic scattering by ground-state He, using the Hylleraas wave function of Eq. (3), is given by

$$F(q) = 2K_i\eta\Big\{2|\Gamma(1+i\eta)|^2 q^{2i\eta-2}\lambda^{-2i\eta}\big[(1+i\eta)\,{}_2F_1(1-i\eta, 1-i\eta;\, 1;\, -\lambda^2 q^{-2}) + (1-i\eta)^2\lambda^2 q^{-2}\,{}_2F_1(2-i\eta, 2-i\eta;\, 2;\, -\lambda^2 q^{-2})\big]$$
$$+ (2i\eta)^3\int_0^\infty b\,db\,J_0(qb)(i\lambda b)^{-4i\eta}\big[(i\lambda b)(i\eta-1)\,\mathfrak{L}_{2i\eta-2,1}(i\lambda b) - (1+i\eta)\,\mathfrak{L}_{2i\eta-1,0}(i\lambda b)\big]^2\Big\}, \qquad (20)$$

where

$$\lambda \equiv 2\alpha/a_0 \quad\text{and}\quad \eta = -Z_i\,e^2(\hbar v_i)^{-1}.$$

Several comments about Eq. (20) are now in order. First of all, the separation of the Glauber amplitude into terms involving hypergeometric functions and the integral over products of modified Lommel functions is a "natural" one. We may break up the full Γ of Eq. (2) in a fashion analogous to the Glauber multiple-scattering expansion,[1] namely,

$$\Gamma(\vec{b};\, \vec{r}_1, \vec{r}_2) = \Gamma_1(\vec{b};\, \vec{r}_1) + \Gamma_2(\vec{b};\, \vec{r}_2) - \Gamma_1(\vec{b};\, \vec{r}_1)\,\Gamma_2(\vec{b};\, \vec{r}_2), \qquad (21)$$

where

$$\Gamma_i(\vec{b};\, \vec{r}_i) \equiv 1 - (|\vec{b} - \vec{s}_i|/b)^{2i\eta}.$$

Equation (21) differs from the usual expansion of $\Gamma(\vec{b};\, \vec{r}_1, \vec{r}_2)$ in two-particle Γ's since each term $\Gamma_i(\vec{b};\, \vec{r}_i)$ contains the collective effects upon the incident particle, not only of the ith bound electron, but also of one proton in the nucleus. The separation of Eq. (21) is dictated by the long-range nature of the Coulomb force. Of course, the sum $\Gamma_1 + \Gamma_2$ contains the effects of single-particle scattering from each of the charged particles comprising the He atom, together with higher-order scattering. If the expansion (21) is used in Eq. (1), then the integrals over the sum $\Gamma_1 + \Gamma_2$ may be obtained directly in closed form using the procedures of

Thomas and Gerjuoy.[4] One immediately obtains the terms in Eq. (20) which involve the hypergeometric functions. Thus, at high energies and small scattering angles where single-particle scattering dominates the amplitude, we may expect the scattering amplitude of Eq. (20) to be well approximated by the terms involving only the hypergeometric functions. Furthermore, for any nonzero incident electron energy it is straightforward to show that the hypergeometric-function contribution to Eq. (20) diverges[4] as $\ln(q^2)$ as $q\to 0$, whereas the integral involving the products of modified Lommel functions is well defined and finite as $q\to 0$. Therefore, the scattering amplitude defined by Eq. (20) diverges as $\ln(q^2)$ as $q\to 0$.

Equation (20) differs from the result to which Franco's procedures would lead in that we have explicitly removed a troublesome δ function in the momentum transfer $\vec{q}$. On the other hand, if we had suspected that the second term in Eq. (4) or (5a) also concealed a δ function which cancelled the δ function stemming from the first term, then we could have retained the first term and proceeded to reduce the second term along the lines which Franco suggests. We would have found, for example, that Eq. (16) would be replaced by

$$\mathfrak{F}(\lambda_1,\lambda_2;q)=2^5(\lambda_1\lambda_2)^{-2}\int_0^\infty b\,db\,J_0(qb)\times[1-(i\lambda_1 b)^{-2i\eta}(i\lambda_2 b)^{-2i\eta}\times\mathfrak{L}_{2i\eta+1,0}(i\lambda_1 b)\,\mathfrak{L}_{2i\eta+1,0}(i\lambda_2 b)] \quad (22)$$

[where Eq. (22) comes from using Eq. (15) for $M(x)$ in Eq. (7)]. Moreover, the functions $\mathfrak{L}_{2i\eta+1,0}(ix)$ in Eq. (22) would have been written out as the sum of two hypergeometric functions [e.g., Eq. (23) of Ref. 9]. However, as we show in the Appendix, each of these hypergeometric functions diverge as e^x for large x. Therefore, even though we implicitly remove the δ function in $\vec{q}$, we would still face the seemingly difficult task of computing the amplitude from a representation involving an infinite integral, the integrand of which required the computation of differences between exponentially divergent functions when the integration variable was large. By identifying the functions $\mathfrak{L}_{\mu,\nu}(ix)$ as modified Lommel functions we have eliminated this problem since we may now compute $\mathfrak{L}_{\mu,\nu}(ix)$ from a valid asymptotic expansion when x is large. Thus, in view of the analytic results in the Appendix, computations of the Glauber amplitude via Eq. (20) should be practical.

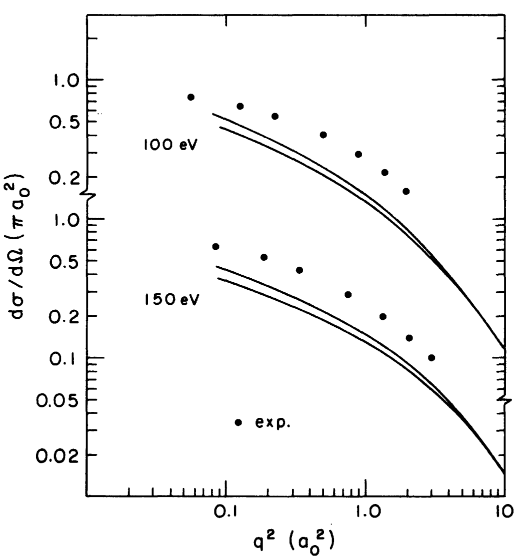

FIG. 1. GA-predicted differential cross sections for e^-+He elastic scattering shown as a function of q^2 for 100- and 150-eV incident electrons. The lower solid curve is obtained using the simple Hylleraas wave function for the He ground state, whereas the upper solid curve is obtained using the Hartree-Fock wave function previously used by Franco. The experimental data are that of Vriens *et al.*, normalized to the data of Chamberlain *et al.*

III. NUMERICAL RESULTS AND CONCLUSIONS

A. e^-+He Elastic Scattering

In order to demonstrate that our analytic techniques for the reduction of the Glauber amplitude are, in fact, practical and useful, we have calculated the GA-predicted elastic scattering amplitude of Eq. (20) for incident electrons. The hypergeometric functions in Eq. (20) were calculated first by applying the linear transformation[14]

$${}_2F_1(a,b;c;z)=(1-z)^{-a}\,{}_2F_1(a,c-b;c;z/[z-1])$$

and then summing the resultant hypergeometric series. The infinite integral involving $J_0(qb)$ and the modified Lommel functions $\mathfrak{L}_{\mu,\nu}(i\lambda b)$ was evaluated by breaking the integration region into two pieces: $0\le b\le R$ and $R\le b<\infty$. The value of R was determined as that value of b for which $\mathfrak{L}_{\mu,\nu}(i\lambda b)$, evaluated by summing simultaneously the hypergeometric series obtained by using Eqs. (A3) and (A4) in Eq. (A6), was well represented by the first few terms of the asymptotic expansion of Eq. (A17). We found that a value of $x=\lambda R\simeq 18$ was adequate for our purposes. Then, in the region $0\le b\le R$, the Lommel functions were evaluated via Eq. (A6) and the integration was performed via Gaussian quadrature. In the asymptotic region, $R\le b<\infty$, the modified Lommel functions were replaced by the first few terms in their asymptotic expansions and the integration was performed analytically.[15] We found that the contribution to the integral in Eq. (20) from the asymptotic region was essentially negligible (less than 1 part in 10^5) at all the incident electron energies and momentum transfers we considered. We remark that Eq. (18) provides a very useful simultaneous check on the integration routine and the numerical generation of the modified Lommel functions; now, however, the asymptotic region $b \geq R$ contributes significantly (~1–5%) to the integral on the left-hand side of Eq. (18) when $q^2/\lambda^2 \gtrsim 0.5$ and $0.1 \leq \eta \leq 2$.

A further word about the generation of the functions $\mathcal{L}_{\mu,\nu}(ix)$ is in order. We found, for example, that the series expansion, Eq. (A6), for the function $\mathcal{L}_{2i\eta-1,0}(ix)$ agreed well with the asymptotic form, Eq. (A17), for $0.1 \leq \eta \leq 2$ and $14 \leq x \leq 20$; from (A17) $\mathcal{L}_{2i\eta-1,0}(ix) \sim (ix)^{2i\eta-2}$, to lowest order. As we mentioned previously, the hypergeometric functions in Eq. (A6) were summed simultaneously; the computations were performed entirely in double precision. Moreover, *both* the real and imaginary parts of Eq. (A6) were required to converge to at least one part in 10^{10}. However, for $x > 20$ where we expect Eq. (A17) to be increasingly valid, the series expansion (A6) does not converge at all well to the asymptotic result. This simply reflects the fact that the expansion parameter in Eq. (A6) is $\frac{1}{4}x^2$, so that extremely high precision is required in order to sum (A6) accurately for large values of x.

In view of the preceeding remarks, we now may establish a tentative criterion under which Franco's procedures may be used conveniently to evaluate the amplitude of Eqs. (5)—provided, of course, the δ function in the momentum transfer first is removed as in Eq. (22). The utility of Franco's procedures is predicated upon the natural assumption that the Glauber amplitude integral over the range $[0,\infty)$ [Eqs. (23) and (24) of Ref. 9] may be replaced by a finite integral over some interval $[0,R]$, where the integrand may be accurately and conveniently computed. In our present example, this assumption is equivalent to the assertion that the amplitude of Eqs. (5) may be computed from Eq. (22), all the while neglecting the asymptotic contribution to the infinite integral in Eq. (22). However, we have already demonstrated that Eq. (22) is just an alternative way of writing Eq. (17) [or Eq. (19)], where we have separated the contribution due to the single-scattering terms. Thus Eq. (22) implicitly contains terms like the integral in Eq. (18). As we mentioned previously, the contribution of the asymptotic region $[R,\infty)$ to the value of the integral on the left-hand side of (18) can be significant. In fact, for very small values of q/λ the right-hand side of Eq. (18) goes asymptotically as $\ln(q/\lambda)$; it is straightforward to show that this logarithmic divergence at small q stems entirely from the asymptotic contribution to the integral on the left-hand side of (18). Thus the region in which Franco's procedures may be conveniently used is roughly determined by those values of the momentum transfer q for which, at fixed incident electron energy, the single-scattering contributions to the amplitude may be well approximated by a finite integral. In the present case, at least, the integral representation for the contribution to the amplitude from higher-order scattering is sufficiently well behaved that these asymptotic problems do not arise. These remarks suggest that in general the single-scattering contribution to the Glauber amplitude should be removed explicitly and evaluated in closed form; the remaining contributions to the amplitude may then, perhaps, be evaluated straightforwardly using the procedures which Franco suggests. This is essentially what we have done in the present case by identifying Eq. (20) as the Glauber scattering amplitude.

In addition to calculating the Glauber amplitude of Eq. (20), we have also recalculated, using these present methods, the e^- +He elastic Glauber amplitude obtained by Franco[6] from a three-dimensional integral representation for the amplitude. Instead of using the simple Hylleraas ground-state wave function of Eq. (3), Franco used a Hartree-Fock wave function by

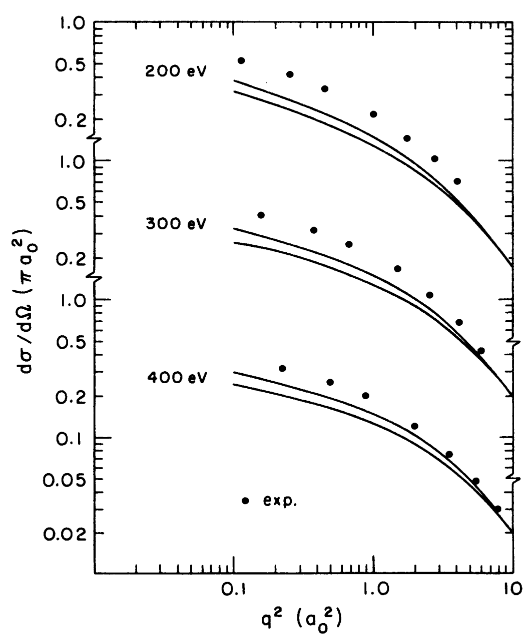

FIG. 2. The same angular distributions as shown in Fig. 1, only now for 200-, 300-, and 400-eV incident electrons.

$$\varphi_i(\vec{r}_1, \vec{r}_2) = (N^2/\pi a_0^3)(e^{-\alpha_1 r_1/a_0} + Ce^{-2\alpha_1 r_1/a_0}) \times (e^{-\alpha_1 r_2/a_0} + Ce^{-2\alpha_1 r_2/a_0}), \qquad (23)$$

where $N=1.484$, $\alpha_1=1.456$, a_0 is the Bohr radius, and $C=0.6$. The results of these two calculations are shown in Figs. 1 and 2, in which we have plotted the GA-predicted differential cross sections (in units of πa_0^2) as a function of q^2 (in units of a_0^2) for incident electron energies of 100, 150, 200, 300, and 400 eV. In each case, the lower solid curve is the GA-predicted angular distribution obtained from Eq. (20), whereas the upper solid curve is obtained by using Eq. (23) in Eq. (1). The experimental data of Vriens *et al.*,[16] renormalized to the small-angle absolute measurements of Chamberlain *et al.*,[17] also are included; at each energy the measured angular distribution covers the range from 5° (leftmost datum point) to 30° (rightmost datum point). We do not present the first Born-predicted angular distributions since they already have been discussed by Franco.[6]

We note that our present Glauber results using the Hartree-Fock ground-state wave function [Eq. (23)] agree well with those obtained with considerably greater numerical effort by Franco.[6] Indeed all the present results shown in Figs. 1 and 2 were calculated in less than 5 min on a *very slow* computer (DEC 1055) using double-precision arithmetic. When compared with experiment, the Glauber predictions obtained from Eq. (23) are seen to be superior to those using the Hylleraas wave function, as we might well expect. However, the difference between the two Glauber predictions is never as large as the difference between the upper curve and experiment. For momentum transfers corresponding to scattering angles greater than 30° the two Glauber predictions are essentially indistinguishable, reflecting the fact that the wide-angle scattering is dominated by the interaction with the He nucleus, and independent of the detailed shape of the electron cloud. Moreover, for an incident electron energy of 400 eV we also find, as expected, that the amplitude of Eq. (20) is well approximated by the hypergeometric-function terms when $q^2a_0^2 < 0.5$. Because the GA-predicted elastic scattering amplitude [using either Eqs. (3) or (23)] diverges as $\ln(q^2)$ as $q \to 0$, we expect these Glauber predictions to overestimate the measured differential cross sections at very small scattering angles. Although the data are all at angles too large ($\geq 5°$) to demonstrate this explicitly, the results shown in Fig. 1 strongly suggest that the Glauber predictions will be larger than the measured differential cross sections at still smaller values of q^2.

The poor agreement between the GA-predicted angular distributions and the data shown in Figs. 1 and 2 is rather disappointing since, from the $e^- + H(1s)$ elastic scattering results,[2] we are lead to expect the Glauber approximation to be most valid at these incident electron energies and scattering angles. Even at 400 eV and $(qa_0)^2 = 0.2$ the Glauber result using Eq. (23) underestimates the measured differential cross section by an approximate factor of 30%. The failure of the Glauber approximation at these scattering angles and energies may simply reflect the fact that even Eq. (23) does not for our purposes adequately represent the shape of the He electron cloud at large distances. Indeed, the results shown in Figs. 1 and 2 seem to confirm this assertion. At low incident electron energies the scattered intensity at small angles is determined predominantly by the large distance behavior of the bound-state wave function. At higher energies, however, the incident electrons are capable of sampling the electron cloud nearer to the nucleus and yet be scattered only through small angles. Thus, the fact that these present Glauber predictions agree best with experiment at high electron energies suggests that we may require an even better wave function than Eq. (23) to obtain good agreement with experiment at these scattering angles.

B. More General Applications

The extension of the foregoing methods to the evaluation of the Glauber amplitude for inelastic scattering by helium targets, or for elastic or inelastic scattering by neutral atoms other than helium, is straightforward along the lines that Franco[9] suggests. In addition, we require a useful reduction of integrals of the class

$$\mathcal{K}_{n,p,m}(\lambda) \equiv \int_0^\infty dt\, t^{-2i\eta-1+n}(t^2+\lambda^2)^{-1-p} J_m(t), \qquad (24)$$

where n, p, and m are all integers ≥ 0 and $n < \frac{7}{2} + 2p$. Although Franco has proposed a general reduction of the integral in Eq. (24), we also may obtain an alternative reduction in terms of the modified Lommel functions described in the Appendix. However, the results of the Appendix [Eq. (A7) in particular] may not be applied directly to the above integral. An alternative reduction of Eq. (24) may be obtained in the following way. We may expand the term $t^n(t^2+\lambda^2)^{-1-p}$ in partial fractions to eliminate excess powers of t in the numerator and then, in each term, replace excess powers of $(t^2+\lambda^2)^{-1}$ by repeated differentiation with respect to λ^2. In this way $\mathcal{K}_{n,p,m}$ may be written as a finite sum of integrals, to each of which we may apply Eq. (A7) of the Appendix. After carrying out the differentiations with respect to λ^2, we will obtain a finite sum of terms involving modified Lommel functions $\mathcal{L}_{2i\eta-n';m'}(i\lambda)$ for the integral $\mathcal{K}_{n,p,m}(\lambda)$. At this point we do not appear to have gained a great deal, aside from the knowledge of the asymptotic behavior of $\mathcal{K}_{n,p,m}(\lambda)$ for large and small λ. However, since the Lommel functions satisfy the recurrence relations discussed in the second part of the Appendix, we need to calculate explicitly via Eq. (A6) only four of the modified Lommel functions [for example, $\mathcal{L}_{2i\eta,0}(i\lambda)$, $\mathcal{L}_{2i\eta,1}(i\lambda)$, $\mathcal{L}_{2i\eta-1,0}(i\lambda)$, $\mathcal{L}_{2i\eta-1,1}(i\lambda)$]; all others may be obtained from these four using the recurrence relations. In this manner, we may calculate easily and conveniently the quantities $\mathcal{K}_{n,p,m}(\lambda)$.

Since no other computations of the Glauber amplitude for multielectron atoms, using either our procedures or those suggested by Franco, have been reported, it is difficult to say *a priori* which procedure will ultimately prove more useful in a more general case when the problem of computing δ functions does not arise. We are confident that the method suggested above for the reduction of Eq. (24), when used in the context of the results of the Appendix, will be practical in actual calculations. However, it may well prove to be the case that these methods will be most useful for establishing the bounds within which one may employ Franco's reduction of Eq. (24), which superficially, at least, is of simpler structure. It should be clear then that further calculations of the Glauber amplitudes for both elastic and inelastic scattering from targets more complex than neutral helium are required in order to establish the utility, not only of these and Franco's procedures, but also of the Glauber approximation itself.

Note added in proof. We recently have received from Franco a report of work prior to publication in which Franco applies his methods (Ref. 9) to the evaluation of the Glauber amplitude for the excitation of the 2^1S state of helium and compares his results with the measured angular distributions. We note that the single-scattering terms in this amplitude again lead to a $\ln(q)$ behavior for the amplitude at small values of the momentum transfer q. Even though the momentum transfer never can be identically zero for inelastic scattering, at high incident particle energies the values of q corresponding to scattering near the forward direction can be quite small. Thus at high incident particle energies and at these small values of q one again must ask if the logarithmic dependence of the single-scattering terms is represented adequately in the numerical calculations of the GA-predicted $2\,^1S$ excitation amplitude. Although Franco does not discuss his numerical techniques for the evaluation of this Glauber amplitude, we remark that for high incident electron energies Franco appears to have evaluated this amplitude at sufficiently large values of q so that the single-scattering terms seem to be represented adequately in his computations.

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MATHEMATICAL APPENDIX

1. Definition of the Function $\mathcal{L}_{\mu,\nu}$

In the first part of this appendix we are concerned with the reduction of the integral

$$\mathcal{G}_{\mu,m}(k) \equiv \int_0^\infty dt\, t^{-\mu}(t^2+k^2)^{-1}J_m(t), \tag{A1}$$

where $k^2>0$ and m is an integer $\geqslant 0$; moreover $\mathrm{Re}(\mu)\neq 0$. We show that the integral $\mathcal{G}_{\mu,m}$ can be expressed in terms of functions $\mathcal{L}_{\mu,m}$, which we shall call "modified Lommel" functions; these functions obey a set of recurrence relations and possess differential properties that make them very useful for our present purposes. These and other properties of the functions $\mathcal{L}_{\mu,\nu}$ are discussed elsewhere in this appendix.

When $-m<\mathrm{Re}(1-\mu)<\frac{7}{2}$, the integral in Eq. (A1) may be evaluated in closed form[18] as

$$\begin{aligned}\mathcal{G}_{\mu,m}(k) = {} & k^{-\mu+m-1}\,2^{-m-1}\,\Gamma\left(\frac{m-\mu+1}{2}\right)\Gamma\left(\frac{1+\mu-m}{2}\right)[\Gamma(1+m)]^{-1}\\ & \times {}_1F_2\left(\frac{m-\mu+1}{2};\frac{m-\mu+1}{2},\ 1+m;\frac{k^2}{4}\right)+2^{-\mu-2}\,\Gamma\left(\frac{m-\mu-1}{2}\right)\left[\Gamma\left(2+\frac{m+\mu-1}{2}\right)\right]^{-1}\\ & \times {}_1F_2\left(1;\,2+\frac{m+\mu-1}{2},\ 2-\frac{m-\mu+1}{2};\frac{k^2}{4}\right).\end{aligned} \tag{A2}$$

Since

$${}_1F_2(a;\,a,\ m+1;\,z)={}_0F_1(m+1;\,z)$$

and[19]

$$I_m(z)=[\Gamma(1+m)]^{-1}(\tfrac{1}{2}z)^m\,{}_0F_1(1+m;\,\tfrac{1}{4}z^2), \tag{A3}$$

the first hypergeometric function in Eq. (A2) reduces to a modified Bessel function. Furthermore, we note that the Lommel function $s_{\mu,\nu}(z)$ is defined by[20]

$$s_{\mu,\nu}(z)=[(\mu+1+\nu)(\mu+1+\nu)]^{-1}z^{\mu+1}$$
$$\times {}_1F_2\left(1;\frac{\mu-\nu+3}{2},\frac{\mu+\nu+3}{2};-\frac{z^2}{4}\right),$$

provided $\mu\pm\nu\neq -1,\ -2,\ldots$. However, in Eq. (A1) $\mathrm{Im}(\mu)$ is nonzero, thus the remaining hypergeometric function in Eq. (A2) can be written as

$$ {}_1F_2\left(1;\,2+\frac{m+\mu-1}{2},\,2-\frac{m-\mu+1}{2};\frac{k^2}{4}\right)$$
$$=(\mu+1+m)(\mu+1-m)(ik)^{-\mu-1}s_{\mu,m}(ik). \quad \text{(A4)}$$

Using Eqs. (A3) and (A4) in Eq. (A2), we find that

$$\mathcal{J}_{\mu,m}(k)=\tfrac{1}{2}k^{-\mu-1}\,\Gamma\left(\frac{1+m-\mu}{2}\right)\left\{\Gamma\left(\frac{1-m+\mu}{2}\right)I_m(k)\right.$$
$$\left.-i^{-\mu-1}2^{1-\mu}\left[\Gamma\left(\frac{m+\mu+1}{2}\right)\right]^{-1}s_{\mu,m}(ik)\right\}, \quad \text{(A5)}$$

where, to obtain (A5), we have used the fact that

$$\frac{(\mu-m+1)(\mu+m+1)}{4}\,\Gamma\left(\frac{m-\mu-1}{2}\right)\left[\Gamma\left(\frac{3+m+\mu}{2}\right)\right]^{-1}$$
$$=-\Gamma\left(\frac{m-\mu+1}{2}\right)\left[\Gamma\left(\frac{1+m+\mu}{2}\right)\right]^{-1}.$$

We now introduce the modified Lommel function $\mathcal{L}_{\mu,\nu}(ik)$ which we define via

$$\mathcal{L}_{\mu,\nu}(ik)\equiv s_{\mu,\nu}(ik)-ie^{i\pi\mu/2}2^{\mu-1}$$
$$\times\Gamma\left(\frac{1+\mu+\nu}{2}\right)\Gamma\left(\frac{1+\mu-\nu}{2}\right)I_\nu(k). \quad \text{(A6)}$$

Hence the integral $\mathcal{J}_{\mu,m}(k)$ defined in Eq. (A1) becomes

$$\int_0^\infty dt\, t^{-\mu}J_m(t)(t^2+k^2)^{-1}$$
$$=-(ik)^{-\mu-1}\left[\Gamma\left(\frac{1+m-\mu}{2}\right)\Big/\Gamma\left(\frac{1+m+\mu}{2}\right)\right]$$
$$\times 2^{-\mu}\,\mathcal{L}_{\mu,m}(ik) \quad \text{(A7)}$$

provided, of course, $-m<\mathrm{Re}(1-\mu)<\frac{7}{2}$. Equation (A6) defines the functions $\mathcal{L}_{\mu,\nu}(ix)$ even when Eq. (A7) is no longer valid.

2. Recurrence Relations for $\mathcal{L}_{\mu,\nu}(ix)$

The Lommel Functions $s_{\mu,\nu}(z)$ and the Bessel functions $I_\nu(z)$ satisfy very similar sets of recurrence relations. Consequently, the modified Lommel functions $\mathcal{L}_{\mu,\nu}(ix)$ defined by Eq. (A6) satisfy recurrence relations similar to those for $s_{\mu,\nu}$. First of all we note that[21] $s_{\mu,\nu}(z)=s_{\mu,-\nu}(z)$ for all ν. However,[22] $I_\nu(z)=I_{-\nu}(z)$ only if ν is an integer. Therefore, from Eq. (A6) we have

$$\mathcal{L}_{\mu,\nu}(ix)=\mathcal{L}_{\mu-\nu}(ix)\ \text{ if, and only if, }\ \nu=0,\,1,\,2\ldots. \quad \text{(A8)}$$

The functions $s_{\mu,\nu}(z)$ satisfy the relation[21]

$$\frac{d}{dz}s_{\mu,\nu}(z)=(\mu+\nu-1)s_{\mu-1,\nu-1}(z)-\frac{\nu}{z}s_{\mu,\nu}(z).$$

From Eq. (A6) we therefore have

$$\frac{d}{dx}\mathcal{L}_{\mu,\nu}(ix)=i(\mu+\nu-1)s_{\mu-1,\nu-1}(ix)-\frac{\nu}{x}s_{\mu,\nu}(ix)$$
$$-ie^{i(\pi/2)\mu}2^{\mu-1}\Gamma\left(\frac{1+\nu+\mu}{2}\right)$$
$$\times\Gamma\left(\frac{1-\nu+\mu}{2}\right)\frac{d}{dx}I_\nu(x). \quad \text{(A9)}$$

However,[23]

$$\frac{d}{dx}I_\nu(x)=I_{\nu-1}(x)-\frac{\nu}{x}I_\nu(x);$$

and

$$\Gamma\left(\frac{1+\mu+\nu}{2}\right)\Gamma\left(\frac{1+\mu-\nu}{2}\right)$$
$$=\frac{\mu+\nu-1}{2}\,\Gamma\left(\frac{1+(\mu-1)+(\nu-1)}{2}\right)\Gamma$$
$$\times\left(\frac{1+(\mu-1)-(\nu-1)}{2}\right).$$

Hence, we may regroup the terms in Eq. (A9) and reapply (A6) to obtain

$$\frac{d}{dx}\mathcal{L}_{\mu,\nu}(ix)=i(\mu+\nu-1)\mathcal{L}_{\mu-1,\nu-1}(ix)$$
$$-\frac{\nu}{x}\mathcal{L}_{\mu,\nu}(ix). \quad \text{(A10)}$$

By similar methods, one also may prove that

$$\mathcal{L}_{\mu+2,\nu}(ix)=(ix)^{\mu+1}-[(\mu+1)^2-\nu^2]\,\mathcal{L}_{\mu,\nu}(ix), \quad \text{(A11)}$$

and that

$$-2i\frac{d}{dx}\mathcal{L}_{\mu,\nu}(ix)=(\mu+\nu-1)\mathcal{L}_{\mu-1,\nu-1}(ix)$$
$$+(\mu-\nu-1)\mathcal{L}_{\mu-1,\nu+1}(ix). \quad \text{(A12)}$$

Moreover, since (A10) holds, it is straightforward to show (proof by induction) that

$$\left(\frac{1}{x}\frac{d}{dx}\right)^m [x^\nu \mathcal{L}_{\mu,\nu}(ix)]$$

$$= \frac{i^m}{\mu+\nu+1}\left(\prod_{p=0}^{m}(\mu+\nu+1-2p)\right) x^{\nu-m}\mathcal{L}_{\mu-m,\nu-m}(ix). \tag{A13}$$

We also note, for example, that Eqs. (A10) and (A12) may be combined to eliminate the term $(d/dx)\mathcal{L}_{\mu,\nu}(ix)$. We emphasize the fact that Eqs. (A10)–(A13) are valid for all μ and ν for which the functions $\mathcal{L}_{\mu,\nu}(ix)$ are well defined.

3. Asymptotic Behavior $\mathcal{L}_{\mu,\nu}(ix)$

The asymptotic behavior of $\mathcal{L}_{\mu,\nu}(ix)$ for small x (μ and ν fixed) may be obtained from Eq. (A6) by retaining only the first few terms in the hypergeometric function expansions of the functions $s_{\mu,\nu}(ix)$ and $I_\nu(x)$. On the other hand, when x is large[24] $I_\nu(x) \sim (2\pi x)^{-1/2} e^x$; moreover, in view of Eq. (A7), we strongly suspect that $s_{\mu,\nu}(ix)$ behaves in a similar fashion. Therefore, we require some relation other than Eq. (A6) as a starting point for developing the asymptotic expansion of $\mathcal{L}_{\mu,\nu}(ix)$ for large x.

First we remark that $\mathcal{L}_{\mu,\nu}(ix)$ can also be expressed in terms of the Lommel function $s_{\mu,\nu}(ix)$, where[21]

$$S_{\mu,\nu}(z) \equiv s_{\mu,\nu}(z) + 2^{\mu-1}\,\Gamma\left(\frac{\mu+1-\nu}{2}\right)\Gamma\left(\frac{\mu+1+\nu}{2}\right) \times\left[\sin\left(\frac{\pi}{2}(\mu-\nu)\right)J_\nu(z) - \cos\left(\frac{\pi}{2}(\mu-\nu)\right)Y_\nu(z)\right]. \tag{A14}$$

If in Eq. (A14) we replace z by $iz = e^{i\pi/2}z$ then, since[19]

$$J_\nu(e^{i\pi/2}z) = e^{i(\pi/2)\nu} I_\nu(z)$$

and[23]

$$Y_\nu(e^{i\pi/2}z) = ie^{i(\pi/2)\nu} I_\nu(z) - (2/\pi)e^{-i\nu\pi/2}K_\nu(z)$$

we have, after rearranging terms,

$$S_{\mu,\nu}(ix) = s_{\mu,\nu}(ix) + 2^{\mu-1}\,\Gamma\left(\frac{1+\mu-\nu}{2}\right)\Gamma\left(\frac{1+\mu+\nu}{2}\right)\left[-ie^{i(\pi/2)\mu}I_\nu(x) + \frac{2}{\pi}e^{-i\nu\pi/2}\cos\left(\frac{\pi}{2}(\mu-\nu)\right)K_\nu(x)\right]. \tag{A15}$$

By comparing (A15) with (A6) we see immediately that

$$\mathcal{L}_{\mu,\nu}(ix) = S_{\mu,\nu}(ix) - 2^{\mu-1}\,\Gamma\left(\frac{1+\mu-\nu}{2}\right)\Gamma\left(\frac{1+\mu+\nu}{2}\right) \times\frac{2}{\pi}e^{-i(\pi/2)\nu}\cos\left(\frac{\pi}{2}(\mu-\nu)\right)K_\nu(x). \tag{A16}$$

The asymptotic behavior of $\mathcal{L}_{\mu,\nu}(ix)$ can be obtained directly from Eq. (A16). For large x, we have[24] $K_n(x) \sim (\pi/2x)e^{-x}$; moreover[21]

$$S_{\mu,\nu}(ix) \sim (ix)^{\mu-1}\left[\sum_{n=0}^{m}\left(\frac{1-\mu+\nu}{2}\right)_n\left(\frac{1-\mu-\nu}{2}\right)_n \times\left(\frac{x}{2}\right)^{-2n} + O(x^{-2m-2})\right], \tag{A17}$$

where $(a)_n$ is the Pochhammer symbol. Thus, if x is sufficiently large so that we may neglect entirely the term in (A16) dependent upon $K_\nu(x)$ then the asymptotic behavior of $\mathcal{L}_{\mu,\nu}(ix)$ is determined by (A17). Since Eq. (A17) also holds for $\mathcal{L}_{\mu,\nu}(ix)$, it should be clear that in Eq. (A6) the function $s_{\mu,\nu}(ix)$ must also diverge as e^x for large x in order to cancel the exponential behavior of $I_\nu(x)$.

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Configuration-Interaction Effects in the Scattering of Electrons by Atoms and Ions of Nitrogen and Oxygen*

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In this paper we report new and improved theoretical electron-impact cross sections involving energy levels of different electronic configurations of atomic nitrogen and oxygen, and some of their ions. The results are expected to be improvements over previously published work, based on a single (ground-state) configuration approximation, because allowance has been made for additional distortion of the target system by the projectile by taking into account the effect of either virtual or real transitions to different terms of excited electronic configurations. The effect of coupling to excited configurations on the total elastic and forbidden cross sections among the ground-state terms of atomic nitrogen and of N IV is discussed in detail. Cross sections are also given for selected transitions to terms of excited configurations in O II, O III, N II, N III, and N IV. Some new autoionizing series in O II and N II are predicted and suggestions are made for their experimental verification. Also, qualitative agreement with recent observations of autodetaching states in atomic oxygen is obtained and the existence of other as yet unobserved states is suggested. The results indicate the need for additional experiments in oxygen and nitrogen and especially a careful measurement of the electron-nitrogen scattering in the energy range 0–5 eV.

I. INTRODUCTION

In a previous paper Smith and Morgan[1] developed a theory for describing transitions, induced by electron impact, between any pair of terms in atomic systems. In this paper we report and discuss the results of the first systematic applications of this theory to the calculation of electron-impact excitation cross sections in atmospheric atoms and their ions. The main thrust of this work is an investigation of (i) the extent to which explicit allowance for different configuration interactions can be used to describe the details of low-energy-electron–complex-atom (ion) scattering and (ii) the degree to which the close-coupling approximation (CCA) can be effectively used to obtain accurate cross sections for a variety of excitation processes. Prior to the work reported here, use of this approximation to investigate the effect of configuration interaction in electron-atom scattering has been explicitly carried out only in the case of simple two- and three-electron systems.[2–4]

The forbidden and total cross sections in atomic nitrogen and oxygen and their ions have been the subject of several model calculations during the last 20 years,[5–14] and of some experimental investigations.[15–18] However, because of algebraic and computational problems, the different theoretical models emphasized either a particular transition or set of transitions, e.g., Seaton,[6] or specific interactions, e.g., Klein and Brueckner,[8] Bauer and Browne,[10] or Temkin.[7] This led to the result that the over-all effect of each type of approximation could not be realistically assessed.

The most intricate calculations to date for low-energy-electron–atmospheric-atom (ion) collisions have employed close coupling within the limitation of a single ground-state configuration approximation (Smith *et al.*[19] henceforth referred to as SC). In their model the eigenfunction expansion of the total wave function for the electron-target system was restricted to only the three terms of the ground-state configuration of the target. More recently, an attempt to allow for configuration interaction via implicit inclusion of some excited terms in ions has been carried out by Eissner and his colleagues.[20] However, the model they used is semiempirical because it relies on adjustable parameters. The present model is totally *ab initio*.

It has been emphasized in Smith, Henry, and