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RADIAL ELECTRIC MULTIPOLE MATRIX ELEMENTS FOR INELASTIC COLLISIONS IN ATOMIC AND NUCLEAR PHYSICS

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PROGRAM SUMMARY

Title of program: CLMINT

Catalogue number: ACCM

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: Burroughs 7700 at Eindhoven University of Technology, Eindhoven, The Netherlands; CDC 175/100 at Utrecht University, Utrecht, The Netherlands

Programming language used: FORTRAN 77

Operating system: MCP (Burroughs); NOS/BE (CDC)

Peripherals used: line printer, card reader

No. of lines in the combined program and test deck: 1544

No. of bits in a word: 52 (Burroughs); 60 (CDC)

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Nature of the physical problem
Solution of the radial Schrödinger equation for inelastic collisions between charged particles requires matrix elements of electric multipole operators in the region of large r values. These matrix elements are in general integrals over a finite interval $[R_1, R_2]$ of a product of Coulomb wave functions and a factor $r^{-\lambda-1}$ [1,2]. Especially in the case of heavy ion collisions at high energy, these are very cumbersome integrals because the integrand is a rapidly oscillating function with a wavelength much smaller than the integration interval. When we choose $R_2 = \infty$, the convergence of the integral is very slow.

Method of solution
If we split up the integrand into a rapidly and slowly varying function of the integration variable r, it is possible to construct an asymptotic series for the integral with the fast oscillating integrand. The remaining integral is easily obtained by Gaussian quadrature. Because we are integrating over large r values (compared to the classical turning points), it is possible to use the familiar WKB-approximation of Coulomb wave functions in the step-by-step integration. The subroutine has been set up to achieve a relative accuracy of 10^{-7}.

Restriction on the complexity of the problem
The subroutine has only been tested for significant l, η and k values i.e. $0 \leqslant l < 2000$, $0 < \eta < 1000$, $0 < k < 50$. The interval $[R_1, R_2]$ can be any part of $[0, \infty)$. When R_1 does not exceed the lowest turning point (especially $R_1 = 0$), only the integrals with the regular Coulomb wave functions $F_l(\eta, \rho)$ are reliable. Furthermore the case $\lambda = 0$ is not included.

Typical running time
The running time depends strongly on the parameters and the lower limit R_1. When R_1 lies in the asymptotic region, as in practical applications, the running time will in general be a fraction of a second but for smaller R_1 values it increases rather rapidly.

References
[1] L.D. Tolsma, Phys. Rev. C20 (1979) 592.
[2] D.H. Feng and A.R. Barnett, Comput. Phys. Commun. 10 (1975) 401.

LONG WRITE-UP

1. Introduction

In the description of inelastic atomic and nuclear scattering of charged particles, the radial Schrödinger equation can be written as a set of coupled integral equations. The partial wave radial functions are decomposed into two linearly independent homogeneous solutions of the differential equations, with more or less slowly varying amplitudes [1]. In the integration region of large r values, only the multiple Coulomb interaction will survive and the homogeneous solutions can be written in terms of Coulomb wave functions. In solving the integral equations on an interval $[R_1, R_2]$ in this region, only radial matrix elements with the general form

$$I_{ll'}^{(\lambda)} = \int_{R_1}^{R_2} X_l(\eta, kr) Y_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^{\lambda+1}} \tag{1}$$

occur. Here $X_l(\eta, kr)$ and $Y_{l'}(\eta', k'r)$ denote Coulomb wave functions and λ corresponds to the electric multipole moment. The quantum numbers of orbital angular momenta l and l' refer to the entrance and exist channels, respectively. A similar convention applies to the wave number of relative motion k and to the Sommerfeld parameter η. The integrals are also of interest in DWBA calculations where $R_1 = 0$ and $R_2 = \infty$ [2].

In the next sections we consider the integrals (1) with the following limitations on the parameters,

η, η', k, k'	real and positive,
l, l'	not negative integer,
λ	positive integer,
$[R_1, R_2]$	part of $[0, \infty)$.

(2)

The Coulomb wave function $X_l(\eta, kr)$ is a solution of the differential equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + 1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2} \right) X_l(\eta, \rho) = 0, \tag{3}$$

where $\rho = kr$. Since there are only two linearly independent solutions, it is sufficient to evaluate the integrals only for the standard real-valued Coulomb wave functions $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$. They behave asymptotically as [3]

$$F_l(\eta, \rho) \underset{\rho \to \infty}{\sim} \sin(\rho - \eta \log(2\rho) + \sigma_l(\eta) - l\pi/2), \quad G_l(\eta, \rho) \underset{\rho \to \infty}{\sim} \cos(\rho - \eta \log(2\rho) + \sigma_l(\eta) - l\pi/2), \tag{4}$$

where the Coulomb phase shift is given by

$$\sigma_l(\eta) = \arg \Gamma(l + 1 + \mathrm{i}\eta). \tag{5}$$

Eq. (3) has a turning point r_T, according to

$$kr_T = \eta + \sqrt{\eta^2 + l(l+1)}, \tag{6}$$

and also r_T' for the primed parameters in (1). These turning points separate two regions of interest. The behaviour of the Coulomb wave function is monotonic at $r < r_T$ but oscillatory at $r > r_T$.

We are mainly interested in the asymptotic region $r_0 < r < \infty$, where r_0 is considerably greater than both the turning points. In this region the integrals are hard to evaluate by standard numerical integration procedures for several reasons.

1) The Coulomb wave functions are calculated by Ricatti expansion or by a continued fraction, both at $l = 0$, after which the actual $F_l(\eta, \rho)$, $G_l(\eta, \rho)$ and derivatives are obtained by recursion [4,5]. These routines are rather time consuming when applied to evaluate the integrals $I_{ll'}^{(\lambda)}$ by numerical quadrature.
2) In many scattering cases, for instance nuclear collisions with medium weight and heavy ions, the integrand of (1) is oscillatory while the integration has to be performed over several hundred or even many thousands of wavelengths and so a step-by-step integration method is practically not feasible.
3) The integral over the last interval, where $R_2 = \infty$, is extremely slowly convergent.

The fundamental concept for the solution of these problems is the elimination of the short wavelength part of the integrand in the asymptotic region by asymptotic expansion of $I_{ll'}^{(\lambda)}$, according to Bellings method [6]. Some other subjects (WKB method, Gaussian quadrature) have to be investigated to make it possible to construct a subroutine, which is able to calculate the integrals (1) in the general case (2).

It is well known that Coulomb wave functions with different l values are connected by several recursion relations. This of course implies recursion relations between integrals $I_{ll'}^{(\lambda)}$ with different l, l' and λ values [7–9]. The utility of the subroutine CLMINT is to generate the initial values for a recursion scheme. In the case $R_1 = 0$, $R_2 = \infty$, the integrals $I_{ll'}^{(\lambda)}$ can be expressed in elementary functions which are much easier to obtain by other methods [7,10].

2. WKB-approximation of Coulomb wave functions

In this section we discuss the approximation of Coulomb wave functions by WKB functions in the asymptotic region [11–15]. The accuracy of the common first order WKB solution is not sufficient for our purposes, so we have to investigate a more general iteration scheme.

The regular and irregular Coulomb wave functions $F_l(\eta, \rho)$, $G_l(\eta, \rho)$ satisfy the differential equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + k(\rho)^2\right) u(\rho) = 0, \quad k(\rho) = \sqrt{1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}}, \tag{7}$$

and behave asymptotically as (4). We consider the solutions at $\rho_T < \rho < \infty$ where the runing point ρ_T is defined by

$$\rho_T = \eta + \sqrt{\eta^2 + l(l+1)}. \tag{8}$$

Introducing the phase–amplitude representation

$$u(\rho) = \frac{\alpha(l, \eta)}{\sqrt{\xi(\rho)}} \sin \phi(\rho), \quad \phi(\rho) = \int \xi(\rho) \mathrm{d}\rho, \tag{9}$$

in eq. (7), yields a differential equation for the amplitude $\xi(\rho)$.

$$\xi(\rho)^2 = k(\rho)^2 + \xi(\rho)^{1/2} \frac{\mathrm{d}^2}{\mathrm{d}\rho^2} \xi(\rho)^{-1/2}. \tag{10}$$

A solution of (10) leads to a Coulomb wave function, but the correct choice of $\alpha(l, \eta)$, and the integration constant in the phase $\phi(\rho)$, must ensure that this solution coincides with $F_l(\eta, \rho)$ or $G_l(\eta, \rho)$.

Now we presuppose the WKB approximation

$$|\xi(\rho)^{1/2}\frac{d^2}{d\rho^2}\xi(\rho)^{-1/2}| \ll k(\rho)^2 \tag{11}$$

which can be shown to be equivalent to the statement that the change of $\xi(\rho)$ over one wavelength $2\pi/k(\rho)$ is much smaller than $\xi(\rho)$ itself. Assuming this, eq. (10) may be solved by iteration.

$$\xi_0(\rho)=1, \quad \xi_n(\rho)=\sqrt{k(\rho)^2+\xi_{n-1}(\rho)^{1/2}\frac{d^2}{d\rho^2}\xi_{n-1}(\rho)^{-1/2}}, \quad n=1,2,\ldots. \tag{12}$$

From eq. (7) it is clear that $k(\rho)=1+\mathcal{O}(\rho^{-1})$ for large ρ, so $\xi_n(\rho)=1+\mathcal{O}(\rho^{-1})$ for every n. Substituting this in (9) and comparing the result with the asymptotic expansion (4), gives us the only possible choice of $\alpha(l,\eta)=1$. Furthermore we see that $k(\rho_T)=0$, so condition (11) might only hold for $\rho>\rho_T$. For large ρ, the left side of (11) vanishes, while the right side approaches one, so the best fit will be obtained in this region.

The only possible distinction between the approximation of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ is the integration constant in the phase of (9), but from (4) we see that they must differ by $\pi/2$. We choose the approximation of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ to be

$$f_l^{(n)}(\eta,\rho)=\xi_n(\rho)^{-1/2}\sin\phi_n(\rho), \quad g_l^{(n)}(\eta,\rho)=\xi_n(\rho)^{-1/2}\cos\phi_n(\rho), \tag{13}$$

where

$$\phi_n(\rho)=\int\xi_n(\rho)d\rho \tag{14}$$

and the integration constant is determined by the condition

$$\phi_n(\rho)\underset{\rho\to\infty}{\sim}\rho-\eta\log(2\rho)+\sigma_l(\eta)-l\pi/2. \tag{15}$$

The first order WKB solutions are immediately found:

$$\xi_1(\rho)=k(\rho)=\frac{1}{\rho}\sqrt{\rho^2-2\eta\rho-l(l+1)},$$

$$\phi_1(\rho)=\int k(\rho)d\rho=\tau(\rho)-\eta\log(\rho-\eta+\tau(\rho))+\eta+\sigma_l(\eta)-l\pi/2$$

$$+\sqrt{l(l+1)}\left\{\arctan\left(\frac{\eta\rho+l(l+1)}{\tau(\rho)\sqrt{l(l+1)}}\right)-\arctan\left(\frac{\eta}{\sqrt{l(l+1)}}\right)\right\}, \tag{16}$$

where we used the abbreviation

$$\tau(\rho)=\rho k(\rho) \tag{17}$$

and the term in curly brackets will be defined to vanish for $l=0$. The second order WKB solutions are somewhat more complicated. From (12) we have

$$\xi_2(\rho)=k(\rho)\sqrt{1+k(\rho)^{-3/2}\frac{d^2}{d\rho^2}k(\rho)^{-1/2}}=k(\rho)+\tfrac{1}{2}k(\rho)^{-1/2}\frac{d^2}{d\rho^2}k(\rho)^{-1/2}+\mathcal{O}(\rho^{-6}). \tag{18}$$

The next iteration, $\xi_3(\rho)$, leads to $\mathcal{O}(\rho^{-5})$ corrections to $\xi_2(\rho)$ so we can omit $\mathcal{O}(\rho^{-6})$ in (18). Substituting the expression for $k(\rho)$ yields the second order approximation for the amplitude:

$$\xi_2(\rho)=\xi_1(\rho)+\frac{1}{4\tau(\rho)^3}\left\{2\eta+\frac{3l(l+1)}{\rho}+\frac{5}{2}\frac{[\eta\rho+l(l+1)]^2}{\rho\tau(\rho)^2}\right\}. \tag{19}$$

The phase $\phi_2(\rho)$ is obtained by integrating (18):

$$\begin{aligned}\phi_2(\rho)&=\phi_1(\rho)+\frac{1}{2}\int k(\rho)^{-1/2}\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}k(\rho)^{-1/2}\mathrm{d}\rho\\&=\phi_1(\rho)-\frac{1}{4}\frac{\eta\rho+l(l+1)}{\tau(\rho)^3}-\frac{1}{2}\int\left[\frac{\mathrm{d}}{\mathrm{d}\rho}k(\rho)^{-1/2}\right]^2\mathrm{d}\rho,\end{aligned} \tag{20}$$

where the last step is a partial integration. The integral in (20) is evaluated as follows:

$$\begin{aligned}\int\left[\frac{\mathrm{d}}{\mathrm{d}\rho}k(\rho)^{-1/2}\right]^2\mathrm{d}\rho&=\frac{1}{4}\int\frac{[\eta\rho+l(l+1)]^2}{\rho\tau^5}\mathrm{d}\rho\\&=\frac{1}{4}\eta^2\int\frac{\rho\mathrm{d}\rho}{\tau^5}+\frac{1}{2}\eta l(l+1)\int\frac{\mathrm{d}\rho}{\tau^5}+\frac{1}{4}l^2(l+1)^2\int\frac{\mathrm{d}\rho}{\rho\tau^5}\\&=\begin{cases}-\frac{1}{6\tau}\left\{\frac{\eta}{2(\rho-2\eta)}+1+\frac{\tau-\rho}{\eta}\right\} & (l=0),\\ -\frac{\eta\rho+l(l+1)}{12\tau^3}+\frac{\eta}{12(\eta^2+l(l+1))}\left\{\frac{\eta-\rho}{\tau}+1\right\}+\frac{1}{4\tau}\\ \quad-\frac{1}{4\sqrt{l(l+1)}}\left\{\arctan\left(\frac{\eta\rho+l(l+1)}{\tau\sqrt{l(l+1)}}\right)-\arctan\left(\frac{\eta}{\sqrt{l(l+1)}}\right)\right\} & (l\neq 0),\end{cases}\end{aligned} \tag{21}$$

where the integration constant is chosen in such a way that this integral vanishes for $\rho\to\infty$. Substituting this result in (2) gives the final expression for $\phi_2(\rho)$:

$$\phi_2(\rho)=\begin{cases}\tau-\eta\log(\rho-\eta+\tau)+\eta+\sigma_0(\eta)+\frac{1}{12\tau}\left\{1+\frac{\tau-\rho}{\eta}-\frac{5}{2}\frac{\eta}{\rho-2\eta}\right\} & (l=0),\\ \tau-\eta\log(\rho-\eta+\tau)+\eta+\sigma_l(\eta)-l\pi/2-\frac{1}{6\tau}-\frac{\eta}{24(\eta^2+l(l+1))}\\ \quad-\frac{\eta\rho+l(l+1)}{24\tau^3}\left\{5-\frac{\tau^2}{\eta^2+l(l+1)}\right\}\\ \quad+\left\{\sqrt{l(l+1)}+\frac{1}{8\sqrt{l(l+1)}}\right\}\left\{\arctan\left(\frac{\eta\rho+l(l+1)}{\tau\sqrt{l(l+1)}}\right)-\arctan\left(\frac{\eta}{\sqrt{l(l+1)}}\right)\right\} & (l\neq 0).\end{cases} \tag{22}$$

From eq. (13) we have

$$f_l^{(n)}(\eta,\rho)^2+g_l^{(n)}(\eta,\rho)^2=1/\xi_n(\rho) \tag{23}$$

and on differentiating eq. (13) we obtain the derivatives

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\rho}f_l^{(n)}(\eta,\rho)&=\xi_n(\rho)g_l^{(n)}(\eta,\rho)-\tfrac{1}{2}f_l^{(n)}(\eta,\rho)\xi_n^{-1}(\rho)\frac{\mathrm{d}}{\mathrm{d}\rho}\xi_n(\rho),\\ \frac{\mathrm{d}}{\mathrm{d}\rho}g_l^{(n)}(\eta,\rho)&=-\xi_n(\rho)f_l^{(n)}(\eta,\rho)-\tfrac{1}{2}g_l^{(n)}(\eta,\rho)\xi_n^{-1}(\rho)\frac{\mathrm{d}}{\mathrm{d}\rho}\xi_n(\rho),\end{aligned} \tag{24}$$

from which we have the Wronskian relation

$$g_l^{(n)}(\eta,\rho)\frac{\mathrm{d}}{\mathrm{d}\rho}f_l^{(n)}(\eta,\rho)-f_l^{(n)}(\eta,\rho)\frac{\mathrm{d}}{\mathrm{d}\rho}g_l^{(n)}(\eta,\rho)=1. \tag{25}$$

We calculate the derivatives (24) starting from $\xi_n(\rho)$, $f_l^{(n)}(\eta,\rho)$, $g_l^{(n)}(\eta,\rho)$ and $\xi_n'(\rho)$, where the latter is given explicitly by

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\xi_1(\rho)=\frac{\eta\rho+l(l+1)}{\rho^2\tau}, \tag{26}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\rho}\xi_2(\rho)=&\frac{1}{\rho\tau}\left\{\eta+\frac{l(l+1)}{\rho}\right\}+\frac{1}{4\tau}\left[\frac{3(\eta-\rho)}{\tau^4}\left\{2\eta+\frac{3l(l+1)}{\rho}+\frac{5}{2}\frac{[\eta\rho+l(l+1)]^2}{\rho\tau^2}\right\}\right.\\ &\left.+\frac{1}{\rho\tau^2}\left[\frac{-3l(l+1)}{\rho}+\frac{5}{2}\frac{\eta\rho+l(l+1)}{\tau^2}\left\{2\eta-\frac{\eta\rho+l(l+1)}{\rho\tau^2}(\tau^2+2\rho(\rho-\eta))\right\}\right]\right]\end{aligned} \tag{27}$$

which simplifies considerably for $l=0$.

Now we have to discuss the accuracy which can be achieved in the approximation of Coulomb wave functions and their derivatives by the expressions above. In the whole treatment of the WKB approximation, there are two ρ-values of interest i.e. $\rho=\rho_T$ and $\rho=\infty$, so we consider the accuracy as a function of η, l and ρ/ρ_T. In table 1 of the test run output we have printed out some first- and second-order WKB functions and the corresponding Coulomb wave functions. From many test runs, we draw the following conclusions:

1) The second order WKB functions are always more accurate than the corresponding first order approximations, while the calculation times are almost equal.
2) Averaged over a large range of parameters l and η and over many ρ-values, the calculation of a WKB function is a factor of about 70 faster compared with the calculation of a Coulomb wave function.
3) For given l, η and ρ, the accuracies of the regular and irregular WKB functions and also of the derivatives are of the same order.
4) The condition

$$\rho/\rho_T>1.5+160/\eta \tag{28}$$

indicates the region where an accuracy of seven figures or more is obtained by second order WKB approximation. In general we can state that the accuracy increases with ρ, l and η.

3. Asymptotic expansion of $I_{ll'}^{(\lambda)}$

In this section we will elaborate the idea of Belling [6] to expand $I_{ll'}^{(\lambda)}$ into an asymptotic series in the lower integration limit R_1, but we taken $R_2=\infty$. Belling uses first order WKB functions to approximate

the integrand, but we will start from the exact Coulomb wave functions, which can be calculated very accurately by methods presented in ref. [4] or [5].

Instead of (13) we put

$$F_l(\eta, \rho) = \xi(\rho)^{-1/2} \sin \phi(\rho), \quad G_l(\eta, \rho) = \xi(\rho)^{-1/2} \cos \phi(\rho) \tag{29}$$

which can be considered to define the amplitude

$$\xi(\rho) = 1/\left[F_l(\eta, \rho)^2 + G_l(\eta, \rho)^2 \right] \tag{30}$$

and also $\sin \phi(\rho)$ and $\cos \phi(\rho)$. By (14) we have the important relation

$$\mathrm{d}\phi(\rho)/\mathrm{d}\rho = \xi(\rho). \tag{31}$$

Now introduce three new functions of l, η, k, l', η', k', λ and r by

$$f(r) = 1/r^{\lambda+1} \sqrt{\xi(kr)\bar{\xi}(k'r)}\,, \tag{32}$$

$$\theta^{\pm}(r) = \phi(kr) \pm \bar{\phi}(k'r), \tag{33}$$

where the bar in $\bar{\xi}$ and $\bar{\phi}$ denotes that these are functions of the primed parameters l', η' and k'. To calculate the integrals (1), it is sufficient to know the following real valued integrals:

$$\begin{aligned}
I_{ll'}^{(\lambda)}1 &= \int_R^\infty F_l(\eta, kr) F_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^{\lambda+1}} = \int_R^\infty f(r) \sin\phi \sin\bar{\phi}\,\mathrm{d}r = \tfrac{1}{2}\left(g_2^-(R) - g_2^+(R)\right), \\
I_{ll'}^{(\lambda)}2 &= \int_R^\infty F_l(\eta, kr) G_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^{\lambda+1}} = \int_R^\infty f(r) \sin\phi \cos\bar{\phi}\,\mathrm{d}r = \tfrac{1}{2}\left(g_1^+(R) + g_1^-(R)\right), \\
I_{ll'}^{(\lambda)}3 &= \int_R^\infty G_l(\eta, kr) G_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^{\lambda+1}} = \int_R^\infty f(r) \cos\phi \cos\bar{\phi}\,\mathrm{d}r = \tfrac{1}{2}\left(g_2^+(R) + g_2^-(R)\right), \\
I_{ll'}^{(\lambda)}4 &= \int_R^\infty G_l(\eta, kr) F_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^{\lambda+1}} = \int_R^\infty f(r) \cos\phi \sin\bar{\phi}\,\mathrm{d}r = \tfrac{1}{2}\left(g_1^+(R) - g_1^-(R)\right),
\end{aligned} \tag{34}$$

in which

$$g_1^{\pm}(R) = \int_R^\infty f(r) \sin\theta^{\pm}(r)\mathrm{d}r, \quad g_2^{\pm}(R) = \int_R^\infty f(r) \cos\theta^{\pm}(r)\mathrm{d}r. \tag{35}$$

Notice that the integrands are well-known functions and that it is not necessary to determine the phases ϕ and $\bar{\phi}$, but only $\sin(\phi \pm \bar{\phi})$ and $\cos(\phi \pm \bar{\phi})$ which is easily done with some trigonometric formulae.

We split up the integrals $g_i^{\pm}(R)$ as follows:

$$g_i^{\pm}(R) = P_i^{\pm}(R) \sin\theta^{\pm}(R) + Q_i^{\pm}(R) \cos\theta^{\pm}(R), \quad i = 1, 2. \tag{36}$$

In equating (35) and (36), we are able to solve for the eight unknown functions $P_i^{\pm}(R)$, $Q_i^{\pm}(R)$. To this end we differentiate both expressions for $g_i^{\pm}(R)$ with respect to R, which yields four sets of two coupled first order differential equations.

$$\frac{\mathrm{d}P_1^{\pm}}{\mathrm{d}R} - \chi^{\pm}(R) Q_1^{\pm}(R) + f(R) = 0, \quad \frac{\mathrm{d}Q_1^{\pm}}{\mathrm{d}R} + \chi^{\pm}(R) P_1^{\pm}(R) = 0, \tag{37}$$

$$\frac{\mathrm{d}Q_2^{\pm}}{\mathrm{d}R} + \chi^{\pm}(R) P_2^{\pm}(R) + f(R) = 0, \quad \frac{\mathrm{d}P_2^{\pm}}{\mathrm{d}R} - \chi^{\pm}(R) Q_2^{\pm}(R) = 0, \tag{38}$$

where we used the notation

$$\chi^{\pm}(R)=\frac{\mathrm{d}}{\mathrm{d}R}\theta^{\pm}(R)=k\xi(kr)\pm k'\bar{\xi}(k'r). \tag{39}$$

Eqs. (37) and (38) have to be solved with the boundary conditions

$$\lim_{R\to\infty}P_i^{\pm}(R)=0, \quad \lim_{R\to\infty}Q_2^{\pm}(R)=0, \quad i=1,2. \tag{40}$$

By choosing

$$P_1^{\pm}(R)=Q_2^{\pm}(R), \quad Q_1^{\pm}(R)=-P_2^{\pm}(R), \tag{41}$$

the sets (37) and (38) become identical, so it suffices to solve (38) and we can suppress the subscripts.

To solve (38) we substitute the series expansion

$$P^{\pm}(R)=A_0^{\pm}(R)+A_2^{\pm}(R)+A_4^{\pm}(R)+\ldots, \quad Q^{\pm}(R)=A_1^{\pm}(R)+A_3^{\pm}(R)+A_5^{\pm}(R)+\ldots, \tag{42}$$

which yields the recursive expression for the successive terms,

$$A_0^{\pm}(R)=-\frac{f(R)}{\chi^{\pm}(R)}, \quad A_m^{\pm}(R)=\frac{(-1)^{m+1}}{\chi^{\pm}(R)}\frac{\mathrm{d}}{\mathrm{d}R}A_{m-1}^{\pm}(R), \quad m\geqslant 1. \tag{43}$$

Using the first order WKB approximations $\phi_1(\rho)$ and $\bar{\phi}_1(\rho)$, we obtain from (33)

$$\theta^{\pm}(R)=(k\pm k')R-\eta\log(2kR)\mp\eta'\log(2k'R)-(l\pm l')\pi/2+\sigma_l(\eta)\pm\sigma_{l'}(\eta')+\mathcal{O}(R^{-1}). \tag{44}$$

Remembering that in actual problems ηk equals $\eta' k'$, we suppose $\eta=\eta'$ whenever $k=k'$. With eq. (44) inserted in eq. (39) we can distinguish three characteristic cases:

$$\begin{aligned}
&\text{a) } \chi^{\pm}(R)=k\pm k'+\mathcal{O}(R^{-1}),\\
&\text{b) } \chi^{-}(R)=\mathcal{O}(R^{-2}), && k=k',\\
&\text{c) } \chi^{-}(R)=0, && k=k' \text{ and } l=l'.
\end{aligned} \tag{45}$$

Substituting this first order expansion in (43) shows that

$$\begin{aligned}
&A_m^{+}(R)=\mathcal{O}(R^{-\lambda-1-m}),\\
&A_m^{-}(R)=\mathcal{O}(R^{-\lambda-1-m}), \quad \text{when } k\neq k',
\end{aligned} \tag{46}$$

and we have a series with descending powers of R, which is expected to converge for sufficiently large R. From (45) we see that when $k=k'$ the series (42) with $\chi^{-}(R)$ might diverge at large R (or is not even defined) because the powers of R are ascending with increasing m, so this case has to be treated in another way. We will come to this later in this paper.

The numerical evaluation of the successive terms of (43) is rather cumbersome because of the appearance of the derivative of the previous term. To solve this problem, we set up an iteration scheme, which was proposed by Belling. To this end we make the substitution

$$A_m^{\pm}(R)=\frac{-f(R)}{\chi^{\pm}(R)}\frac{\beta_m^{\pm}(R)}{\left(R\chi^{\pm}(R)\right)^m} \tag{47}$$

and try to calculate $\beta_m^{\pm}(R)$. With (43) we find the relation for $\beta_m^{\pm}(R)$ to be

$$\begin{aligned}
&\beta_0^{\pm}(R)=1,\\
&\beta_m^{\pm}(R)=\Psi_m^{\pm}(R)\beta_{m-1}^{\pm}(R)+(-1)^{m+1}R\frac{\mathrm{d}}{\mathrm{d}R}\beta_{m-1}^{\pm}(R),
\end{aligned} \tag{48}$$

where

$$\Psi_m^{\pm}(R) = (-1)^{m+1}\left\{1 - m + R\frac{\chi^{\pm m}}{f}\frac{\mathrm{d}}{\mathrm{d}R}\left(\frac{f}{\chi^{\pm m}}\right)\right\} \tag{49}$$

is a known function of the parameters and R. Henceforth we leave out the superscript on $\beta_m^{\pm}(R)$ and $\Psi_m^{\pm}(R)$. From (45), (46) and (47) we have $\beta_m(R) = \mathcal{O}(1)$, so for sufficiently large R this β_m tends to a constant and the derivative in (48) will vanish. As a zeroth order approximation for β_m we have

$$\beta_0^{(0)} = 1, \quad \beta_m^{(0)} = \Psi_m \beta_{m-1}^{(0)} \tag{50}$$

which can be calculated successively. From this we make an approximation for the derivatives of the β_m's

$$\beta_0^{(0)'} = 0, \quad \beta_m^{(0)'} = \Psi_m \beta_{m-1}^{(0)'} + \Psi_m' \beta_{m-1}^{(0)} \tag{51}$$

and with these a first order approximation for the β_m's

$$\beta_0^{(1)} = 1, \quad \beta_m^{(1)} = \Psi_m \beta_{m-1}^{(1)} + (-1)^{m+1} R \beta_{m-1}^{(0)'}. \tag{52}$$

To increase the accuracy we make another iteration:

$$\beta_0^{(0)''} = 0, \quad \beta_m^{(0)''} = \Psi_m \beta_{m-1}^{(0)''} + 2\Psi_m' \beta_{m-1}^{(0)'} + \Psi_m'' \beta_{m-1}^{(0)}, \tag{53}$$

$$\beta_0^{(1)'} = 0, \quad \beta_m^{(1)'} = \Psi_m \beta_{m-1}^{(1)'} + \Psi_m' \beta_{m-1}^{(1)} + (-1)^{m+1}\left\{\beta_{m-1}^{(0)'} + R\beta_{m-1}^{(0)'}\right\}, \tag{54}$$

$$\beta_0^{(2)} = 1, \quad \beta_m^{(2)} = \Psi_m \beta_{m-1}^{(2)} + (-1)^{m+1} R \beta_{m-1}^{(1)'}, \tag{55}$$

in which $\beta_m^{(2)}$ will be the final approximation of β_m. Writing out explicitly the $\beta_m^{(2)}$ with $m = 0, 1, 2, 3$ and comparing with the exact formula (48) will show that the approximation of β_m by $\beta_m^{(2)}$ is exact up to $m = 3$. That is to say, the first approximated term is $A_4^{\pm}(R)$.

The calculation of $\beta_m^{(2)}$ by (50)–(55) is not trivial because of the appearance of $\Psi_m^{\pm}(R)$ and derivatives for every m. Introducing the functions $\tilde{\Psi}_m^{\pm}(R)$

$$\tilde{\Psi}_m^{\pm}(R) = (-1)^m \Psi_m^{\pm}(R) = m - 1 + R\left\{m\frac{\chi^{\pm'}}{\chi^{\pm}} - \frac{f'}{f}\right\}, \tag{56}$$

we see that

$$\tilde{\Psi}_m^{\pm}(R) = \alpha(R) + m\epsilon^{\pm}(R) \tag{57}$$

which has only a linear dependence on m. With (57) we also have

$$\frac{\mathrm{d}}{\mathrm{d}R}\tilde{\Psi}_m^{\pm}(R) = \alpha'(R) + m\epsilon^{\pm}(R)', \tag{58}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}R^2}\tilde{\Psi}_m^{\pm}(R) = \alpha''(R) + m\epsilon^{\pm}(R)'', \tag{59}$$

but $\alpha(R)$, $\epsilon^{\pm}(R)$ and derivatives are constants at a given set of parameters and at a given R. To calculate these, we first define a new function

$$\gamma(R) = \xi(kR) = \left[F_l(\eta, kR)^2 + G_l(\eta, kR)^2\right]^{-1} \tag{60}$$

and also $\bar{\gamma}(R)$ for the primed parameters. With this notation we have

$$\chi^{\pm}(R) = k\gamma(R) \pm k'\bar{\gamma}(R), \quad f(R) = R^{-\lambda-1}\left(\gamma(R)\bar{\gamma}(R)\right)^{-1/2}. \tag{61}$$

From (60) we have the derivative

$$B_l(\eta, k, R) = \frac{\mathrm{d}}{\mathrm{d}R}\gamma(R) = -2\gamma(R)^2(FF' + GG'), \tag{62}$$

where F' is a shorthand notation for $\mathrm{d}F_l(\eta, kR)/\mathrm{d}R$, etc. The Coulomb wave function routines from refs. [4], [5] also return the derivatives with respect to $\rho = kR$. With the differential equation (3) we can calculate the derivatives of any order. With the next sequence of formulae we are able to construct an expression for $\tilde{\Psi}_m^{\pm}(R)$. The idea is that every newly introduced function is calculated in this sequence.

$$H_l(\eta, k, R) = B_l(\eta, k, R)/\gamma(R), \tag{63}$$

$$A^{\pm}(R) = \chi^{\pm\prime}/\chi^{\pm} = \left[kB_l(\eta, k, R) \pm k'B_{l'}(\eta', k', R)\right]/\chi^{\pm}(R), \tag{64}$$

$$f'(R)/f(R) = -(\lambda+1)/R + \tfrac{1}{2}\left(H_l(\eta, k, R) + H_{l'}(\eta', k', R)\right), \tag{65}$$

$$\tilde{\Psi}_m^{\pm}(R) = m + \lambda + R\left\{mA^{\pm}(R) + \tfrac{1}{2}\left(H_l(\eta, k, R) + H_{l'}(\eta', k', R)\right)\right\}. \tag{66}$$

In the same way we can proceed to calculate the first and second derivatives of (66). This is straightforward, but for reference purposes we write down the sequence which leads to the derivatives needed:

$$C_l(\eta, k, R) = \frac{\mathrm{d}}{\mathrm{d}R}B_l(\eta, k, R) = 2\gamma(R)\left[H_l^2(\eta, k, R) - \gamma(R)(FF'' + F'^2 + GG'' + G'^2)\right], \tag{67}$$

$$D_l(\eta, k, R) = \frac{\mathrm{d}}{\mathrm{d}R}H_l(\eta, k, R) = \frac{C_l(\eta, k, R)}{\gamma(R)} - H_l^2(\eta, k, R), \tag{68}$$

$$I^{\pm}(R) = \left[kC_l(\eta, k, R) \pm k'C_{l'}(\eta', k', R)\right]/\chi^{\pm}(R), \tag{69}$$

$$\frac{\mathrm{d}}{\mathrm{d}R}A^{\pm}(R) = I^{\pm}(R) - A^{\pm}(R)^2, \tag{70}$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}R}\tilde{\Psi}_m(R) &= \tfrac{1}{2}\left\{H_l(\eta, k, R) + H_{l'}(\eta', k', R) + R\left(D_l(\eta, k, R) + D_{l'}(\eta', k', R)\right)\right\} \\ &\quad + m\left\{A^{\pm}(R) + R\left(I^{\pm}(R) - A^{\pm}(R)^2\right)\right\},\end{aligned} \tag{71}$$

$$\begin{aligned}J_l(\eta, k, R) &= \frac{\mathrm{d}}{\mathrm{d}R}C_l(\eta, k, R) \\ &= C_l(\eta, k, R)H_l(\eta, k, R) + 2\gamma(R)\left\{2H_l(\eta, k, R)D_l(\eta, k, R)\right. \\ &\quad - B_l(\eta, k, R)(FF'' + F'^2 + GG''G'^2) \\ &\quad \left. -\gamma(R)(FF''' + 3F'F'' + GG''' + 3G'G'')\right\},\end{aligned} \tag{72}$$

$$\begin{aligned}E_l(\eta, k, R) &= \frac{\mathrm{d}}{\mathrm{d}R}D_l(\eta, k, R) \\ &= \frac{1}{\gamma(R)}\left\{J_l(\eta, k, R) - C_l(\eta, k, R)H_l(\eta, k, R)\right\} - 2H_l(\eta, k, R)D_l(\eta, k, R),\end{aligned} \tag{73}$$

$$K^{\pm}(R) = \left[kJ_l(\eta, k, R) \pm k'J_{l'}(\eta', k', R)\right]/\chi^{\pm}(R), \tag{74}$$

$$\frac{\mathrm{d}}{\mathrm{d}R}I^{\pm}(R) = K^{\pm}(R) - A^{\pm}(R)I^{\pm}(R), \tag{75}$$

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}R^2}\tilde{\Psi}_m^{\pm}(R) &= D_l(\eta, k, R) + D_{l'}(\eta', k', R) + \tfrac{1}{2}R\left(E_l(\eta, k, R) + E_{l'}(\eta', k', R)\right) \\ &\quad + m\left\{R\left(K^{\pm}(R) - A^{\pm}(R)I^{\pm}(R)\right) + 2\left(I^{\pm}(R) - A^{\pm}(R)^2\right)\left(1 - RA^{\pm}(R)\right)\right\}.\end{aligned} \tag{76}$$

After the analytical treatment we wrote a numerical procedure in order to calculate the $I_{ll'}^{(\lambda)}$ by asymptotic expansion. The next consideration was how to investigate the convergence of the asymptotic series and how to check on the accuracy to which the $I_{ll'}^{(\lambda)}$ could be approximated by the method of calculation, described in this section. To this end we remark that there exist many recursion relations between the integrals with different l, l' and λ values [7–9]. We choose the following one:

$$\frac{k(l+l'+\lambda+3)\sqrt{(l+2)^2+\eta^2}}{(l+2)(2l+3)} I_{l+2,l'+1}^{(\lambda)} + \eta k\left\{\frac{1}{l'+1} - \frac{l'+\lambda+1}{(l+1)(l+2)}\right\} I_{l+1,l'+1}^{(\lambda)}$$
$$+ \frac{k(l'-l+\lambda)\sqrt{(l+1)^2+\eta^2}}{(l+1)(2l+3)} I_{l,l'+1}^{(\lambda)} - \frac{k'}{l'+1}\sqrt{(l'+1)^2+\eta'^2}\, I_{l+1,l'}^{(\lambda)} = \frac{X_{l+1}(\eta, kR) Y_{l'+1}(\eta', k'R)}{R^{\lambda+1}}. \tag{77}$$

We can calculate the four integrals by the asymptotic expansion and substitute them in the left-hand side of (77). This result is compared with the right-hand side of (77). The analytical development, however, is separated into a $\chi^+(R)$ and a $\chi^-(R)$ part and it would be interesting to check on these independently. With eq. (34) it is easy to see that there is a recursion relation between the integrals $g_l^{\pm}(R)$, similar to (77), but with a different right-hand side.

In table 2 of the test run output an example is given of a test run, made in this way. The order of printout is $g_1^+(R)$, $g_1^-(R)$, $g_2^+(R)$, $g_2^-(R)$. From many test runs we can summarize some conclusions:

1. The series (42) with $\chi^+(R)$ always converges for large R, but even for R just above the turning point.
2. The series with $\chi^-(R)$ converges when $|k-k'|R$ is sufficiently large. This is clear from (47), where the denominator is a power of $R\chi^+ \approx (k-k')R$. In some applications this gives rise to a severe problem, because $|k-k'|R$ is of the order 10^{-1}–10^{-4}, so the χ^--series will diverge. Remeber that the χ^--series is not defined when $k = k'$.
3. At a given integration limit R and parameters k, η, l, k', η', l', λ, the χ^+-series is always more accurate than the χ^--series, when both converge. The χ^--series also uses much more terms, as will be apparent.
4. The striking feature of this routine is the convergence and the accuracy of the χ^+-series. This series is connected with the θ^+-integrals (see (35)) which are the constituent parts of $I_{ll'}^{(\lambda)}$, responsible for the fast oscillatory behaviour of the integrand. We only need to consider further the θ^--integrals, which will be done in the next section.

4. Determination of θ^--integrals by Gaussian quadrature

In the previous section, we have pointed out how θ^--integrals can be evaluated, whenever $|k-k'|$ is not too small. Now we investigate the complementary problem, where k and k' are equal or almost equal. We will consider the integrals

$$g_1^- = \int_{R_1}^{R_2} f(r) \sin\theta^-(r)\mathrm{d}r, \quad g_2^- = \int_{R_1}^{R_2} f(r)\cos\theta^-(r)\mathrm{d}r. \tag{78}$$

The functions $f(r)$ and $\theta^-(r)$ behave as

$$f(r) = \frac{1}{r^{\lambda+1}}\left(1+\mathcal{O}\left(\frac{1}{r}\right)\right), \quad \theta^-(r) = (k-k')r + \ldots \quad (r \text{ large}), \tag{79}$$

so the integrand is oscillatory with a wavelength $2\pi/|k-k'|$ but when $k = k'$ the $\theta^-(r)$ tends to a constant

and there is no oscillation at all. Since we assume $|k-k'|$ sufficiently small, the integrand of g_i^- is a smooth function of r and we can use a simple Gaussian quadrature formula

$$\int_a^b \phi(y)\mathrm{d}y = \tfrac{1}{2}(b-a)\sum_{i=1}^{20} w_i\phi(y_i) + \delta, \quad 0 < w_i < 1,$$
$$y_i = \tfrac{1}{2}(b-a)x_i + \tfrac{1}{2}(b+a), \qquad -1 < x_i < 1. \tag{80}$$

The abscissas x_i and the weight factor w_i are tabulated in ref. [3]. The absolute error δ is given by

$$\delta = \frac{(b-a)^{41}(20!)^4}{41(40!)^3}\phi^{(40)}(\xi), \quad a < \xi < b, \tag{81}$$

$$\delta = \beta(b-a)^{41}\phi^{(40)}(\xi), \quad \beta = 1.573 \times 10^{-72}. \tag{82}$$

Now we try to choose a step size $b-a$ in such a way that some relative error, 10^{-q}, will not be exceeded. At first we assume $|k-k'|$ small, and to be more precise

$$b - a \ll 2\pi/|k-k'| \tag{83}$$

so the factors $\sin\theta^-(r)$ and $\cos\theta^-(r)$ will behave smoothly on $[a, b]$ and are almost constant. In the calculation of the step size, we can replace them by 1, as long as (83) holds. Furthermore, we assume r sufficiently large, so we can approximate $f(r)$ by $r^{-\lambda-1}$. From (82) we then have

$$\delta = \beta\frac{(\lambda+40)!}{\lambda!}\left(\frac{b-a}{\xi}\right)^{41}\frac{1}{\xi^\lambda} < \beta\frac{(\lambda+40)!}{\lambda!}\left(\frac{b}{a}-1\right)^{41}a^{-\lambda}. \tag{84}$$

Suppose we have integrated up to $r = a$. We then want to calculate a step size $b-a$, to integrate over the subsequent interval $b-a$.

If we put

$$b = pa \quad (p > 1), \tag{85}$$

we have for the relative error ϵ in the next interval

$$\epsilon = \left|\delta\Big/\int_a^b \frac{\mathrm{d}y}{y^{\lambda+1}}\right| < \beta\frac{(\lambda+40)!}{(\lambda-1)!}(p-1)^{41}\frac{p^\lambda}{p^\lambda-1}. \tag{86}$$

Remark that at this point we have to make the restriction $\lambda \neq 0$. With the abbreviation

$$\alpha(\lambda) = \beta(\lambda+40)!/(\lambda-1)! \tag{87}$$

and with $p^\lambda \geqslant p$, we have

$$\epsilon < \alpha(\lambda)p(p-1)^{40}. \tag{88}$$

If p is near to one (say $p < 2$) we can omit this factor in (88), but for large p we have $p^\lambda \simeq p^\lambda - 1$ and we can omit $p^\lambda/(p^\lambda-1)$ in (86). This increases the exponent in (88) by 1. So, if we want $\epsilon < 10^{-q}$, we find

$$p = 1 + \sqrt[41]{10^{-q}/\alpha(\lambda)}. \tag{89}$$

With (85) we have

$$b - a = (p-1)a, \tag{90}$$

so with increasing a, the step size increases too. This is especially interesting if we want to integrate up to infinity. Actual p-values, calculated by (89), are between 2 and 3.

When we want to integrate up to infinity, it is important to choose the step size as large as possible, for the integrals are very slowly convergent. Because of the factor $r^{-\lambda-1}$, the contribution to the integrals descends in every step. If we have integrated step-by-step up to r^*, we may already have achieved an accuracy of say 10^{-s}, with $s < q$. In that case we may integrate up to R_2 (eventually $R_2 = \infty$) with an accuracy of 10^{-q+s}. When we use this value in (89), we come up with a larger p-value. If we have integrated up to r^* we can estimate the remaining part by

$$\int_{r^*}^{R_2} f(r) \sin\theta^-(r) \mathrm{d}r \approx \int_{r^*}^{R_2} \sin\theta^-(r) \frac{\mathrm{d}r}{r^{\lambda+1}} < \int_{r^*}^{R_2} \frac{\mathrm{d}r}{r^{\lambda+1}} = \lambda^{-1}\left(r^{*-\lambda} - R_2^{-\lambda}\right). \tag{91}$$

The integral itself is estimated by

$$I^* = \int_{R_1}^{r^*} f(r) \sin\theta^-(r) \mathrm{d}r, \tag{92}$$

so we already have an accuracy of

$$10^{-s} = \left|\left(r^{*-\lambda} - R_2^{-\lambda}\right)/\lambda I^*\right| \tag{93}$$

but this is better seen as an upper limit. Instead of 10^{-q} in (89), we use now 10^{-q+s}. This can increase p much, especially when a high accuracy is desired.

In increasing the step size it might occur that condition (83) is not fulfilled anymore. In that case we choose

$$b - a = 2\pi/|k - k'| \tag{94}$$

in all the remaining intervals and integrate with a 20-point formula. In this way we come up with the desired accuracy of 10^{-q}, for it is the limiting case of the estimation made above. If we integrate however over many wavelengths, the contributions of the wavelengths at large r values are calculated much too accurately for the same reason as above. We now cannot increase the step size as in the previous case and so we choose the complementary solution and decrease the order of the Gaussian formula to a 10-point or a 5-point formula. This subject will not be treated in detail, because it is along the same lines as the estimation above.

Up to here we have considered the integration over the asymptotic region and its peculiarities. To complete the integration procedure we extend the allowed R_1-values to $R_1 = 0$.

We start the integration in general with a 20-point Gaussian quadrature in R_1 until the θ^+-integrals can be calculated by asymptotic expansion. Additionally, the θ^--integrals are evaluated by the method of this section, where wee use WKB functions wherever possible. If R_1 is less than both turning points, only $I_{l'}^{(\lambda)}1$ will be reliable.

5. Notes on the program

The subroutine CLMINT calculates the integrals $I_{ll'}^{(\lambda)}$, as defined in (34). The calling sequence is CALL CLMINT(DR1, DR2, DETA1, DK1, L1, DETA2, DK2, L2, LAMBDA, DCLM, CONV, IACC). Here the convention is made that a D as a first figure indicates DOUBLE PRECISION type. The arguments in the call have the following meaning

DR1, DR2 — Lower and upper integration limits. If DR2 is less than DR1, the upper limit will be assumed infinite.

DETA1...LAMBDA	Parameters.
DCLM	The integrals are returned in array DCLM(4).
CONV	Logical variable. If CONV = .FALSE. after return, then there is an illegal parameter in the call or something went wrong in the calculation.
IACC	Integer chosen from 0 or 1. For general purposes one takes IACC = 0, but on putting IACC = 1, the accuracy will increase somewhat.

The subroutine uses the routines BELLIN, GAUSS, INTEGR, COULOM, STEED, RICCAT, WKB and DPHASE. These subroutines use two COMMON blocks, named XX and YY. The subroutine COULOM can be used independently and is a modified version of the routines from refs. [4,5]. The calling sequence is CALL COULOM(DRHO, DETA, L, DF, DFP, DG, DGP, CONV) and it generates the Coulomb wave functions. Here DF = $F_l(\eta, \rho)$, DFP = $\mathrm{d}F_l(\eta, \rho)/\mathrm{d}\rho$, etc. Also here the logical CONV indicates the convergence of the routine. Two other routines are included, that is WKB1 and WKB2, which calculate the first and second order WKB functions and derivatives by the method of section 2.

A test deck is included which prints Coulomb wave functions and the corresponding WKB approximations. The second test deck makes the check on BELLIN with the aid of a recursion relation as was discussed in section 3.

6. Discussion

In developing the routine, we always kept in mind that it should work best for large r values. That is why WKB functions are matched to the Coulomb wave functions at $\rho = \infty$ and is the reason for making the asymptotic expansion around infinity. Also the Gaussian formulae are chosen so as to produce the maximum interval length at infinity. In this asymptotic region, the routine is fast and accurate, compared to any step-by-step method. It will be clear that this is the most interesting region with respect to applications in nuclear physics, because at the lower r values there is still a nuclear potential and the homogeneous solutions are not Coulomb wave functions. There is also the interesting feature that the routine works best for heavy ions with high energy, for then η and k are large and $|k - k'|$ is very small. Because of the large k and k', the χ^+ series will converge rapidly, and already in the very neighbourhood of the turning point. It is just with these parameters that a numerical quadrature will fail because of the immense number of steps. When $|k - k'|$ is small, the θ^- integrals have a slowly-oscillating integrand is and the intervals of the Gaussian quadrature can be very large. In the case of $^{84}\mathrm{Kr} + ^{238}\mathrm{U}$ the wavelength of the θ^- integrand is of the order of 10^3 fm and we can integrate from the turning point (≈ 10 fm for $l = 0$) up to $r = 2000$ in eight steps. When we consider atomic collisions, the level distances are not very small compared to the kinetic energy of the colliding particles and $|k - k'|$ is sufficiently large to enable both the χ^+ and the χ^- series to converge. The most difficult application is in light ion reactions for then the χ^- series just diverges but $|k - k'|$ is rather large, so we have to integrate the θ^- integrals with 20 points per wavelength, which is severely time consuming, if we want to integrate up to infinity. In this case it is better to use $R_2 = 3000$ instead of $R_2 = \infty$ and approximate the integral up to infinity by the one obtained with $R_2 = 3000$. The accuracy will then be less than 7D but the calculation time will remain reasonable.

We recall once more that the evaluation of these integrals by closed expressions or by recursion relations is always superior to this routine. This routine only provides the $I_{ll'}^{(\lambda)}$ when there is no other way out. It, for instance, generates the initial values of a recursion scheme.

Many test runs have been made on the WKB approximation, the asymptotic expansion and the Gaussian quadrature. The WKB approximations were simply compared with the exact values, generated by a Coulomb wave function routine. The other routines were first tested by the substitution of $I_{ll'}^{(\lambda)}$ in a

recursion relation as was discussed before. Another method is to evaluate the right hand side of

$$\int_{R_1}^{R_2} = \int_{R_1}^{R} + \int_{R}^{R_2} \tag{95}$$

for different R values. This test, however, did not bring any new insight into the accuracy which can be achieved. As a third test we used the closed expression

$$\int_0^\infty F_l(\eta, kr) F_{l+1}(\eta, kr) \frac{\mathrm{d}r}{r^2} = \frac{k}{2|l+1+\mathrm{i}\eta|} \tag{96}$$

which showed that the integration below the turning point is crucial for the accuracy at large l values ($l \approx 1000$). As a final test we compared the results of CLMINT with the integrals obtained from the program of Samuel and Smilansky [10] in the quadrupole case. These integrals are

$$\int_0^\infty F_l(\eta, kr) F_{l'}(\eta', k'r) \frac{\mathrm{d}r}{r^3}, \quad l' = l-2, l, l+2. \tag{97}$$

There was a correspondence of 7D and this is just the accuracy claimed by Samuel and Smilansky.

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TEST RUN OUTPUT

Table 1

REGULAR COULOMB WAVE FUNCTION AND WKB APPROXIMATIONS AT 3*TURNINGPOINT

DETA	L	COULOM	WKB1	WKB2
1	1	-.1057887397D+01	-.1060805533D+01	-.1057639164D+01
1	10	-.2013681176D+00	-.2002627181D+00	-.2013720354D+00
1	100	-.8466177272D+00	-.8465538451D+00	-.8466177302D+00
1	1000	-.8919967881D+00	-.8920024201D+00	-.8919967881D+00
10	1	.1056700829D+01	.1056335580D+01	.1056701221D+01
10	10	.4408548097D+00	.4399960787D+00	.4408554858D+00
10	100	.1001653272D+00	.1000465597D+00	.1001653318D+00
10	1000	.9889057332D+00	.9889089511D+00	.9889057332D+00
100	1	-.7157823466D+00	-.7158868118D+00	-.7157823453D+00
100	10	-.1106351663D+01	-.1106350415D+01	-.1106351660D+01
100	100	.5441642610D+00	.5440802766D+00	.5441642635D+00
100	1000	-.5518213252D+00	-.5518315023D+00	-.5518213252D+00
1000	1	-.2059096758D+00	-.2058962478D+00	-.2059096758D+00
1000	10	-.1093514413D+00	-.1093378419D+00	-.1093514413D+00
1000	100	.1088063909D+01	.1088061443D+01	.1088063909D+01
1000	1000	.1079402300D+01	.1079403739D+01	.1079402300D+01

Table 2

CONVERGENCE AND ACCURACY CHECK OF BELLIN WITH A RECURSION RELATION

AND AS A FUNCTION OF THE LOWER LIMIT R

```
 DETA1 = .18000D+03
   DK1 = .40000D+02
    L1 =    40
 DETA2 = .14400D+03
   DK2 = .50000D+02
    L2 =    45
LAMBDA =     2
 DTURN =     9
```

R	LEFT HAND SIDE	RIGHT HAND SIDE	REL. DIFF.
54			
	.5431830995D-05	.5431830995D-05	.13D-10
	.4492142174D-05	.4492142542D-05	.82D-07
	.4154134779D-05	.4154134780D-05	.27D-10
	-.5155800061D-05	-.5155800531D-05	.91D-07
45			
	.3948285558D-05	.3948285558D-05	-.36D-12
	-.7742652824D-05	-.7742653255D-05	.56D-07
	.1134371270D-04	.1134371270D-04	.52D-10
	.9182596447D-05	.9182597521D-05	.12D-06
36			
	.2332061763D-04	.2332061763D-04	.16D-09
	-.2285451543D-04	-.2285451429D-04	-.50D-07
	-.5956609584D-05	-.5956609584D-05	-.57D-10
	-.7550075452D-05	-.7550071587D-05	-.51D-06
27			
	.5339512417D-04	.5339512421D-04	.73D-09
	.1485579010D-04	.1485580211D-04	.81D-06
	-.2683006289D-04	-.2683006290D-04	.11D-09
	.5788099216D-04	.5788088379D-04	-.19D-05
18			
	-.2216526523D-03	-.2216526525D-03	.96D-09
	-.3328158856D-04	-.3328183167D-04	.73D-05
	-.3950380848D-04	-.3950380913D-04	.16D-07
	-.2226747172D-03	-.2226718864D-03	-.13D-04
9			
	NO CONVERGENCE IN BELLIN		
	.4677916297D-02	.4668716554D-02	-.20D-02
	NO CONVERGENCE IN BELLIN		
	-.6705181619D-02	-.6705000823D-02	-.27D-04