Generalized oscillator strength and Coulomb excitation

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Coulomb interaction is characterized by two nondimensional fundamental quantities: the Sommerfeld parameter η and the adiabaticity parameter $\xi=\eta_f-\eta_i$. In this different approach, we choose these variables to describe the behavior of the generalized oscillator strength (GOS). The expression we obtain is valid for scattering of electrons, positrons, and nuclei by arbitrary targets. We present asymptotic expansions, in the quantal and semiclassical approximation, of the electric dipole GOS.

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I. INTRODUCTION

We develop a method of analysis to study the *generalized oscillator strength* (GOS)

$$f(K)=\frac{E_{if}}{4}\frac{k_i}{k_f}K^2\frac{d\sigma^{CBe}(i\rightarrow f)}{d\Omega}, \tag{1.1}$$

in the Coulomb excitation of atomic systems [1].

The GOS represents the dynamical response of the atomic system to momentum transfer from a moving charged particle. The GOS information, for both the valence and inner-shell excitations of atoms and molecules, is of great interest in areas ranging from astrophysics and laser development to radiation biology.

The difference in our approach resides in the choice of the nondimensional variables η_i and ξ, and the deflection angle θ [2,3], to describe the behavior of GOS. The expression we obtain is valid for the scattering of electrons and nuclei by arbitrary targets.

The parameter η_i measures the strength of the interaction, while the parameter ξ gives an estimate of the collision time, and thus measures whether the process is *impulsive* ($\xi\ll 1$) or *adiabatic* ($\xi\gg 1$). We show in this paper a very important property that the limiting value of the GOS, as ξ goes to zero, is the optical oscillator strength (OOS). This limiting behavior of GOS may be used to put the *relative* experimental differential cross section (DCS) on an *absolute* scale [4–6].

The scalar $\hbar K$ denotes the magnitude of the momentum change vector, $\hbar\mathbf{K}=\hbar\mathbf{k_i}-\hbar\mathbf{k_f}$, when a particle is scattered through an angle θ. The squared magnitude of the vector $\mathbf{K}$ is then given by

$$\begin{aligned}K^2a_0^2&=k_i^2+k_f^2-2k_ik_f\cos(\theta)\\&=\left(\frac{Z_1Z_2M}{\eta_i\eta_f}\right)^2[\xi^2+4\eta_i\eta_f\sin^2(\theta/2)]\\&=ME_i\left[2-\frac{E_{if}}{E_i}-2\left(1-\frac{E_{if}}{E_i}\right)^{1/2}\cos(\theta)\right],\end{aligned} \tag{1.2}$$

where a_0 is the Bohr radius.

The dimensionless Sommerfeld parameter η_i is defined by

$$\eta_i=\frac{Z_1Z_2e^2}{\hbar v_i}=\frac{Z_1Z_2M}{k_i}=Z_1Z_2\sqrt{\frac{M}{E_i}}, \tag{1.3}$$

where Z_1 (Z_2) is the charge number of the projectile (atomic system), v_i is the relative velocity, k_i is the wave number measured in a_0^{-1} units, M is the reduced mass in electron-mass units, and E_i is the initial kinetic energy of relative motion measured in rydbergs (13.6 eV). The dimensionless adiabaticity parameter ξ is defined by

$$\begin{aligned}\xi=\eta_f-\eta_i=\eta_i\left[\left(1-\frac{E_{if}}{E_i}\right)^{-1/2}-1\right]\\=Z_1Z_2\sqrt{\frac{M}{E_i}}\left[\left(1-\frac{E_{if}}{E_i}\right)^{-1/2}-1\right],\end{aligned} \tag{1.4}$$

where the indices i and f refer to the initial and final states, respectively, and $E_{if}=E_i-E_f$ is the energy loss of the projectile measured in rydbergs.

The traditional approach is to analyze the behavior of GOS as a function of K or K^2 [7–16]. Since K combines into *one variable*, the distinct contributions of *three variables*: θ, η_i, and ξ or alternatively θ, E_i, and E_{if}, the mathematical analysis of GOS has been difficult, to say the least. Mzesane and co-workers have used this approach to conduct in-depth studies of GOS, for electron-impact excitation of neutral atoms (see Refs. [17,18], and references therein).

Some of the ground work for the present paper derives from earlier papers [19,20], henceforth referred to as I and II, respectively.

We begin our discussion with the quantal expression [21,22] of the electric dipole differential excitation cross section,

$$\frac{d\sigma^{CBe}(i\rightarrow f)}{d\Omega}=\frac{9Z_1^2M^2f_0}{4\pi k_i^2E_{if}}\frac{d\hat{f}_{E1}(\theta,\eta_i,\xi)}{d\Omega}a_0^2, \tag{1.5}$$

which determines the angular distribution of inelastically scattered particles in Coulomb excitation [2,3]. The differential cross section is obtained by asssuming the validity of the first-order time-independent perturbation theory, i.e., the Coulomb-Bethe approximation. We define the quantity $Z_1^2M^2f_0$, in Eq. (1.5) as the generalized OOS corresponding

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to transition $i \to f$. Notice that in the case of electron- or positron-impact excitation, $Z_1=1$ and $M=1$.

The differential excitation function is given by

$$\frac{d\hat{f}_{E1}(\theta,\eta_i,\xi)}{d\Omega}=\frac{8\pi^3\eta_i\eta_f}{9\xi^2}\frac{e^{-\pi\xi}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\times\frac{d}{dx}\left(-x\frac{d}{dx}\left|{}_2F_1(-i\eta_i,-i\eta_f;1;x)\right|^2\right). \tag{1.6}$$

We can convert the repulsive case ($\eta_i>0$) to the attractive case ($\eta_i<0$) by simply switching the signs of η_i, η_f, and ξ. The only, but crucial, effect of this transformation is to replace the factor of $\exp(-\pi\xi)$, for repulsive potentials, by a factor of $\exp(+\pi\xi)$, for attractive potentials, in which ξ is positive. Throughout the paper we consider ξ and θ positive.

The argument x is defined by

$$x=-4\sin^2(\theta/2)\frac{\eta_i\eta_f}{\xi^2}=-4\sin^2(\theta/2)\frac{(1-E_{if}/E_i)^{1/2}}{[1-(1-E_{if}/E_i)^{1/2}]^2}, \tag{1.7}$$

where θ is the deflection angle of the scattered particle. Gauss's hypergeometric function ${}_2F_1(a,b;c;z)$ is defined by

$${}_2F_1(a,b;c;z)=\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{n!(c)_n}z^n, \tag{1.8}$$

within the circle of convergence $|z|<1$ and by analytic continuation elsewhere. Henceforth, we omit the subscripts and write ${}_2F_1(\cdots)$ simply as $F(\cdots)$. We used the symbolic computation program MAPLE VI [23] to help us with the algebraic manipulations.

II. GENERALIZED OSCILLATOR STRENGTH

By substituting Eqs. (1.2), (1.5), and (1.6) into Eq. (1.1), we obtain

$$f(\theta,\eta_i,\xi)=\frac{\pi^2}{2}f_0Z_1^2M^2\xi^{-2}[\xi^2+4\eta_i\eta_f\sin^2(\theta/2)]\times\frac{e^{-\pi\xi}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\frac{d}{dx}\times\left(-x\frac{d}{dx}\left|{}_2F_1(-i\eta_i,-i\eta_f;1;x)\right|^2\right). \tag{2.1}$$

We perform differentiation in the previous equation using Eq. (15.2.2) of Ref. [25] and, after some manipulation, we obtain (Paper II)

$$\begin{aligned}f(\theta,\eta_i,\xi)={}&\frac{\pi^2}{2}f_0Z_1^2M^2\eta_i\eta_f\xi^{-2}[\xi^2+4\eta_i\eta_f\sin^2(\theta/2)]\\&\times\frac{e^{-\pi\xi}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\{2\,\mathrm{Re}[F(1-i\eta_i,\\&1-i\eta_f;2;x)F(i\eta_i,i\eta_f;1;x)]\\&+x[\mathrm{Re}\{(1-i\eta_i)(1-i\eta_f)F(2-i\eta_i,\\&2-i\eta_f;3;x)F(i\eta_i,i\eta_f;1;x)\}\\&-2\eta_i\eta_f|F(1-i\eta_i,1-i\eta_f;2;x)|^2]\}.\end{aligned} \tag{2.2}$$

For neutral targets ($Z_2=0$), the parameters ξ, η_i, and η_f vanish, and the argument x is finite for $E_i \gg E_{if}$. In this case, the hypergeometric functions reduce to elementary functions, and one can show that

$$f(\theta,0,0)=f_0Z_1^2M^2, \tag{2.3}$$

for arbitrary values of the colliding energy E_i. This limit is known as the Lassettre limit theorem [7].

For ionized targets ($Z_2\neq 0$), this functional form of GOS is suitable for colliding energies $E_i \to E_{if}$, that is the argument $x\to 0$. The parameters ξ and η_f, on the other hand, tend to infinity, whereas η_i remains finite.

We also obtain an equivalent definition of GOS, appropriate for $\xi\to 0$, i.e., the condition $E_i \gg E_{if}$ and ionized targets. The definition below is also suitable for $\xi \not\to 0$, with $\eta_i,\eta_f \to\infty$. We use the analytic continuations (15.3.5) and (15.3.6) of Ref. [25], and some intricate manipulation (Paper I) yields

$$\begin{aligned}f(\theta,\eta_i,\xi)={}&\pi^2f_0Z_1^2M^2e^{-\pi\xi}\frac{\eta_i\eta_f}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\Bigg\{\frac{|\Gamma(\mathrm{i}\,\xi)|^2}{|\Gamma(1+\mathrm{i}\eta_i)|^2\Gamma(1+\mathrm{i}\eta_f)|^2}[\mathrm{Im}(e_1-e_3)-\mathrm{Re}(e_4)]\\&+\mathrm{Im}\left(\frac{t^{-\mathrm{i}\xi}\Gamma^2(\mathrm{i}\xi)}{\Gamma^2(1-\mathrm{i}\eta_i)\Gamma^2(1+\mathrm{i}\eta_f)}(e_2-e_5)\right)-\mathrm{Re}\left(\frac{t^{-\mathrm{i}\xi}\Gamma^2(\mathrm{i}\xi)}{\Gamma^2(1-\mathrm{i}\eta_i)\Gamma^2(1+\mathrm{i}\eta_f)}(e_6)\right)\\&+t\Bigg[\frac{|\Gamma(\mathrm{i}\,\xi)|^2}{|\Gamma(1+\mathrm{i}\eta_i)|^2\Gamma(1+\mathrm{i}\eta_f)|^2}[\mathrm{Im}(e_3)+\mathrm{Re}(e_4)]+\mathrm{Im}\left(\frac{t^{-\mathrm{i}\xi}\Gamma^2(\mathrm{i}\xi)}{\Gamma^2(1-\mathrm{i}\eta_i)\Gamma^2(1+\mathrm{i}\eta_f)}(e_5)\right)\\&+\mathrm{Re}\left(\frac{t^{-\mathrm{i}\xi}\Gamma^2(\mathrm{i}\xi)}{\Gamma^2(1-\mathrm{i}\eta_i)\Gamma^2(1+\mathrm{i}\eta_f)}(e_6)\right)\Bigg]\Bigg\},\end{aligned} \tag{2.4}$$

where

$$t=\frac{\xi^2}{\xi^2+4\eta_i\eta_f\sin^2(\theta/2)}=\frac{[1-(1-E_{if}/E_i)^{1/2}]^2}{[1-(1-E_{if}/E_i)^{1/2}]^2+4\sin^2(\theta/2)(1-E_{if}/E_i)^{1/2}}, \tag{2.5}$$

and

$$e_1=-\eta_iF(1+i\eta_i,1-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t)+\eta_fF(1+i\eta_i,1-i\eta_f;1-i\xi;t)\times F(-i\eta_i,1+i\eta_f;1+i\xi;t), \tag{2.6}$$

$$e_2=-\eta_fF(1+i\eta_i,1-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t)+\eta_iF(1+i\eta_i,1-i\eta_f;1-i\xi,t)\times F(1+i\eta_i,-i\eta_f;1-i\xi;t), \tag{2.7}$$

$$e_3=-\eta_iF(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t)+\eta_fF(2+i\eta_i,1-i\eta_f;1-i\xi;t)\times F(-i\eta_i,1+i\eta_f;1+i\xi;t), \tag{2.8}$$

$$e_4=\eta_i\eta_f[F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t)+F(2+i\eta_i,1-i\eta_f;1-i\xi;t)\times F(-i\eta_i,1+i\eta_f;1+i\xi;t)-2F(1-i\eta_i,1+i\eta_f;1+i\xi;t)F(1+i\eta_i,1-i\eta_f;1-i\xi;t)], \tag{2.9}$$

$$e_5=-\eta_fF(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t)+\eta_iF(2+i\eta_i,1-i\eta_f;1-i\xi;t)\times F(1+i\eta_i,-i\eta_f;1-i\xi;t), \tag{2.10}$$

$$e_6=\eta_f^2F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t)+\eta_i^2F(2+i\eta_i,1-i\eta_f;1-i\xi;t)F(1+i\eta_i,-i\eta_f;1-i\xi;t)-2\eta_i\eta_fF^2(1+i\eta_i,1-i\eta_f;1-i\xi;t). \tag{2.11}$$

The above expression has the advantage that all of the hypergeometric functions are evaluated at t, a variable bounded between zero and one, which is small provided the condition

$$\xi^2\ll 4\eta_i\eta_f\sin^2\left(\frac{\theta}{2}\right) \tag{2.12}$$

holds. Over most of the angular range available, this condition can be met for small enough ξ, so Eq. (2.4) is ideal for taking the limit $\xi\to 0$. A problem arises, however, when $\theta=0$ or $E_i=E_{if}$, since, in that case, $t\equiv 1$. If $E_i=E_{if}$, one should use Eq. (2.2). Accordingly, we distinguish the cases $\theta=0$ and $\theta\neq 0$. Figure 1 displays the variable t as a function of θ for different values of ξ and η_i.

III. ANGLE $\theta=0$

We can take the limit as $\theta\to 0$ in Eq. (2.2), provided we also assume that $\xi\neq 0$, i.e., the collision is inelastic. Under these conditions, $x=0$ and, since all the hypergeometric functions have the value of unity, we obtain

$$f(0,\eta_i,\xi)=f_0Z_1^2M^2\pi^2\eta_i\eta_f\frac{e^{-\pi\xi}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)} \tag{3.1}$$

for ionized targets.

We consider the following possibilities.

(1) The initial kinetic energy $E_i\gg E_{if}$. It is then straightforward to show that $\xi/\eta_i\ll 1$; see the definition (1.4) of ξ. If, in addition, we have $\pi\eta_i\ll 1$, then Eq. (3.1) reduces to

$$f(0,\eta_i,\xi)\approx f_0Z_1^2M^2e^{-\pi\xi}\left(1-\frac{\pi^2\eta_i^2}{3}\right), \tag{3.2}$$

to a second order in $\pi\eta_i$. The same result was obtained by Ancarani [16], using the standard approach of considering GOS a function of K. Obviously $f(0,0,0)=f_0Z_1^2M^2$.

(2) The initial kinetic energy $E_i\to E_{if}$, i.e., $E_f\to 0$. Here, the parameters $\xi,\eta_f\to\infty$, whereas η_i remains finite; see the definitions (1.3) and (1.4) of η_i and ξ, respectively. The asymptotic behavior of $f(0,\eta_i,\xi)$ as $\xi\to\infty$ is different for repulsive and attractive potentials. It diverges linearly with ξ in the case of attractive potentials, and converges to zero for repulsive ones

$$f(0,\eta_i,\xi\to\infty)\approx 2f_0Z_1^2M^2\pi^2\eta_i\frac{e^{-\pi\eta_i}}{\sinh\pi(\eta_i)}\times\begin{cases}\xi\to\infty, & \text{attractive}\\ \xi e^{-2\pi\xi}\to 0, & \text{repulsive.}\end{cases} \tag{3.3}$$

(3) One may encounter situations in which it might be correct to assume that η_i, $\eta_f\to\infty$, and ξ is finite (semiclassical approximation). This is the case of highly charged ions being excited by incoming heavy particles. In such a limit, we have the asymptotic behavior

$$f^{class}(0,\eta_i\to\infty,\xi)\approx 4f_0Z_1^2M^2\pi^2\times\begin{cases}\eta_i^2e^{-2\pi\eta_i}\to 0, & \text{attractive}\\ e^{-2\pi\xi}\eta_i^2e^{-2\pi\eta_i}\to 0, & \text{repulsive.}\end{cases} \tag{3.4}$$

IV. ANGLE $\theta\neq 0$

The GOS is a rather complicated function of its parameters θ, η_i, and ξ. To study its asymptotic behavior, we distinguish three cases, as in $\theta=0$.

A. No energy loss ($\xi\to 0$)

The energy loss by the projectile, $E_{if}=E_i-E_f$, is small compared to its initial energy E_i. We use Eq. (2.4) and, upon application of Eqs. (6.1.29) and (6.1.31) of Ref. [25], we find

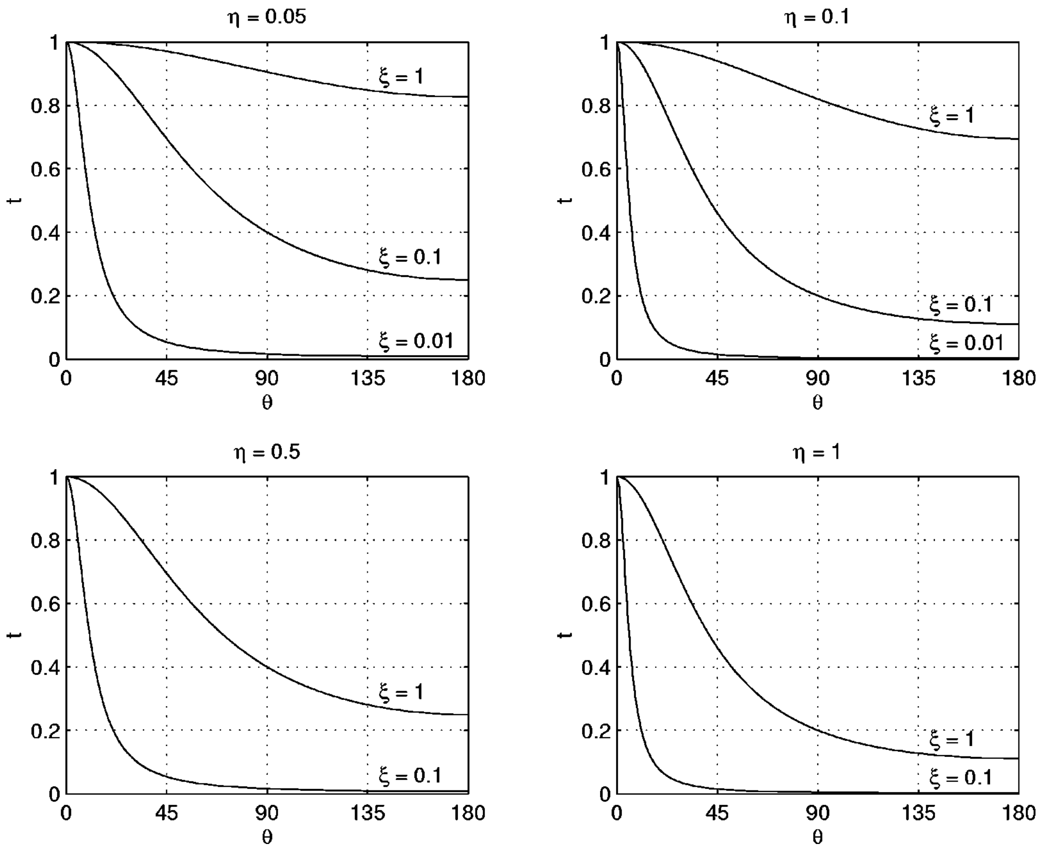

FIG. 1. $t=\xi^2/[4\eta(\eta+\xi)\sin^2(\theta)]$ as a function of the deflection angle θ in degrees. We use the variable name $\eta_i=\eta$ and express η_f as $\eta+\xi$. For small values of ξ, the variable t is small compared to unity except for a narrow interval around $\theta=0$. At $\theta=0$, $t\equiv 1$ for all η and ξ.

$$f(\theta,\eta_i,\xi)=f_0Z_1^2M^2\frac{\pi\xi}{\sinh(\pi\xi)}e^{-\pi\xi}\Bigg\{\mathrm{Im}\left(\frac{e_1-e_3}{\xi^2}\right)-\mathrm{Re}\left(\frac{e_4}{\xi^2}\right)+\mathrm{Im}\left[e^{i\varphi}\left(\frac{e_2-e_5}{\xi^2}\right)\right]-\mathrm{Re}\left[e^{i\varphi}\frac{e_6}{\xi^2}\right]+t\left[\mathrm{Im}\left(\frac{e_3}{\xi^2}\right)+\mathrm{Re}\left(\frac{e_4}{\xi^2}\right)+\mathrm{Im}\left(e^{i\varphi}\frac{e_5}{\xi^2}\right)+\mathrm{Re}\left(e^{i\varphi}\frac{e_6}{\xi^2}\right)\right]\Bigg\}, \quad (4.1)$$

where the phase φ is given by

$$\varphi=\arg\left[-\frac{t^{-i\xi}\Gamma^2(1+i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}\right]=\pi+\alpha, \quad (4.2)$$

$$\alpha=-\xi\ln\left(\frac{\xi^2}{\xi^2+4\eta_i\eta_f\sin^2(\theta/2)}\right)+2\arg\Gamma(1+i\xi)-2\arg\Gamma(1-i\eta_i)-2\arg\Gamma(1+i\eta_f), \quad (4.3)$$

and the parameter t by Eq. (2.5).

Since $E_i \gg E_{if}$, $\xi/\eta_i \ll 1$, and $\xi \ll 1$. It is therefore a good approximation to neglect the energy loss completely and consider the limit $\xi\to 0$. We also consider angles θ, such that $t=\xi^2/[4\eta_i\eta_f\sin^2(\theta/2)]\ll 1$.

Since we have factorized the expression (4.1) into subexpressions, all of which have finite limits as $\xi\to 0$, we may take the limits of each factor separately and combine them afterwards. We expand the six subexpressions (2.6)–(2.11) as a series in ξ, making sure to take into account the additional factors of ξ, due to the relation between the variables $\eta_f=\eta_i+\xi$. Upon substitution of these asymptotic forms into Eq. (4.1), we find

$$f(\theta,\eta_i,\xi)\approx f_0Z_1^2M^2\frac{\pi\xi}{\sinh(\pi\xi)}\times e^{-\pi\xi}\Bigg\{\cos(\alpha)+\frac{1}{2\sin^2(\theta/2)}[1-\cos(\alpha)]-\frac{\xi}{2\sin^2(\theta/2)}\sin(\alpha)+\frac{\xi^2}{8\sin^4(\theta/2)}\times\left[3[1-\cos(\alpha)]-\frac{1}{4\sin^2(\theta/2)}\right]\Bigg\}, \quad (4.4)$$

where

$$\alpha=\xi\ln\left(\frac{4\eta_i^2\sin^2(\theta/2)}{\xi^2}\right). \quad (4.5)$$

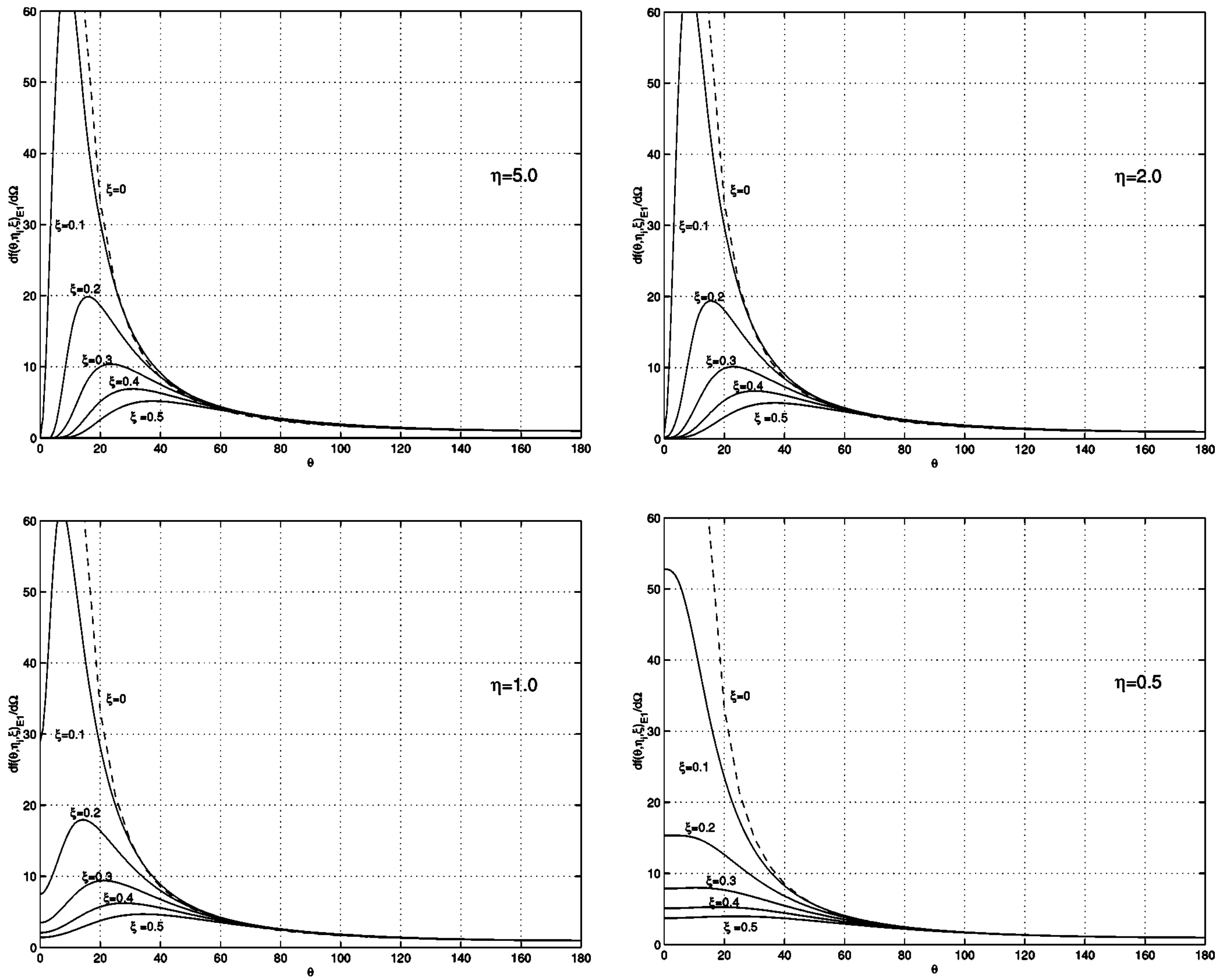

FIG. 2. The differential $E1$ excitation function $d\hat{f}_{E1}(\eta,\xi,\theta)/d\Omega$ for various values of η ($\eta_i=\eta$) as a function of the deflection angle θ in degrees. $-$, quantal expression; $--$, classical expression. The limit as $\xi \rightarrow 0$ is independent of η. The plots are normalized so that $d\hat{f}_{E1}(\theta=180°)/d\Omega=1$. With this normalization, there is no distinction between the repulsive and attractive cases.

Notice, of course, that we are left with the intensely anticlimactic result $f(\theta,\eta_i,\xi)\rightarrow f_0 Z_1^2 M^2$ as $\xi\rightarrow 0$.

In the limit of $\xi^2/(4\eta_i\eta_f \sin^2(\theta/2) \ll 1$, the differential excitation function (1.6) reduces to

$$\frac{d\hat{f}_{E1}(\theta,\eta_i,\xi)}{d\Omega}\approx\frac{4}{9}\frac{\pi}{\sin^2(\theta/2)}\frac{\pi\xi}{\sinh(\pi\xi)} \times e^{-\pi\xi}\left\{\cos(\alpha)+\frac{1}{2\sin^2(\theta/2)}[1-\cos(\alpha)] -\frac{\xi}{2\sin^2(\theta/2)}\sin(\alpha)+\frac{\xi^2}{8\sin^4(\theta/2)} \times\left[3[1-\cos(\alpha)]-\frac{1}{4\sin^2(\theta/2)}\right]\right\}. \tag{4.6}$$

For $\xi\rightarrow 0$, one obtains from Eq. (4.6) the formula

$$\frac{d\hat{f}_{E1}(\theta,\eta_i,0)}{d\Omega}=\frac{4}{9}\frac{\pi}{\sin^2(\theta/2)}, \tag{4.7}$$

which coincides exactly with the classical result quoted by Alder *et al.* (see Secs. II E.71 and II A.29 of Ref. [24]). The behavior of the quantal expression, and its convergence to the classical expression is illustrated in Fig. 2.

Figure 3 shows the normalized exact GOS, $f(\theta,\eta_i,\xi)/f_0 Z_1^2 M^2$, for *attractive* potentials [replace exp $(-\pi\xi)$ by $\exp(+\pi\xi)$ in Eq. (4.1)], and different values of η_i and ξ. For small ξ, the GOS tends to the optical oscillator strength $f_0 Z_1^2 M^2$, as expected. As η_i increases, the contribution from small angles decreases. Figure 4 displays the approximate GOS, given by Eq. (4.4), as well the exact one, for $\eta_i=0.5$ and $\xi=0.1$. The approximate form is in excellent agreement with the exact GOS, for angles greater than 40°, i.e., $\xi^2/4\eta_i^2\sin^2(\theta/2)\leqslant 0.024$.

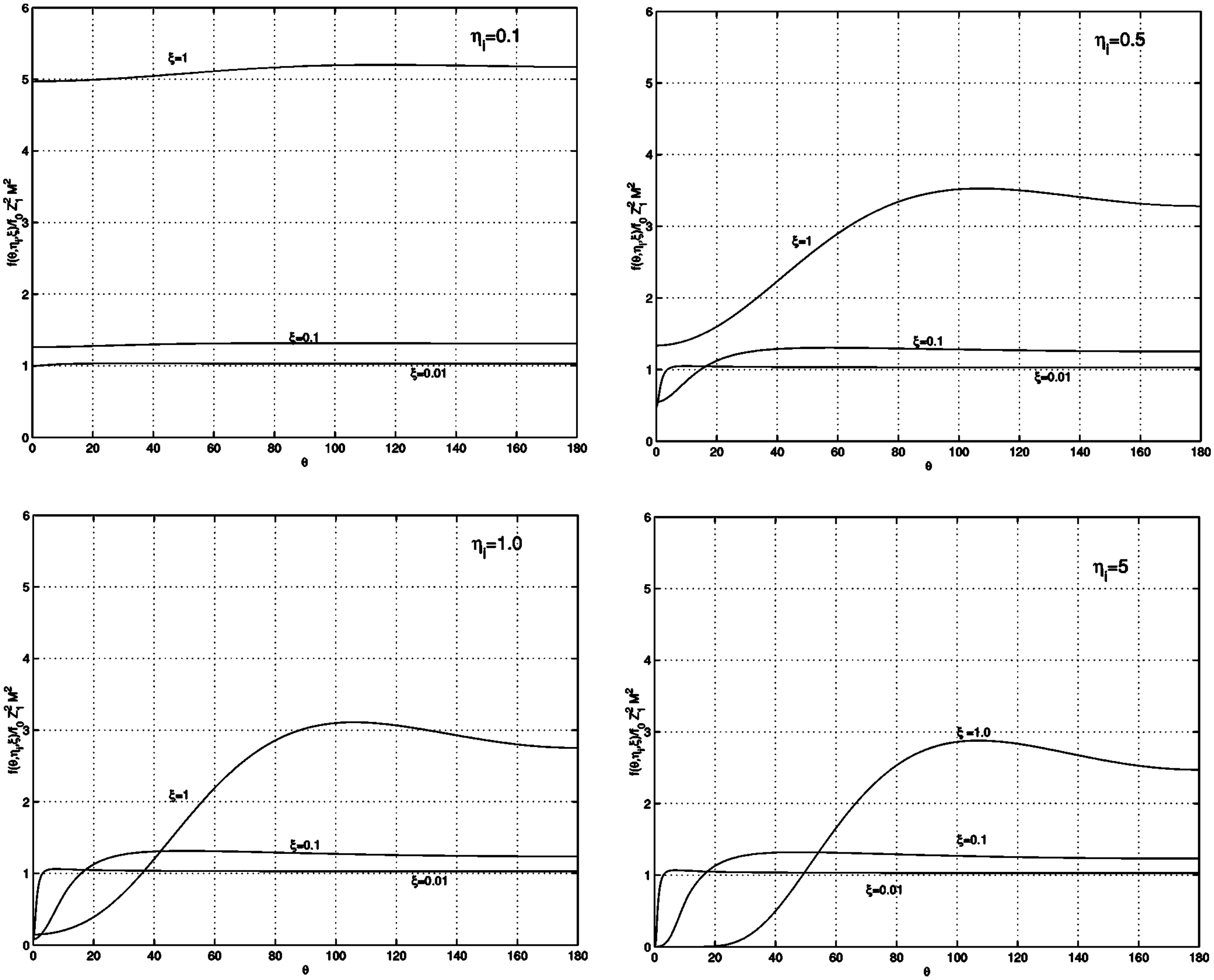

FIG. 3. Quantal GOS, for an attractive Coulomb field, for various values of η_i and ξ [Eq. (4.1)]. The normalized function $f(\theta,\eta_i,\xi)/f_0Z_1^2M^2$ plotted as a function of the deflection angle θ in degrees.

B. Total-energy loss ($\xi\rightarrow\infty$)

The projectile transfers a large proportion of its energy to the target in the collision. In this case, $E_i\rightarrow E_{if}$ implies $\xi,\eta_f\rightarrow\infty$ and η_i finite. We begin with Eq. (2.2) and, using results derived in Paper II, we distinguish between the attractive and repulsive potentials

$$f(\theta,\eta_i,\xi)\approx 2f_0Z_1^2M^2\pi^2\eta_i\frac{e^{-\pi\eta_i}}{\sinh(\pi(\eta_i)}g(\theta,\eta_i)\times\begin{cases}\xi\rightarrow\infty, & \text{attractive}\\ \xi e^{-2\pi\xi}\rightarrow 0, & \text{repulsive,}\end{cases}\tag{4.8}$$

where

$$\begin{aligned}g(\theta,\eta_i)=\mathrm{Re}[{}_1F_1(1-i\eta_i,2;z_0)\,{}_1F_1(i\eta_i,1;-z_0)\\+2i\eta_i(1-i\eta_i)\sin^2\left(\frac{\theta}{2}\right){}_1F_1(2-i\eta_i,3;z_0\\\times{}_1F_1(i\eta_i,1;-z_0)]+4\eta_i^2\sin^2\left(\frac{\theta}{2}\right)\\\times|{}_1F_1(1-i\eta_i,2;z_0)|^2,\end{aligned}\tag{4.9}$$

and $z_0=4\,\mathrm{i}\eta_i\sin^2(\theta/2)$. In Figs. 5 and 6, we show the quotient $f(\theta,\eta_i,\xi)/f(0,\eta_i,\xi)$, calculated using the exact quantal expressions (2.2) for $\theta\neq 0$ and (3.1) for $\theta=0$, and the asymptotic expression $g(\theta,\eta_i)=f(\theta,\eta_i,\xi\rightarrow\infty)/f(0,\eta_i,\xi\rightarrow\infty)$. With this normalization of $f(\theta,\eta_i,\xi)$, there is no distinction between the repulsive and attractive cases.

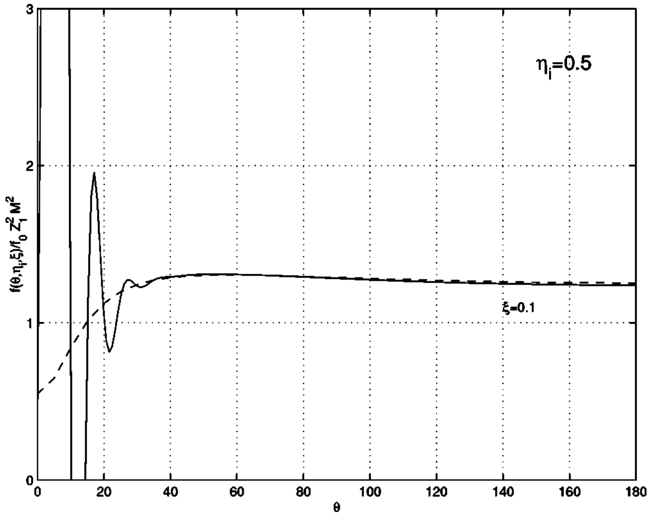

FIG. 4. Normalized GOS, for an attractive Coulomb field, as a function of the deflection angle θ in degrees. $--$, quantal expression (4.1); $-$, approximate expression (4.4) corresponding to $\xi \to 0$.

C. Semiclassical approximation: $\eta_i, \eta_f \to \infty$, $\xi = \eta_f - \eta_i$ finite

In the quantal expression (2.4), we let $\eta_i, \eta_f \to \infty$, with the restriction that $\xi = \eta_f - \eta_i$ remains finite, which leads to (Paper I)

$$f^{class}(\theta, \eta_i \to \infty, \xi) \approx f_0 Z_1^2 M^2 \xi^2 e^{-\pi\xi} \frac{1}{\sin^2(\theta/2)} \times \left\{ \cos^2(\theta/2) K_{i\xi}^2\left(\frac{\xi}{\sin(\theta/2)}\right) + K_{i\xi}^{\prime 2}\left(\frac{\xi}{\sin(\theta/2)}\right) \right\}, \tag{4.10}$$

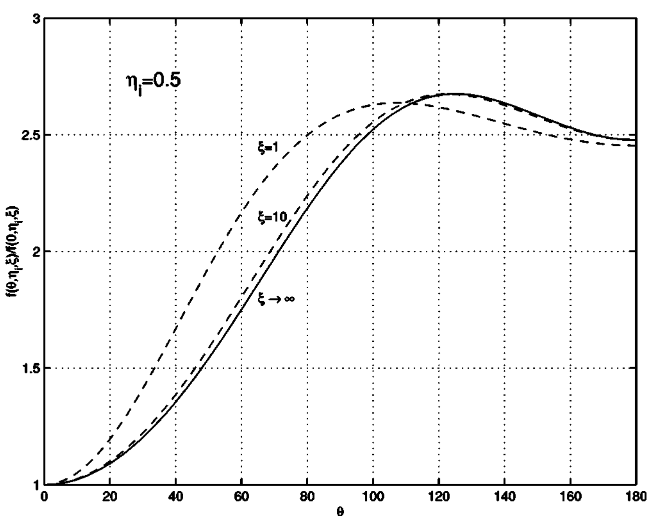

FIG. 5. Quantal GOS, for an attractive Coulomb field, for large values of ξ. Normalized function $f(\theta, \eta_i, \xi)/f(0, \eta_i, \xi)$ plotted as a function of the deflection angle θ in degrees. $--$, quantal expression (2.2); $-$, asymptotic expression (4.8). With this normalization, there is no distinction between the repulsive and attractive cases.

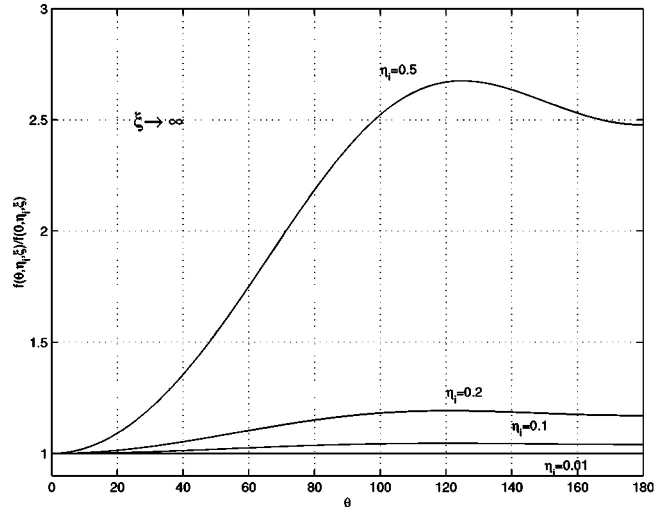

FIG. 6. Normalized asymptotic GOS ($\xi \to \infty$), plotted as a function of the deflection angle θ in degrees, for increasing values of η_i [Eq. (4.8)].

where $K_\nu(z)$ is the modified Bessel function of the second kind, and $K'_\nu(z)$ is its derivative with respect to its argument z. It is straightforward to show, using the relations (9.6.8), (9.6.9), and (9.6.27) of Ref. [25], that $f^{class}(\theta, \eta_i \to \infty, \xi) \to f_0 Z_1^2 M^2$ as $\xi \to 0$.

Figures 7 and 8 show the correspondence of the quantum-mechanical (2.4) and the semiclassical results (4.10) for *attractive* potentials [replace $\exp(-\pi\xi)$ by $\exp(+\pi\xi)$ in the corresponding formulas]. Figure 9 illustrates the singular behavior, at $\theta = 0$, of the semiclassical approximation as $\xi \to 0$, namely,

$$\frac{f^{class}(\theta, \eta_i \to \infty, \xi)}{f_0 Z_1^2 M^2} = \begin{cases} 0, & \text{for} \quad \theta = 0 \\ 1, & \text{for} \quad \theta \neq 0. \end{cases} \tag{4.11}$$

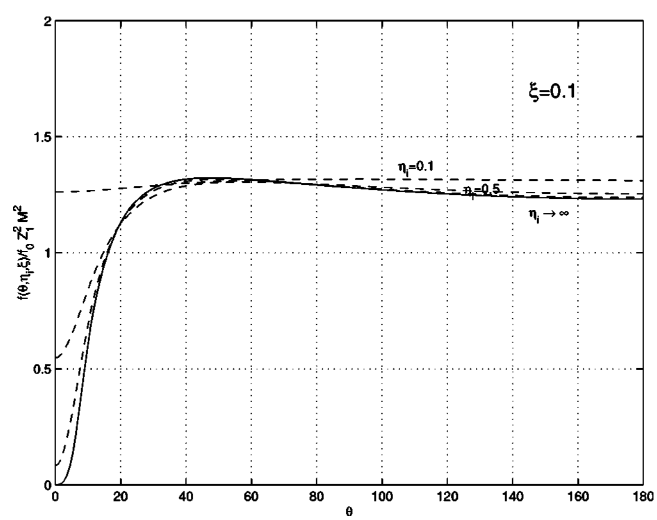

FIG. 7. Normalized GOS, for an attractive Coulomb field, plotted as a function of the deflection angle θ in degrees, for $\xi = 0.1$ and increasing values of η_i. $--$, quantal expression (2.4); $-$, semiclassical expression (4.10). The case $\eta_i = 1.0$ is almost indistinguishable from the $\eta_i \to \infty$ case, except at very small angles.

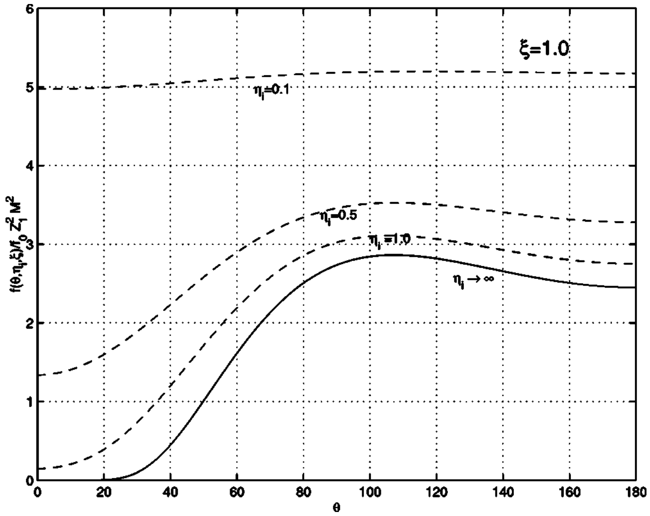

FIG. 8. Normalized GOS, for an attractive Coulomb field, plotted as a function of the deflection angle θ in degrees, for $\xi=1$ and increasing values of η_i. $--$, quantal expression (2.4); $-$, semiclassical expression (4.10).

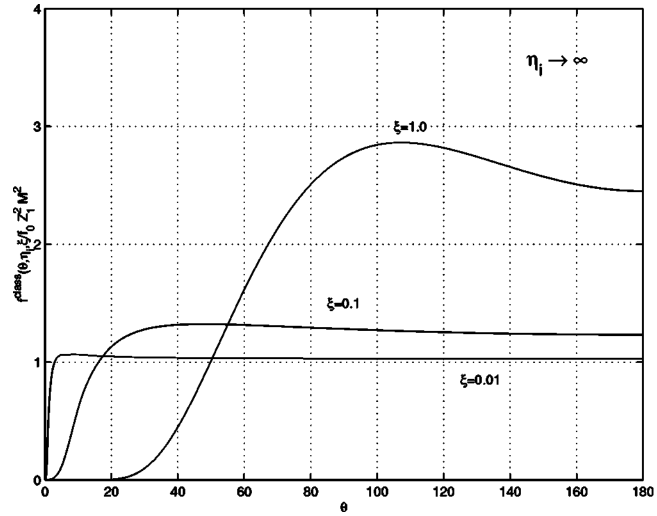

FIG. 9. Normalized asymptotic GOS ($\eta_i\to\infty$), plotted as a function of the deflection angle θ in degrees, for decreasing values of ξ [Eq. (4.10)]. As $\xi\to 0$, $f^{class}(\theta,\eta_i,\xi)/f_0 Z_1^2 M^2$ tends to one for $\theta\neq 0$ and zero for $\theta=0$.

The present calculations have been performed as an initial step in a more general investigation of GOS and Coulomb excitation. Future work will include the systematic application and testing our formulation to the available data on charged particles. We plan to improve our study of the asymptotic behavior of GOS by considering the Coulomb-Born approximation, which will investigate the importance of electron-exchange effects. A further extension could come from studying relativistic effects in the Born series approach, which should be particularly relevant for the excitation or ionization of heavy-atomic targets.

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[1] H.A. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).
[2] L. C. Biedenharn and P. J. Brussaard, *Coulomb Excitation* (Clarendon Press, Oxford, 1965).
[3] K. Alder and A. Winther, *Coulomb Excitation* (Academic Press, New York, 1966).
[4] C. Backx, R.R. Tol, G.R. Wight, and M.J. VanderWiel, J. Phys. B: At., Mol. Phys. **8**, 2050 (1975).
[5] M. Ismail and P.J. Teubner, J. Phys. B **28**, 4149 (1995).
[6] X.W. Fan and K.T. Leung, Phys. Rev. A **62**, 062703 (2000).
[7] E.N. Lassettre, A. Skerbele, and M.A. Dillon, J. Chem. Phys. **50**, 1829 (1969).
[8] M. Inokuti, Rev. Mod. Phys. **43**, 297 (1971).
[9] K.N. Klump and E.N. Lassetre, J. Chem. Phys. **68**, 886 (1978).
[10] S.J. Buckman, C.J. Noble, and P.J.O. Teubner, J. Phys. B: At., Mol. Phys. **12**, 3077 (1979).
[11] W.M. Huo, J. Chem. Phys. **71**, 1593 (1979).
[12] R.A. Bonham and R.R. Goruganthu, J. Chem. Phys. **84**, 3068 (1986).
[13] K. Sakimoto and Y. Itikawa, Phys. Rev. A **40**, 3646 (1989).
[14] L. U. Ancarani, in Proceedings of the First Europhysics Study Conference on Photon and Electron Collisions with Atoms and Molecules, Roma, Italy, 1992.
[15] J. Mitroy, J. Phys. B **26**, 2201 (1993).
[16] L. U. Ancarani, Ph.D. dissertation, University of Cambridge, 1994 (unpublished).
[17] A.Z. Msezane, Z. Felfli, M.Ya. Amusia, Z. Chen, and L.V. Chernysheva, Phys. Rev. A **65**, 054701 (2002).
[18] A.Z. Msezane, Z. Felfli, and D. Bessis, Phys. Rev. A **65**, 050701(R) (2002).
[19] M.D. Thorsley and M.C. Chidichimo, J. Math. Phys. **42**, 1921 (2001).
[20] M.C. Chidichimo and M.D. Thorsley, J. Math. Phys. **42**, 5371 (2001).
[21] C.J. Mullin and E. Guth, Phys. Rev. **82**, 141 (1951).
[22] R. Huby and H.C. Newns, Proc. Phys. Soc., London, Sect. A **64**, 619 (1951).
[23] M.B. Monagan, K.O. Geddes, K. M. Heal, G. Labahn, S. M. Vorkoetter, J. McCarron, and P. DeMarco, *The Maple Programming Guide* (Waterloo Maple Inc., Waterloo, ON, Canada, 2001).
[24] K. Alder, A. Bohr, T. Huus, B. Mottelson, and A. Winther, Rev. Mod. Phys. **28**, 432 (1956).
[25] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I.A. Stegun (Dover, New York, 1972).