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Further series expansions of the solutions of the confluent hypergeometric equation

P Kay and J A Reissland

Department of Physics, University of Essex, Colchester, Essex, UK

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Abstract. A convenient series expansion of the solutions of the confluent hypergeometric equation is developed for angular momentum quantum numbers $l = 2$ and 3 . Following a procedure proposed by Kuhn, the expansion coefficients are deduced for the two independent solutions which may then be combined to give a series representation of the eigenfunctions. The results are couched in terms suitable for application to physical situations involving hydrogenic wavefunctions.

The Coulomb (Whittaker) functions are written in terms of the Kuhn asymptotic series expansion with respect to a parameter related to the principal quantum number. The irregular part of these solutions has been shown by Ham to be divergent. Alternative solutions are evaluated to test the validity of Kuhn's series.

The solutions are applied to find electron energy eigenvalues in the neighbourhood of a positive ion of finite size. Boundary conditions as used in model potential calculations are imposed and the results are given in a general form from which the parameters for the model potential of a particular ion may be obtained.

1. Introduction

The work of Kuhn (1951), Ham (1957) and Wannier (1943) on the generation of solutions of the confluent hypergeometric equation enables Shaw (1968) to develop a successful model of the potential in the neighbourhood of a metallic ion. In particular, Kuhn produces numerical values of the expansion coefficients for the first two angular momentum quantum numbers ($l = 0, 1$). These coefficients provide solutions for atoms with s and p electrons and in a form suitable for use with the physical boundary conditions.

In order to extend Shaw's method to atoms with s , p , d and f electrons it is necessary to develop the corresponding series solutions of the hydrogenic wave equation. Since the equation is of more general interest than the special use we have made of it, we have presented the extensions of Kuhn's analysis to give the series solutions for $l = 2$ and $l = 3$.

The relevant space is divided into two regions; inside the ionic radius and outside the ionic radius. The boundary conditions are to match the logarithmic derivative of the 'interior' and 'exterior' solutions; that is we need expressions for ψ_I , ψ_E , $\partial\psi_I/\partial r$ and $\partial\psi_E/\partial r$ where ψ_I is the interior and ψ_E the exterior solution.

To find the derivative, it is convenient to represent it directly as a series expansion with its own coefficients—hence two sets of expansion coefficients are generated to obtain the logarithmic derivative for the exterior solution. The interior solution is dependent on the model chosen to describe the potential for values of r less than the ionic radius. This work is concerned with the series expansions of the exterior solutions

for which the eigenvalue equation of interest is the radial part of the hydrogenic wave equation.

The accuracy of these asymptotic series for the irregular solution are assessed by comparison with two other series, one due to Ham and the other obtained from an alternative expansion discussed in § 3.

As an example, the solutions are applied to fit the boundary conditions with the Shaw form of the interior solution. The results are obtained in the form from which the model potential parameters for particular ions may be obtained. These represent a considerable extension to the table of Shaw (1968).

2. Analytical basis

Using Hartree units ($\hbar = e = m_e = 1$), the hydrogenic radial wave equation may be written

$$\frac{d^2 U^{(l,n)}}{dr^2} - \left(\frac{l(l+1)}{r^2} - \frac{2Z}{r} + \frac{Z^2}{n^2} \right) U^{(l,n)} = 0 \tag{2.1}$$

where $n \equiv Z/|2E|^{1/2}$ and Z is the ionic charge. Equation (2.1) may be easily transformed to the confluent hypergeometric equation (see for example Slater 1960).

If we substitute $z = (8ZR)^{1/2}$ and $U^{(l,n)} = (z/2)V^{(l,n)}$, equation (2.1) reduces to

$$\nabla_l V^{(l,n)} - n^{-2}(z/2)^4 V^{(l,n)} = 0 \tag{2.2}$$

where ∇_l is the Bessel operator of index l :

$$\nabla_l \equiv z^2 \frac{d^2}{dz^2} + z \frac{d}{dz} + z^2 - (2l+1)^2.$$

Kuhn (1951) has shown that $V^{(l,n)}$ may be written as a series in n^{-2} thereby permitting each term in the series to be substituted into (2.2) and solved separately. That is, we have

$$U^{(l,n)}(z) = \sum_{k=0}^{\infty} n^{-2k} U_k^l(z) \tag{2.3}$$

where $U_k^l(z) \equiv (z/2)V_k^l(z)$. Taking this together with (2.2) we see

$$\nabla_l V_0^l(z) = 0 \tag{2.4a}$$

and

$$\nabla_l V_k^l(z) = (z/2)^4 V_{k-1}^l(z). \tag{2.4b}$$

Equations (2.4) lead to an infinite set of differential equations which may be solved to yield the coefficients $V_k^l(z)$ as required for equation (2.3). Equation (2.4a) which is Bessel's equation of index $2l+1$ has the general solution $V_0^l(z) = C_{2l+1}(z)$ where

$$C_{2l+1}(z) = \alpha J_{2l+1}(z) + \beta Y_{2l+1}(z), \tag{2.5}$$

α and β being arbitrary constants. Using this solution and the standard recurrence relations for Bessel functions, we can find any $V_k^l(z)$.

Values of α and β may be chosen to satisfy the boundary condition at infinity. One solution of interest that tends to zero as z approaches infinity (${}^0V^{(l,n)}(z)$) may be obtained

by putting $\alpha = 1$ and $\beta = 0$. Kuhn proposed a second independent solution (${}^1V^{(l,n)}(z)$) with $\alpha = 0$ and $\beta = 1$. However Ham (1957) showed subsequently that the resulting series diverged and that the correct other solution was

$${}^1V^{(l,n)}(z) = \lim_{m \rightarrow l} \left(\frac{(\Gamma(n+m+1)/\Gamma(n-m))J_{2m+1}^n(z) \cos(2m+1)\pi - J_{-2m-1}^n(z)}{\sin(2m+1)\pi} \right) = N_{2l+1}^n(z) \quad (2.6)$$

where $J_{2l+1}^n(z) = {}^0V^{(l,n)}(z)$.

To avoid the tedious reduction of high order Bessel functions, Kuhn proposed an alternative generating procedure to find $V_k^l(z)$. He replaced $V_0^l(z)$ by

$$V_0^l(z) = \sum_{i=m}^M a_i^0 (z/2)^{2i+1} C_0 + \sum_{i=n}^N b_i^0 (z/2)^{2i} C_1 \quad (2.7a)$$

and wrote

$$V_1^l(z) = \sum_{i=m}^{M+2} a_i^1 (z/2)^{2i+1} C_0 + \sum_{i=n}^{N+2} b_i^1 (z/2)^{2i} C_1 \quad (2.7b)$$

where a_i^0 and b_i^0 are known but a_i^1 and b_i^1 may be deduced from equation (2.4b) by invoking the identities

$$\nabla_l((z/2)^q C_0) = -4q(z/2)^{q+1} C_1 + [q^2 - (2l+1)^2](z/2)^q C_0 \quad (2.8a)$$

$$\nabla_l((z/2)^q C_1) = 4q(z/2)^{q+1} C_0 + [(q-1)^2 - (2l+1)^2](z/2)^q C_1. \quad (2.8b)$$

Similarly the values of $V_k^l(z)$ may be found for $k = 2, 3, 4$, etc.

Notwithstanding Ham's proof, that in general we should take (2.6) rather than $Y_{2l+1}(z)$, he also showed that in the case applicable to our equation, Kuhn's procedure does provide an approximate asymptotic solution. He also gives a convergent series solution which we consider later. We have used the Kuhn procedure to develop the asymptotic series expansions of the two solutions ($\alpha = 0, \beta = 1$ and $\alpha = 1, \beta = 0$ in equation (2.5)). Linear combinations of these two solutions can be constructed to satisfy the boundary conditions and whose energy eigenvalues would correspond to the energy levels of an electron in the neighbourhood of a free ion (called free-ion-term values). Thus we arrive at

$$U^{(l,n)}(z) = n^{-l-1} \Gamma(n+l+1) [\cos(n-l+1)\pi {}^0U^{(l,n)}(z) + \sin(n-l+1)\pi {}^1U^{(l,n)}(z)]. \quad (2.9)$$

The derivatives of the two independent solutions may be defined as

$${}^0D^{(l,n)}(z) = \frac{z}{2} \frac{d}{dz} {}^0U^{(l,n)}(z) = \sum_{k=0}^{\infty} n^{-2k} {}^0D_k^l(z) \quad (2.10)$$

where

$${}^0D_k^l(z) \equiv \frac{z}{2} \frac{d}{dz} {}^0U_k^l(z),$$

and similarly for ${}^1D^{(l,n)}(z)$. Kuhn has given values for the coefficients ${}^0U_k^l(z)$, ${}^0D_k^l(z)$, ${}^1U_k^l(z)$ and ${}^1D_k^l(z)$ for $l = 0$ and $l = 1$. However the $D_k(z)$ are easily deduced from the

corresponding $U_k^l(z)$; using (2.10) and the general expression for $U_k^l(z)$ corresponding to those for $k = 0, 1$ in equation (2.7),

$$D_k^l(z) = \sum_{i=-\infty}^{+\infty} [(i+1)a_i^k + b_i^k](z/2)^{2i+2} C_0 + [ib_i^k - a_{i-1}^k](z/2)^{2i+1} C_1. \quad (2.11)$$

Thus we quote the values of only ${}^0U_k^l(z)$ and ${}^1U_k^l(z)$ for $l = 2$ and $l = 3$. These coefficients are most conveniently written in tabular form as in table 1.

We found Kuhn's tables of values of the functions ${}^0U^{(l,n)}(z)$, ${}^0D^{(l,n)}(z)$, ${}^1U^{(l,n)}(z)$ and ${}^1D^{(l,n)}(z)$ a useful check on our analysis and we have evaluated tables of the corresponding quantities for $l = 2$ and $l = 3$ for values of z in the range 3.5 to 7. These are available from the authors on request.

3. The expansion coefficients

We have evaluated the coefficients for a six term series ($k = 0$ to 5) and they are shown in table 1.

Table 1. Showing values of the coefficients a_j^k and b_j^k appearing in equations (2.7) and (2.11); the powers of ten are shown in parenthesis. (For some purposes these are required to a greater accuracy than shown here, they are available from the authors.)

$l = 2$						
k	0	1	2	3	4	5
i	-2	0	2	3	3	3
a_i^k	-24	1	-2.916667(-2)	-3.158069(-3)	4.778439(-4)	-3.690176(-4)
a_{i+1}^k	6	-8.333333(-2)		9.645062(-5)	-3.185626(-5)	2.460117(-4)
a_{i+2}^k					2.893519(-5)	-5.736307(-5)
a_{i+3}^k						4.615851(-6)
a_{i+4}^k						-3.348980(-8)
b_i^k	24	-1	6.250000(-2)	3.158069(-3)	-4.778439(-4)	3.690176(-4)
b_{i+1}^k	-18	5.833333(-1)	-3.472222(-3)	-1.080247(-3)	5.574846(-4)	-4.305205(-4)
b_{i+2}^k	1				-1.483962(-4)	1.496175(-4)
b_{i+3}^k					2.009388(-6)	-2.048427(-5)
b_{i+4}^k						6.363062(-7)
$l = 3$						
k	0	1	2	3	4	5
i	-3	-1	1	3	4	4
a_i^k	-720	18	-0.375	8.482143(-3)	6.881063(-4)	-1.111813(-4)
a_{i+1}^k	+240	-5	0.05	-9.645062(-5)	-4.099151(-5)	6.948829(-5)
a_{i+2}^k	-12	8.333333(-2)				-7.428994(-6)
a_{i+3}^k						3.348980(-8)
b_i^k	720	-18	0.375	-1.562500(-2)	-6.881063(-4)	1.111813(-4)
b_{i+1}^k	-600	14	-0.2375	1.658951(-3)	2.858383(-4)	-1.250789(-4)
b_{i+2}^k	+72	-1.083333	3.472222(-3)		-2.009389(-6)	3.290803(-5)
b_{i+3}^k	-1					-8.372449(-7)

We have made various checks on the accuracy and stability of the Kuhn series representation of the solution of equation (2.1), ie on the validity of equations (2.7) with the coefficients given by table 1.

The first of these checks was to evaluate the series given by Ham for ${}^1V^{(l,n)}(z)$. This may be carried out using the Kuhn reduction method involving only C_0 and C_1 or by direct evaluation involving high order Bessel functions. Over most of the range of n and z of interest we found excellent agreement between the Kuhn and Ham series. However, the higher order terms in the Ham series for $l = 2$ and $l = 3$ involve small differences between large terms. Even if the arithmetic is carried out with eleven significant figures, it is inadequate and large random discrepancies are introduced. Thus, although in principle the series is sound, in practice it is difficult to maintain accuracy when it is used.

As an alternative procedure we can evaluate the limit in equation (2.6) to find the irregular solution. If in (2.6) we write

$$J_{2m+1}^n(z) = \frac{(z/2)^{2m+1} e^{-z^2/8n}}{\Gamma(2m+2)} M(m+1-n, 2m+2, z^2/4n) \tag{3.1}$$

where

$$M(a, b, x) = 1 + \sum_{n=1}^{\infty} \left(\prod_{i=0}^{n-1} \frac{a+i}{b+i} \right) \frac{x^n}{n!} \tag{3.2}$$

we may evaluate the limit by writing $m \equiv l + \epsilon$ and find asymptotic expansions for each of the terms. Since asymptotic expansions may be multiplied or added together, $N_{2m+1}^n(z)$ may be reduced to the form

$$N_{2l+2\epsilon+1}^n(z) \simeq f(l) + O(\epsilon), \tag{3.3}$$

where (writing $d \ln \Gamma(x)/dx|_s \equiv \psi(s)$)

$$f(l) = \frac{e^{-z^2/8n}}{2\pi} \left[\frac{\Gamma(n+l+1)}{\Gamma(n-l)} \frac{M}{\Gamma(2l+2)} (z/2n)^{2l+1} \left(\psi(n+l+1) + \psi(n-l) - 2\psi(2l+2) \right) \right. \\ \left. + 2 \ln(z/2n) + \frac{l}{M} \frac{\partial M}{\partial l} \right] + (z/2)^{-2l-1} \xi_l^0 X [-2 \ln(z/2) - \xi_l^1 + Y/X] \tag{3.4}$$

in which for brevity $M \equiv M(l+1-n, 2l+2, z^2/4n)$, ξ_l^0 and ξ_l^1 are defined by

$$\frac{1}{\Gamma(-2l-2\epsilon)} = \xi_l^0 \epsilon (1 - \xi_l^1 \epsilon) \tag{3.5}$$

and take the values $\xi_0^0 = -2$, $\xi_1^0 = -4$, $\xi_2^0 = -48$, $\xi_3^0 = -1440$, $\xi_0^1 = 1.154431$, $\xi_1^1 = -1.845569$, $\xi_2^1 = -3.012235$ and $\xi_3^1 = -3.745569$. X and Y are given by

$$X \equiv -\frac{1}{2} \sum_{n=2l+1}^{\infty} \left[(a+2l) \prod_{i=0}^{n-1} \left(\frac{a+i}{b+i} \right) \right] \frac{x^n}{n!} \tag{3.6a}$$

$$Y \equiv 1 + \sum_{n=1}^{2l} \left[\prod_{i=0}^{n-1} \left(\frac{a+i}{b+i} \right) \frac{x^n}{n!} \right] + \frac{1}{2} \sum_{n=2l+1}^{\infty} \left[(a+2l) \prod_{i=0}^{n-1} \left(\frac{a+i}{b+i} \right) \right] \\ \times \left[\sum_{i=0}^{n-1} \left(\frac{1}{a+i} - \frac{2}{b+i} \right) + \frac{1}{a+2l} \right] \frac{x^n}{n!} \tag{3.6b}$$

with $a = -n-l$, $b = -2l$ and the primes on the product and summation indicate that $i = 2l$ is to be excluded. In these expressions

$$\sum_{n=1}^{2l} \left(\prod_{i=0}^{n-1} \frac{a+i}{b+i} \right) \frac{x^n}{n!} \equiv 0 \quad \text{for } l = 0. \tag{3.7}$$

Thus allowing $\epsilon \rightarrow 0$ we get,

$$N_{2l+1}^n(z) = f(l) \tag{3.8}$$

where $N_{2l+1}^n(z)$ is now defined in terms of an absolutely convergent power series for all n and l except when $(n+l) = 0, 1, 2, \dots$

We have evaluated $N_{2l+1}^n(z)$ by equation (3.8) and by the Kuhn procedure for values of n ranging upwards from 1.2 and values of z from 3.5 to 7.5 in steps of 0.5. As is expected from the form of the expressions the error in the Kuhn series (estimated by evaluating the next term in the series) decreases rapidly with increasing n and with decreasing z . We took the worst physically relevant values and the salient features of the comparison are shown in table 2. The $l = 0$ case produces the only significant differences but $n = 1.27$ is the end of the range where the equations in the following section can be solved rather than corresponding to a physical energy eigenvalue. The lowest n corresponding to an actual s state eigenvalue is higher than 1.3, so even for $l = 0$ there need be little fear of errors arising from the Kuhn series. For other l , the accuracy is clearly more than adequate and these findings, together with the similar results for the more extensive range we have investigated, provide convincing evidence to justify the use of the Kuhn expansion with the coefficients as given in table 1.

Table 2. Showing parts of the check on the accuracy of Kuhn's asymptotic expansion. Values of n shown in bold type are the smallest values of relevance to the model potential calculation in §4. The *error estimate* is the magnitude of the next term in the Kuhn expansion.

	$N_{2l+1}^n(z)$ (Kuhn)	Error estimate	$N_{2l+1}^n(z)$ (equation (3.8))
$l = 0, \quad n = \mathbf{1.27}, \quad z = 5$	0.499913	0.0001	0.499867
$l = 1, \quad n = \mathbf{2.1}, \quad z = 5$	-0.019377	0.000001	-0.019377
$l = 2, \quad n = \mathbf{3.1}, \quad z = 5$	-0.438982	0.000001	-0.438981
$l = 3, \quad n = \mathbf{4.1}, \quad z = 5$	-1.153740	0.000001	-1.153742

4. The potential in the neighbourhood of a positive ion—a model

The Shaw (1968) potential is set up as a constant well-depth, $A_l(E)$, for r less than a model ionic radius $R_M(l)$ and the Coulomb potential for r greater than $R_M(l)$, as shown in figure 1.

The energy eigenvalue equation for the region outside $R_M(l)$ is equation (2.1) while the corresponding interior equation has solutions which are the modified spherical Bessel functions

$$\psi_l(r) = \alpha_l r j_l(\alpha_l r) \quad r < R_M(l) \tag{4.1}$$

where $\alpha_l^2 \equiv 2(A_l + E)$. The boundary conditions are to match the logarithmic derivatives of the solutions for the two regions where they meet at $r = R_M(l)$. The previous sections

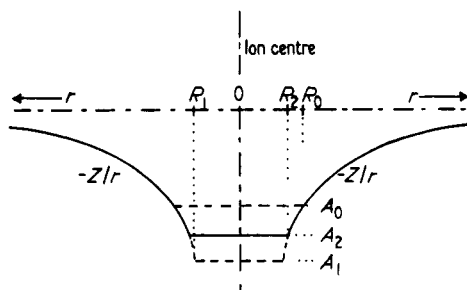


Figure 1. The optimized model potential.

have dealt with the exterior region and the corresponding logarithmic derivative of the interior solution is

$$\left(\frac{1}{\psi_l} \frac{\partial \psi_l}{\partial r} \right)_{r < R_M(l)} = \frac{\alpha_l R_M(l) j_{l-1}(\alpha_l R_M(l))}{j_l(\alpha_l R_M(l))} - l \quad (4.2)$$

(see Eise and Reissland 1973). Shaw also imposed an optimization condition

$$A_l = \frac{Z}{R_M(l)} \quad (4.3)$$

which ensures that the wavefunction is as smooth as possible by avoiding an artificial discontinuity at the boundary. This condition also has the advantage that the model permits a different ionic radius for each l (see figure 1) thus defining a more flexible model than the earlier version in which R_M had to be arbitrarily chosen and was the same for all l . A further implication of this optimization is that it is no longer an approximation to neglect higher order l contributions to the total wavefunction but a consequence of the model that only l values up to the largest l value of the core electrons need be included (Shaw 1968).

The exterior equation has solutions at only certain energies, the free-ion-term values, thus the boundary conditions should be imposed for only these energy values. However, this would mean working through the whole procedure for every new case (including minor changes in conditions which affect the crystal not just those that affect the individual ions). Rather than do this it is more convenient to solve for the well-depths $A_l(E)$ for a range of values of E without specifying the ion and then read particular cases from the resulting tabulation. For a given l , there are a unique set of solutions E against A_l , the different members of the set corresponding to functions with a different number of nodes. We have evaluated three from each set and these are labelled curves 1, 2 and 3 in table 3. A particular ion is characterized by its known energy levels (E_{ns} , E_{np} , etc, where n is the principal quantum number), hence the use of these together with the tables enables potential parameters appropriate to a specific ion to be deduced. Three curves are required since the electrons of interest in a metallic crystal are those close to the Fermi level and we require to interpolate from the free-ion-term data to get the potential for the Fermi level electron. Thus to find $A_0(E_F)$ we take three measured s state energy levels for the particular ion, find the three corresponding $A_0(E_{ns})$ values from table 3(a) one from each curve, and then interpolate for $A_0(E_F)$.

For example, consider the potential parameters for aluminium. From spectroscopic tables we find the s state energy levels of the free Al^{+++} . The corresponding $A_0(E_{ns})$ may be read from table 3(a) which yields

$$\begin{aligned} E_{3s} &= -0.1162Z^2 & A_0(E_{3s}) &= 0.1565Z^2 \\ E_{4s} &= -0.0523Z^2 & A_0(E_{4s}) &= 0.1349Z^2 \\ E_{5s} &= -0.0298Z^2 & A_0(E_{5s}) &= 0.1246Z^2. \end{aligned}$$

But we wish to find the parameters for an electron at $E_F (= -0.1081Z^2$ in aluminium)

Table 3. Parts a, b, c and d show values of A_l/Z^2 against E/Z^2 . The range is limited to that of physical interest, namely that corresponding to values of $ZR_M(l)$ lying between 2 and 20. For $l = 2$ and $l = 3$ (parts c and d), the rate of change of the potential parameters with E_l/Z is so rapid for small $ZR_M(l)$ that tables with a uniform energy interval do not show the values of A_l/Z^2 in this region. Footnotes indicate the values just beyond those of the table, computed at smaller increments in the energy.

(a) $l = 0$										
Curve 1										
E/Z^2	0	2	4	6	8	10	12	14	16	18
-0.04			0.0489	0.0515	0.0541	0.0568	0.0594	0.0621	0.0648	0.0675
-0.06	0.0702	0.0729	0.0757	0.0785	0.0813	0.0841	0.0869	0.0898	0.0927	0.0956
-0.08	0.0986	0.1015	0.1045	0.1075	0.1106	0.1136	0.1167	0.1199	0.1230	0.1262
-0.10	0.1294	0.1326	0.1359	0.1392	0.1425	0.1459	0.1492	0.1526	0.1561	0.1596
-0.12	0.1631	0.1666	0.1702	0.1738	0.1774	0.1811	0.1848	0.1885	0.1923	0.1961
-0.14	0.1999	0.2038	0.2077	0.2116	0.2156	0.2196	0.2237	0.2278	0.2319	0.2361
-0.16	0.2404	0.2446	0.2489	0.2532	0.2576	0.2621	0.2666	0.2711	0.2756	0.2802
-0.18	0.2849	0.2896	0.2943	0.2992	0.3040	0.3089	0.3139	0.3189	0.3239	0.3290
-0.20	0.3342	0.3394	0.3447	0.3500	0.3554	0.3608	0.3663	0.3719	0.3775	0.3832
-0.22	0.3890	0.3948	0.4007	0.4066	0.4127	0.4188	0.4249	0.4312	0.4375	0.4438
-0.24	0.4503	0.4568	0.4634	0.4702	0.4769	0.4838	0.4907	0.4978	0.5049	0.5121
-0.26	0.5194	0.5268	0.5343	0.5419	0.5496	0.5574	0.5653	0.5733	0.5814	0.5896
-0.28	0.5979	0.6064	0.6150	0.6236	0.6325	0.6414	0.6505	0.6597	0.6690	0.6785
-0.30	0.6881	0.6979	0.7078	0.7179	0.7281	0.7385	0.7491			
Curve 2										
E/Z^2	0	1	2	3	4	5	6	7	8	9
-0.03	0.0487	0.0513	0.0540	0.0568	0.0597	0.0627	0.0658	0.0691	0.0724	0.0759
-0.04	0.0795	0.0832	0.0870	0.0910	0.0951	0.0994	0.1037	0.1083	0.1129	0.1178
-0.05	0.1228	0.1279	0.1332	0.1387	0.1444	0.1502	0.1562	0.1624	0.1688	0.1754
-0.06	0.1822	0.1892	0.1965	0.2040	0.2117	0.2197	0.2279	0.2364	0.2452	0.2543
-0.07	0.2637	0.2734	0.2835	0.2939	0.3047	0.3159	0.3275	0.3395	0.3520	0.3649
-0.08	0.3783	0.3923	0.4068	0.4220	0.4377	0.4541	0.4713	0.4891	0.5078	0.5274
-0.09	0.5479	0.5693	0.5919	0.6155	0.6405	0.6667	0.6944	0.7237	0.7547	0.7876
-0.10	0.8225									
Curve 3										
E/Z^2	0	5	10	15	20	25	30	35	40	45
-0.020		0.0493	0.0518	0.0544	0.0571	0.0600	0.0630	0.0661	0.0695	0.0730
-0.025	0.0767	0.0806	0.0848	0.0891	0.0937	0.0986	0.1037	0.1091	0.1148	0.1208
-0.030	0.1271	0.1336	0.1406	0.1478	0.1554	0.1634	0.1718	0.1805	0.1897	0.1993
-0.035	0.2093	0.2199	0.2310	0.2426	0.2548	0.2677	0.2812	0.2954	0.3104	0.3263
-0.040	0.3431	0.3609	0.3797	0.3997	0.4210	0.4437	0.4680	0.4939	0.5218	0.5517
-0.045	0.5840	0.6189	0.6569	0.6982	0.7434	0.7930	0.8480			

Table 3—continued

(b) $l = 1$										
Curve 1										
E/Z^2	0	5	10	15	20	25	30	35	40	45
-0.035								0.0493	0.0502	0.0510
-0.040	0.0519	0.0527	0.0536	0.0545	0.0554	0.0563	0.0572	0.0581	0.0590	0.0599
-0.045	0.0608	0.0617	0.0626	0.0636	0.0645	0.0654	0.0664	0.0674	0.0683	0.0693
-0.050	0.0703	0.0713	0.0722	0.0732	0.0742	0.0753	0.0763	0.0773	0.0784	0.0794
-0.055	0.0805	0.0815	0.0826	0.0837	0.0848	0.0859	0.0870	0.0881	0.0892	0.0904
-0.060	0.0915	0.0927	0.0938	0.0950	0.0962	0.0974	0.0986	0.0998	0.1010	0.1023
-0.065	0.1035	0.1048	0.1061	0.1074	0.1087	0.1100	0.1113	0.1127	0.1140	0.1154
-0.070	0.1168	0.1182	0.1196	0.1210	0.1225	0.1239	0.1254	0.1269	0.1284	0.1299
-0.075	0.1315	0.1330	0.1346	0.1362	0.1378	0.1394	0.1411	0.1428	0.1445	0.1462
-0.080	0.1479	0.1497	0.1515	0.1532	0.1551	0.1569	0.1588	0.1607	0.1626	0.1646
-0.085	0.1666	0.1686	0.1706	0.1727	0.1748	0.1769	0.1791	0.1813	0.1835	0.1858
-0.090	0.1881	0.1904	0.1928	0.1952	0.1977	0.2002	0.2027	0.2053	0.2080	0.2107
-0.095	0.2134	0.2162	0.2190	0.2219	0.2249	0.2279	0.2310	0.2342	0.2374	0.2407
-0.100	0.2440	0.2475	0.2510	0.2546	0.2583	0.2621	0.2660	0.2699	0.2740	0.2783
-0.105	0.2826	0.2870	0.2916	0.2963	0.3012	0.3062	0.3114	0.3168	0.3224	0.3282
-0.110	0.3342	0.3404	0.3469	0.3536	0.3607	0.3680	0.3758	0.3839	0.3924	0.4014
-0.115	0.4109	0.4209	0.4317	0.4431	0.4554	0.4686	0.4828	0.4984	0.5154	0.5342
-0.120	0.5551	0.5787	0.6057	0.6370	0.6743	0.7199	0.7781	0.8575	0.9783	
Curve 2										
E/Z^2	0	5	10	15	20	25	30	35	40	45
-0.020										0.0493
-0.025	0.0511	0.0531	0.0551	0.0571	0.0592	0.0613	0.0636	0.0658	0.0682	0.0706
-0.030	0.0730	0.0756	0.0782	0.0809	0.0837	0.0865	0.0895	0.0925	0.0956	0.0988
-0.035	0.1022	0.1056	0.1091	0.1128	0.1166	0.1205	0.1246	0.1288	0.1332	0.1377
-0.040	0.1425	0.1474	0.1525	0.1578	0.1634	0.1693	0.1754	0.1818	0.1886	0.1957
-0.045	0.2032	0.2111	0.2196	0.2285	0.2381	0.2484	0.2594	0.2713	0.2843	0.2985
-0.050	0.3141	0.3315	0.3510	0.3732	0.3988	0.4291	0.4659	0.5123	0.5746	0.6670
-0.055	0.8369									
Curve 3										
E/Z^2	0	2	4	6	8	10	12	14	16	18
-0.016						0.0500	0.0515	0.0530	0.0546	0.0562
-0.018	0.0578	0.0595	0.0613	0.0631	0.0650	0.0669	0.0688	0.0708	0.0729	0.0750
-0.020	0.0772	0.0794	0.0817	0.0840	0.0865	0.0889	0.0915	0.0941	0.0968	0.0996
-0.022	0.1024	0.1054	0.1084	0.1115	0.1147	0.1180	0.1215	0.1250	0.1287	0.1324
-0.024	0.1364	0.1404	0.1446	0.1490	0.1535	0.1582	0.1631	0.1682	0.1736	0.1791
-0.026	0.1849	0.1911	0.1975	0.2042	0.2113	0.2188	0.2267	0.2351	0.2441	0.2537
-0.028	0.2639	0.2750	0.2869	0.2998	0.3140	0.3296	0.3470	0.3665	0.3886	0.4141
-0.030	0.4442	0.4806	0.5263	0.5871	0.6758	0.8322				

Table 3—continued

(c) $l = 2$										
Curve 1										
E/Z^2	0	2	4	6	8	10	12	14	16	18
-0.032					0.0499	0.0504	0.0508	0.0513	0.0517	0.0521
-0.034	0.0526	0.0531	0.0535	0.0540	0.0545	0.0549	0.0554	0.0559	0.0564	0.0569
-0.036	0.0574	0.0579	0.0585	0.0590	0.0595	0.0601	0.0606	0.0612	0.0618	0.0623
-0.038	0.0629	0.0635	0.0641	0.0648	0.0654	0.0660	0.0667	0.0674	0.0680	0.0687
-0.040	0.0695	0.0702	0.0709	0.0717	0.0724	0.0732	0.0740	0.0748	0.0757	0.0765
-0.042	0.0774	0.0783	0.0792	0.0801	0.0811	0.0820	0.0830	0.0840	0.0851	0.0861
-0.044	0.0872	0.0883	0.0894	0.0905	0.0917	0.0929	0.0941	0.0954	0.0966	0.0979
-0.046	0.0992	0.1006	0.1019	0.1034	0.1048	0.1063	0.1078	0.1093	0.1108	0.1125
-0.048	0.1141	0.1158	0.1175	0.1193	0.1211	0.1230	0.1249	0.1269	0.1290	0.1311
-0.050	0.1333	0.1355	0.1379	0.1403	0.1429	0.1455	0.1483	0.1511	0.1542	0.1574
-0.052	0.1607	0.1643	0.1681	0.1721	0.1764	0.1811	0.1861	0.1916	0.1977	0.2045
-0.054	0.2122	0.2210	0.2313	0.2438	0.2596	0.2809	0.3134	0.3788	†	
† E/Z^2	-0.05540	-0.05545	-0.05550	-0.05555						
A_2/Z^2	0.3788	0.4121	0.4720	0.7551						
Curve 2										
E/Z^2	0	1	2	3	4	5	6	7	8	9
-0.020			0.0496	0.0502	0.0507	0.0512	0.0518	0.0523	0.0529	0.0534
-0.021	0.0540	0.0546	0.0552	0.0557	0.0564	0.0570	0.0576	0.0582	0.0588	0.0594
-0.022	0.0601	0.0607	0.0614	0.0620	0.0627	0.0634	0.0641	0.0648	0.0655	0.0662
-0.023	0.0669	0.0676	0.0684	0.0691	0.0699	0.0707	0.0715	0.0723	0.0731	0.0739
-0.024	0.0747	0.0756	0.0764	0.0773	0.0782	0.0791	0.0800	0.0809	0.0819	0.0828
-0.025	0.0838	0.0848	0.0858	0.0868	0.0879	0.0889	0.0900	0.0911	0.0922	0.0934
-0.026	0.0945	0.0957	0.0970	0.0982	0.0995	0.1008	0.1021	0.1034	0.1048	0.1062
-0.027	0.1077	0.1091	0.1107	0.1122	0.1138	0.1155	0.1172	0.1189	0.1207	0.1225
-0.028	0.1244	0.1264	0.1284	0.1305	0.1326	0.1349	0.1372	0.1397	0.1422	0.1448
-0.029	0.1476	0.1504	0.1535	0.1566	0.1600	0.1636	0.1673	0.1713	0.1756	0.1803
-0.030	0.1852	0.1907	0.1966	0.2033	0.2106	0.2190	0.2287	0.2402	0.2542	0.2721
-0.031	0.2969	0.3364	0.4309	‡						
‡ E/Z^2	-0.03120	-0.03121	-0.03122	-0.03123	-0.03124					
A_2/Z^2	0.4309	0.4520	0.4802	0.5220	0.6001					
Curve 3										
E/Z^2	0	8	16	24	32	40	48	56	64	72
-0.0140		0.0502	0.0510	0.0518	0.0526	0.0535	0.0543	0.0552	0.0560	0.0569
-0.0148	0.0578	0.0588	0.0597	0.0607	0.0617	0.0627	0.0637	0.0647	0.0658	0.0668
-0.0156	0.0679	0.0690	0.0702	0.0713	0.0725	0.0738	0.0750	0.0762	0.0775	0.0789
-0.0164	0.0802	0.0816	0.0830	0.0845	0.0860	0.0875	0.0891	0.0907	0.0924	0.0941
-0.0172	0.0959	0.0977	0.0996	0.1015	0.1035	0.1055	0.1077	0.1099	0.1122	0.1146
-0.0180	0.1171	0.1197	0.1224	0.1252	0.1282	0.1313	0.1346	0.1380	0.1417	0.1456
-0.0188	0.1498	0.1543	0.1591	0.1643	0.1700	0.1762	0.1832	0.1910	0.2000	0.2104
-0.0196	0.2228	0.2383	0.2587	0.2885	0.3426	§				
§ E/Z^2	-0.01992	-0.01994	-0.01996	-0.01998	-0.01999					
A_2/Z^2	0.3426	0.3664	0.4016	0.4666	0.5387					

Table 3—continued

(d) $l = 3$										
Curve 1										
E/Z^2	0	4	8	12	16	20	24	28	32	36
-0.0250		0.0499	0.0501	0.0503	0.0505	0.0507	0.0509	0.0511	0.0513	0.0516
-0.0254	0.0518	0.0520	0.0522	0.0524	0.0526	0.0529	0.0531	0.0533	0.0535	0.0537
-0.0258	0.0540	0.0542	0.0544	0.0546	0.0549	0.0551	0.0553	0.0556	0.0558	0.0560
-0.0262	0.0563	0.0565	0.0568	0.0570	0.0573	0.0575	0.0578	0.0580	0.0583	0.0586
-0.0266	0.0588	0.0591	0.0593	0.0596	0.0599	0.0601	0.0604	0.0607	0.0610	0.0612
-0.0270	0.0615	0.0618	0.0621	0.0624	0.0626	0.0629	0.0632	0.0635	0.0638	0.0641
-0.0274	0.0644	0.0647	0.0651	0.0654	0.0657	0.0660	0.0663	0.0666	0.0670	0.0673
-0.0278	0.0676	0.0680	0.0683	0.0686	0.0690	0.0693	0.0697	0.0700	0.0704	0.0707
-0.0282	0.0711	0.0715	0.0718	0.0722	0.0726	0.0730	0.0734	0.0738	0.0742	0.0746
-0.0286	0.0750	0.0754	0.0758	0.0762	0.0767	0.0771	0.0775	0.0780	0.0784	0.0789
-0.0290	0.0793	0.0798	0.0803	0.0808	0.0813	0.0818	0.0823	0.0828	0.0833	0.0838
-0.0294	0.0844	0.0849	0.0855	0.0861	0.0866	0.0872	0.0878	0.0884	0.0891	0.0897
-0.0298	0.0904	0.0910	0.0917	0.0924	0.0931	0.0939	0.0946	0.0954	0.0962	0.0970
-0.0302	0.0979	0.0987	0.0997	0.1006	0.1016	0.1026	0.1036	0.1047	0.1059	0.1071
-0.0306	0.1083	0.1097	0.1111	0.1126	0.1142	0.1159	0.1178	0.1198	0.1220	0.1245
-0.0310	0.1273	0.1306	0.1345	0.1394	0.1459	0.1561	0.1869			
E/Z^2	-0.0312400	-0.0312420	-0.0312440	-0.0312445	-0.0312450					
A_3/Z^2	0.1869	0.1936	0.2093	0.2478	0.3124					
Curve 2										
E/Z^2	0	4	8	12	16	20	24	28	32	36
-0.0164		0.0501	0.0504	0.0508	0.0512	0.0516	0.0519	0.0523	0.0527	0.0531
-0.0168	0.0535	0.0539	0.0543	0.0547	0.0551	0.0555	0.0560	0.0564	0.0568	0.0573
-0.0172	0.0577	0.0582	0.0586	0.0591	0.0595	0.0600	0.0605	0.0610	0.0615	0.0620
-0.0176	0.0625	0.0630	0.0636	0.0641	0.0647	0.0652	0.0658	0.0663	0.0670	0.0675
-0.0180	0.0682	0.0687	0.0694	0.0700	0.0707	0.0715	0.0721	0.0729	0.0734	0.0741
-0.0184	0.0748	0.0756	0.0763	0.0771	0.0779	0.0788	0.0796	0.0805	0.0814	0.0823
-0.0188	0.0833	0.0842	0.0852	0.0863	0.0873	0.0885	0.0896	0.0908	0.0921	0.0934
-0.0192	0.0947	0.0961	0.0976	0.0992	0.1009	0.1027	0.1046	0.1066	0.1087	0.1111
-0.0196	0.1137	0.1165	0.1197	0.1233	0.1274	0.1324	0.1384	0.1464	0.1579	0.1788 [¶]
¶ E/Z^2	-0.019960	-0.019970	-0.019980	-0.019980	-0.019990	-0.019995				
A_3/Z^2	0.1788	0.1880	0.2021	0.2296	0.2631					
Curve 3										
E/Z^2	0	4	8	12	16	20	24	28	32	36
-0.0114								0.0498	0.0504	0.0510
-0.0118	0.0516	0.0523	0.0529	0.0536	0.0542	0.0549	0.0556	0.0563	0.0570	0.0578
-0.0122	0.0585	0.0593	0.0601	0.0609	0.0617	0.0625	0.0634	0.0643	0.0652	0.0662
-0.0126	0.0671	0.0681	0.0691	0.0702	0.0713	0.0724	0.0735	0.0747	0.0760	0.0773
-0.0130	0.0788	0.0801	0.0813	0.0831	0.0847	0.0864	0.0882	0.0901	0.0921	0.0943
-0.0134	0.0966	0.0991	0.1019	0.1049	0.1083	0.1120	0.1164	0.1215	0.1277	0.1357
-0.0138	0.1468	0.1651	0.2245	*						
* E/Z^2	-0.013880	-0.013882	-0.013884	-0.013884	-0.013886	-0.013888				
A_3/Z^2	0.2245	0.2347	0.2491	0.2731	0.3369					

and this may be found by interpolation using these three s state values. Quadratic interpolation yields $A_0(E_F) = 0.1544Z^2$ for aluminium. The procedure is repeated for $A_1(E_F)$ using p state energies and table 3(b). For ions containing d and f electrons

tables 3(c and d) are used also. Hence a set of parameters may be found for the model potential of any ion for which sufficient spectroscopic data are available. We have carried this out for 27 elements and the results are available on request. Optimized model potential parameters (up to $l = 2$) including other factors have been discussed in some detail by Appapillai and Williams (1973). Here, however, we are primarily concerned with improving and extending the solutions of the equations involved in establishing the details of the potential.

5. Conclusions

We have demonstrated that the Kuhn representation of the solutions of the confluent hypergeometric equation is accurate for values of $l = 0, 1, 2$ and 3 in the region $n > n_l$ and $z < z_l$ where n_l and z_l are such that the whole range of physical interest lies within this region.

The solutions may be used to deduce potential parameters for electrons in the influence of positive ions and we have prepared a general table from which the potential parameters of the Shaw model may be obtained if the ionic electronic energy states are known. Since these are known accurately for a large number of ions, the method is useful for band structure calculations for electrons in solids, for lattice dynamical calculations in metals (where the electrons influence the vibrations of the ions), etc.

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