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Numerical Calculation of the Limiting Properties of Coulomb Excitation Functions*

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We present techniques for evaluating the coefficients of the leading terms for both the high ($\xi = 0$) and low ($\xi \gg 1$) energy limits of classical nuclear Coulomb excitation. Results are given for ion-induced electric and magnetic transitions up to $\lambda = 10$ that are required for astrophysical calculations of the effectiveness of certain stellar environments in enhancing the radiative deexcitation rates of important long-lived isomeric states.

1. INTRODUCTION

In calculating the classical Coulomb process [1–3] of inducing excited-state transitions in a heavy target nucleus by the time-varying electromagnetic field of an incoming *ion* projectile (that does not "penetrate" the nucleus), the problem can be conveniently separated into: (i) a purely nuclear part that depends only on the internal details of the transition, and (ii) the external details of the relative motion of the target and the projectile during their mutual electromagnetic interaction. The work presented here is motivated by the recent interest in calculating the effectiveness of inelastic charged-particle collisions in the stellar interior [4–6] in enhancing the spontaneous radiative-decay rates of long-lived isomeric states [7–9] formed in various processes of nucleosynthesis. Most isomers of interest are encountered in studies of branching in the path of heavy element formation by slow neutron capture (the so-called *s*-process) [9, 10].

In the case of both electric and magnetic transition types, the semiclassical cross section for exciting a given transition in the target nucleus is proportional to a quantity known as the Coulomb excitation function [1]. These functions in turn depend only on a dimensionless parameter, ξ, which is a measure of the relative energy change of the incident projectile during the encounter. The limit $\xi \to 0$ physically corresponds to a "sudden" collision with negligible energy change, while the other extreme of $\xi \gg 1$ obtains for a slow adiabatic collision in which the projectile gives up a significant fraction of its initial energy. These important Coulomb excitation

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functions, $f_{E\lambda}(\xi)$ and $f_{M\lambda}(\xi)$, for electric and magnetic excitation of multipole order λ are given [1] explicitly as

$$f_{E\lambda}(\xi) = \frac{4\pi^2}{(2\lambda + 1)^2} \sum_{\substack{\mu=-\lambda \\ (\mu+\lambda,\text{even})}}^{+\lambda} A(\lambda, \mu) \int_0^{\pi} | I_{\lambda,\mu}(\theta, \xi)|^2 \frac{\cos(\theta/2)}{[\sin(\theta/2)]^3} \, d\theta \tag{1}$$

and

$$f_{M\lambda}(\xi) = \frac{4\pi^2}{\lambda^2(2\lambda + 1)^2} \sum_{\substack{\mu=-\lambda \\ (\mu+\lambda,\text{even})}}^{+\lambda} \frac{1}{A(\lambda, \mu)} \int_0^{\pi} | I_{\lambda+1,\mu}(\theta, \xi)|^2 \left(\cot \frac{\theta}{2}\right)^2 \frac{\cos(\theta/2)}{[\sin(\theta/2)]^3} \, d\theta, \tag{2}$$

where

$$A(\lambda, \mu) \equiv \frac{(\lambda - \mu)! \, (\lambda + \mu)!}{[(\lambda - \mu)!! \, (\lambda + \mu)!!]^2},$$

and the classical orbit integrals are defined as

$$I_{\lambda,\mu}(\theta, \xi) \equiv \int_{-\infty}^{\infty} \exp[i\xi(\epsilon \sinh \omega + \omega)] \frac{[\cosh \omega + \epsilon + i(\epsilon^2 - 1)^{1/2} \sinh \omega]^{\mu}}{(\epsilon \cosh \omega + 1)^{\lambda+\mu}} \, d\omega \tag{3}$$

for $\epsilon = 1/\sin(\theta/2)$. Thus, the Coulomb excitation functions are seen to be somewhat complicated quantities to evaluate numerically, since they involve performing the indicated double integrals for each value of ξ.

For approximate applications in the anticipated astrophysical context, averages of the Coulomb excitation rates over a Maxwell–Boltzmann distribution of relative velocities [4, 5] can be easily performed [6] for the limiting cases of $\xi = 0$ and $\xi \gg 1$. However, the wide variety of multipole orders and types encountered by Ward [9] (e.g., E3, M3, E4, E5, E6, M7, E8, E10) demands an *automated* extension of the very limited $\xi = 0$ results of Alder *et al.* [1], and of the $\xi \gg 1$ results of Brussaard, *et al.* [11]. This work provides it. In Section 2 we present the manipulations required to evaluate numerically the leading coefficients of $f_{\pi\lambda}(\xi = 0)$; and in Section 3 we show the much more extensive considerations required to obtain the asymptotic behavior of $f_{\pi\lambda}(\xi \gg 1)$ and contrast our numerical results with those of Brussaard *et al.* [11].

2. The $\xi = 0$ Limit

For high projectile temperatures and/or small excitation energies we are interested in the quantities $f_{E\lambda}(0)$ and $f_{M\lambda}(0)$. We follow the notation of Alder *et al.* [1] during our development and for electric transitions examine the function

$$\mathcal{I}_{\lambda,\mu}(E\lambda, \xi) \equiv \int_0^{\pi} | I_{\lambda,\mu}(\theta, \xi)|^2 \frac{\cos(\theta/2)}{[\sin(\theta/2)]^3} \, d\theta, \tag{4}$$

where the orbit integral is given in this limiting case by

$$I_{\lambda,\mu}(\theta, \xi = 0) = \int_{-\infty}^{\infty} \frac{[\cosh \omega + \epsilon + i(\epsilon^2 - 1)^{1/2} \sinh \omega]^{\mu}}{(\epsilon \cosh \omega + 1)^{\lambda+\mu}} \, d\omega. \tag{5}$$

Note that the $\xi = 0$ limit of a sudden collision has removed the troublesome oscillating exponential factor from the integrand of the orbit integrals. The integral in (5) can now be performed explicitly [1] to give

$$I_{\lambda,\mu}(\theta, \xi = 0) = (2\pi/\epsilon)^{1/2} (\lambda - 1)! \, (\epsilon^2 - 1)^{-\lambda/2+1/4} \, P_{\mu-1/2}^{-\lambda+1/2}(1/\epsilon), \tag{6}$$

where P_{α}^{β} is the Legendre function of half-integer and negative order. For the particular values of α and β in (6), these functions are in fact terminating series in elementary functions of the angle θ. Although the resulting trigonometric expressions allow the indivdiual $\mathscr{I}_{\lambda,\mu}$ to be evaluated explicitly in closed form, the general cases for these integrals are much more readily evaluated numerically by the following transformations to rapidly convergent series. Changing variables in (4) to $x = \sin(\theta/2)$ and using (6) results in

$$\mathscr{I}_{\lambda,\mu}(E\lambda, \xi = 0) = 4\pi[(\lambda - 1)!]^2 \int_0^1 \frac{x^{2\lambda-3}}{(1 - x^2)^{\lambda-1/2}} \, | P_{\mu-1/2}^{-\lambda+1/2}(x)|^2 \, dx. \tag{7}$$

Following a similar prescription for the magnetic transitions, we find that the required quantity

$$\mathscr{I}_{\lambda,\mu}(M\lambda, \xi) \equiv \int_0^{\pi} | I_{\lambda,\mu}(\theta, \xi)|^2 \frac{\cos(\theta/2)[\cot(\theta/2)]^2}{[\sin(\theta/2)]^2} \, d\theta \tag{8}$$

can be easily transformed into

$$\mathscr{I}_{\lambda,\mu}(M\lambda, \xi = 0) = 4\pi[(\lambda - 1)!]^2 \int_0^1 \frac{x^{2\lambda-5}}{(1 - x^2)^{\lambda-3/2}} \, | P_{\mu-1/2}^{-\lambda+1/2}(x)|^2 \, dx. \tag{9}$$

Furthermore, since we evaluate these integrals *numerically*, it is quite useful to transform the Legendre functions as [12]

$$| P_{\mu-1/2}^{-\lambda+1/2}(x)|^2 = \left(\frac{1 - x^2}{4}\right)^{\lambda-1/2} \left[\frac{F(\lambda + \mu, \lambda - \mu; \lambda + \tfrac{1}{2}; (1 - x)/2)}{\Gamma(\lambda + \tfrac{1}{2})}\right]^2, \tag{10}$$

where Γ is the usual gamma function and F is Gauss' hypergeometric function defined by

$$F(a, b; c; z) = \sum_{l=0}^{\infty} \frac{(a)_l \, (b)_l \, z^l}{l! \, (c)_l} \tag{11}$$

for the Pochhammer symbol $(a)_l \equiv \Gamma(a + l)/\Gamma(a)$. This series is absolutely convergent for all $| z | < 1$ and is therefore quite useful for computational purposes since the argument in (7) is bounded by $0 \leqslant (1 - x)/2 \leqslant \tfrac{1}{2}$.

Assembling all of these results and using the general Eqs. (1) and (2) for the Coulomb excitation functions, the complete expressions for evaluating the $\xi = 0$ limit become

$$f_{E\lambda}(\xi = 0) = B(\lambda) \sum_{\substack{\mu=0 \\ (\lambda+\mu,\text{even})}}^{\lambda} A(\lambda, \mu) \left(1 - \frac{1}{2}\delta_{\mu,0}\right) \times \int_0^1 x^{2\lambda-3} \left[F\left(\lambda + \mu, \lambda - \mu; \lambda + \frac{1}{2}; \frac{1-x}{2}\right)\right]^2 dx \tag{12}$$

and

$$f_{M\lambda}(\xi = 0) = \frac{B(\lambda)}{(2\lambda+1)^2} \sum_{\substack{\mu=0 \\ (\mu+\lambda,\text{odd})}}^{\lambda} \frac{(1 - \frac{1}{2}\delta_{\mu,0})}{A(\lambda, \mu)} \times \int_0^1 x^{2\lambda-3}(1-x^2) \left[F\left(\lambda + \mu + 1, \lambda - \mu + 1; \lambda + \frac{3}{2}; \frac{1-x}{2}\right)\right]^2 dx, \tag{13}$$

where $\delta_{\mu,0}$ is the Kronecker delta symbol and where we have defined the quantity

$$B(\lambda) \equiv \frac{64\pi^3}{4^\lambda(2\lambda+1)^2} \left[\frac{(\lambda-1)!}{\Gamma(\lambda + \frac{1}{2})}\right]^2.$$

An additional point to note is that the use of $f_{\pi\lambda}(\xi = 0)$ for small ξ is actually correct to *first order* in ξ since

$$[\partial f_{\pi\lambda}(\xi)/\partial\xi]_{\xi=0} = 0. \tag{14}$$

This result is most easily established by noting that the properties (i) $I_{\lambda,\mu}(\theta, -\xi) = I_{\lambda,-\mu}(\theta, \xi)$, and (ii) $A(\lambda, -\mu) = A(\lambda, \mu)$ [in conjunction with merely reversing the order of the summations in (1) and (2)] show that $f_{\pi\lambda}(\xi) = f_{\pi\lambda}(-\xi)$. Thus we have that the Coulomb excitation functions are *continuous* and *even* functions of ξ, and simple Taylor series expansions of $f_{\pi\lambda}(\pm\xi)$ about $\xi = 0$ confirm (14) and show that

$$f_{\pi\lambda}(\xi) = f_{\pi\lambda}(\xi = 0) + \mathcal{O}(\xi^2) \ldots .$$

Equation (14) is demonstrated numerically by the $\lambda \geqslant 2$ curves of Alder *et al.* [1, Fig. II.4].

The numerical results obtained from evaluating expressions (12) and (13) for electric and magnetic transitions up through $\lambda = 10$ are those given in Table I. The required integrals were evaluated by application of a simple 32-point Gauss–Legendre quadrature scheme (which gave agreement to at least six digits with the three analytical results given below) over the interval [0, 1], and the hypergeometric functions appearing in the integrands were calculated by straightforward term-by-term series expansions at each point. To give confidence in the general accuracy of the results in the table, we

TABLE I

$\xi \to 0$ Limit of the Coulomb Excitation Functions[a]

Multipole order (λ)	$f_{E\lambda}(\xi = 0)$	$f_{M\lambda}(\xi = 0)$
1	—[b]	—[b]
2	0.8954	0.1936
3	3.797(−2)	4.495(−3)
4	2.861(−3)	2.317(−4)
5	2.865(−4)	1.760(−5)
6	3.413(−5)	1.686(−6)
7	4.571(−6)	1.889(−7)
8	6.666(−7)	2.365(−8)
9	1.037(−7)	3.224(−9)
10	1.696(−8)	4.693(−10)

[a] Note that $r(s) \equiv r \times 10^s$.
[b] Both f_{E1} and f_{M1} diverge logarithmically as $\xi \to 0$.

may compare them to the only three cases to have been integrated analytically. The results as given by Alder *et al.* [1] are

$$f_{E2}(0) = \frac{8\pi^2}{25}\left(\frac{\pi^2}{16} - \frac{1}{3}\right) = 0.895424...,$$

$$f_{E3}(0) = \frac{8\pi^2}{49}\left(\frac{8}{45} - \frac{\pi^2}{64}\right) = 0.0379721...,$$

and

$$f_{M2}(0) = \frac{8\pi^2}{25}\left(\frac{\pi^2}{16} - \frac{5}{9}\right) = 0.193585... .$$

They have also given the additional numerically calculated point [1, Table II.4, p. 459],

$$f_{E4}(0) = 0.002862.$$

For $\lambda = 1$, (12) and (13) show that the excitation functions diverge logarithmically in the limit $\xi \to 0$. The excellent numerical agreement between the exact values given above and the corresponding ones listed in Table I is evident and thus adds confidence to the remainder of the computed results shown there.

3. Calculation of the $\xi \gg 1$ Asymptotic Limit

(a) *General Development*

This asymptotic limit of the Coulomb excitation process corresponds to physical effects of low projectile temperatures and/or large transition energies that result in a slow adiabatic collision. Unfortunately, as we see in the rather lengthy discussion which follows, obtaining the appropriate limiting behavior will be mathematically *and* computationally much more difficult than for the $\xi = 0$ case. The physically important feature of the excitation functions for ion projectiles will be their resulting exponential decrease [$\propto \exp(-2\pi\xi)$] for large values of ξ, which reflects the adiabatic character of the collision process.

We initially follow the work of Brussaard *et al.* [11] and Ter-Martirosyan [13] and consider the orbit integral (3). For $\xi \gg 1$ the exponential in the integrand is a very rapidly varying function of ω. We therefore use the method of steepest descent and shift the path of integration over the point of stationary phase $\omega_0 = -i\pi + i \arctan[(\epsilon^2 - 1)^{1/2}]$, where $d/d\omega\ (\epsilon \sinh \omega + \omega) = 0$, and the resulting noncanceling contribution to the integral is sharply peaked at ω_0. It is important to note that the remaining slowly varying part of the integrand may also have poles at some of these points of stationary phase. Expanding all of the terms in the integrand about $\rho \equiv \omega - \omega_0$, we have correct to *third* order in ρ [13]

$$I_{\lambda,\mu}(x, \xi) \simeq \exp\left(-\pi\xi - \frac{\xi x^3}{3}\right) \int_{-\infty}^{\infty} \exp\left(-\frac{x\rho^2}{2} + \frac{i\rho^3}{6}\right) \times \frac{[-\rho(1 + x^2)^{1/2}]^{\mu}}{[-(\rho/2)(\rho + 2ix)]^{\lambda+\mu}}\, d\rho, \tag{15}$$

where $x \equiv (\epsilon^2 - 1)^{1/2}$, and we have taken $x - \arctan x \simeq -x^3/3$ since $\xi \gg 1$. To show the explicit dependence on the important quantity ξ, we now change variables in (15) to $s = x\xi^{1/3}$ and $y = \rho\xi^{1/3}$, and the approximate expression for $I_{\lambda,\mu}$ then reads

$$I_{\lambda,\mu}(s\xi^{-1/3}, \xi) = 2^{\lambda} \exp(-\pi\xi - s^3/3)\, \xi^{(2\lambda-1)/3} Q(\mu - \lambda, -\lambda - \mu; s), \tag{16}$$

where we have put the factor $(1 + s^2\xi^{-2/3}) \simeq 1$ for $\xi \gg 1$. The additional function, Q, in (16) will prove to be the key to all of our subsequent development, and is defined as [11]

$$Q(k, m; s) \equiv i^{-k-m} \int_{-\infty}^{\infty} \exp\left(-\frac{sy^2}{2} + \frac{iy^3}{6}\right) y^k (y + 2is)^m\, dy, \tag{17}$$

where k and m are positive or negative integers. From definition (17) we see that the Q-functions are *real* and can be written in the alternate form

$$Q(k, m; s) = 2 \int_0^{\infty} \exp\left(-\frac{sy^2}{2}\right) y^k (y^2 + 4s^2)^{m/2} \times \cos\left[\frac{y^3}{6} + m \tan^{-1}\left(\frac{2s}{y}\right) - \frac{\pi}{2}(k + m)\right] dy, \tag{18}$$

where for $k \leqslant -1$ we must augment (18) to properly account (in the Cauchy principal-value sense) for the pole on the path of integration at $y = 0$.

To obtain the appropriate forms for the complete excitation functions, $I_{\lambda,\mu}$ in (16) must now be integrated over all possible scattering angles as in (4) and (8). Since $s = \xi^{1/3} \cot(\theta/2)$, this gives for electric transitions

$$\mathscr{I}_{\lambda,\mu}(E\lambda,\ \xi \gg 1) \simeq 2\xi^{(4\lambda-4/3)} \exp(-2\pi\xi)\, 4^{\lambda} \times \int_0^{\infty} \exp\left(-\frac{2s^3}{3}\right) [Q(\mu - \lambda, -\lambda - \mu; s)]^2\, s\, ds \tag{19}$$

and for magnetic transitions

$$\mathscr{I}_{\lambda,\mu}(M\lambda,\ \xi \gg 1) \simeq 2\xi^{(4\lambda-6/3)} \exp(-2\pi\xi)\, 4^{\lambda} \times \int_0^{\infty} \exp\left(-\frac{2s^3}{3}\right) [Q(\mu - \lambda, -\lambda - \mu; s)]^2\, s^3\, ds. \tag{20}$$

The asymptotic expansion coefficients are now defined as

$$\Omega(E\lambda) \equiv \xi^{(4-4\lambda/3)} \exp(2\pi\xi)\, f_{E\lambda}(\xi \gg 1), \tag{21}$$

and

$$\Omega(M\lambda) \equiv \xi^{(2-4\lambda/3)} \exp(2\pi\xi)\, f_{M\lambda}(\xi \gg 1). \tag{22}$$

Using the general expressions for the excitation functions given previously, we obtain the final results:

$$\Omega(E\lambda) = C(\lambda) \sum_{\substack{\mu=-\lambda \\ (\mu+\lambda,\text{even})}}^{+\lambda} A(\lambda, \mu) \times \int_0^{\infty} \exp\left(-\frac{2s^3}{3}\right) [Q(\mu - \lambda, -\lambda - \mu; s)]^2\, s\, ds, \tag{23}$$

and

$$\Omega(M\lambda) = \frac{4C(\lambda)}{\lambda^2} \sum_{\substack{\mu=-\lambda \\ (\mu+\lambda,\text{odd})}}^{+\lambda} \frac{1}{A(\lambda, \mu)} \times \int_0^{\infty} \exp\left(-\frac{2s^3}{3}\right) [Q(\mu - \lambda - 1, -\lambda - 1 - \mu; s)]^2\, s^3\, ds, \tag{24}$$

where

$$C(\lambda) \equiv 8\pi^2 4^{\lambda}/(2\lambda + 1)^2.$$

The only obstacle that now remains to be overcome is the evaluation of the *double* integrals required [compare, for example, Eqs. (17) and (23)]. Were it not for the fact

that any general Q-function as defined by (17) can be reduced to linear combinations of only *four* basic Q-functions, the numerical evaluation of these integrals would be a most tedious and prohibitively time-consuming task.

(b) *Reduction of the Q-Functions*

Again initially following the work of Brussaard *et al.* [11], we now examine the behavior of the general Q-functions defined in (17). As was remarked in the previous section, their numerical evaluation would be prohibitive were it not for the fact that they can be reduced to expressions involving only polynomials in powers of s and s^{-1} times the following four basis functions:

$$Q(1, 0; s), \qquad Q(0, 0; s), \qquad Q(-1, 0; s), \qquad \text{and} \qquad Q(0, -1; s).$$

The pattern for these important reductions can be seen by considering the integral definition (17) for the Q-functions. Since for our particular physical problem of Coulomb excitation the quantities k and m are specifically $k = \mu - \lambda$ and $m = -\lambda - \mu$, the fact that $-\lambda \leqslant \mu \leqslant +\lambda$ means that k and m are initially bounded by $-2\lambda \leqslant k, m \leqslant 0$. Thus, we see that what is required for the general reductions are recursion relations that will raise the general values for k to $+1$, 0, or -1 and m to 0 or -1.

The most general recursion relation is obtained by a simple integration by parts in (17) to give

$$Q(k, m; s) = (m + 1)^{-1}[-kQ(k - 1, m + 1; s) - \tfrac{1}{2}Q(k + 1, m + 2; s)] \qquad \text{for } m \leqslant -2. \tag{25}$$

This relation can then be applied repeatedly to increase the value of m (at the expense of lowering k) until $m = -1$. The last allowed iteration at $m = -2$ will thus be expressed in terms of Q-functions with $m = -1$ and with $m = 0$. Note that (25) results in the accumulation of only *constant* coefficients. To bridge the gap at $m = -1$, the expression for $Q(k, -1; s)$ must be reduced by a partial-fraction expansion of the integrand in (17) for $k < 0$ as

$$\frac{y^k}{y + 2is} = \frac{(-2is)^k}{y + 2is} - \sum_{l=1}^{|k|} (-2is)^{l-1-|k|}\, y^{-l} \tag{26}$$

[14, p. 168]. This expansion shows that

$$Q(k, -1; s) = (-2s)^k\, Q(0, -1; s) - \sum_{l=1}^{|k|} (-2s)^{k+l-1}\, Q(-l, 0; s) \qquad \text{for } k \leqslant -1. \tag{27}$$

Since k is negative in this case, we see that (26) introduces negative powers of s into

the accumulated recursion coefficients. For k > 0 we must use repeated synthetic division to yield

$$\frac{y^k}{y+2is} = \frac{(-2is)^k}{y+2is} + \sum_{l=1}^{k-1} (-2is)^l \, y^{k-1-l}. \tag{28}$$

The third important recursion relation then becomes

$$Q(k, -1; s) = (-2s)^k \, Q(0, -1; s) + \sum_{l=0}^{k-1} (-2s)^l \, Q(k-1-l, 0; s) \quad \text{for} \quad k \geqslant 2, \tag{29}$$

thus introducing *positive* powers of the variable s. Recursion relations (25), (27), and (29) will reduce a general Q-function to a polynomial in s times $Q(0, -1; s)$ plus polynomials in s times Q-functions of the form $Q(\pm k, 0; s)$. Relations are therefore needed to raise or lower the index $\pm k$ into the range $k = 1, 0$ or $+1$. Using (17) for $m = 0$, an integration by parts gives

$$Q(k, 0; s) = (k+1)^{-1}[-sQ(k+2, 0; s) - \tfrac{1}{2}Q(k+3, 0; s)], \quad \text{for} \quad k \leqslant -2, \tag{30}$$

which will eventually reduce any $Q(k, 0; s)$ for $k \leqslant -2$ to combinations of $Q(1, 0; s)$, $Q(0, 0; s)$, and $Q(-1, 0; s)$. To *lower* k, we merely let $k \to k - 3$ in (30) to trivially obtain

$$Q(k, 0; s) = -2sQ(k-1, 0; s) - 2(k-2)Q(k-3, 0; s) \quad \text{for} \quad k \geqslant 2. \tag{31}$$

The five recursion relations (25), (27), (29), (30), and (31) thus suffice to reduce *any* general Q-function to its appropriate expansion in terms of the four basis functions.

This very tedious reduction has been done *algebraically* only for the Q-functions generated for transition multipole orders up through $\lambda = 4$ as given by Chattarji and Brussaard [15]. Since Coulomb deexcitation of long-lived s-process isomeric states [9] requires these reductions up to $\lambda = 10$ (note that the number of Q-functions to be reduced for each value of λ goes as $\lambda + 1$), the five recursion relations were programmed to numerically accumulate the coefficients of the resulting polynomials multiplying each basis function in the expansion.

As an example of the numerical technique involved in these reductions, in Fig. 1 we have schematically illustrated the reduction pattern for the function $Q(-2, -14; s)$ which is one of the nine functions needed to calculate the asymptotic expansion coefficients for $\lambda = 8$. The shaded square indicates the starting point at $k = -2$ and $m = -14$. The "axes" are labeled for all of the intermediate values of k and m encountered during the reduction. The *dashed* squares represent all of the intervening Q-functions generated (most of them several times each) in the reduction by the use of (25); the *solid* squares are the functions that result from the last allowed application of (25) yielding $m = 0$ or -1. The last four remaining recursion relations to be used in the final reduction of the solid squares to the four basic Q-functions (indicated by

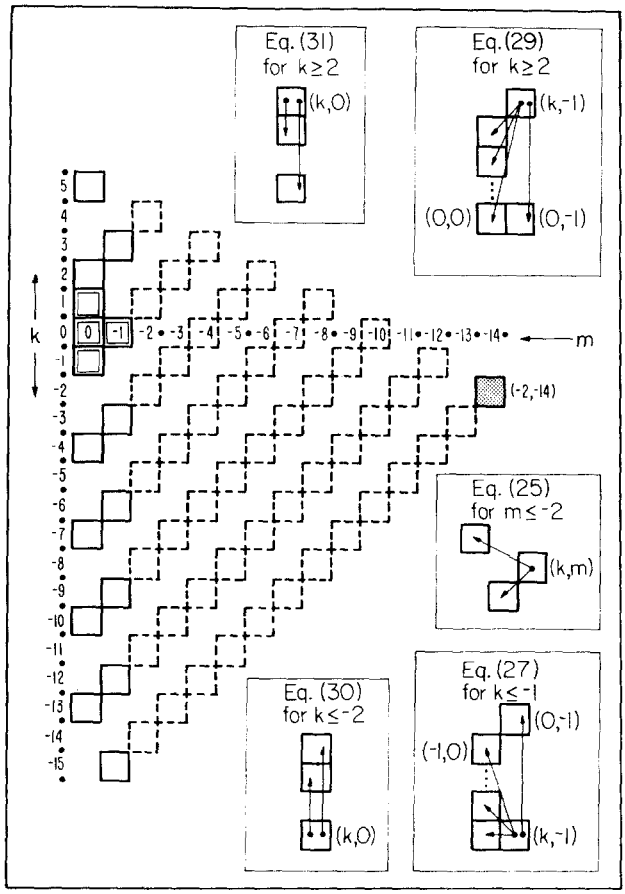

FIG. 1. The recursion relations given in the text (shown in the five insets) used to reduce the general function $Q(-2, -14; s)$ (the shaded square) to linear combinations of polynomials in s times the four basic Q-functions (indicated by the doubly boxed squares). For the range in intervening values of k and m, the dashed squares are the intermediate Q-functions encountered along the way solely by application of (25), and the solid squares mark the Q-functions which must then be reduced by the remaining four recursion relations as shown.

the four doubly boxed squares) are also schematically illustrated in the various insets in Fig. 1. We first use (27) and (29) to reduce those cases with $m = -1$ directly to $Q(0, -1; s)$ and forms with $m = 0$. The final steps use (31) to lower the only remaining forms with $m = 0$ and $k \geqslant 2$ and (30) to raise $k \leqslant -2$ and $m = 0$ for a complete expansion. The numerical reduction program made use of these symmetries to perform first column-wise reductions in the matrix "array" suggested by the figure, followed by row-wise reductions (accumulating along the way all of the resulting polynomials in s) to the four basis functions. Although much of the theory given here was discussed by Brussaard *et al.* [11], our explicit development of the required five basic recursion relations along with the *numerical* techniques for achieving the reduc-

tions is obviously much faster and more flexible than their hand-calculated algebraic reductions (only attempted up through $\lambda = 4$). Since reductions for up to $\lambda = 10$ were required, the algebraic technique would have been so tedious as to have been prohibitive for our purposes.

In Table II we have given the explicit numerical values of the coefficients of each polynomial multiplier of the four basic Q-functions generated in the reductions for $\lambda = 4$. The entries in each row correspond to the coefficients of the power of s indicated on the left. The polynomial described by a given column multiplies the basis function given at the top of that column. Particular attention has been paid to minimizing the accumulated round-off error inherent in such recursive calculations. The particular results of our calculations for $\lambda \leqslant 4$ were found to agree *exactly* with the hand-calculated reductions of Chattarji and Brussaard [15]. For example, they obtained as the expansion for $Q(-6, -2; s)$:

$$\begin{aligned} Q(-6, -2; s) = &\left(\frac{3}{64} s^{-6} + \frac{1}{64} s^{-3} + \frac{1}{120}\right) Q(1, 0; s) \\ &+ \left(\frac{3}{64} s^{-5} + \frac{7}{320} s^{-2} + \frac{1}{60} s\right) Q(0, 0; s) \\ &- \left(\frac{3}{64} s^{-7} + \frac{1}{32} s^{-4} + \frac{1}{96} s^{-1}\right) Q(-1, 0; s) \\ &+ \frac{3}{64} s^{-7} Q(0, -1; s). \end{aligned} \tag{32}$$

Comparison with our corresponding result in Table II shows that it agrees exactly with the *rational* coefficients given in (32).

(c) *The Four Basic Q-Functions*

Using the form (18) we can immediately write down the real integral representations of the four basis functions required for their evaluation by Gauss–Hermite numerical quadrature as

$$Q(1, 0; s) = 2 \int_0^\infty \exp\left(\frac{-s\omega^2}{2}\right) \omega \sin\left(\frac{\omega^3}{6}\right) d\omega, \tag{33}$$

$$Q(0, 0; s) = 2 \int_0^\infty \exp\left(\frac{-s\omega^2}{2}\right) \cos\left(\frac{\omega^3}{6}\right) d\omega, \tag{34}$$

$$Q(-1, 0; s) = \pi - 2 \int_0^\infty \exp\left(\frac{-s\omega^2}{2}\right) \omega^{-1} \sin\left(\frac{\omega^3}{6}\right) d\omega, \tag{35}$$

and

$$Q(0, -1; s) = \int_0^\infty \frac{\exp(-s\omega^2/2)}{\omega^2 + 4s^2} \left[4s \cos\frac{\omega^3}{6} - 2\omega \sin\frac{\omega^3}{6}\right] d\omega. \tag{36}$$

TABLE II

Reduction to Polynomial Coefficients of the Four Basic Q-Functions for $\lambda = 4$

LAMBDA = 4 , MU = -4

Q(-8, 0;S)

	Q(1,0;S)	Q(0,0;S)	Q(-1,0;S)	Q(0,-1;S)
	*	*	*	*
S**(0)	4.46428570-03	0.0	0.0	0.0
S**(1)	0.0	1.6964286D-02	0.0	0.0
S**(2)	0.0	0.0	2.08333330-02	0.0
S**(3)	4.7619048D-03	0.0	0.0	0.0
S**(4)	0.0	9.5238095D-03	0.0	0.0

LAMBDA = 4 , MU = -2

Q(-6, -2;S)

	Q(1,0;S)	Q(0,0;S)	Q(-1,0;S)	Q(0,-1;S)
	*	*	*	*
S**(-7)	0.0	0.0	-4.68750000-02	4.68750000-02
S**(-6)	4.68750000-02	0.0	0.0	0.0
S**(-5)	0.0	4.6875000D-02	0.0	0.0
S**(-4)	0.0	0.0	-3.12500000-02	0.0
S**(-3)	1.56250000-02	0.0	0.0	0.0
S**(-2)	0.0	2.18750000-02	0.0	0.0
S**(-1)	0.0	0.0	-1.04166670-02	0.0
S**(0)	8.3333333D-03	0.0	0.0	0.0
S**(1)	0.0	1.6666667D-02	0.0	0.0

LAMBDA = 4 , MU = 0

Q(-4, -4;S)

	Q(1,0;S)	Q(0,0;S)	Q(-1,0;S)	Q(0,-1;S)
	*	*	*	*
S**(-7)	0.0	0.0	-1.56250000-01	1.56250000-01
S**(-6)	1.56250000-01	0.0	0.0	0.0
S**(-5)	0.0	1.5625000D-01	0.0	0.0
S**(-4)	0.0	0.0	-5.20833330-02	-5.20833330-02
S**(-2)	0.0	2.0833333D-02	0.0	0.0

LAMBDA = 4 , MU = 2

Q(-2, -6;S)

	Q(1,0;S)	Q(0,0;S)	Q(-1,0;S)	Q(0,-1;S)
	*	*	*	*
S**(-7)	0.0	0.0	-4.68750000-02	4.68750000-02
S**(-6)	4.68750000-02	0.0	0.0	0.0
S**(-5)	0.0	4.6875000D-02	0.0	0.0
S**(-4)	0.0	0.0	0.0	-3.12500000-02
S**(-3)	-1.56250000-02	0.0	0.0	0.0
S**(-2)	0.0	-9.37500000-03	0.0	0.0
S**(-1)	0.0	0.0	0.0	1.04166670-02
S**(0)	8.3333333D-03	0.0	0.0	0.0

LAMBDA = 4 , MU = 4

Q(0, -8;S)

	Q(1,0;S)	Q(0,0;S)	Q(-1,0;S)	Q(0,-1;S)
	*	*	*	*
S**(0)	4.46428570-03	0.0	0.0	0.0
S**(1)	0.0	-8.03571430-03	0.0	0.0
S**(2)	0.0	0.0	0.0	2.08333330-02
S**(3)	-4.7619048D-03	0.0	0.0	0.0

The additional term π in (35) represents the contribution from the pole at $\omega = 0$, and the remaining term is the Cauchy principal value of the integral. One additional numerical complication arises, however, because we must integrate the reduced Q-functions from 0 to ∞ [see Eqs. (23) and (24)]. As was mentioned in the last subsection, the resulting polynomials in our reduction scheme often contain *negative* powers of s. Thus for small s (<1) each basis function must first be expressed as a power series in s [11]:

$$Q(l, 0; s) = \sum_{n=0}^{\infty} \frac{(s/2)^n}{n!} Q(2n + l, 0; 0) \qquad \text{for} \quad l = -1, 0, \text{or } 1, \tag{37}$$

and

$$Q(0, -1; s) = \sum_{n=0}^{\infty} \sum_{l=0}^{n} \frac{(-1)^{n+l}}{l!} 2^{n-2l} s^n Q(3l - n - 1, 0; 0), \tag{38}$$

where we have integrated the expansions term by term using the definition (17). For further details see [11]. When these expansions are used, the negative powers of s indeed cancel exactly as they should (since physically we know the integrals over the Q-functions must be finite). When checking the results of Brussaard *et al.* [11] for these expansion coefficients, we found their values for $Q(0, -1; s)$ to be the victim of severe round-off error for the (negative) coefficients of the powers: $s^{3n-1, 3n-2}$ (for $n = 1, 2, \ldots$) greater than about s^{15}, because they are computed as the differences of many nearly equal large numbers. Since our calculations were carried out to $\sim$27 decimal digits (double precision on the CDC 7600 at Lawrence Berkeley Laboratory), we believe that this problem has been successfully avoided.

In numerically evaluating the four basis functions for large values of s ($\gtrsim 1$), the integral definitions (33)–(36) were used, while for small values of s they were evaluated using the series expansions (37) and (38). Expressions (33)–(36) were numerically integrated with a 64-point Gauss–Hermite quadrature scheme which gave agreement to six significant digits with the direct series expansions at the $s = 1$ matching point. Note that these integral definitions become increasingly easier to evaluate for larger values of s since the exponentials in the integrands rapidly cut off the remaining troublesome oscillating factors. For $s = 0$, these integrals can be performed analytically to yield the results [16]

$$Q(1, 0; 0) = 2^{2/3} 3^{1/6} \Gamma(\tfrac{2}{3}),$$

$$Q(0, 0; 0) = \frac{4\pi}{Q(1, 0; 0)\, 3^{1/2}},$$

and

$$Q(-1, 0; 0) = Q(0, -1; 0) = 2\pi/3.$$

As $s \to \infty$, all of the integrals in (33)–(36) vanish and we are left with only

$$Q(-1, 0; \infty) = \pi.$$

The explicit behavior of these basis functions is illustrated graphically in Brussaard *et al.* [11].

(d) *Numerical Results*

To illustrate the general behavior of the Q-functions, we have shown in Fig. 2 the Q-functions that contribute to $\lambda = 4$. The range has been limited to $0 \leqslant s \leqslant 5$ since the required integrals over the squares of the Q-functions are all weighted in the integrand with the factor $\exp(-2s^3/3) \simeq 6 \times 10^{-37}$ for $s = 5$. Further examination of the integrands in (19) and (20) shows the greatest weight to be given to values of the Q-function near $s \simeq (\frac{1}{2})^{1/3}$ and $(\frac{3}{2})^{1/3}$. Note that at $s = 0$, eq. (17) shows that all of the Q-functions for a given λ are equal, since the result is *independent* of μ.

Once the Q-functions have been reduced for each contributing value of μ for a given λ, the required integrals in (23) and (24) were performed numerically by repeated

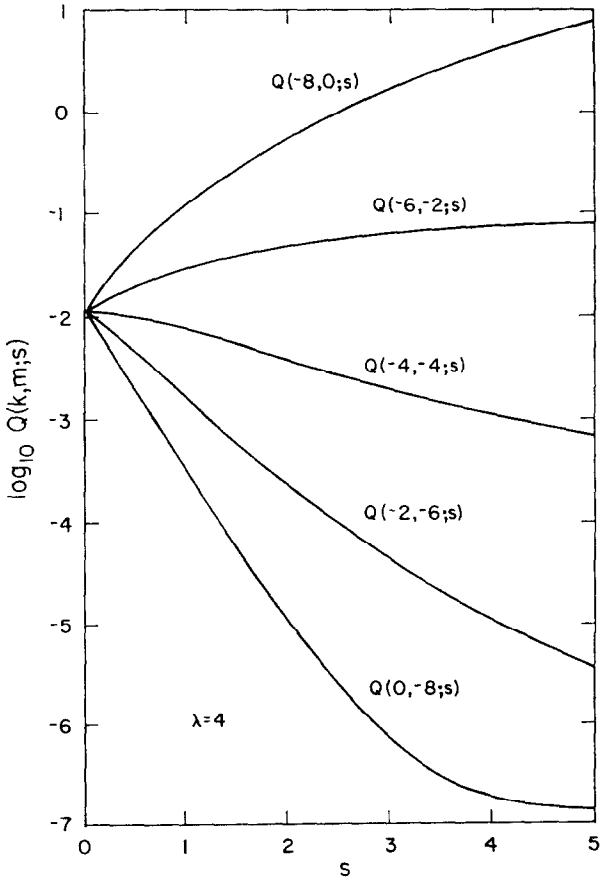

FIG. 2. The *five* Q-functions (as a function of s) needed for $\lambda = 4$ transitions.

application of 32-point Gauss quadratures over the interval $0 \leqslant s \leqslant 5$. Note that (23) and (24) show that the Q-functions computed at the quadrature points for the evaluation of $\Omega(E\lambda)$ can be stored and used for the subsequent evaluation of $\Omega[M(\lambda+1)]$ without having to recompute them. The final results for the asymptotic expansion coefficients $\Omega(E\lambda)$ and $\Omega(M\lambda)$ are as given in Table III up through $\lambda = 10$. The

TABLE III

Asymptotic Expansion Coefficients for the $\xi \gg 1$ Limit of the Coulomb Excitation Functions[a]

Multipole order (λ)	$\Omega(E\lambda)$	$\Omega(M\lambda)$
1	63.65	3.912
2	18.81	0.4287
3	4.547	5.605(−2)
4	0.8860	6.973(−3)
5	0.1417	7.834(−4)
6	1.901(−2)	7.848(−5)
7	2.177(−3)	7.011(−6)
8	2.162(−4)	5.610(−7)
9	1.887(−5)	4.043(−8)
10	1.463(−6)	2.640(−9)

[a] Note that $r(s) = r \times 10^s$.

division of the integration interval into six such panels was found to give six-digit agreement with the analytical result for $\Omega(E1)$ given below. As an additional check, the coefficients $\Omega(E3)$, $\Omega(E8)$, $\Omega(M2)$, and $\Omega(M7)$ were recomputed using 12 divisions for the 32-point quadratures and the results were in complete agreement with those obtained with only six panels as given in Table III. The only reliable benchmark for checking these results comes from the *analytic* expression available only for $E1$ transitions [1]:

$$f_{E1}(\xi \gg 1) \simeq 32\pi^3/9(3)^{1/2} \exp(-2\pi\xi) \tag{39}$$

or

$$\Omega(E1) = 32\pi^3/9(3)^{1/2} = 63.64971\ldots. \tag{40}$$

Our corresponding result in Table III was actually calculated to be 63.649704, in excellent agreement with (40). However, the results (rounded back to four significant digits) of Brussaard *et al.* [11] were

$\Omega(E1) = 63.65$, $\Omega(M1) = 3.912$, $\Omega(E2) = 18.81$, $\Omega(M2) = 0.9053$,

and $\Omega(E3) = 7.254$.

Note the large disagreement with our values for $\Omega(E3)$ and $\Omega(M2)$ shown in Table III. In the light of the round-off errors in their tabulations mentioned earlier (not to mention the *numerous* errors in the text of their paper), we believe our results to be the correct ones, since all of the values in Table III were calculated by the same general numerical program using extended precision arithmetic.

One final point about the asymptotic expansion coefficients can be illustrated [2] by multiplying the only numerical data available in Alder *et al.* [1] by $\exp(2\pi\xi)$ and the appropriate power of ξ [see Eqs. (21) and (22)] such that the resulting value as $\xi \to \infty$ becomes our asymptotic constant. The solid curves in Fig. 3 show the result

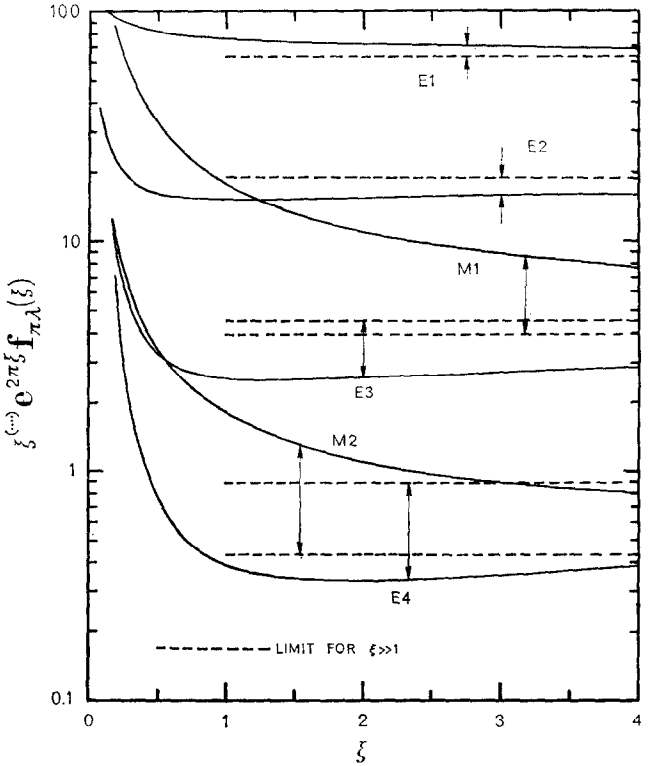

FIG. 3. Multiplication of the excitation functions by $\exp(2\pi\xi)$ and the proper power of ξ (see the text) such that the asymptotic values approach finite constants (the dashed lines connected with arrows to the proper curves). The solid curves were calculated from the numerical results of Alder *et al.* [1].

of such a transformation. The arrows connect each curve with its appropriate asymptotic value (dashed line) from Table III. One sees that the $E\lambda$ curves flatten out sooner ($\xi \sim 1$) than the $M\lambda$ curves. From these (admittedly somewhat limited) comparisons it would seem that use of the asymptotic expansions down to $\xi \sim 1$ should probably be good to within a factor of two for the $E\lambda$ cases but may underestimate the exact results for $M1$ and $M2$ transitions by up to a factor of 5 at $\xi = 1$.

4. Conclusions

Owing to the wide variety of electric and magnetic transition orders required for astrophysical studies, we have systematically performed calculations of the expansion coefficients of the limiting cases of the classical Coulomb excitation functions up through $\lambda = 10$. The transformations to numerically tractable forms have been presented for both sudden ($\xi = 0$) and adiabatic ($\xi \gg 1$) collisions with particular attention paid to developing the properties of the recursion relations required for programming the $\xi \gg 1$ evaluation. Considerable disagreement was found between our work and that of Brussaard *et al.* [11] for values of the $\xi \gg 1$ asymptotic expansion coefficients for $\lambda \geqslant 2$.

The numerical values of the expansion coefficients presented in this work can now be used (with more than adequate accuracy for the anticipated astrophysical applications) to calculate Coulomb deexcitation rates in stellar interiors. The thermonuclear averages over a Maxwellian distribution of relative target–projectile energies can be explicitly performed for the extreme cases of $\xi \to 0$ (high temperatures) and $\xi \gg 1$ (low temperatures), and intermediate cases can be smoothly interpolated [6] between these limits as a function of stellar temperature. Since these deexcitation rates will vary over many (tens!) of orders of magnitude as the projectile temperature ranges from 10^8 to 10^{10}K [6], the moderate errors of a factor of only 2 to 5 induced by using our limiting cases are negligible in the astrophysical context.

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