# ANALYTIC PERTURBATION THEORY FOR SCREENED COULOMB POTENTIAL: FULL CONTINUUM WAVE FUNCTION*

By A. Bechler†

Institute of Theoretical Physics, University of Warsaw**

and J. Mc Ennan***, R. H. Pratt

Department of Physics, University of Pittsburgh, Pittsburgh, PA 15260, USA

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An analytic perturbation theory developed previously is used to find a continuum screened-Coulomb wave function characterized by definite asymptotic momentum. This wave function satisfies an inhomogeneous partial differential equation which is solved in parabolic coordinates; the solution depends on both parabolic variables. We calculate partial wave projections of this solution and show that we can choose to add a solution of the homogeneous equation such that the partial wave projections become equal to the normalized continuum radial function found previously. However, finding the unique solution with given asymptotic linear momentum will require either using boundary conditions to determine the unique needed solution of the homogeneous equation or equivalently specifying the screened-Coulomb phase-shifts.

## 1. Introduction

In the analytic perturbation theory developed recently [1, 2] nonrelativistic radial wave functions for screened-Coulomb potentials have been found. The method is based on the following expansion of the potential

$$V(r) = -\frac{a}{r}(1+\lambda V_1 r+\lambda^2 V_2 r^2+ \ldots), \tag{1}$$

whera $a = \alpha Z$ with $\alpha$ — the fine-structure constant and $Z$ — the atomic number. $\lambda (\approx \alpha Z^{1/3})$ is a small parameter characterizing the screening and $V_k$ are the expansion coefficients

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** Address: Instytut Fizyki Teoretycznej UW, Hoża 69, 00-681 Warszawa, Poland.

*** Present address: 14112 Castle Boulevard, Apt. 103, Silver Spring, Maryland 20904, USA.

which are of the order of unity. The series (1) converges rapidly in the interior of an atom i.e. for $\lambda r < 1$. Screened radial wave functions for both bound and continuum states are given as series in $\lambda$ and give good approximation to the exact wave functions known numerically in the interior of an atom. The screened radial wave function found in Refs [1, 2] have been further used to the calculation of photoeffect cross-section in the non-relativistic dipole approximation [3]. The results agree with numerical nonrelativistic dipole calculations and also with the full relativistic screened calculations for photon energies up to 100 keV. This unexpected agreement with the relativistic results is due to various cancellations which occur between relativistic and multipole effects in the expression for the total cross-section [7]. It thus appears that the results of Ref. [3] are very good in the energy range for which the major contribution to the matrix element arises within the interior of an atom. One anticipates that the perturbation theory described in Ref. [1] should be useful for any atomic process for which the contribution to the matrix element is dominated by the contribution from the interior of an atom.

In this note we want to demonstrate the application of the analytic perturbation theory to the problem of the screened continuum wave function describing an electron moving with given asymptotic momentum $\boldsymbol{k} = (0, 0, k)$ and with the kinetic energy $T = k^2/2m$. This solution of the Schrödinger equation is needed for the description of the processes such as electron bremsstrahlung, annihilation of a positron with an atomic electron etc. In particular, analytic calculations of the screened bremsstrahlung cross-section are now in progress.

As in the point-Coulomb case we use parabolic coordinates. We find that corrections to the point-Coulomb wave function satisfy inhomogeneous partial differential equations with their left-hand side given by the Schrödinger differential operator with the Coulomb potential. Solutions of these equations can be easily found with the use of connections between contiguous confluent hypergeometric functions [4, 5].

Corrections to the point-Coulomb function in the first, second and third order in $\lambda$ are found in Section 2. In Section 3 we calculate partial wave projections of our solution for arbitrary $l$ and discuss the solution of the homogeneous equation which should be added to the particular solution obtained in Section 2. This solution can be chosen so that the partial wave projection of inhomogeneous plus homogeneous solution is equal to the radial wave function found in Ref. [2]. However, to obtain the unique wave function characterized by definite asymptotic momentum one would have to add an additional homogeneous solution to produce the proper but unknown phase-shifts. Nevertheless, the present solution can be used in the calculations of features of atomic processes which do not depend on this phase information.

## *2. Solution of the Schrödinger equation in parabolic coordinates*

Together with the expansion of the potential (1) we assume expansion of the energy in the form

$$T = T_c + \frac{a^2}{2}\left(\lambda \frac{V_1}{a} c_1 + \lambda^2 \frac{V_2}{a^2} c_2 + \lambda^3 \frac{V_3}{a^3} c_3 + \dots\right) = T_c + \delta T, \tag{2}$$

where the parameters $c_i$ are in principle arbitrary. It has been pointed out in Ref. [1] that the description of many atomic processes may be considerably simplified with the use of the expansion (2). In atomic units the Schrödinger equation can now be written as

$$(-\tfrac{1}{2}\Delta + V_c - T_c)\psi = (\delta T - \delta V)\psi, \tag{3}$$

where $V_c = -a/r$ is the point-Coulomb potential and $\delta V = V - V_c$. Expanding the wave function

$$\psi = \psi_c + \lambda B_1 + \lambda^2 B_2 + \lambda^3 B_3 + \ldots, \tag{4}$$

where $\psi_c$ is the point-Coulomb solution, we get in the first order in $\lambda$

$$(-\tfrac{1}{2}\Delta + V_c - T_c)B_1 = (aV_1 + \tfrac{1}{2}aV_1c_1)\psi_c. \tag{5}$$

Choosing now $c_1 = -2$ we can put $B_1 = 0$ and therefore we have no first order correction to the wave function, as in the case of the radial functions [1, 2] (see also Ref. [6]).

Picking up second order terms in (3) we get

$$(-\tfrac{1}{2}\Delta + V_c - T_c)B_2 = (aV_2r + \tfrac{1}{2}V_2c_2)\psi_c. \tag{6}$$

Normalizing on the energy scale we can write for the point-Coulomb wave function

$$\psi_c(\boldsymbol{r}) = \frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi\nu_c/2}\Gamma(1-i\nu_c)M(i\nu_c, 1; ik_c(r-z))e^{ik_cz}, \tag{7}$$

where $T_c = k_c^2/2$, $\nu_c = a/k_c$ and $M(a, b; x)$ is the regular confluent hypergeometric function. To find the solution to Eq. (6) we use parabolic variables defined by $\xi = r+z$, $\eta = r-z$ and we write the wave function $\psi$ in the form

$$\psi(\eta, \xi) = e^{ik_c(\xi-\eta)/2}w(\eta, \xi). \tag{8}$$

Using further the dimensionless variables $y = ik_c\xi$ and $x = ik_c\eta$ we can write the general equation (3) in the form

$$\left[x\frac{\partial^2}{\partial x^2} + (1-x)\frac{\partial}{\partial x} - i\nu_c + y\frac{\partial^2}{\partial y^2} + (1+y)\frac{\partial}{\partial y}\right]w(x, y)$$

$$= \frac{1}{2k_c^2}(x+y)(\delta T - \delta V)w(x, y). \tag{9}$$

From (7) we see that

$$w_c(x, y) = \frac{k_c^{1/2}}{\ldots}\, e^{\pi\nu_c/2}\Gamma(1-i\nu_c)M(i\nu_c, 1; x) \tag{10}$$

and using (6) we get in the second order

$$\left[x\frac{\partial^2}{\partial x^2}+(1-x)\frac{\partial}{\partial x}-iv_c+y\frac{\partial^2}{\partial y^2}+(1+y)\frac{\partial}{\partial y}\right]w_2$$

$$=\frac{1}{2k_c}(x+y)\left[\frac{aV_2}{2ik_c}(x+y)+\tfrac{1}{2}V_2c_2\right]w_c. \tag{11}$$

Using now the well known relations between contiguous confluent hypergeometric functions [5, 6]

$$xM(a,b;x)=aM(a+1,b;x)+(b-2a)M(a,b;x)+(a-b)M(a-1,b;x), \tag{12}$$

we write Eq. (11) as

$$\mathscr{D}_{iv_c}w_2=\frac{k_c^{1/2}}{(2\pi)^{3/2}}e^{\pi v_c/2}\Gamma(1-iv_c)\sum_{n=-2}^{2}\alpha_n^2(iv_c,y)M(iv_c+n,1;x), \tag{13}$$

where we denote by $\mathscr{D}_{iv_c}$ the partial differential operator on the L.H.S. of (11), and $\alpha_n^2$ are polynomials in $y$ of the order $2-|n|$:

$$\alpha_{-2}^2=-\frac{iaV_2}{4k_c^3}(iv_c-1)(iv_c-2),$$

$$\alpha_{-1}^2=-\frac{iaV_2}{k_c^3}(iv_c-1)^2+\frac{V_2c_2(iv_c-1)}{4k_c^2}-\frac{iaV_2(iv_c-1)}{2k_c^3}y,$$

$$\alpha_0^2=-\frac{iaV_2}{4k_c^3}(2-6v_c^2-6iv_c)+\frac{1-2iv_c}{2k_c^2}\frac{V_2c_2}{2}+\left[-\frac{iaV_2}{2k_c^3}(1-2iv_c)+\frac{V_2c_2}{4k_c^2}\right]y-\frac{iaV_2}{4k_c^3}y^2,$$

$$\alpha_1^2=-\frac{iaV_2}{k_c^3}v_c^2+\frac{iv_cV_2c_2}{4k_c^2}+\frac{aV_2v_c}{2k_c^3}y,\qquad \alpha_2^2=-\frac{iaV_2}{4k_c^3}iv_c(iv_c+1). \tag{14}$$

The right-hand side can be further expressed in terms of the Laguerre polynomials $M(-n,1;-y)$ due to the relations

$$M(0,1;-y)=1,\qquad -M(0,1;-y)+M(-1,1;-y)=y,$$

$$2M(0,1;-y)-4M(-1,1;-y)+2M(-2,1;-y)=y^2. \tag{15}$$

Using (15) we write equation (13) as

$$\mathscr{D}_{iv_c}w_2=-\frac{V_2}{2k_c^2}iv_c(c_2+1-iv_c-3v_c^2)W(0,0)+\frac{V_2}{2k_c^2}iv_c(1-iv_c)W(-1,-1)$$

$$-\frac{V_2}{4k_c^2}(1-iv_c)[c_2-2iv_c(1-2iv_c)]W(0,-1)-\frac{V_2}{4k_c^2}iv_c(1-iv_c)(2-iv_c)W(0,-2)$$

$$+\frac{V_2}{4k_c^2}\, iv_c[c_2+2iv_c(1+2iv_c)]W(0,1)$$

$$+\frac{V_2}{4k_c^2}\, v_c^2(1+iv_c)W(0,2)+\frac{V_2}{4k_c^2}\,[c_2+2iv_c(1+2iv_c)]W(-1,0)$$

$$+\frac{V_2}{2k_c^2}\, v_c^2 W(-1,1)-\frac{V_2}{2k_c^2}\, iv_c W(-2,0), \tag{16}$$

where

$$W(m,n)=\frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi v_c/2}\Gamma(1-iv_c)M(m,1;-y)M(iv_c+n,1;x). \tag{17}$$

One can also arrive at the equation (16) by writing (10) as

$$w_c(x,y)=\frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi v_c/2}\Gamma(1-iv_c)M(0,1;-y)M(iv_c,1;x) \tag{10a}$$

and then using the relation (12) with respect to the variable $y$. In the R.H.S. of (16) we have now two types of terms:

1) terms proportional to $W(0,0)$ and $W(-1,-1)$ which are solutions of the homogeneous equation $D_{iv_c}f=0$,

2) terms proportional to $W(n,m)$ with $n\neq m$.

The part of the solution for $w_2$ which produces the second type of terms can be easily found due to the obvious relation

$$\mathscr{D}_{iv_c}W(n,m)=(m-n)W(n,m). \tag{18}$$

On the other hand part of $w_2$ which produces terms of the first type can be also obtained in a simple manner with the use of the method described in Refs [2, 6]. Differentiating the homogeneous equation

$$\mathscr{D}_{iv_c}W(n,n)=0 \tag{19}$$

with respect to $iv_c$ we get

$$\mathscr{D}_{iv_c}\frac{\partial}{\partial(iv_c)}\, W(n,n)=W(n,n). \tag{20}$$

Taking into account (18) and (20) we see that the solution of the inhomogeneous equation (16) is given by

$$w_2^{\mathrm{inh}}(x,y)=-\frac{V_2}{2k_c^2}\, iv_c(c_2+1-iv_c-3v_c^2)\frac{\partial}{\partial(iv_c)}\, W(0,0)$$

$$+\frac{V_2}{2k_c^2}\, iv_c(1-iv_c)\frac{\partial}{\partial(iv_c)}\, W(-1,-1)+\frac{V_2}{4k_c^2}\,(1-iv_c)\,[c_2-2iv_c(1-2iv_c)]W(0,-1)$$

$$+\frac{V_2}{8k_c^2}\,iv_c(1-iv_c)(2-iv_c)W(0,-2)+\frac{V_2}{4k_c^2}\,iv_c[c_2+2iv_c(1+2iv_c)]W(0,1)$$

$$+\frac{V_2}{8k_c^2}\,v_c^2(1+iv_c)W(0,2)+\frac{V_2}{4k_c^2}\,[c_2+2iv_c(1+2iv_c)]W(-1,0)$$

$$+\frac{V_2}{4k_c^2}\,v_c^2W(-1,1)-\frac{V_2}{4k_c^2}\,iv_cW(-2,0). \tag{21}$$

Equation (21) can be written in the compact form

$$w_2^{\mathrm{inh}}(x,y)=\sum_{m\neq n}\beta_{mn}^2(v_c)W(m,n)+\sum_{m=0,1}\beta_m^2(v_c)\frac{\partial}{\partial(iv_c)}\,W(-m,-m), \tag{22}$$

where the coefficients $\beta_{mn}^2$ can be arranged in the five-dimensional matrix

$$[\beta_{mn}^2]=\begin{array}{cc} & n\rightarrow \\ m\downarrow & \begin{bmatrix} 0 & 0 & \beta_{-20}^2 & 0 & 0\\ 0 & 0 & \beta_{-10}^2 & \beta_{-11}^2 & 0\\ \beta_{0,-2}^2 & \beta_{0,-1}^2 & 0 & \beta_{01}^2 & \beta_{02}^2\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}\end{array}. \tag{23}$$

Third order terms in the equation (9) give

$$\mathscr{D}_{iv_c}w_3(x,y)=\frac{1}{2k_c^2}\,(x+y)\frac{V_3}{2a}\,[c_3-v_c^2(x+y)^2]W(0,0). \tag{24}$$

Using the relation (12) several times we get

$$\mathscr{D}_{iv_c}w_3=-\frac{V_3v_c^4}{4a^3}\,2iv_c\left[\frac{c_3}{v_c^2}-(4-3iv_c-5v_c^2)\right]W(0,0)$$

$$-\frac{V_3v_c^4}{4a^3}(1-iv_c)6iv_cW(-1,-1)-\frac{V_3v_c^4}{4a^3}\,(1-iv_c)\left[\frac{c_3}{v_c^2}-\tfrac{3}{2}(4-6iv_c-5v_c^2)\right]W(0,-1)$$

$$-\frac{V_3v_c^4}{4a^3}\,3(1-iv_c)^2(2-iv_c)W(0,-2)+\frac{V_3v_c^4}{4a^3}\,\tfrac{1}{2}(1-iv_c)(2-iv_c)(3-iv_c)W(0,-3)$$

$$+\frac{V_3v_c^4}{4a^3}\,iv_c\left[\frac{c_3}{v_c^2}-\tfrac{3}{2}(3+4iv_c+5v_c^2)\right]W(0,1)+\frac{V_3v_c^4}{4a^3}\,3iv_c(1+iv_c)^2W(0,2)$$

$$
\begin{aligned}
&- \frac{V_3 v_c^4}{4a^3} \tfrac{1}{2}\, iv_c(1+iv_c)(2+iv_c)W(0,3) + \frac{V_3 v_c^4}{4a^3}\left[\frac{c_3}{v_c^2} - 3(2+iv_c-3v_c^2)\right] W(-1,0) \\
&- \frac{V_3 v_c^4}{4a^3} \tfrac{3}{2}(1-iv_c)(2-iv_c)W(-1,-2) + \frac{V_3 v_c^4}{4a^3}\, 6iv_c(1+iv_c)W(-1,1) \\
&- \frac{V_3 v_c^4}{4a^3} \tfrac{3}{2}\, iv_c(1+iv_c)W(-1,2) + \frac{V_3 v_c^4}{4a^3}\, 6(1+iv_c)W(-2,0) \\
&+ \frac{V_3 v_c^4}{4a^3}\, 3(1-iv_c)W(-2,-1) - \frac{V_3 v_c^4}{4a^3}\, 3iv_c W(-2,1) - \frac{V_3 v_c^4}{4a^3}\, 3W(-3,0).
\end{aligned}
\tag{25}
$$

The solution of this equation can be written immediately:

$$
\begin{aligned}
w_3^{\text{inh}}(x,y) = &- \frac{V_3 v_c^4}{4a^3}\, 2iv_c\left[\frac{c_3}{v_c^2} - (4-3iv_c-5v_c^2)\right]\frac{\partial}{\partial(iv_c)} W(0,0) \\
&- \frac{V_3 v_c^4}{4a^3}\, 6iv_c(1-iv_c)\frac{\partial}{\partial(iv_c)} W(-1,-1) + \frac{V_3 v_c^4}{4a^3}(1-iv_c)\left[\frac{c_3}{v_c^2} - \tfrac{3}{2}(4-6iv_c-5v_c^2)\right] W(0,-1) \\
&+ \frac{V_3 v_c^4}{4a^3} \tfrac{3}{2}(1-iv_c)^2(2-iv_c)W(0,-2) - \frac{V_3 v_c^4}{4a^3} \tfrac{1}{6}(1-iv_c)(2-iv_c)(3-iv_c)W(0,-3) \\
&+ \frac{V_3 v_c^4}{4a^3}\, iv_c\left[\frac{c_3}{v_c^2} - \tfrac{3}{2}(3+4iv_c-5v_c^2)\right] W(0,1) + \frac{V_3 v_c^4}{4a^3} \tfrac{3}{2}\, iv_c(1+iv_c)^2 W(0,2) \\
&- \frac{V_3 v_c^4}{4a^3} \tfrac{1}{6}\, iv_c(1+iv_c)(2+iv_c)W(0,3) + \frac{V_3 v_c^4}{4a^3}\left[\frac{c_3}{v_c^2} - 3(2+iv_c-3v_c^2)\right] W(-1,0) \\
&+ \frac{V_3 v_c^4}{4a^3} \tfrac{3}{2}(1-iv_c)(2-iv_c)W(-1,-2) + \frac{V_3 v_c^4}{4a^3}\, 3iv_c(1+iv_c)W(-1,1) \\
&- \frac{V_3 v_c^4}{4a^3} \tfrac{1}{2}\, iv_c(1+iv_c)W(-1,2) + \frac{V_3 v_c^4}{4a^3}\, 3(1+iv_c)W(-2,0) \\
&+ \frac{V_3 v_c^4}{4a^3}\, 3(1-iv_c)W(-2,-1) - \frac{V_3 v_c^4}{4a^3}\, iv_c W(-2,1) - \frac{V_3 v_c^4}{4a^3}\, W(-3,0).
\end{aligned}
\tag{26}
$$

This solution can also be written in the compact form

$$
w_3^{\text{inh}}(x,y) = \sum_{m \neq n} \beta_{mn}^3(v_c) W(m,n) + \sum_{m=0,1} \beta_m^3(v_c) \frac{\partial}{\partial(iv_c)} W(-m,-m), \tag{27}
$$

where the coefficients $\beta^3_{mn}$ can be arranged in the matrix form

$$[\beta^3_{mn}] = \begin{bmatrix} 0 & 0 & 0 & \beta^3_{-30} & 0 & 0 & 0 \\ 0 & 0 & \beta^3_{-2-1} & \beta^3_{-20} & \beta^3_{-21} & 0 & 0 \\ 0 & \beta^3_{-1-2} & 0 & \beta^3_{-10} & \beta^3_{-11} & \beta^3_{-12} & 0 \\ \beta^3_{0-3} & \beta^3_{0-2} & \beta^3_{0-1} & 0 & \beta^3_{01} & \beta^3_{02} & \beta^3_{03} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{28}$$

### 3. *Partial wave projections of $w^{\text{inh}}$*

In this section we calculate partial wave projections of the solution of the inhomogeneous equation and discuss the solution of the homogeneous equation which should be added to $w^{\text{inh}}$. We start in second order, where the quantity we are looking for is

$$B_{2l}(r) = \int_0^\pi d\vartheta \sin \vartheta e^{ik_c z} w_2^{\text{inh}}(x, y) P_l(\cos \vartheta). \tag{29}$$

The details of the calculation are given in the Appendix. Using (21) and formulae (A9)–(A11) in the Appendix we find

$$B_{2l}(r) = 2\frac{k_c^{1/2}}{(2\pi)^{3/2}} \frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)} e^{\pi v_c/2}(2ik_c r)^l e^{-ik_c r}$$

$$\times \frac{V_2 v_c^2}{4a^2} \{-\tfrac{1}{2} iv_c(l+1+iv_c)(l+2+iv_c)M(-2)+(l+1+iv_c)[c_2+2iv_c(2iv_c+1)]M(-1)$$

$$+(l+1-iv_c)[c_2+2iv_c(2iv_c-1)]M(1)+\tfrac{1}{2} iv_c(l+1-iv_c)(l+2-iv_c)M(2)\}$$

$$+2\frac{k_c^{1/2}}{(2\pi)^{3/2}} \frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)} e^{\pi v_c/2}(2ik_c r)^l e^{-ik_c r} \frac{V_2 v_c^2}{4a^2}$$

$$\times \Big\{-iv_c[3v_c^2+l(l+1)-c_2][i\pi+2\psi(l+1-iv_c)]M(0)+2iv_c[3v_c^2+l(l+1)-c_2]$$

$$\times \frac{\partial}{\partial(iv_c)} M(0)+2iv_c \frac{l(l+1)}{1-iv_c} M(0)\Big\}, \tag{30}$$

where $M(n) = M(l+1-iv_c-n, 2l+2; 2ik_c r)$ and $\psi$ is the logarithmic derivative of the $\Gamma$-function $\psi = \Gamma'/\Gamma$. The term in (30) which contains solution of the homogeneous radial equation $M(0)$ and its $v_c$-derivative $\partial/\partial(iv_c)M(0)$ results from the derivative terms in (21). The first expression in the second bracket can be written as

$$[3v_c^2+l(l+1)-c_2]\left[\varrho_l-\frac{iv_c}{2}\psi(l+1-iv_c)-\frac{iv_c}{2}\psi(l+1+iv_c)\right], \tag{31}$$

where

$$\varrho_l = 1-\frac{2\pi v_c}{e^{2\pi v_c}-1}+\sum_{n=0}^{l}\frac{2v_c^2}{n^2+v_c^2}, \tag{32}$$

(cf. Ref. [2] formula (13)). $\varrho_l$ gives the real part of (31) and the imaginary part contributes to the phase-shift (see formula (40) below). Expression (30) has to be compared with the second order normalized radial wave function [2]. It is given by (formulae (11a) and (12) in Ref. [2])

$$R_{2l} = r^l e^{-ik_c r}A_2(r),$$

$$A_2(r) = -\frac{V_2 v_c^2}{4a^2}\Big\{\tfrac{1}{2}\, iv_c(l+1+iv_c)\,(l+2+iv_c)M(-2)$$

$$-(l+1+iv_c)\,[c_2+2iv_c(2iv_c+1)]M(-1)-[3v_c^2(2l+3)-2(l+1)c_2]M(0)$$

$$-2iv_c[3v_c^2+l(l+1)-c_2]\,\frac{\partial}{\partial(iv_c)}\,M(0)-(l+1-iv_c)\,[c_2+2iv_c(2iv_c+1)]M(1)$$

$$-\tfrac{1}{2}\, iv_c(l+1-iv_c)\,(l+2-iv_c)M(2)\Big\}, \tag{33a}$$

and the normalization factor is

$$N_2 = \left(\frac{k_c}{k}\right)^{1/2} N_c\,\frac{V_2 v_c^2}{4a^2}\,\{l(l+1)\,(2l+1)+[3v_c^2+l(l+1)-c_2]\,(\varrho_l-2l-1)\} \tag{33b}$$

(with the factor $(k_c/k)^{1/2}$ we normalize on the energy scale [2]). $N_c$ is the point-Coulomb normalization of the continuum wave function

$$N_c = 2(2k_c)^l|\Gamma(l+1+iv_c)|e^{\pi v_c/2}/\Gamma(2l+2). \tag{34}$$

We see that terms with $M(n)$, $n \neq 0$ in $B_{2l}$ reproduce exactly analogous terms in the radial wave function. Also the derivative term is the same in $B_{2l}$ and $R_{2l}$ and the only part of $B_{2l}$ which requires modification is that containing $M(0)$. The real part of (31) gives part of the normalization contribution (32). First, we shall find the solution of the homogeneous equation (9) whose partial wave projection will cancel the terms $2v_c^2 l(l+1)/(1-iv_c)M(0)$. Looking at the formulae (A9) and (A10) we see that the desired solution is

$$H_1^{(2)} = -\frac{V_2 v_c^2}{2a^2}\, iv_c[W(-1,\,-1)-W(0,0)]. \tag{35}$$

The terms left unaccounted for in (33a), including the remaining normalization contribution, are

$$\frac{k_c^{1/2}}{(2\pi)^{3/2}}\frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)}e^{\pi v_c/2}(2ik_cr)^l e^{-ik_cr}M(0)\frac{V_2v_c^2}{4a^2}$$

$$\times\{-(3v_c^2-c_2)(2l+1)+[3v_c^2(2l+3)-2(l+1)c_2]\}$$

$$=\frac{k_c^{1/2}}{(2\pi)^{3/2}}\frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)}e^{\pi v_c/2}(2ik_cr)^l e^{-ik_cr}M(0)\frac{V_2v_c^2}{4a^2}(6v_c^2-c_2). \tag{36}$$

This expression can be included by adding the additional solution of the homogeneous equation

$$H_2^{(2)} = \frac{V_2v_c^2}{4a^2}(6v_c^2-c_2)W(0,0). \tag{37}$$

Hence, up to the second order, we must add the following solution of the homogeneous equation

$$w_2^{\mathrm{hom}} = \frac{V_2v_c^2}{2a^2}\left[\left(3v_c^2+iv_c-\frac{c_2}{2}\right)W(0,0)-iv_cW(-1,-1)\right] \tag{38}$$

if we are to project out precisely the radial wave functions determined previously, and the second order wave function takes on the form

$$B_2(\boldsymbol{r}) = e^{ik_cz}(w_2^{\mathrm{inh}}+w_2^{\mathrm{hom}}), \tag{39}$$

However, this is not yet the particular solution characterized by definite asymptotic momentum since we did not take into account the phase-shifts. In fact we must have

$$\int_0^\pi d\vartheta \sin\vartheta\,\psi_k(\boldsymbol{r})P_l(\cos\vartheta) = 2i^l e^{i\delta_l}R_l(r). \tag{40}$$

Assuming now the existence of perturbation expansions for $R_l$ normalization constant and $\delta_l$ (apart from an overall $l$-independent term) we see that we have included in $\psi_k$ only the solution of the homogeneous equation which contributes to the normalization corrections on the R.H.S. of (40). If, apart from an $l$-independent term, $\delta_l = \delta_{cl}+\lambda\delta_l^{(1)}+\lambda^2\delta_l^{(2)}+\dots$ where $\delta_{cl}$ is the point-Coulomb phase-shift, then on the R.H.S. of (40) we must also have terms of the type $i\delta_l^{(2)}M(0)$ and this requires that an additional solution of the homogeneous equation be added to $\psi_k$. But, since we do not know the screened phase-shifts, this solutiǒn of the homogeneous equation cannot be specified. This trouble is, of course, connected with the incorrect behaviour of our perturbative wave functions for $r \to \infty$ (they are good approximations only in the interior of an atom) and so cannot directly be used to determine the phase-shifts. On the other hand our perturbative solution of definite asymptotic momentum also behaves incorrectly at large distances, so that the necessary solution of the homogeneous equation cannot be directly determined from the requirement that the wave function behaves like a plane wave plus outgoing spherical waves.

In the third order we have

$$B_{3l} = \int_0^\pi d\vartheta \sin\vartheta e^{ik_c z} w_3^{\mathrm{inh}}(x, y) P_l(\cos\vartheta)$$

$$= 2\frac{k_c^{1/2}}{(2\pi)^{3/2}} \frac{\Gamma(l+1-i\nu_c)}{\Gamma(2l+2)} e^{\pi\nu_c/2}(2ik_c r)^l e^{-ik_c r} \frac{V_3\nu_c^4}{4a^3}$$

$$\times\{-\tfrac{1}{6}(l+1+i\nu_c)(l+2+i\nu_c)(l+3+i\nu_c)M(-3)+\tfrac{3}{2}(1+i\nu_c)(l+1+i\nu_c)(l+2+i\nu_c)M(-2)$$

$$+\tfrac{1}{2}(l+1+i\nu_c)\left[-15i\nu_c(1+i\nu_c)+3l(l+1)-6+2\frac{c_3}{\nu_c^2}\right]M(-1)$$

$$+\tfrac{1}{2}(l+1-i\nu_c)\left[15i\nu_c(1-i\nu_c)+3l(l+1)-6+2\frac{c_3}{\nu_c^2}\right]M(1)$$

$$+\tfrac{3}{2}(1-i\nu_c)(l+1-i\nu_c)(l+2-i\nu_c)M(2)-\tfrac{1}{6}(l+1-i\nu_c)(l+2-i\nu_c)(l+3-i\nu_c)M(3)\}$$

$$+2\frac{k_c^{1/2}}{(2\pi)^{3/2}} \frac{\Gamma(l+1-i\nu_c)}{\Gamma(2l+2)} e^{\pi\nu_c/2}(2ik_c r)^l e^{-ik_c r} \frac{V_3\nu_c^4}{4a^3}$$

$$\times\left\{-6i\nu_c\frac{l(l+1)}{1-i\nu_c}M(0)+2i\nu_c\left[-5\nu_c^2+1-3l(l+1)-\frac{c_3}{\nu_c^2}\right]\frac{\partial}{\partial(i\nu_c)}M(0)\right.$$

$$\left.-i\nu_c\left[-5\nu_c^2+1-3l(l+1)-\frac{c_3}{\nu_c^2}\right][i\pi+2\psi(l+1-i\nu_c)]M(0)\right\}. \tag{41}$$

Again, the term containing $M(0)$ and $\partial/\partial(i\nu_c)M(0)$ results from the derivative term in (26). The third term in the second bracket can be written as

$$\left[-5\nu_c^2+1-3l(l+1)-\frac{c_3}{\nu_c^2}\right]\left[\varrho_l-\frac{i\nu_c}{2}\psi(l+1-i\nu_c)-\frac{i\nu_c}{2}\psi(l+1+i\nu_c)\right]M(0), \tag{42}$$

and its real part contributes to the normalization of the third order radial function [2]. Expression (41) has to be compared with the third order normalized radial function (Ref. [2] formulae (11b) and (13)).

$$A_3(r) = -\frac{V_3\nu_c^4}{4a^3}\left\{-\tfrac{1}{6}(l+1+i\nu_c)(l+2+i\nu_c)(l+3+i\nu_c)M(-3)\right.$$

$$+\tfrac{1}{2}(l+1+i\nu_c)\left[-15i\nu_c(1+i\nu_c)+3l(l+1)-6+2\frac{c_3}{\nu_c^2}\right]M(-1)$$

$$+\tfrac{3}{2}(1+i\nu_c)(l+1+i\nu_c)(l+2+i\nu_c)M(-2)$$

$$-\left[10v_c^2(l+2)+\tfrac{1}{3}(l+1)(8l^2-13l-6)-2(l+1)\frac{c_3}{v_c^2}\right]M(0)$$

$$+2iv_c\left[-5v_c^2+1-3l(l+1)-\frac{c_3}{v_c^2}\right]\frac{\partial}{\partial(iv_c)}M(0)$$

$$+\tfrac{1}{2}(l+1-iv_c)\left[15iv_c(1-iv_c)+3l(l+1)-6+2\frac{c_3}{v_c^2}\right]M(1)$$

$$\left.+\tfrac{3}{2}(1-iv_c)(l+1-iv_c)(l+2-iv_c)M(2)-\tfrac{1}{6}(l+1-iv_c)(l+2-iv_c)(l+3-iv_c)M(3)\right\}, \quad (43a)$$

and the third order normalization

$$N_3 = -\left(\frac{k_c}{k}\right)^{1/2} N_c \frac{V_3v_c^4}{4a^3}\left\{\tfrac{5}{3}l(l+1)(2l+1)\right.$$

$$\left.+\left[-5v_c^2-3l(l+1)+1-\frac{c_3}{v_c^2}\right](2l+1-\varrho_l)\right\}. \quad (43b)$$

We again see that the terms with $M(n)$, $n \neq 0$ in (41) are the same as analogous terms in (43a) and also the derivative terms are identical in both formulae. Now we may find the solution of the homogeneous equation, partial wave projection of which cancels the term $-6iv_cl(l+1)/(1-iv_c)M(0)$ in (41). From (A9) and (A10) we see that the desired solution is

$$H_1^{(3)} = \frac{V_3v_c^4}{4a^3}\,6iv_c[W(-1,-1)-W(0,0)]. \quad (44)$$

It follows from (42) and (43b) that part of the normalization contribution is already included in (41) and terms unaccounted for, including remaining part of the normalization, are given by

$$\frac{k_c^{1/2}}{(2\pi)^{3/2}}\frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)}e^{\pi v_c/2}(2ik_cr)^le^{-ik_cr}\frac{V_3v_c^4}{4a^3}$$

$$\times\left\{-10v_c^2(l+2)-\tfrac{1}{3}(l+1)(8l^2-13l-6)-2(l+1)\frac{c_3}{v_c^2}-\tfrac{5}{3}l(l+1)(2l+1)\right.$$

$$\left.-[-5v_c^2+1-3l(l+1)](2l+1)-(2l+1)\frac{c_3}{v_c^2}\right\}M(0)$$

$$=\frac{k_c^{1/2}}{(2\pi)^{3/2}}\frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)}e^{\pi v_c/2}(2ik_cr)^le^{-ik_cr}\frac{V_3v_c^4}{4a^3}\left[-15v_c^2+1+\tfrac{1}{3}l(l+1)-\frac{c_3}{v_c^2}\right]M(0). \quad (45)$$

This expression is equal to the partial wave projection of

$$H_2^{(3)} = \frac{V_3 v_c^4}{4a^3}\left\{\left[-15v_c^2+1-\frac{c_3}{v_c^2}-\tfrac{1}{3}(1-iv_c)\right]W(0,0)+\tfrac{1}{3}(1-iv_c)W(-1,-1)\right\}. \tag{46}$$

Hence

$$w_3^{\mathrm{hom}} = H_1^{(3)}+H_2^{(3)} = \frac{V_3 v_c^4}{4a^3}\left\{\left(-15v_c^2-\tfrac{17}{3}\,iv_c+\tfrac{2}{3}-\frac{c_3}{v_c^2}\right)W(0,0)\right.$$

$$\left.+\tfrac{1}{3}(17iv_c+1)W(-1,-1)\right\}, \tag{47}$$

and finally

$$B_3(r) = e^{ik_0 z}(w_3^{\mathrm{inh}}+w_3^{\mathrm{hom}}). \tag{48}$$

## 4. Conclusions

We have tried to find the perturbation expansion of a screened continuum wave function characterized by definite asymptotic linear momentum. The Schrödinger equation for a screened-Coulomb potential was solved in parabolic coordinates; partial wave projections of the solution found correspond to the radial wave functions of Ref. [2]. However, this solution is not yet the desired solution which would include further homogeneous terms which produce the phase-shifts (cf. Eq. (40)) on projections. The problem of finding the screened phase-shifts in this perturbation scheme still remains open. Nevertheless, the wave function found in this paper is adequate for certain calculations which do not depend on this phase-shift information, for example the calculation of the bremsstrahlung energy spectrum integrated over angles.

## APPENDIX

Here we calculate the partial wave projections of $B_2$ and $B_3$. Since

$$B_i = e^{ik_c z} w_i(x, y)$$

we see that basic quantity is

$$W_l(m, n) = \int_{-1}^{1} du\, e^{ik_c r u} P_l(u)\frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi v_c/2}\Gamma(1-iv_c)M(m, 1; -y)M(iv_c+n, 1; x), \tag{A1}$$

where $u = \cos\vartheta$, $z = r\cos\vartheta$ and $P_l(u)$ is the Legendre polynomial. For the point-Coulomb solution i.e. for $m = n = 0$ we get radial wave function of the hydrogen atom.

$$W_l(0, 0) = \frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi v_c/2}\, 2(2ik_c r)^l e^{-ik_c r}\frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)}M(l+1+iv_c, 2l+2; 2ik_c r). \tag{A2}$$

Next, we calculate $W_l(m,n)$ for $m = -1$ and negative integer $n\,(n = -\mu = 0, -1, -2, \ldots)$. Applying Kummer's identity [4, 5] to $M(x)$ we have

$$W_l(-1, -\mu) = \frac{k_c^{1/2}}{(2\pi)^{3/2}}\, e^{\pi\nu_c/2}\Gamma(1-i\nu_c)e^{ik_c r}$$

$$\times \int_{-1}^{1} du P_l(u) M(-1, 1; -y) M(1+\mu-i\nu_c, 1; x). \tag{A3}$$

This integral will be calculated with the use of the Mellin–Barnes type contour integral representation [4] of the confluent hypergeometric function

$$M(a, c; x) = \frac{1}{2\pi i}\,\frac{\Gamma(c)}{\Gamma(a)} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{\Gamma(-s)\Gamma(a+s)}{\Gamma(c+s)}(-x)^s ds \tag{A4}$$

with $\gamma < 0$. Substituting (A4) into (A3) and using explicit form of the polynomial $M(-1, 1; -y)$ we get

$$W_l(-1, -\mu) = N\,\frac{e^{ik_c r}}{\Gamma(1+\mu-i\nu_c)}\,\frac{1}{2\pi i}\int_C ds\,\frac{\Gamma(-s)\Gamma(1+\mu-i\nu_c+s)}{\Gamma(1+s)}$$

$$\times (ik_c r)^s \int_{-1}^{1} du P_l(u)\,[1+2ik_c r - ik_c r(1-u)]\,(1-u)^s, \tag{A5}$$

where the variables $x$ and $y$ have been expressed in terms of the integration variable $u$, $C$ denotes the integration contour (cf. (A4)) and $N = k_c^{1/2}(2\pi)^{-3/2}e^{\pi\nu_c/2}\Gamma(1-i\nu_c)$. Since

$$\int_{-1}^{1} P_l(u)\,(1-u)^s du = 2^{s+1}\,\frac{\Gamma(1+s)\Gamma(l-s)}{\Gamma(-s)\Gamma(l+2+s)}, \tag{A6}$$

equation (A5) becomes

$$W_l(-1, -\mu) = 2N\,\frac{e^{ik_c r}}{\Gamma(1+\mu-i\nu_c)}\,\frac{1}{2\pi i}\left\{\int_C ds\,\frac{\Gamma(l-s)\Gamma(1+\mu-i\nu_c+s)}{\Gamma(l+2+s)}(2ik_c r)^s\right.$$

$$+ \int_C ds\,\frac{\Gamma(l-s)\Gamma(1+\mu-i\nu_c+s)}{\Gamma(l+2+s)}(2ik_c r)^{s+1}$$

$$\left. + \int_C ds\,\frac{\Gamma(l-1-s)\,(1+s)^2\Gamma(1+\mu-i\nu_c+s)}{\Gamma(l+3+s)}(2ik_c r)^{s+1}\right\}. \tag{A7}$$

In the first integral in (A7) we introduce new integration variable $s' = s-l$ and in the second and third integrals $s'' = s-l+1$.

Then

$$W_l(-1,-\mu) = 2N \frac{(2ik_c r)^l e^{ik_c r}}{\Gamma(1+\mu-iv_c)} \frac{1}{2\pi i} \left\{ \int_{C'} ds \frac{\Gamma(-s)\Gamma(l+1+\mu-iv_c+s)}{\Gamma(2l+2+s)} (2ik_c r)^s \right.$$

$$\left. + \int_{C''} ds \frac{\Gamma(-s)\,[(l+s)^2 - s(2l+1+s)]\Gamma(l+\mu-iv_c+s)}{\Gamma(2l+2+s)} (2ik_c r)^s \right\}. \tag{A8}$$

Using the identity

$$(l+s)^2 - s(2l+1+s) = l(l+1) + \mu - iv_c - (l+\mu-iv_c+s)$$

and comparing with (A4) we find

$$W_l(-1,-\mu) = [l(l+1)+\mu-iv_c]2N \frac{(2ik_c r)^l e^{-ik_c r}}{\Gamma(2l+2)}$$

$$\times \frac{\Gamma(l+\mu-iv_c)}{\Gamma(1+\mu-iv_c)} M(l+2-\mu+iv_c, 2l+2; 2ik_c r). \tag{A9}$$

We still need partial wave projections of $W(m,n)$ with $m=0,-2,-3$. In the same way as for $W(-1,-\mu)$ we get

$$W_l(0,-\mu) = 2N \frac{(2ik_c r)^l e^{-ik_c r}}{\Gamma(2l+2)} \frac{\Gamma(l+1+\mu-iv_c)}{\Gamma(1+\mu-iv_c)}$$

$$\times M(l+1-\mu+iv_c, 2l+2; 2ik_c r), \tag{A10}$$

$$W_l(-2,-\mu) = N[l^2(l-1)^2 + 2(2l^2+l+\mu-iv_c)(l-1+\mu-iv_c)]$$

$$\times \frac{(2ik_c r)^l e^{-ik_c r}}{\Gamma(2l+2)} \frac{\Gamma(l-1+\mu-iv_c)}{\Gamma(1+\mu-iv_c)} M(l+3-\mu+iv_c, 2l+2; 2ik_c r), \tag{A11}$$

$$W_l(-3,-\mu) = \tfrac{1}{3} N\{l^2(l-1)^2(l-2)^2 + 3[3l^2(l-1)^2$$

$$+2(l+\mu-iv_c)(l-1+\mu-iv_c)]\,(l-2+\mu-iv_c)\}$$

$$\times \frac{(2ik_c r)^l e^{-ik_c r}}{\Gamma(2l+2)} \frac{\Gamma(l-2+\mu-iv_c)}{\Gamma(1+\mu-iv_c)} M(l+4-\mu+iv_c, 2l+2; 2ik_c r). \tag{A12}$$

Results (A9)–(A11) are sufficient for calculating partial wave projection of $w_2^{\text{inh}}$ and $w_3^{\text{inh}}$. We include also the result for $m=1$ to indicate the type of the result for $m>0$.

$$W_l(1,\mu) = 2N \frac{(-2ik_c r)^l e^{-ik_c r}}{\Gamma(2l+2)} \frac{\Gamma(l+\mu+iv_c)}{\Gamma(\mu+iv_c)} M(l+\mu+iv_c, 2l+2; 2ik_c r). \tag{A13}$$

We see that the formula for $m>0$ contains the factor $(-1)^l$ which is absent in (A9)–(A12). In each case when $m=n$ the partial wave projection is proportional to the point-Coulomb radial function

$$(2ik_c r)^l e^{-ik_c r} M(l+1+iv_c, 2l+2; 2ik_c r).$$

This result is, in fact, true for any $m = n$. To prove it let us assume that $\psi_k$ is a regular solution of the Schrödinger equation, not necessarily well behaved at infinity

$$[\Delta - 2V(r) + k^2]\psi_k = 0. \tag{A14}$$

Its partial wave projection $R_l(r)$ is given by

$$R_l(r) = \tfrac{1}{2}\, i^{-l} e^{-i\delta_l} \int_0^\pi d\vartheta \sin\vartheta\, \psi_k(\boldsymbol{r}) P_l(\cos\vartheta). \tag{A15}$$

We want to prove that for any such $\psi_k$ $R_l$ satisfies the homogeneous radial Schrödinger equation which, we know, is true for the particular $\psi_k$ given asymptotically by a plane wave plus outgoing spherical waves

$$\left[\frac{1}{r}\frac{d^2}{dr^2} r - \frac{l(l+1)}{r^2} - 2V(r) + k^2\right] R_l(r) = \mathscr{D}_{k,l} R_l = 0. \tag{A16}$$

We have

$$\mathscr{D}_{k,l} R_l = \tfrac{1}{2}\, i^{-l} e^{-i\delta_l} \int_0^\pi d\vartheta \sin\vartheta\, \mathscr{D}_{k,l} \psi_k(\boldsymbol{r}) P_l(\cos\vartheta). \tag{A17}$$

The right-hand side of this equation can be split into two parts

$$\text{R.H.S.} = \tfrac{1}{2}\, i^{-l} e^{-i\delta_l} \int_0^\pi d\vartheta \sin\vartheta \left[\frac{1}{r}\frac{d^2}{dr^2} r - 2V(r) + k^2\right] \psi_k(\boldsymbol{r})$$

$$\times P_l(\cos\vartheta) + \tfrac{1}{2}\, i^{-l} e^{-i\delta_l} \int_0^\pi d\vartheta \sin\vartheta\, \psi_k(\boldsymbol{r}) \frac{1}{r^2 \sin\vartheta} \frac{\partial}{\partial\vartheta} \sin\vartheta \frac{\partial}{\partial\vartheta} P_l(\cos\vartheta). \tag{A18}$$

Integrating the second expression twice by parts we get

$$\mathscr{D}_{k,l} R_l = \tfrac{1}{2}\, i^{-l} e^{-i\delta_l} \int_0^\pi d\vartheta \sin\vartheta \left[\frac{1}{r}\frac{d^2}{dr^2} r\right.$$

$$\left. + \frac{1}{r^2 \sin\vartheta} \frac{\partial}{\partial\vartheta} \sin\vartheta \frac{\partial}{\partial\vartheta} - 2V(r) + k^2\right] \psi_k(\boldsymbol{r}) P_l(\cos\vartheta), \tag{A19}$$

and due to (A14) we obtain (A16). Since for $V = -a/r$ the only regular solution of the radial equation is given by $r^l \exp(-ikr) M(l+1+iv, 2l+2; 2ikr)$ we have thus demonstrated that the partial wave projection of $W(m, m)$ is of this form.

Therefore we put ($m > 0$, integer)

$$W_l(-m, -m) = 2^{l+1} (ik_c r)^l e^{-ik_c r} \frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)} D_l M(l+1+iv_c, 2l+2; 2ik_c r) \tag{A20}$$

and then we find

$$D_l = \frac{\Gamma(2l+2)}{2^{l+1}l!}\,\frac{1}{\Gamma(l+1-i\nu_c)}\int_{-1}^{1} du\,\frac{\partial^l}{\partial\varrho^l}\,[e^{\varrho u}W(-m,\,-m)]_{\varrho=0}P_l(u), \tag{A21}$$

where $\varrho = ik_c r$. In view of (17) we have

$$e^{\varrho u}W(-m,\,-m) = Ne^{\varrho u}M(-m,1;\,-y)M(i\nu_c-m,\,1;\,x). \tag{A22}$$

Using now explicit form of the polynomial $M(-y)$

$$M(-m,1;\,-y) = \sum_{k=0}^{m}\frac{(-m)_k}{(k!)^2}\,(-1)^k\varrho^k(1+u)^k, \tag{A23}$$

and the integral representation of $M(x)$ [4]

$$M(i\nu_c-m,1;x) = \frac{1}{\Gamma(i\nu_c-m)_\Gamma(1-i\nu_c+m)}\int_0^1 d\xi e^{\varrho(1+u)\xi}\xi^{i\nu_c-m-1}(1-\xi)^{-i\nu_c+m} \tag{A24}$$

we get

$$D_l = N\,\frac{\Gamma(2l+2)}{2^{l+1}l!}\,\frac{1}{\Gamma(l+1-i\nu_c)}\sum_{k=0}^{m}\frac{(-m)_k(-1)^k}{(k!)^2}$$

$$\times\,\frac{1}{\Gamma(i\nu_c-m)\Gamma(1-i\nu_c+m)}\int_{-1}^{1} du(1+u)^kP_l(u)$$

$$\times\int_0^1 d\xi\xi^{i\nu_c-m-1}(1-\xi)^{-i\nu_c+m}\,\frac{\partial^l}{\partial\varrho^l}\,\{e^{\varrho[u(1-\xi)+\xi]}\varrho^k\}_{\varrho=0}. \tag{A25}$$

After some calculations (A25) takes on the form

$$D_l = N\,\frac{\Gamma(2l+2)}{2^{l+1}l!}\,\frac{1}{\Gamma(l+1-i\nu_c)}\sum_{k=0}^{m}\frac{(-m)_k(-1)^k}{(k!)^2}\binom{l}{k}$$

$$\times\,\frac{1}{\Gamma(i\nu_c-m)\Gamma(1-i\nu_c+m)}\int_0^1 d\xi\xi^{i\nu_c-m-1}(1-\xi)^{-i\nu_c+m}$$

$$\times\int_{-1}^{1} du(1+u)^k[u(1-\xi)+\xi]^{l-k}P_l(u). \tag{A26}$$

In the $u$ integral only the $l$-th power of $u$ contributes and in view of the relation

$$\int_{-1}^{1} du u^l P_l(u) = \frac{2^{l+1}(l!)^2}{\Gamma(2l+2)} \tag{A27}$$

we finally get

$$D_l = \frac{N}{\Gamma(l+1-iv_c)\Gamma(1+m-iv_c)} \sum_{k=0}^{m} (-m)_k(-1)^k \binom{l}{k}^2 \Gamma(l-k+m-iv_c). \tag{A28}$$

Formulae (A20) and (A28) reproduce our previous results for $W_l(-m, -m)$ with $m = 0, 1, 2, 3$. In the same way we put ($m \geqslant 1$, integer)

$$W_l(m, m) = N2^{l+1}(ik_c r)^l e^{-ik_c r} \frac{\Gamma(l+1-iv_c)}{\Gamma(2l+2)} C_l M(l+1+iv_c, 2l+2; 2ik_c r). \tag{A29}$$

Then

$$C_l = \frac{\Gamma(2l+2)}{2^{l+1}l!} \frac{1}{\Gamma(l+1-iv_c)} \int_{-1}^{1} du P_l(u) \frac{\partial^l}{\partial \varrho^l} [e^{\varrho u} W(m, m)]_{\varrho=0}. \tag{A30}$$

Using Kummer's identity we write $W(m, m)$ in the form

$$W(m, m) = Ne^{-y} M(1-m, 1; y) M(iv_c+m, 1; x). \tag{A31}$$

Substituting (A31) into (A30) and performing the calculations in the same way as previously we find

$$C_l = \frac{N(-1)^l}{\Gamma(iv_c+m)\Gamma(l+1-iv_c)} \sum_{k=0}^{m} (1-m)_k(-1)^k \binom{l}{k} \Gamma(iv_c+m+l-k). \tag{A32}$$

For $m \neq n$ we need only note that, for instance, $W(-m, -n)$ ($m, n > 0$, integer) is a solution of the homogeneous equation with L.H.S. given by Eq. (9) but with $iv_c$ replaced by $iv_c+m-n$. Therefore

$$W_{iv_c}(-m, -n) = W_{iv_c+m-n}(-m, -m), \tag{A33}$$

where the $v_c$-dependence has been indicated by the subscript. Using (A33) we find at once

$$W_l(-m, -n) = N \cdot 2^{l+1}(ik_c r)^l e^{-ik_c r} \frac{}{\Gamma(2l+2)\Gamma(n+1-iv_c)}$$

$$\times M(l+1+m-n+iv_c, 2l+2; 2ik_c r) \sum_{k=0}^{m} (-m)_k(-1)^k \binom{l}{k}^2 \Gamma(l+n+1-k-iv_c), \tag{A34}$$

and

$$W_l(m, n) = N \cdot 2^{l+1}(ik_c r)^l e^{-ik_c r} \frac{(-1)^l}{\Gamma(2l+2)\Gamma(n+i\nu_c)}$$

$$\times M(l+1-m+n+i\nu_c, 2l+2; 2ik_c r) \sum_{k=0}^{m} (1-m)_k(-1)^k \binom{l}{k}^2 \Gamma(i\nu_c+n+l-k). \qquad \text{(A35)}$$

## REFERENCES

[1] J. Mc Ennan, L. Kissel, R. H. Pratt, *Phys. Rev.* **A13**, 532 (1976); E **A13**, 2325 (1976).
[2] J. Mc Ennan, L. Kissel, R. H. Pratt, *Phys. Rev.* **A14**, 521 (1976).
[3] S. D. Oh, J. Mc Ennan, R. H. Pratt, *Phys. Rev.* **A14**, 1428 (1976).
[4] H. Bateman, A. Erdelyi, *Higher Transcendental Functions*, Vol. 1, McGraw-Hill Book Company, New York, Toronto, London 1953.
[5] M. Abramowitz, I. Stegun, *Handbook of Mathematical Functions*, Dover Publications, Inc., New York 1965.
[6] A. Bechler, *Ann. Phys.* (USA) **108**, 49 (1977).
[7] Validity of the nonrelativistic dipole approximation is discussed in A. Ron, R. H. Pratt, H. K. Tseng, *Chem. Phys. Lett.* **47**, 377 (1977).