PHYSICAL REVIEW C VOLUME 23, NUMBER 6 JUNE 1981

Recurrence relations for distorted-wave Born approximation Coulomb excitation integrals and their use in coupled channel calculations

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(Received 17 November 1980)

Coupled channel calculations for heavy ion inelastic scattering can be alleviated through the use of integrals involving the product of two Coulomb functions, regular or irregular, with some inverse power of the radius, the range of the integration going from the point where the nuclear potential is weak to infinity. These integrals can be obtained by recurrence relations, starting with at most four of them which must be obtained by some method already described in the literature.

[NUCLEAR REACTIONS HI inelastic scattering. Treatment of Coulomb interaction above Coulomb barrier.]

I. INTRODUCTION

Coupled channel calculations for heavy ion inelastic scattering usually involve many partial waves as well as long-range numerical integration.[1] The Coulomb potential generates coupling potentials which decrease only as $r^{-\lambda-1}$ for a transfer of angular momentum λ; when the numerical integration is stopped at R, the induced error is of the order of $R^{-\lambda}$. In the following, we shall consider a decrease in r^{-6} as sufficiently quick; we shall thus consider the problem for λ ranging from 1–4 only. This limitation is rather arbitrary; problems are crucial for $\lambda=1$ and 2, less important for $\lambda=3$, and already negligible for $\lambda=4$.

The use of an iteration procedure such as the "Equations Couplées en Itérations Séquentielles"[2] of the program ECIS shows that the distorted-wave Born approximation (DWBA) is enough for the upper half or two-thirds of the values of the total spin J. Furthermore, the nuclear potential has some effects only for the few lower values of J in this region; for larger values of J, the numerical integration can be replaced by analytical methods such as those published by Alder *et al.*[3] and Biedenharn *et al.*[4] more than twenty years ago. For the lower values of J, where coupled channel calculations should be used, the knowledge of integrals for products of $r^{-\lambda-1}$ with regular or irregular Coulomb functions from the matching point R to infinity can eliminate the largest part of the error in $R^{-\lambda}$, and allows the use of a shorter range of numerical integration for the coupling equations.

In Sec. II, the ECIS method will be presented in order to show how such integrals can be used. The ECIS method has the advantage of telling us from which value of the total spin J the DWBA results can replace those of coupled equations. Its Green's function formulation is the easiest way to introduce the use of Coulomb corrections. This will be done in Sec. III, where details will be given on their use in the differential and the integral procedures, as well as in the usual coupled equation techniques, in such a way as to achieve the same accuracy as in the numerical integration.

In Sec. IV, we show how some recurrence equations of Ref. 3 can be generalized to integrals of products of regular and irregular Coulomb functions from a finite radius to infinity. A tedious use of these recurrence relations allows us to express any integral, depending upon λ, l_i, l_j, in terms of integrals with $\lambda=1$, $l_i=l_j$, and the Coulomb functions at the starting radius of the integration. The integrals with $\lambda=1, l_i=l_j$ are not of direct physical interest in this problem, but they are related to relativistic corrections. They are obtained by recurrence relations, starting with four of them, for which direct methods[5] are available. They are computed beforehand and all the other integrals are expressed in terms of them by "local recurrence relations."

In Sec. V, we present an analytic derivation of these local recurrence relations; they can be simplified in an interesting manner for "reorientation" integrals, namely when the wave numbers of the two Coulomb functions are the same. Results in heavy ion calculations are given in Sec. VI; however, Coulomb corrections are also shown to be necessary in proton and deuteron scattering. The relation between the present method and that of other authors is also discussed.

II. HEAVY ION INELASTIC SCATTERING AND THE ECIS METHOD

The problems linked with Coulomb inelastic scattering arise whenever a heavy target is bom-

barded by charged projectiles, including protons and alpha particles. However, they are more important for heavy ions; for instance, a matching radius of 60 fm and 300 J values were needed for the inelastic scattering of 50–60 MeV ^{18}O on Ni when the excitation of the first 2^+ state was taken into account.[1] In order to illustrate the physical problems encountered, let us consider the scattering of ^{16}O on ^{28}Si at 56 MeV, when the excitation of the first 2^+ state of ^{28}Si is described in the framework of the rotational model.[6]

A. The rotational model

The interaction between ^{16}O and ^{28}Si is represented by an optical potential:

$$V(\vec{r},\hat{r}')=Vf_r(\vec{r},\hat{r}')+iWf_i(\vec{r},\hat{r}')+V_C(\vec{r},\hat{r}'), \quad (1)$$

where

$$f(\vec{r},\hat{r}')=\left[1+\exp\left(\frac{r-R(\theta)}{a}\right)\right]^{-1} \quad (2)$$

is a Woods-Saxon form factor. The radius

$$R(\theta)=R_0[1+\beta_2 Y_2^0(\theta)] \quad (3)$$

depends upon the angle θ between the position $\vec{r}$ of ^{16}O and the intrinsic axis of symmetry $\hat{r}'$ of the target. The Coulomb potential $V_C(\vec{r},\hat{r}')$ is the one generated by a uniformly charged volume, the surface of which is described by $R^C(\theta)$, similar to (3).

The optical potential (1) can be expanded into multipoles

$$V(\vec{r},\hat{r}')=4\pi\sum_\lambda V_\lambda(r)Y_\lambda^\mu(\hat{r})Y_\lambda^{\mu*}(\hat{r}'). \quad (4)$$

In the rotational model, this expansion is usually obtained by a Gauss-Legendre integration over $\cos\theta$; in the vibrational model, derivatives of the form factor with respect to R_0 are used.

The multipoles of the Coulomb potential are

$$V_\lambda^C(r)=\frac{ZZ'}{\Omega}\int_0^\pi \sin\theta P_\lambda(\cos\theta)d\theta\int_0^{R^C(\theta)}\frac{r_<^\lambda}{r_>^{\lambda+1}}r'^2dr', \quad (5)$$

where ZZ' is the product of charges, Ω the volume of the charge distribution, and $r_>$ and $r_<$ are the larger and the smaller of the two values r and r', respectively. The first few terms in this multipole expansion are

$$V_0^C=\frac{ZZ'}{r},\quad V_2^C=\frac{3}{5}\left(\frac{5}{4\pi}\right)^{1/2}\frac{R_0^{C2}ZZ'\beta_2}{r^3},\quad V_4^C=\frac{9}{28\pi}\frac{R_0^{C4}\beta_2^2}{r^5} \quad (6)$$

for values of r much larger than R_0^C.

B. The coupled equations

The total wave function, describing projectile and target, is expanded into multipoles:

$$|\psi\rangle=\sum_{l,I,J}\frac{1}{r}y_{l,I,J}(r)i^l[Y_l^m(\hat{r})|\psi_{IM}\rangle]_J, \quad (7)$$

where $|\psi_{IM}\rangle$ is the target wave function. When projected on all possible $[Y_l^m(\hat{r})|\psi_{Im}\rangle]_J$, the Schrödinger equation reduces to separate sets of four coupled equations for each value of J:

$$y_i''+\sum_j V_{ij}y_j=0, \quad (8)$$

$$V_{ij}=\left(k_i^2-\frac{l_i(l_i+1)}{r^2}\right)\delta_{ij}-\frac{2m}{\hbar^2}\sum_\lambda g_{ij}^\lambda V_\lambda(r), \quad (9)$$

where

$$g_{ij}^\lambda=i^{l_i-l_j}(-)^{J+\lambda}(2\lambda+1)[(2l_i+1)(2l_j+1)(2I_i+1)(2I_j+1)]^{1/2}\begin{pmatrix}l_i & l_j & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}I_i & I_j & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}l_i & l_j & \lambda\\ I_j & I_i & J\end{Bmatrix} \quad (10)$$

is a geometrical factor which reduces to $\delta_{l_il_j}\delta_{I_iI_j}$ for $\lambda=0$. For a given total angular momentum J, the parity is $(-)^J$ and the coupled functions are

y_0 for the 0^+ state with $l=J$,

y_1, y_2, y_3 for the 2^+ state with $l=J-2$, J, and $J+2$. (11)

This system of four second-order linear equations has four solutions which vanish at $r=0$ as requested by (7). The usual method is to compute four independent solutions and obtain their linear combination such that

$$y_0\xrightarrow[r\to\infty]{} F_{l_0}+C_0(G_{l_0}+iF_{l_0}),$$
$$y_i\xrightarrow[r\to\infty]{} C_i(G_{l_0}+iF_{l_i}), \quad (12)$$

F_l and G_l being the known solutions for a point charge Coulomb field. This method requires a numerical integration up to the point where the equations are no longer coupled and where the potentials reduce to the Coulomb one. For heavy ions, this point is located quite far away, since the multipoles decrease as $r^{-\lambda-1}$. It can be shown through Wronskian relations[2] that neglecting the λ multipoles from point R to infinity generates an error of the order $R^{-\lambda}$.

C. The ECIS method

The ECIS method is an iteration procedure which allows us to find only the solution (12) for the system of equations (8). It is not convergent

in all cases, but it is in many situations of physical interest. It becomes less advantageous for small systems of equations and situations where more than one solution (12) is needed, because the sum of the spins of the particle and the target is larger than $\frac{1}{2}$.

Let us write the system of equations (8) as

$$y_i'' + V_{ii} y_i = -\mu \sum_{j \neq i} V_{ij} y_j , \tag{13}$$

with $\mu = 1$, and consider an expansion of the solution in powers of μ. The zeroth-order solution is obtained for $\mu = 0$ and reduces to

$$\begin{aligned} y_0^{(0)} &= y_0^{\text{opt}} \xrightarrow[r\to\infty]{} F_{l_0} + C_0^{(0)}(G_{l_0} + iF_{l_0}) , \\ y_i^{(0)} &= 0 , \end{aligned} \tag{14}$$

where y_0^{opt} is the usual optical solution of the uncoupled equation for y_0.

In the first iteration, Eq. (13) for $y_1^{(1)}$ is considered with $y_0^{(0)}$ only in the second number. To obtain $y_1^{(1)}$, one needs the optical solution y_1^{opt} of the homogeneous equation and any solution $\bar{y}_1$ of the inhomogeneous equation. The solution $y_1^{(1)}$ is the linear combination $\bar{y}_1 + \alpha y_1^{\text{opt}}$ with α such that the asymptotic behavior (12) is fulfilled; it then reduces to a purely outgoing wave with a coefficient $C_1^{(1)}$. It is then possible to compute $y_2^{(1)}$ with $y_0^{(0)}$ and $y_1^{(1)}$ in the second member; the use of $y_1^{(1)}$ will lead to a result which is not the pure first order result in μ and depends upon the sequence along which the equations are iterated. For example, in a 0-1-2 phonon calculation within the framework of the vibrational model, the first iteration can give quite a good result for the two-phonon state, which has not direct coupling with the ground state, as long as the one-phonon state has been computed first. The first iteration ends by solving the equation for y_0 with all the $y_i^{(1)}$ in the second member. In general, in the nth iteration y_i is given by the solution of

$$\begin{aligned} y_i^{(n)''} + V_{ii} y_i^{(n)} = &- \sum_{\substack{0<j<i \text{ if } i\neq 0 \\ 0<j \text{ if } i=0}} V_{ij} y_j^{(n)} \\ &- \sum_{\substack{j=0 \text{ and } j>i \\ i\neq 0}} V_{ij} y_j^{(n-1)} , \end{aligned} \tag{15}$$

$$y_i^{(n)} \xrightarrow[r\to\infty]{} F_{l_i}\delta_{i0} + C_i^{(n)}(G_{l_i} + iF_{l_i}) . \tag{16}$$

After the first iteration, the process is started again, leading to a new set of results $C_i^{(2)}$. If $|C_i^{(2)} - C_i^{(1)}|$ is less than a given value for all i, the set of equations is regarded as solved; if not, a new iteration is done. From the fourth iteration a symmetric Padé approximant can be constructed with the $C_i^{(n)}$ for a given i, and the test between successive iterations can be replaced by evaluation of the Padé approximant with and without its last term. On the contrary, if the second iteration was sufficient for a given value of the total spin J, one can stop at the first iteration for larger values of J. "Sequential effects" apart, the result of the first iteration is identical to that of a DWBA calculation.

This method has been successful in nucleon scattering, chiefly for the study of polarization effects[7] which introduce first derivatives in the nondiagonal potentials. It can break down for coupling potentials which are too large, and at low energy.

D. The Green's function and the integral method

The method described above is the differential version of the ECIS method. It necessitates the computation of the optical solutions of the uncoupled equations. In the integral version of the ECIS method, one also needs the "irregular solutions" y_i^{irr} of the uncoupled equations, defined by

$$y_i^{\text{irr}} \xrightarrow[r\to\infty]{} G_{l_i} + iF_{l_i} , \tag{17}$$

which are easily obtained by backward integration. With these two solutions, one can build the Green's function

$$g_i(r,r') = \frac{1}{k_i} y_i^{\text{opt}}(r_<) y_i^{\text{irr}}(r_>) \tag{18}$$

which is the solution, regular at the origin and purely outgoing, of the inhomogeneous equation with $\delta(r-r')$ on the right-hand side. The solution of the system (15) with boundary conditions (16) is

$$\begin{aligned} y_i^{(n)}(r) &= y_i^{\text{opt}}(r)\delta_{i0} + \int_0^\infty g_i(r,r') \sum_{j\neq i} V_{ij}(r') y_j^{(n)}(r')\, dr' \\ &= y_i^{\text{opt}}(r)\delta_{i0} + \frac{1}{k_i} y_i^{\text{opt}}(r) \int_r^\infty y_i^{\text{irr}}(r') \sum_{j\neq i} V_{ij}(r') y_j^{(n)}(r')\, dr' + \frac{1}{k_i} y_i^{\text{irr}}(r) \int_0^r y_i^{\text{opt}}(r') \sum_{j\neq i} V_{ij}(r') y_j^{(n)}(r')\, dr' \end{aligned} \tag{19}$$

and the coefficient of the outgoing wave is

$$C_i^{(n)} = C_0^{(0)}\delta_{i0} + \frac{1}{k_i}\int_0^\infty y_i^{\mathrm{opt}}(r')\sum_{j\neq i} V_{ij}(r')y_j^{(m)}(r')\,dr' . \tag{20}$$

The sequence of iterations through which these solutions are obtained is identical with the one described above in connection with Eq. (15); the summations and the values of the iteration index m on the right-hand side are the same as in the latter. Note that $y_i^{\mathrm{irr}}(r)$ replaces the information contained in $V_{ii}(r)$, which no longer appears explicitly. Equations (19) and (20) show clearly where and how Coulomb corrections should be introduced in order to avoid the errors coming from the use of some finite matching radius R instead of infinity.

At this point, two comments of a technical nature are in order. First, accurate, equal step methods have been described to solve single[8] and coupled[2] second-order differential equations. Numerov or modified Numerov methods lead to an error of the order h^4 when a step h is used; they deal with $\xi(x) = y(x) - (h^2/12)y''(x)$ instead of $y(x)$. To use Coulomb corrections with convenience we will have to discard the method of matching[2] which uses the values of $\xi(R \pm h)$ and to go back to the use of the function and its first derivative at point R, given by

$$y'(R) = \frac{1}{24h}\{14[\xi(R+h) - \xi(R-h)] + \xi(R-2h) - \xi(R+2h)\} . \tag{21}$$

Second, the evaluation of integrals with a Green's function is not straightforward. To obtain

$$y(r) = \frac{1}{k}\int_0^\infty y^{\mathrm{opt}}(r_<)y^{\mathrm{irr}}(r_>)f(r')\,dr' \tag{22a}$$

at the point $r = nh$, one can use[2]

$$y(nh) = \frac{h}{k}\left[y^{\mathrm{irr}}(nh)\sum_{i=1}^{n} y^{\mathrm{opt}}(ih)f(ih) + y^{\mathrm{opt}}(nh)\sum_{i=n+1}^{\infty} y^{\mathrm{irr}}(ih)f(ih)\right] - \frac{h^2}{12}f(nh), \tag{22b}$$

because

$$\int_{nh}^{(n+1)h} f(r)\,dr = \frac{h}{2}[f(nh) + f((n+1)h)] + \frac{h^2}{12}[f'(nh) - f'((n+1)h)], \tag{22c}$$

with an error of the order h^5. Such a simple method gives accurate results because $f(r)$ and its first derivative vanish at the origin and at infinity; the correction term in h^2 of (22b) comes from the discontinuity of the derivative of the Green's function at $r = r'$. Such details must be kept in mind if Coulomb corrections are to be introduced without destroying the accuracy of the computation.

The ECIS method, as described above, has been used successfully for heavy ions inelastic scattering with many partial waves and large matching points.[6,9,10]

III. COULOMB CORRECTIONS

When Coulomb deformation is taken into account with no special care, a large matching radius (50 or 100 fm) must be used. For small total spins, many iterations are needed. In the case of ^{16}O on ^{28}Si at 56 MeV with a convergence parameter 10^{-4}, five iterations are necessary up to $J = 10$, six or seven up to $J = 30$, three up to $J = 50$, and only one above. Then, if sequential effects are neglected, the inelastic scattering described by (20) is the pure DWBA result. For some larger value, 55 or 60, one can consider that the wave function is no more distorted by the nuclear potential; it is the asymptotic region of J values. We shall refer to small J values as the nuclear region.

A. The asymptotic region

When the nuclear potential does not matter, the optical solutions of the diagonal equations are the regular Coulomb functions $F_{l_i}(\eta_i; k_i r)$. The deformed Coulomb potential is $\alpha r^{-\lambda-1}$ only for r larger than the Coulomb radius. However, this expression of the coupling potential can be extended to the origin in the integral (20) because the wave functions are very small.

So, the result is

$$C_i^{(1)} = \frac{1}{k_i}\int_0^\infty \frac{\alpha}{r^{\lambda+1}}F_{l_i}(\eta_i, k_i r)F_{l_0}(\eta_0, k_0 r)\,dr . \tag{23}$$

Such integrals have already been studied,[3,4] but we need to generalize them. Because $\eta_j k_j = \eta_i k_i$, we shall use

$$\bar{k} = (k_i k_j)^{1/2}, \quad \epsilon = (k_i/k_j)^{1/2}, \quad \bar{\eta} = (\eta_i \eta_j)^{1/2}, \tag{24}$$

and define the integrals

$$M(H, K, R)_{l_i l_j}^{-\lambda-1} = \int_{kR}^\infty \frac{1}{\rho^{\lambda+1}}H_{l_i}(\epsilon^{-1}\bar{\eta}, \epsilon\rho)K_{l_j}(\epsilon\bar{\eta}, \epsilon^{-1}\rho)\,d\rho , \tag{25}$$

where H and K are the regular or the irregular Coulomb function or any combination of them. With these notations, (23) becomes

$$C_i^{(1)} = \frac{\alpha\bar{k}^\lambda}{k_i}M(F, F, 0)_{l_i l_0}^{-\lambda-1} . \tag{26}$$

These integrals are real. This first order result does not respect unitarity. However, the coupled

channel problem can be formulated differently, in terms of the reactance matrix K, which is the coefficient of the irregular function (instead of the outgoing function) in the solution, with the normalized regular function in one channel only. This K matrix is built with integrals (26) between all the equations, and the C matrix is $K(1-iK)^{-1}$.

This method takes into account reorientation effects, gives some effects for the incident channel, and maintains unitarity. In the absence of reorientation effects, the matrix elements K_{00} and K_{ij} vanish and the C matrix is

$$C_{00}=\frac{i\sum_j K_{0j}K_{j0}}{1+\sum_j K_{0j}K_{j0}}, \quad C_{ij}=\frac{iK_{i0}K_{0j}}{1+\sum_j K_{0j}K_{j0}},$$
$$C_{0i}=\frac{K_{0i}}{1+\sum_j K_{0j}K_{j0}}, \quad C_{i0}=\frac{K_{i0}}{1+\sum_j K_{0j}K_{0j}}. \tag{27}$$

Neglecting the denominator, this expression for C_{00} has been used[11] to derive a long range imaginary optical potential to fit the elastic scattering.

Coulomb functions are not used in the asymptotic region. The integrals (26) vary regularly and the matrix C can be interpolated easily with respect to J.

B. The nuclear region with the integral method

For lower J values, where the numerical integration is needed, there must be some matching radius R beyond which the mixture of regular and irregular Coulomb functions does not change significantly. All the functions which appear in (19) and (20) can be replaced by their asymptotic forms,

$$V_{ij}(r)\to\sum_\lambda \alpha_{ij}^\lambda r^{-\lambda-1}, \tag{28a}$$
$$y_i^{\rm opt}(r)\to F_i+C_i^{(0)}(G_i+iF_i), \tag{28b}$$
$$y_i^{\rm irr}(r)\to G_i+iF_i, \tag{28c}$$
$$y_i^{(n)}(r)\to F_i\delta_{i0}+C_i^{(n)}(G_i+iF_i). \tag{28d}$$

The infinite integral of (19) can be replaced by

$$\int_r^\infty y^{\rm irr}(r')\sum_{j\neq i}V_{ij}(r')y_j^{(m)}(r')\,dr' = \int_r^R y^{\rm irr}(r')\sum_{j\neq i}V_{ij}(r')y_j^{(m)}(r')\,dr'+A, \tag{29}$$

and (20) becomes

$$C_i^{(n)}=\frac{1}{k_i}\int_0^R y_i^{\rm opt}(r')\sum_{j\neq i}V_{ij}(r')y_j^{(m)}(r')\,dr'+\frac{1}{k_i}B, \tag{30}$$

with

$$A=\sum_{j\neq i}\sum_\lambda \alpha_{ij}^\lambda \bar{k}^\lambda[M(H^{(+)},F,R)_{i,j}^{-\lambda-1}\delta_{j0}+C_j^{(m)}M(H^{(+)},H^{(+)},R)_{i,j}^{-\lambda-1}], \tag{31a}$$

$$B=\sum_{j\neq i}\sum_\lambda \alpha_{ij}^\lambda \bar{k}^\lambda\{[M(F,F,R)_{i,j}^{-\lambda-1}+C_i^{(0)}M(H^{(+)},F,R)_{i,j}^{-\lambda-1}]\delta_{j0} + [M(F,H^{(+)},R)_{i,j}^{-\lambda-1}+C_i^0M(H^{(+)},H^{(+)},R)_{ij}^{-\lambda-1}]C_j^{(m)}\}. \tag{31b}$$

Here $H^{(+)}$ is the outgoing Coulomb function $G+iF$. Corrections for finite step size are easily performed by neglecting the last value of the potential in Eq. (22) and replacing $M(H,K,R)_{i,j}^{-\lambda-1}$ by

$$M(H,K,R)_{i,j}^{-\lambda-1}+\frac{h}{2}\left(\rho^{-\lambda-1}H_iH_j+\frac{h}{6}\frac{d}{dr}(\rho^{-\lambda-1}H_iH_j)\right). \tag{32}$$

In this way, one takes into account the first-order effect of the nondiagonal Coulomb potential between R and infinity. The diagonal deformed Coulomb potential is taken into account when computing $y_i^{\rm opt}(r)$ and $y_i^{\rm irr}(r)$; at the matching point, the regular and irregular Coulomb functions are replaced by $\bar{F}_i(R)$ and $\bar{G}_i(R)$, respectively, which are given by

$$\bar{F}_i(R)=F_i\left(1-\sum_\lambda \alpha_{ii}^\lambda\frac{\bar{k}^\lambda}{k_i}M(G,F,R)_{ii}^{-\lambda-1}\right) + G_i\sum_\lambda \alpha_{ii}^\lambda\frac{\bar{k}^\lambda}{k_i}M(F,F,R)_{ii}^{-\lambda-1},$$
$$\bar{G}_i(R)=G_i\left(1+\sum_\lambda \alpha_{ii}^\lambda\frac{\bar{k}^\lambda}{k_i}M(F,G,R)_{ii}^{-\lambda-1}\right) \times F_i\sum_\lambda \alpha_{ii}^\lambda\frac{\bar{k}^\lambda}{k_i}M(G,G,R)_{ii}^{-\lambda-1}. \tag{33}$$

At the level of approximation used in (28)–(31), these functions are the solutions of the diagonal equations which reduce to the regular and irregular Coulomb functions at infinity. Their difference with Coulomb functions generates higher-order

corrections in (28)–(31), which should be neglected if R is sufficiently large.

C. The differential version of ECIS and the usual coupled channel method

In the differential version of the ECIS method, the optical solutions $y_i^{\rm opt}$ are obtained as above, using values (33) instead of the pure Coulomb functions at the matching radius. The solution $y_i^{(n)}$ of the inhomogeneous equation (15) is the linear superposition of a numerical solution $\bar{y}_i$ of the inhomogeneous equation and the optical solution $y_i^{\rm opt}$, such that, at the matching radius,

$$y_i^{(n)} = \bar{y}_i + \alpha y_i^{\rm opt} = \bar{F}_i(R)\left(\delta_{i0} + \frac{A}{k_i}\right) + \left(C_i^{(n)} - \frac{B}{k_i}\right)[\bar{G}_i(R) + i\bar{F}_i(R)]. \quad (34)$$

Here, A and B are the integrals (31) without the correction (32). This expression is easily obtained by comparison with the integral method; A/k_i is the component of the regular Coulomb function which remains at the matching point and B/k_i is the missing part in the phase shift.

Coulomb corrections can be used also in the usual method of coupled equations, in which n independent solutions are obtained. The matching conditions can be written as the solution of a linear system of $2n$ equations; with the Wronskian relations of the Coulomb functions, this system reduces[2] to dimension n. But this reduction is not possible if one matches directly with the "corrected" functions. It is best to compute an "uncorrected" $\bar{C}$ matrix with plain regular and irregular Coulomb functions and to obtain the corrected C matrix afterwards,

$$\sum_i \left(\delta_{ji} + \sum_\lambda \alpha_{ji}^\lambda \frac{\bar{k}^\lambda}{k_j} M(F, H^{(+)}, R)_{ji}^{-\lambda-1} + \sum_m \bar{C}_{jm} \sum_\lambda \alpha_{mi}^\lambda \frac{\bar{k}^\lambda}{k_m} M(H^{(+)}, H^{(+)}, R)_{mi}^{-\lambda-1}\right) C_{ii}$$
$$= -\sum_\lambda \alpha_{ji}^\lambda \frac{\bar{k}^\lambda}{k_j} M(F, F, R)_{ji}^{-\lambda-1} + \sum_i C_{ji}\left(\delta_{ii} - \sum_\lambda \alpha_{ii}^\lambda \frac{\bar{k}^\lambda}{k_i} M(H^{(+)}, F, R)_{i,i}^{-\lambda-1}\right). \quad (35)$$

With the iteration method, the second iteration is enough for some J value; from there, the computation can be continued with one iteration only. The asymptotic region begins five or ten J values above. No such indication of a shift to the asymptotic region can be found when the usual coupled channel method is used.

IV. RECURRENCE RELATIONS ON COULOMB INTEGRALS

As shown in the last section, knowledge of the integrals (25) allows us the use of a smaller matching radius. They can be computed one by one,[5] but this is tedious and can be done only above some minimum matching radius, which increases with the angular momentum.

Recurrence relations do not allow us to directly pick up a given integral. However, they can be used to obtain, with very high precision, some simple integrals which we shall call the "stored integrals," and to derive some "local recurrence" expressing the wanted integrals in terms of the stored ones.

A. Recurrence relations

Recurrence relations of Coulomb functions can be used to generalize formula (2.B.64) of Ref. 3 to the integrals (25). One obtains

$$x_1 \frac{|l_j+1+i\eta_j|}{\eta_j(l_j+1)} M(H,K,R)_{l_i,l_j+1}^{-\lambda-1} + x_2 \frac{|l_i+i\eta_i|}{\eta_i l_i} M(H,K,R)_{l_i-1,l_j}^{-\lambda-1} - x_3 \frac{|l_i+1+i\eta_i|}{\eta_i(l_i+1)} M(H,K,R)_{l_i+1,l_j}^{-\lambda-1}$$
$$- x_4 \frac{|l_j+i\eta_j|}{\eta_j l_j} M(H,K,R)_{l_i,l_j-1}^{-\lambda-1} - \left(\frac{x_1}{l_j+1} + \frac{x_2}{l_i} - \frac{x_3}{l_i+1} - \frac{x_4}{l_j}\right) M(H,K,R)_{l_i l_j}^{-\lambda-1} \quad (36)$$
$$- \frac{1}{\bar{\eta}}[x_1(l_j-\lambda) + x_2 l_i - x_3(l_i+1) - x_4(l_j+\lambda+1)] M(H,K,R)_{l_i l_j}^{-\lambda-2}$$
$$= \frac{x_1+x_4}{\bar{\eta}} \frac{1}{R^{\lambda+1}} H_{l_i}(\epsilon^{-1}\eta, \epsilon R) K_{l_j}(\epsilon\eta, \epsilon^{-1}R) + \frac{x_1+x_2+x_3+x_4}{\bar{\eta}} \int_R^\infty \frac{1}{\rho^{\lambda+1}} \left(\frac{d}{d\rho} H_{l_i}(\epsilon^{-1}\eta, \epsilon\rho)\right) K_{l_j}(\epsilon\eta, \epsilon^{-1}\rho) d\rho,$$

where x_1, x_2, x_3, and x_4 are arbitrary constants. Independent recurrence relations may be obtained by using various values of the x's such that $x_1+x_2+x_3+x_4=0$. For $R=0$, when triangular relations between

l_i, l_j, and λ are fulfilled, the extra term in the second member disappears, and the equation is exactly the one of Ref. 3. For $R \neq 0$ and an arbitrary Coulomb function H and K, the recurrence relation differs from the previous one only by this inhomogeneous term in the second member.

Other recurrence relations can be obtained by combining those derived from (36) as in Ref. 3; the result differs by an inhomogeneous term. Of particular interest are the recurrence relations between integrals with the same value for λ and for the difference $q = l_j - l_i$. There are three-term relations for $\lambda = q = 0$ and $\lambda = |q| = 1$, four-term relations for $\lambda = |q| > 1$, and five-term relations for $\lambda \neq |q|$.

B. Stored integrals

In practice, we are interested in the integrals with $\lambda \leq 4$. They can be expressed through local recurrences in terms of the integrals with some fixed value of λ and q. Integrals with the chosen values for λ and q are evaluated beforehand, also by recurrence relations, with the best precision possible. One cannot choose the monopole integrals $\lambda = q = 0$, nor the integrals for which $\lambda = |q|$, because their recurrence involves less than five terms. We choose $q = 0$ to obtain symmetric expressions for the local recurrences with respect to the exchange of l_i and l_j. We choose $\lambda = 1$ with the hope that the expressions will be simpler. These integrals for $\lambda = 1$, $q = 0$ are not used by themselves in this problem for parity reasons. However, for $k_i = k_j$ they are related to relativistic corrections, as we shall see later.

The recurrence relation between five integrals with $\lambda = 1$, $q = 0$ is quite complicated. Instead, we can use

$$\left(\frac{2l-1}{2l+1}\right)(l+1)^2 |\, l+i\eta_i \,|\, |\, l+i\eta_j \,| \, M(H,K,R)_{l-1,\,l-1}{}^{-2} - \left[\eta_i \eta_j \left[\, l^2 + (l+1)^2 \right] + l^2(l+1)^2 \left(\frac{\eta_i}{\eta_j} + \frac{\eta_j}{\eta_i}\right)\right] M(H,K,R)_{l,l}{}^{-2}$$

$$+ \left(\frac{2l+3}{2l+1}\right) l^2 |\, l+1+i\eta_i \,| \,|\, l+1+i\eta_j \,| \;\; M(H,K,R)_{l+1,\,l+1}{}^{-2}$$

$$= -2\eta_j (l+1) |\, l+i\eta_i \,| \, M(H,K,R)_{l-1,\,l}{}^{-2} + 2\eta_i \, l \,|\, l+1+i\eta_j \,| \, M(H,K,R)_{l,\,l+1}{}^{-2}$$

$$- l(l+1)^2 \eta_j \, \frac{|\, l+i\eta_i \,|}{\bar{\eta}} \, \frac{1}{R^2} \, H_{l-1} K_l + l^2 (l+1) \eta_i \, \frac{|\, l+1+i\eta_j \,|}{\bar{\eta}} \, \frac{1}{R^2} \, H_l K_{l+1} \,, \qquad (37a)$$

which is an inhomogeneous three-term recurrence relation, the inhomogeneous terms of which can be obtained from another three-term recurrence relation, which is

$$2 |\, l+i\eta_i \,| \, |\, l+1+i\eta_j \,| \, M(H,K,R)_{l-1,\,l}{}^{-2} - \left[4\eta_i \eta_j + (l+1)\left((2l+1)\frac{\eta_i}{\eta_j} + (2l+3)\frac{\eta_j}{\eta_i}\right)\right] M(H,K,R)_{l,\,l+1}{}^{-2}$$

$$+ 2 |\, l+1+i\eta_i \,| \, |\, l+2+i\eta_j \,| \, M(H,K,R)_{l+1,\,l+2}{}^{-2}$$

$$= -(2l+1)\eta_i \frac{|\, l+1+i\eta_j \,|}{\bar{\eta}} \frac{1}{R^2} H_l K_l + (2l+3)\eta_j \frac{|\, l+1+\eta_i \,|}{\bar{\eta}} \frac{1}{R^2} H_{l+1} K_{l+1} \,. \qquad (37b)$$

The monopole integral could be used; we avoid it because $M(F,F,0)_{l,\,l}{}^{-1}$ has a logarithmic singularity when $k_i = k_j$.

The four integrals $M(H,K,R)_{0,\,0}{}^{-2}$, $M(H,K,R)_{1,\,1}{}^{-2}$, $M(H,K,R)_{0,\,1}{}^{-2}$, and $M(H,K,R)_{1,\,2}{}^{-2}$ are needed to start the recurrence. As the last one can be expressed in terms of $M(H,K,R)_{0,\,1}{}^{-1}$ and $M(H,K,R)_{1,\,0}{}^{-1}$, these starting values involve only the angular momenta 0 and 1. They can be obtained by integration[5] of the product of the asymptotic expansions[12] at the matching point. For $l = 0$, and $\eta < 30$, this asymptotic expansion can be used only[13] for $R_m \geq 5\eta/3 + 7.5$; for larger values of η, a look at the asymptotic formula shows a quadratic variation of the lower radius; $R_m \geq 0.06\,\eta^2$ seems to be a safe limit. To use a smaller matching point R, a numerical integration between R and R_m is necessary; with these starting values we can obtain the integrals $M_{l,\,l}{}^{-2}$ through the recurrence relations (37) for any R, whereas the direct computation[5] can be used only from some value of R which increases with angular momentum as $(\eta^2 + l^2)^{1/2}$.

This procedure is convenient for $M(G,G,R)_{l,\,l}{}^{-2}$, which increases quickly with l, and for $M(G,F,R)_{l,\,l}{}^{-2}$ and $M(F,G,R)_{l,\,l}{}^{-2}$, which remain of the same order of magnitude when η_j and η_i are not very different. On the contrary, $M(F,F,R)_{l,\,l}{}^{-2}$, which decreases with l, is not given accurately. The downward recurrences, starting from zero values for the integrals and using the usual procedure of downward recurrence for the regular Coulomb function of the inhomogeneous terms, give a very accurate value of the integral

from the origin to the matching point; then $M(F,F,R)_{l,l}^{-2}$ is obtained by taking the difference with $M(F,F,0)_{l,l}^{-2}$, which is needed anyway in the asymptotic region.

The integrals $M(F,F,0)_{l_i,l_j}^{-\lambda-1}$ have been extensively studied,[3,4] and can be expressed in terms of hypergeometric functions of two variables. Here one only needs

$$M(F,F,0)_{ll}^{-2}=\frac{\pi}{2}\frac{\bar{\eta}}{sh\pi(\eta_j-\eta_i)}\left\{\frac{\exp(\pi(\eta_j-\eta_i)/2)}{(2l+1)\eta_j}\left(\frac{\eta_i}{\eta_j}\right)^l\left|\frac{\Gamma(l+1+i\eta_j)}{\Gamma(l+1+i\eta_i)}\right|-\frac{\exp(\pi(\eta_i-\eta_j)/2)}{(2l+1)\eta_i}\left(\frac{\eta_j}{\eta_i}\right)^l\left|\frac{\Gamma(l+1+i\eta_i)}{\Gamma(l+1+i\eta_j)}\right|\right.$$
$$\left.+\frac{\eta_j-\eta_i}{\bar{\eta}^2}\exp\frac{\pi}{2}(\eta_i-\eta_j)\,\mathrm{Re}\left[\left(\frac{\eta_j-\eta_i}{2}\right)^{i(\eta_j-\eta_i)}\eta_i^{i\eta_j}\eta_j^{-i\eta_i}\exp i(\sigma_l(\eta_i)-\sigma_l(\eta_j))\frac{1}{\Gamma(l-i\eta_j+i\eta_i)}\right.\right.$$
$$\left.\left.\times F_3\left(-l_i+i\eta_i,-l_j-i\eta_j,l+1+i\eta_i,l+1-i\eta_j,2-i\eta_j+i\eta_i;\frac{\eta_j-\eta_i}{2\eta_j},\frac{\eta_i-\eta_j}{2\eta_i}\right)\right]\right\} \tag{38}$$

where $\sigma_l(\eta)$ is the Coulomb phase shift. For large angular momenta, more and more terms are necessary to evaluate the hypergeometrical function F_3. So, the recurrence relations (36) and (37) are also useful in this case.

In a forward recurrence, the starting values $M(F,F,0)_{0,0}^{-2}$ and $M(F,F,0)_{1,1}^{-2}$ are obtained by (38); $M(F,F,0)_{0,1}^{-2}$ and $M(F,F,0)_{1,2}^{-2}$ can be expressed in terms of $M(F,F,0)_{0,0}^{-1}$ and $M(F,F,0)_{1,1}^{-1}$, for which the closed expression[3] is a hypergeometric function with the argument $(\eta_j-\eta_i)^2/(\eta_j+\eta_i)^2$. Such a recurrence was found to be quite stable. However, for a maximum l value such that $l_{\max}|\eta_j-\eta_i|>3(\eta_j+\eta_i)$, the downward recurrence was found to be better. The upward recurrence (37) is more stable if $\eta_i>\eta_j$, the downward one if $\eta_i<\eta_j$, but the role of η_i and η_j can be exchanged. The downward recurrence is started with

$$M(F,F,0)_{L+1,L+1}^{-2}=M(F,F,0)_{L,L}^{-2}=0\,,$$
$$M(F,F,0)_{L+1,L+2}^{-2}=\frac{\eta_i}{\eta_j}\frac{|L+1+i\eta_i|}{|L+1+i\eta_j|}M(F,F,0)_{L,L+1}^{-2}\,. \tag{39}$$

All the values are normalized by using the computed value of $M(F,F,0)_{0,1}^{-2}$; then the increasing solution of the homogeneous recurrence (37a) must be added to the $M(F,F,0)_{l,l}^{-2}$. In fact, the first part of (37a) can be rewritten as follows

$$\frac{1}{2l+1}\left(\frac{\eta_i}{\eta_i}(l+1)^2|\,l+i\eta_i\,|X_l-l^2|\,l+1+i\eta_j\,|X_{l+1}\right).$$
$$X_l=(2l-1)\frac{\eta_i}{\eta_j}|\,l+i\eta_j\,|M(F,F,0)_{l-1,l-1}^{-2}$$
$$-(2l+1)|\,l+i\eta_i\,|M(F,F,0)_{l,l}^{-2}\,. \tag{40}$$

A solution of the homogeneous system is obtained with $X_l=0$. It is

$$M(F,F,0)_{ll}^{-2}=\frac{1}{2l+1}\left(\frac{\eta_i}{\eta_j}\right)^l\left(\frac{\Gamma(l+1+i\eta_j)}{\Gamma(l+1+i\eta_i)}\right). \tag{41}$$

The other one differs by the exchange of η_i and η_j. The linear combination of the increasing solution with the values obtained in the recurrence is fixed, using (38) to obtain $M(F,F,0)_{0,0}^{-2}$. So, when downward recurrences are used, only two integrals must be obtained from the closed formulas.

C. Local recurrences

The general recurrence relation (36) has been used to express all the integrals $M(H,K,R)_{l_i,l_j=l_i+q}^{-\lambda-1}$ in terms of the stored $M(H,K,R)_{l,l}^{-2}$ for $\lambda=1,2,3,4$ and $0\geq q\geq\lambda$, $q+\lambda$ even; negative values of q are obtained by permutation of (η_i,η_j) and (l_i,l_j). These local recurrences depend upon the chosen l value. The integrals $M(H,K,R)_{l,l}^{-2}$ exist for $l\geq 0$; the integrals $M(H,K,R)_{l_i,l_i+q}^{-\lambda-1}$ exist only for $l_i\geq\frac{1}{2}(\lambda-q)$. So we derive local recurrences expressing $M(H,K,R)_{l_i,l_i+q}^{-\lambda-1}$ in terms of the four successive $M(H,K,R)_{l,l}^{-2}$, starting with $l=l_i+\frac{1}{2}(q-\lambda)=\frac{1}{2}(l_j+l_i-\lambda)$. These recurrences are obtained by tedious manipulations of (36). In a first step, those manipulations generate inhomogeneous terms which include Coulomb functions for various angular momenta. In a second step, recurrence relations for Coulomb functions are used to express the inhomogeneous term with H_{l_i}, K_{l_j} and their derivative, or, as it appeared better, H_{l_i+1}, K_{l_j+1}. The local recurrence relations are then

$$M(H,K,R)^{\lambda-1}_{l_i,\,l_j=l_i+q}=\sum_{i=1}^{4}\alpha_i(l_i,\lambda,q)\,M(H,K,R)_{l+i,\,l+i,\,l=1/2(l_i+l_j-\lambda)-1}{}^{-2}$$

$$+\beta_1(l_i,\lambda,q,R)H_{l_i}K_{l_j}+\beta_2(l_i,\lambda,q,R)H_{l_i}K_{l_j+1}$$

$$+\beta_3(l_i,\lambda,q,R)H_{l_i+1}K_{l_j}+\beta_4(l_i,\lambda,q,R)H_{l_i+1}K_{l_j+1}\,. \tag{42}$$

The quantities $\alpha_i(l_i,\lambda,q)$ and $\beta_i(l_i,\lambda,q,R)$ are quite simple for $\lambda=2$, but more and more complicated with increasing values of λ. The simplest ones are

$\lambda=2,\ q=0$,

$$\alpha_1(l,2,0)=-\frac{1}{2\bar{\eta}}\,\frac{(l+1)(2l-1)}{l(2l+1)}\,|\,l+i\eta_i\,|\,|\,l+i\eta_j\,|\,,$$

$$\alpha_2(l,2,0)=\frac{1}{2\bar{\eta}}\left[\left(\frac{\eta_i}{\eta_j}+\frac{\eta_j}{\eta_i}\right)l(l+1)+\eta_i\eta_j\,\frac{2l^2+2l-1}{l(l+1)}\right],$$

$$\alpha_3(l,2,0)=-\frac{1}{2\bar{\eta}}\,\frac{l(2l+3)}{(l+1)(2l+1)}\,|\,l+1+i\eta_i\,|\,|\,l+1+i\eta_j\,|\,,$$

$$\alpha_4(l,2,0)=0\,, \tag{43}$$

$$\beta_1(l,2,0,R)=\left(\frac{1}{\bar{k}R}\right)^2\left[l-\frac{1}{2}+\frac{1}{\bar{\eta}\bar{k}R}\,l(l+1)(l+\tfrac{1}{2})\right],$$

$$\beta_2(l,2,0,R)=-\left(\frac{1}{\bar{k}R}\right)^2\frac{l}{2n_f}\,|\,l+1+i\eta_j\,|\,,$$

$$\beta_3(l,2,0,R)=-\left(\frac{1}{\bar{k}R}\right)\frac{l}{2n_i}\,|\,l+1+i\eta_i\,|\,,$$

$\lambda=2,\ q=2$,

$$\alpha_1(l,2,2)=-\frac{2l+1}{6\eta_j}\left(\frac{\eta_i}{\eta_j}\right)^{1/2}|\,l+1+i\eta_j\,|\,|\,l+2+i\eta_j\,|\,,$$

$$\alpha_2(l,2,2)=\frac{2l+3}{6\bar{\eta}(2l+5)}\,\frac{|\,l+2+i\eta_j\,|}{|\,l+1+i\eta_i\,|}\left(6\eta_i{}^2(l+2)+\frac{\eta_i{}^2}{\eta_j{}^2}(2l+5)(l+1)^2+(l+1)(4l^2+19l+23)\right),$$

$$\alpha_3(l,2,2)=-\frac{1}{6\bar{\eta}}\,\frac{|\,l+2+i\eta_i\,|}{|\,l+1+i\eta_i\,|}\left(3\eta_i\eta_j(2l+3)+2\,\frac{\eta_j}{\eta_i}(l+1)(l+3)^2+\frac{\eta_i}{\eta_j}(l+1)(4l^2+19l+23)\right),$$

$$\alpha_4(l,2,2)=\frac{(2l+7)(l+1)}{3\bar{\eta}(2l+5)}\,\frac{|\,l+2+i\eta_i\,|\,|\,l+3+i\eta_i\,|\,|\,l+3+i\eta_j\,|}{|\,l+1+i\eta_i\,|}\,, \tag{44}$$

$$\beta_1(l,2,2,R)=\left(\frac{1}{\bar{k}R}\right)^2\frac{1}{6(l+3)}\left[4l^3+16l^2+7l-21+\left(\frac{1}{\bar{\eta}\bar{k}R}\right)(l+1)(l+2)(l+3)(2l+3)(2l+5)\right],$$

$$\beta_2(l,2,2,R)=-\left(\frac{1}{\bar{k}R}\right)^2\frac{(l+2)(4l^2+17l+21)}{6\eta_j(l+3)}\,|\,l+3+i\eta_j\,|\,,$$

$$\beta_3(l,2,2,R)=-\left(\frac{1}{\bar{k}R}\right)^2\frac{l+2}{6\eta_j(l+3)}\left[\eta_i\eta_j(4l^2+17l+3)\right.$$

$$\left.+(l+1)(l+3)\left(\frac{\eta_i}{\eta_j}(l+1)(2l+3)+2\,\frac{\eta_j}{\eta_i}(l+3)^2\right)\right]\frac{1}{|\,l+1+i\eta_i\,|}\,,$$

$$\beta_4(l,2,2,R)=\left(\frac{1}{\bar{k}R}\right)^2\eta_i\,\frac{(2l+3)(l+2)}{6\eta_j(l+3)}\left((2l+1)+\frac{2}{\bar{\eta}\bar{k}R}(l+1)(l+3)^2\right)\frac{|\,l+3+i\eta_j|}{|\,l+1+i\eta_i\,|}\,.$$

The b's are polynomials in $\bar{\eta}(kR)$ starting with the second degree. Such formulas can be used for $\eta_i = \eta_j$, except in the case $\lambda = q = 1$, in which $\eta_i^2 - \eta_j^2$ appears in the denominator. We shall see in the next section that different formulas can be derived for $\eta_i = \eta_j$, with $\alpha_1(l, \lambda, q) = \alpha_4(l, \lambda, q) = 0$.

Recurrence relations similar to (36) can be found in the literature.[14, 15] In Ref. 14, they have been written in a matrix form which allows us to express any integral in terms of four of them with l_i and l_i+1, l_f and l_f+1, and a fixed value of λ. In Ref. 15, the recurrence relations are used upwards and downwards for a fixed value of λ.

V. ANALYTIC DERIVATION OF LOCAL RELATIONS

The coefficients of the relation (42) can be obtained directly. In practice, the derivation which we shall describe now leads to less precise results and longer computation times than the use of final expressions like those given in (44) and (45). But, it shows the existence of three-term recurrence relations for given values of λ and q when $\eta_i = \eta_j$.

A. General formulation

To prove the relation

$$\int_{\rho_0}^{\infty} \frac{1}{\rho^{\lambda+1}} H_{l_i}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l_j}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) d\rho$$

$$= \sum_{i=1}^{4} \alpha_i \int_{\rho_0}^{\infty} \frac{1}{\rho^2} H_{l+i}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l+1}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) d\rho$$

$$+ \sum_{i=1}^{4} \beta_i(\rho_0) F_i(\rho_0) , \qquad (45)$$

with

$$F_1(\rho) = H_{l_i}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l_j}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) ,$$

$$F_2(\rho) = H_{l_i}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l_j+1}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) ,$$

$$F_3(\rho) = H_{l_i+1}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l_j}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) , \qquad (46)$$

$$F_4(\rho) = H_{l_i+1}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) K_{l_j+1}(\epsilon\bar{\eta}, \epsilon^{-1}\rho) ,$$

we use the recurrence relation

$$\frac{2l+1}{\epsilon}\left(\bar{\eta} + \frac{l(l+1)}{\rho}\right) H_{l_i}(\epsilon^{-1}\eta, \epsilon\rho)$$

$$= l\,|l+1+i\eta_i|\, H_{l_i+1}(\epsilon^{-1}\bar{\eta}, \epsilon\rho)$$

$$+ (l+1)\,|l+i\eta_i|\, H_{l_i-1}(\epsilon^{-1}\bar{\eta}, \epsilon\rho) \qquad (47)$$

and the similar one for K to express H_{l+i} and K_{l+i} in terms of H_{l_i}, H_{l_i+1} and K_{l_j}, K_{l_j+1}. This transformation generates as coefficients of $F_j(\rho)$ some polynomials $A_{ji}(\rho)$ in ρ^{-1}. Expression (45) reads

$$\int_{\rho_0}^{\infty} \sum_{i=1}^{4} C_i(\rho) F_i(\rho) = \sum_{i=1}^{4} \beta_i(\rho_0) F_i(\rho_0) , \qquad (48)$$

with

$$C_i(\rho) = \delta_{i1}\rho^{-\lambda-1} - \sum_{j=1}^{4} \alpha_j A_{ji}(\rho) = \sum_{n=2}^{N} C_i^n \rho^{-n} ,$$

$$\beta_i(\rho) = \sum_n \beta_i^n \rho^{-n} . \qquad (49)$$

Differentiating with respect to ρ_0, we get

$$\beta_i^{n-1} = N_i(n)^{-1}\left(C_i^n + \sum_j M_{ij}\beta_j^n\right) , \qquad (50)$$

where $N(n)$ is a diagonal matrix

$$N(n) = \begin{pmatrix} n-l_i-l_j-3 & 0 & 0 & 0 \\ 0 & n-l_i+l_j-1 & 0 & 0 \\ 0 & 0 & n+l_i-l_j-1 & 0 \\ 0 & 0 & 0 & n+l_i+l_j+1 \end{pmatrix} \qquad (51)$$

and

$$M = \begin{pmatrix} \bar{\eta}\left(\frac{1}{l_i+1}+\frac{1}{l_j+1}\right) & \frac{1}{\epsilon}\frac{|l_j+1+i\eta_j|}{l_j+1} & \epsilon\frac{|l_i+1+i\eta_i|}{l_i+1} & 0 \\ -\frac{1}{\epsilon}\frac{|l_j+1+i\eta_j|}{l_j+1} & \bar{\eta}\left(\frac{1}{l_i+1}-\frac{1}{l_j+1}\right) & 0 & \epsilon\frac{|l_i+1+i\eta_i|}{l_i+1} \\ -\epsilon\frac{|l_i+1+i\eta_i|}{l_i+1} & 0 & \bar{\eta}\left(-\frac{1}{l_i+1}+\frac{1}{l_j+1}\right) & \frac{1}{\epsilon}\frac{|l_j+1+i\eta_j|}{l_j+1} \\ 0 & -\epsilon\frac{|l_i+1+i\eta_i|}{l_i+1} & -\frac{1}{\epsilon}\frac{|l_j+1+i\eta_j|}{l_j+1} & \bar{\eta}\left(-\frac{1}{l_i+1}-\frac{1}{l_j+1}\right) \end{pmatrix} . \qquad (52)$$

The $C_i(\rho)$'s are polynomials in ρ^{-1}, starting from ρ^{-2} and ending at ρ^{-N}; their coefficients are linear functions of the α's. The expansion coefficients of $\beta_i(\rho)$ are obtained from (50) starting from β_i^{N-1}, unless $N_i(n)=0$, which happens if $l_j=l_i+q$ with $q>0$ for $N_3(q+1)$; in this case β_3^q is not defined and must be considered also as an unknown on which the β_i^η's obtained afterward will depend. As there is no $C_i^{\,1}$, we obtain the α's by solving the linear system of equations

$$C_i^{\,2}+\sum_j M_{ij}\beta_j^\eta(\alpha,\beta_2^q)=0\,,$$
$$C_3^{q+1}+\sum_j M_{ij}\beta_j^{q+1}(\alpha)=0\,. \tag{53}$$

The order of the polynomials increases with λ and also with q. Moreover, it depends on the value of l chosen in (45). Any integral can be expressed with any l value, but it is clear that the final result is simpler when $l_i, l_j, l+i$ are closer.

B. Degenerate case $\eta_i=\eta_j$

The determinant of the matrix (52) is

$$\det\{M\}=\left(\frac{\eta_i}{\eta_j}-\frac{\eta_j}{\eta_i}\right)^2 \tag{54}$$

and this matrix is of rank 2 when $\eta_i=\eta_j$. So, if (50) is used to compute the $\beta_i^{\,1}$'s, there are only two of them which are independent. Consequently, the relation (46) holds with $\alpha_1=\alpha_4=0$ when $\eta_i=\eta_j$ and the first term of the polynomial expansion of the $\beta_i(\rho)$'s is ρ^{-1}.

In this way, a recurrence relation between three integrals with fixed λ and q can be derived. The one with $l_i=l_j$ and $\lambda=1$ is

$$\begin{aligned}(2l-1)(l^2+\eta^2)M(H,K,R)_{l-1,l-1}^{\;-2}&-(2l+1)(2l^2+2l+1+2\eta^2)M(H,K,R)_{l,l}^{\;-2}+(2l+3)[(l+1)^2+\eta^2]M(H,K,R)_{l+1,l+1}^{\;-2}\\
&=\frac{1}{\rho_0}\frac{2l+1}{(l+1)^2}\left((l+1)^2+\eta^2-\frac{\eta}{\rho_0}(l^2-1)(2l+1)-\frac{1}{\rho_0^{\,2}}l^2(l+1)^2(2l+1)\right)H_lK_l\\
&+\frac{1}{\rho_0}\frac{2l+1}{(l+1)^2}|l+1+i\eta|\left(-\eta+\frac{1}{\rho_0}l^2(l+1)\right)(H_lK_{l+1}+H_{l+1}K_l)+\frac{1}{\rho_0}\frac{2l+1}{(l+1)^2}[(l+1)^2+\eta^2]H_{l+1}K_{l+1}\end{aligned} \tag{55}$$

can be used to simplify (43) and (44):

$$\lambda=2,\ q=0,\ \alpha_1=\alpha_4=0\,,$$
$$\alpha_2(l,2,0)=-\frac{(2l+1)[(l+1)^2+\eta^2]+2\eta^2}{2\eta l(l+1)}\,,$$
$$\alpha_3(l,2,0)=\frac{(2l+3)[(l+1)^2+\eta^2]}{2\eta l(l+1)}\,,$$
$$\beta_1(l,2,0;R)=\frac{1}{kR}\frac{1}{2\eta l(l+1)}\left((l+1)^2+\eta^2+\frac{\eta}{kR}(l+1)\right)\,,$$
$$\beta_2(l,2,0,R)=\beta_3(l,2,0,R)=-\frac{1}{kR}\frac{|l+1+i\eta|}{2l(l+1)}\,,$$
$$\beta_4(l,2,0,R)=\frac{(l+1)^2+\eta^2}{2kRl(l+1)}\,, \tag{56}$$

$$\lambda=2,\ q=2,\ \alpha_1=\alpha_4=0\,,$$
$$\alpha_2(l,2,2)=-\frac{2l+3}{6\eta}\frac{|l+2+i\eta|}{|l+1+i\eta|}\,,$$
$$\alpha_3(l,2,2)=\frac{2l+5}{6\eta}\frac{|l+2+i\eta|}{|l+1+i\eta|}\,,$$

$$\beta_1(l,2,2,R)=\frac{1}{6\eta kR(l+1)(l+3)}\times\left[\eta^2+(l+3)\left(\frac{3\eta}{kR}-l-2\right)\right]\,,$$
$$\beta_2(l,2,2,R)=-\frac{1}{kR}\frac{|l+3+i\eta|}{6(l+1)(l+3)}\,,$$
$$\beta_3(l,2,2,R)=\frac{1}{6kR(l+1)(l+3)|l+1+i\eta|}\times\left(3l^2+12l+11-\eta^2+\frac{l+3}{\eta kR}[4(l+1)(l+2)^2-(2l+5)\eta^2]\right)\,,$$
$$\beta_4(l,2,2,R)=-\frac{1}{kR}\frac{[(l+1)(l+2)-\eta^2]}{6\eta(l+1)(l+3)}\frac{|l+3+i\eta|}{|l+1+i\eta|}\,. \tag{57}$$

For the dipole integral, the limit $\eta_i=\eta_j$ cannot be used, due to a denominator $\eta_i^{\,2}-\eta_j^{\,2}$. We obtain

$$\lambda=1,\ q=1,\ \alpha_1=\alpha_4=0,$$

$$\alpha_2(l,1,1)=-\frac{2l+3}{2\eta}\frac{(l+2)^2+\eta^2}{|l+1+i\eta|},$$

$$\alpha_3(l,1,1)=\frac{2l+5}{2\eta}\frac{(l+2)^2+\eta^2}{|l+1+i\eta|},$$

$$\beta_1(l,1,1,R)=\frac{1}{kR}\frac{1}{2(l+1)},$$

$$\beta_2(l,1,1,R)=-\frac{1}{\eta kR}\frac{l+2}{2(l+1)}|l+2+i\eta|, \tag{58}$$

$$\beta_3(l,1,1,R)=\frac{1}{\eta kR}\frac{(l+1)(l+2)^3+\eta^2(l^2+l-1)}{2(l+1)(l+2)|l+1+i\eta|},$$

$$\beta_4(l,1,1,R)=\frac{1}{kR}\frac{2l+3}{2(l+1)(l+2)}\frac{|l+2+i\eta|}{|l+1+i\eta|}\times\left(1+\frac{(l+1)(l+2)^2}{\eta kR}\right).$$

The integral

$$M(F,F,0)_{ll}{}^{-2}=\frac{1}{2l+1}\left(\frac{\pi}{2}-\mathrm{Im}\psi(l+1+i\eta)\right), \tag{59}$$

where ψ, the logarithmic derivative of the Γ function, can be used to evaluate the other integrals $M(F,F,0)_{l_il_j}^{\lambda-1}$; their expressions are simple[16] but cannot be generalized to finite integrals.

C. Relations with relativistic corrections

We want to underline the relations between Coulomb corrections and the differences between relativistic and nonrelativistic Coulomb phase shifts. The Dirac equation in an external field can be written as a Schrödinger equation for the large components

$$\left(\Delta-\frac{1}{2}\frac{1}{E+m-V}(\Delta V)-\frac{3}{4}\frac{1}{(E+m-V)^2}(\vec{\nabla}V)\cdot(\vec{\nabla}V)-\frac{1}{E+m-V}\vec{\sigma}\frac{(\vec{\nabla}V)}{i}\times\vec{\nabla}+V^2-2EV+k^2\right)\psi=0, \tag{60}$$

where ψ is the wave function multiplied by $(E+m-V)^{-1/2}$. The potential in this equation could be expanded into multipoles as shown for the rotational model in Sec. II. The vector product term is of standard use[7] in proton inelastic scattering with a deformed spin-orbit potential.

Let us consider the use of (60) for electron scattering on a point charge. The potential is $-z/r$ and the Schrödinger equation is

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+\frac{2zE}{r}+k^2\right)\psi+\left(\frac{z^2}{r^2}-\frac{1}{E+m-V}\frac{z}{r^3}(\vec{L}\vec{\sigma})-\frac{3}{4}\frac{1}{(E+m-V)^2}\frac{1}{r^4}\right)\psi=0. \tag{61}$$

The first part of this equation generates the pure Coulomb phase shift $\sigma_l=\arg\Gamma(l+1+i\eta)$ with $\eta=-zE/k$. The first correction term generates a correction $z^2M(F,F,0)_{l,l}{}^{-2}$ and the second one, if V is neglected in the denominator, a correction $-k(E+m)^{-1}z(\vec{L}\cdot\vec{\sigma})M(F,F,0)_{l,l}{}^{-3}$. The result is

$$\delta=\arg\Gamma(l+1+i\eta)+\frac{z^2}{2l+1}\left(\frac{\pi}{2}-\mathrm{Im}\psi(l+1+i\eta)\right)-\frac{zk}{E+m}\frac{\vec{L}\vec{\sigma}}{2l(l+1)(2l+1)}[(2l+1)-\eta\pi+2\eta\psi(l+1+i\eta)], \tag{62}$$

which must be compared with the relativistic phase shift[17]

$$e^{2i\delta_r}=\frac{x+i\eta m/E}{\gamma+i\eta}\frac{\Gamma(\gamma+1+i\eta)}{\Gamma(\gamma+1-i\eta)}e^{i\pi(l-\gamma)}, \tag{63}$$

where $\gamma^2=l^2-z^2$ and $x=-1-(\vec{L}\cdot\vec{\sigma})$. The expansion in l^{-1} of (63) coincides with (62) for the term zl^{-1}. The differences between the z^2l^{-1} terms are

$$\Delta_+=z^2\left[\frac{1}{2l+1}\left(1-\frac{E}{E+m}\frac{1}{l+1}\right)-\frac{1}{2(l+1)}\right],$$

$$\Delta_-=z^2\left[\frac{1}{2l+1}\left(1+\frac{E}{E+m}\frac{1}{l}\right)-\frac{1}{2l}\right] \tag{64}$$

and vanishes for $E=m$.

We can conclude that the method described here could be used to study the inelastic and the elastic scattering of a relativistic charged particle. The difference between relativistic and corrected nonrelativistic Coulomb phase shifts is small for large l values. This difference should also be small for low l values with a matching at a finite radius.

VI. RESULTS

The Coulomb corrections as described here have been introduced in the codes ECIS78 and ECIS79. In the latter only, the parameters of optical potentials and the deformations can be introduced in the manner that is usual for heavy ion reactions; furthermore, formulas (56) and (57) are used instead of (43) and (44) in the degenerate case.

A. Heavy ions

The scattering of ^{16}O on ^{28}Si with inclusion of the effects due to the first 2^+ state of ^{28}Si has been studied in the rotational model.[6] We have chosen a potential derived in this study and done the calculation without Coulomb corrections for

matching radii of 13.5, 20, 30, 50, and 75 fm. There is no difference in the drawing of the inelastic cross section for matching radii of 50 and 75 fm. The curve obtained with 30 fm shows small differences for angles smaller than 25°. These differences can be seen up to 50° (or 60°) when the matching radius is at 20 (or 13.5) fm. The elastic cross section and the backward inelastic scattering are not significantly changed.

When Coulomb corrections are included with a matching point of 13.5 fm, the result is identical with the one obtained previously for the largest matching point. The result is independent of the choice of the matching point when Coulomb corrections are taken into account. The value of 13.5 fm corresponds to the radius plus 12 times the diffuseness; that is, the matching radius used when there is no Coulomb deformation (slightly more than the radius plus ten times the diffuseness because the rotational model is used).

Requesting a precision of 10^{-5}, the computation is stopped at $J=52$, 79, 120, 201 for matching radii of 13.5, 20, 30, and 50 fm without Coulomb corrections, but $J=250$ is not enough for a matching radius of 75 fm without Coulomb corrections. The shift to only one iteration occurs at $J=45$, 63, 76, and 78 but there are only 3 iterations from $J=32$ in all cases. Even if it seems that the asymptotic region is not well defined by the criterion of only one iteration, the stability of the J value for which there are only three iterations shows that it is because the required precision was so high. Anyway, J's larger than 120 do not show up in the results. Various curves obtained in this test for the inelastic scattering below 90° are shown in Fig. 1, which shows results in the rotational model with the parameters of Table I.

A more interesting test is the scattering of ^{16}O on ^{74}Ge, for which curves obtained with different matching radii have been published.[9] The results of such calculations, without Coulomb corrections and with matching radii of 40, 60, and 100 fm are shown on Fig. 2. The computation stops at $J=205$, 310, and 525 for a precision of 10^{-5} in these cases. The computation with Coulomb corrections using the nuclear matching point 15 fm (potential radius plus 12 times the diffuseness)

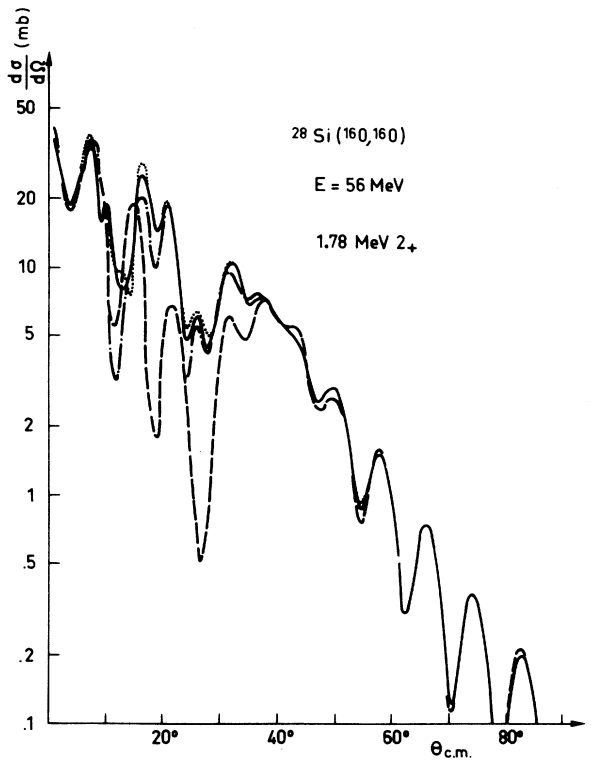

FIG. 1. Results in the rotational model with the parameters of Table I. The plain curve is obtained with Coulomb corrections and a matching radius of 13.5 fm. The other curves are obtained without Coulomb corrections, the dashed one with a matching point at 13.5 fm, the dash-dot one with 20 fm, and the dotted one with 30 fm.

agrees quite well with the conventional calculations using a matching point at 100 fm, except between 5° and 10°, where the curve is sensitive to very high partial waves. The dashed curve at the right is the DWBA result and shows that coupled channel effects are mostly the nuclear ones. The elastic cross section depends slightly on the matching radius: the maximum of the cross section divided by Rutherford's cross section at 54° decreases from 1.1690 to 1.1325 when the matching radius is changed from 15 to 100 fm without Coulomb corrections; these values are 1.1269, 1.1310, and 1.1320 with Coulomb cor-

TABLE I. Optical potential parameters. The imaginary potential for protons is a surface one; in this case $\beta_4=0.044$ and $\beta_6=-0.012$ are included. The β_2 of the Coulomb potential for ^{74}Ge is 0.208.

	V		a	W	H_i	a_i	V_{ls}	r_{ls}	q_{ls}	β_2
$^{16}O+^{28}Si$	50.0	1.245	0.539	5.25	1.245	0.539				−0.223
$^{16}O+^{74}Ge$	24.4	1.360	0.430	36.6	1.270	0.420				0.234
$p+^{238}U$	57.05	1.19	0.73	11.43	1.220	0.720	8.0	1.1	0.65	0.238

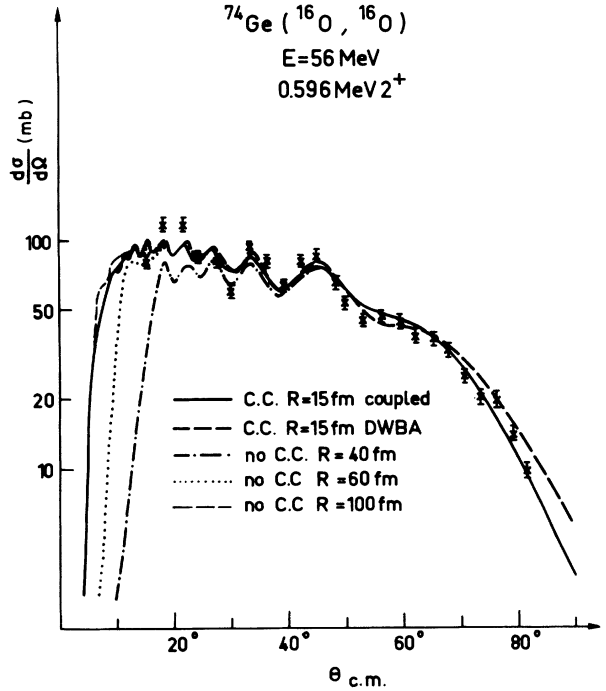

FIG. 2. Results in the second-order vibrational model with the parameters of Table I. The plain curve is obtained with Coulomb corrections at a matching radius of 15 fm. The other ones are obtained without Coulomb corrections; the dashed-dot one with a matching point at 40 fm, the dotted one with 60 fm, and the dashed one with 100 fm. For the last one the difference with the plain curve might come from long range integration. For large angles, the dashed line shows effects of coupled channels.

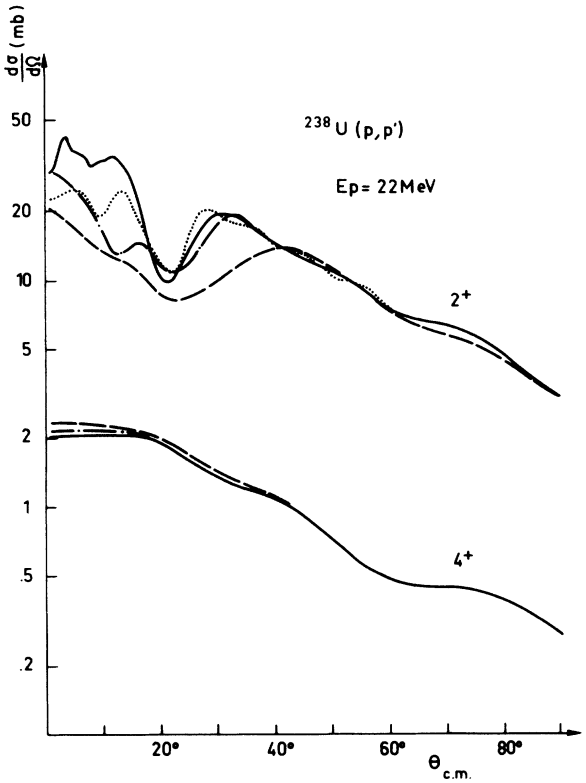

FIG. 3. Results in the rotational model with the parameters of Table I, taking into account the 0^+-2^+-4^+ coupling without spin-orbit deformation. The plain curve has been obtained with Coulomb corrections at 15 fm and 191 values of J. The dashed and the dash-dot curves are obtained without Coulomb corrections and a matching radius at 20 and 30 fm, respectively. In this last case 31 values of J were used. The dotted curve is obtained with Coulomb corrections, a matching radius at 15 fm, and only 31 values of J.

rections and matching radii at 15, 20, and 25 fm, respectively.

B. Proton scattering

Coulomb corrections are needed also for inelastic scattering of light particles in a heavy target. As an example, let us consider the scattering of protons on ^{238}U at 22 MeV.[18] The nuclear matching radius is 15 fm, whereas a value of 30 fm was used in Ref. 18. The cross section obtained with 20 fm is also shown on Fig. 3 by the dashed curve.

The value of 30 fm is not large enough because the curve obtained with 50 fm differs below 30°. The plain curve is obtained with Coulomb corrections and a matching radius of 15 fm. It differs from the 50 fm results below 16°. The computation with Coulomb corrections stops with 191 values of J, whereas the usual computation with 30 fm stops with 31 values of J. The dotted curve is the result obtained with Coulomb corrections and only 31 J values. The series of S matrices are too sharply truncated and there are more oscillations in the curve. This shows that very high partial waves must be taken into account, even if all the 191 ones used in the plain curve are not necessary.

This example shows that the importance of Coulomb corrections is not restricted to heavy ion inelastic scattering. It should often be included for deuterons, and, *a fortiori*, in α-particle inelastic scattering.

C. Comparison with other approaches

In one of the most usual approaches to heavy ion inelastic scattering,[15,19] the wave function is written as a superposition of ingoing and outgoing waves of which the coefficients are unknown new functions. The coefficients of the outgoing waves are related among themselves by slowly varying potentials and with the coefficients of the ingoing

waves by quickly varying terms which are dropped in a first approximation. This implies

$$M(F,F,R)^{-\lambda-1}_{l_i l_j} = M(G,G,R)^{-\lambda-1}_{l_i l_j} ,$$

$$M(F,G,R)^{-\lambda-1}_{l_i l_j} = -M(G,F,R)^{-\lambda-1}_{l_i l_j} , \quad (65)$$

which is approximately true for heavy ion but not for proton scattering. The integral $M(G,G,R)^{-\lambda-1}_{l_i l_j}$ becomes very large with respect to $M(F,F,R)^{-\lambda-1}_{l_i l_j}$ in the transition region between the nuclear region and the asymptotic one; we chose to use (65) if $M(G,G,R)^{-\lambda-1}_{l_i l_j}$ is larger than the wave number.

The coupling between ingoing and outgoing waves can be taken into account in higher approximations.[20] For very heavy ions, this procedure converges quickly,[21] but the method described here is no more suitable, due to too large wave numbers. However, it should be noted that iterations on the coupling between ingoing and outgoing waves are more time consuming than the ones described here, and that the use of Padé approximants[2] gives good results up to six times the radius of convergence.

When the bombarding energy is decreased down to the Coulomb barrier, the iteration procedure described here does not work any longer; results are not stable with respect to the matching radius. However, the usual coupled equations with the use of (35) are fairly independent of the matching radius. This difference of behavior comes from higher-order effects; it should disappear if the B term of Eq. (30) is not taken into account when the $C_i^{(n)}$'s are used to compute (31) if the integral of Eq. (30) is negligible.

ACKNOWLEDGMENTS

The author is indebted to J. Letourneux who carefully read the manuscript.

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