NOTES ON THE TWO-CENTRE PROBLEM IN WAVE MECHANICS

II. SOME NEW SOLUTIONS OF THE WAVE EQUATION

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Although solutions of the general equations of the two-centre problem, which are sufficient for the purpose of numerical calculation, have been given by various investigators, they are often very slowly convergent for certain ranges of the parameter p in terms of which the solutions are most simply expressed. There is therefore a need of more rapidly convergent solutions. In the present paper certain solutions which depend on the confluent hypergeometric equation are discussed and their use illustrated.

The problem reduces to the solution of two differential equations which we write in the forms*

$$(\lambda^2-1)\frac{d^2f}{d\lambda^2}+2(m+1)\lambda\frac{df}{d\lambda}+[A+m(m+1)-p^2\lambda^2+2l'p\lambda]f=0 \qquad (1)$$

and

$$(\mu^2-1)\frac{d^2f}{d\mu^2}+2(m+1)\mu\frac{df}{d\mu}+[A+m(m+1)-p^2\mu^2+2lp\mu]f=0, \qquad (2)$$

in which $2lp\equiv R(N_1-N_2)$, $2l'p\equiv R(N_1+N_2)$; R is the distance between the nuclei, the charges on which are N_1 and N_2, and, since we may take $N_1>N_2$, l is positive. In these equations the range of λ is $1\leqslant\lambda\leqslant\infty$, that of μ is $-1\leqslant\mu\leqslant1$ and m is a positive integer; further the equations have an essential singularity at infinity and regular singularities at -1 and $+1$ at which the exponents in both cases are $-m$ and 0.

1. Consider the function

$$R_{r,l',m}\equiv(-2p)^{-r}\Gamma(l'-r)\,y^{r-m}\int e^{-yz}(z+p)^{r+l'}(z-p)^{r-l'}\,dz, \qquad (3)$$

which, as will be seen later, is related to the confluent hypergeometric function, where the contour in the z plane is such that the integrand resumes its original value on completing the contour. For convenience in writing, the suffixes l' and m in $R_{r,l',m}$ will be omitted in future.

* Baber and Hassé, *Proc. Cambridge Phil. Soc.* 31 (1935), 564. Marrack, *Proc. Cambridge Phil. Soc.* 35 (1939), 44.

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If $$S_r \equiv (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int e^{-yz}\,z(z+p)^{r+l'}\,(z-p)^{r-l'}\,dz$$

with the same contour then, since

$$0 = (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m-1}\int \frac{d}{dz}\left[e^{-yz}(z+p)^{r+l'}\,(z-p)^{r-l'}\right]dz$$

$$= (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m-1}\int e^{-yz}(z+p)^{r+l'-1}\,(z-p)^{r-l'-1}\,(2rz-2l'p)\,dz$$

$$-(-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int e^{-yz}(z+p)^{r+l'}\,(z-p)^{r-l'}\,dz$$

$$= -\frac{1}{p(l'-r)}\,(rS_{r-1}-l'pR_{r-1})-R_r,$$

it follows that $$rS_{r-1} = l'pR_{r-1}-(l'-r)pR_r. \tag{4}$$

Again, since

$$0 = (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int \frac{d}{dz}\left[e^{-yz}\,z(z+p)^{r+l'}\,(z-p)^{r-l'}\right]dz$$

$$= R_r - yS_r + (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int e^{-yz}(z+p)^{r+l'-1}\,(z-p)^{r-l'-1}$$

$$\times\,[2r(z^2-p^2)-2l'pz+2rp^2]\,dz,$$

it follows that $$0 = R_r - yS_r + 2rR_r + \frac{l'y}{l'-r}\,S_{r-1} - \frac{rpy}{l'-r}\,R_{r-1},$$

so that, using (4), we have

$$\frac{R_r}{py} = \frac{(r+1-l')}{(r+1)\,(2r+1)}\,R_{r+1} + \frac{l'R_r}{r(r+1)} - \frac{(r+l')}{r(2r+1)}\,R_{r-1}. \tag{5}$$

Further, by differentiating (3), we obtain

$$\frac{1}{p}\,\frac{dR_r}{dy} = \frac{r-m}{py}\,R_r - \frac{1}{p}\,S_r,$$

so that from (4) and (5) we have

$$\frac{1}{p}\,\frac{dR_r}{dy} = -\frac{(r+1+m)\,(r+1-l')}{(r+1)\,(2r+1)}\,R_{r+1} - \frac{l'm}{r(r+1)}\,R_r - \frac{(r+l')\,(r-m)}{r(2r+1)}. \tag{6}$$

The differential equation satisfied by R_r is

$$y^2\frac{d^2R_r}{dy^2} + 2(m+1)\,y\,\frac{dR_r}{dy} + \{-p^2y^2+2l'py-(r-m)\,(r+m+1)\}\,R_r = 0. \tag{7}$$

To prove this we take the left-hand side of (7), which is equal to

$$(-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int e^{-yz}(z+p)^{r+l'}\,(z-p)^{r-l'}\,Z\,dz,$$

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where
$$\begin{aligned} Z &= y^2z^2 - 2(m+1)yz - (r-m)(r+m+1) + 2pl'y - p^2y^2 \\ &\quad + (r-m)(r-m-1) + 2(m+1)(r-m) - 2(r-m)zy \\ &= y^2(z^2-p^2) - 2y(r+1)z + 2yl'p \\ &= y^2(z^2-p^2) - y(r+1-l')(z+p) - y(r+1+l')(z-p), \end{aligned}$$

so that it equals

$$-(-2p)^{-r}\Gamma(l'-r)\,y^{r-m+1}\int\frac{d}{dz}[e^{-yz}(z+p)^{r+l'+1}(z-p)^{r-l'+1}]\,dz = 0.$$

If we write $R_r = y^{-(m+1)}W$, the differential equation satisfied by W is, if we put $2py = w$,

$$w^2\frac{d^2W}{dw^2} + \left[-\frac{w^2}{4} + l'w + \tfrac{1}{4} - (r+\tfrac{1}{2})^2\right]W = 0,$$

so that W is Whittaker's function $W_{l',r+\frac{1}{2}}(2py)$.

Therefore $R_r = y^{-(m+1)}W_{l',r+\frac{1}{2}}(2py)$, which gives its connection with the confluent hypergeometric function.

2. If in (1) we now put $y = 1+\lambda$, this equation becomes

$$\begin{aligned} (y^2-2y)\frac{d^2f}{dy^2} + 2(m+1)(y-1)\frac{df}{dy} \\ + \{A + m(m+1) + 2l'py - p^2y^2 + 2p^2y - 2l'p - p^2\}f = 0 \end{aligned}$$

so that, if $f = \Sigma\alpha_r R_r$ then, using (7), we have

$$\begin{aligned} 0 = \Sigma\alpha_r\Big\{&[(r-m)(r+m+1) + A + m(m+1) - p^2 + 2p^2y - 2l'p]\,R_r \\ &- 2(m+1)\frac{dR_r}{dy} - 2y\frac{d^2R_r}{dy^2}\Big\}, \end{aligned} \tag{8}$$

and, using (7) again, the last two terms in the curly brackets in (8) are equal to

$$\frac{2(m+1)}{y}\frac{dR_r}{dy} - 2p^2yR_r + 4l'pR_r - \frac{2(r-m)(r+m+1)R_r}{y},$$

so that (8) may be written

$$\Sigma\alpha_r\left\{R_r[A + r(r+1) - p^2 + 2l'p] + \frac{2(m+1)}{y}\frac{dR_r}{dy} - \frac{2(r-m)(r+m+1)}{y}R_r\right\} = 0. \tag{9}$$

With the aid of (5) and (6), equation (9) reduces to

$$\Sigma\alpha_r\left\{R_r[A + r(r+1) - p^2] - 2p\frac{(r+1-l')(r+1+m)}{2r+1}R_{r+1} + 2p\frac{(r+l)(r-m)}{2r+1}R_{r-1}\right\} = 0,$$

so that the recurrence relation for α_r is

$$\alpha_r[A + r(r+1) - p^2] - 2p\frac{(r-l')(r+m)}{2r-1}\alpha_{r-1} + 2p\frac{(r+1+l')(r+1-m)}{2r+3}\alpha_{r+1} = 0. \tag{10}$$

Thus equation (1) is satisfied by a series of the form $\Sigma\alpha_r R_r(1+\lambda)$ provided that this series converges in the range $1 \leqslant \lambda \leqslant \infty$ (or $2 \leqslant y \leqslant \infty$) and that (10) is satisfied.

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In order that $R_r(y)$ may be finite in the range 2 to ∞ we must take a contour starting from $z = +\infty$, where the value of the integrand is zero, going round $z = p$ in the positive direction and returning to $z = +\infty$, where the value of the integrand is again zero.

For *large positive* values of r the integrand is finite at $z = p$, so that the contour can be reduced to a straight line from $z = p$ to $z = \infty$ circling $z = p$ closely in a positive direction, and thereby changing the value of the integrand by $e^{2i(r-l')\pi}$, and returning to $z = \infty$, so that

$$R_r = (-2p)^{-r}\,[e^{2i(r-l')\pi} - 1]\,\Gamma(l'-r)\,y^{r-m}\int_p^\infty e^{-yz}(z+p)^{r+l'}(z-p)^{r-l'}\,dz.$$

Now the single maximum of the integrand occurs when $yz \doteq 2r$ approximately, r being large, so that we put $yz = 2rt$, thereby making the maximum occur at $t = 1$. On evaluating the dominant term of the transformed integral it can be shown that the integral is asymptotically equal to $y^{-(2r+1)}\,\Gamma(2r+1)$. Hence, since $\Gamma(l'-r)\sin(l'-r)\pi = \pi/\Gamma(r-l'+1)$,

$$R_r \sim (-2p)^{-r}\,(-)^{r-l'+\frac{1}{2}}\,2\pi y^{-r-m-1}\,\Gamma(2r+1)/\Gamma(r-l'+1).$$

By using the asymptotic formula for $\Gamma(x)$ when x is large it can be proved that, when r is large,

$$\Gamma(2r+1)/\{\Gamma(r-l'+1)\,\Gamma(r+l'+\tfrac{1}{2})\} \sim 2^{2r}2^{\frac{1}{2}}(2\pi)^{-\frac{1}{2}},$$

whence finally
$$R_r \sim (-)^{-l'-\frac{1}{2}}\,2^{r+1}\pi^{\frac{1}{2}}p^{-r}y^{-r-m-1}\,\Gamma(r+l'+\tfrac{1}{2}). \qquad (11)$$

For *large negative* values of r the most convenient contour is the imaginary axis and the half of the circle at infinity for which the real part of z is positive. The integral over this semi-circle vanishes, so that

$$R_r = (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}\int_{i\infty}^{-i\infty} e^{-yz}(z+p)^{r+l'}(z-p)^{r-l'}\,dz,$$

or, with $z = ipt$,

$$R_r = (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}(-)^{r-l'-\frac{1}{2}}\,p^{2r+1}\int_{-\infty}^{\infty} e^{-ipyt}(1+t^2)^r\left(\frac{1+it}{1-it}\right)^{l'}dt. \qquad (11a)$$

The integrand of the above integral is real and is an even function of t, as can be proved by changing the variable from t to θ, where $t = \tan\theta$, so that the integral is $2\int_0^\infty (1+t^2)^r\,\Re(t)\,dt$, where $\Re(t)$ is the real part of $e^{-ipyt}\{(1+it)/(1-it)\}^{l'}$. If we write $r = -k$, where $k > 0$, and split up the range of integration into two parts, it follows that the portion arising from the range $k^{-\frac{1}{3}} \leqslant t < \infty$ is less in numerical value than

$$2\int_{k^{-1/3}}^\infty (1+t^2)^{-k}\,dt < 2\int_{k^{-1/3}}^\infty k^{\frac{1}{3}}t(1+t^2)^{-k}\,dt = \frac{k^{\frac{1}{3}}}{k-1}\,(1+k^{-\frac{2}{3}})^{-k+1},$$

which for large k is very small compared with $k^{-\frac{1}{3}}$.

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As regards $2\int_0^{k^{-1/3}} R(t)\,(1+t^2)^{-k}\,dt$, this lies between

$$2\alpha\int_0^{k^{-1/3}} (1+t^2)^{-k}\,dt \quad \text{and} \quad 2\beta\int_0^{k^{-1/3}} (1+t^2)^{-k}\,dt,$$

where α and β are the greatest and least values of $\Re(t)$ in the range $0 \leqslant t \leqslant k^{-\frac{1}{3}}$. Putting $tk^{\frac{1}{2}} = \phi$, we have

$$\int_0^{k^{-1/3}} (1+t^2)^{-k}\,dt = \frac{1}{k^{\frac{1}{2}}}\int_0^{k^{1/6}} \left(1+\frac{\phi^2}{k}\right)^{-k} d\phi,$$

and as $k \to \infty$ this behaves like $k^{-\frac{1}{2}}\int_0^{\infty} e^{-\phi^2}d\phi = \frac{1}{2}\pi^{\frac{1}{2}}k^{-\frac{1}{2}}$ by Tannery's theorem. Since α and β tend to unity as $k \to \infty$, it follows that the dominant term of the integral in (H1 a) for large k is $\pi^{\frac{1}{2}}k^{-\frac{1}{2}}$. Hence, for large negative r,

$$\begin{aligned} R_r &= (-2p)^{-r}\,\Gamma(l'-r)\,y^{r-m}(-)^{r-l'-\frac{1}{2}}p^{2r+1}\pi^{\frac{1}{2}}(-r)^{-\frac{1}{2}} \\ &= (-)^{-l'-\frac{1}{2}}\,2^{-r}p^{r+1}y^{r-m}\pi^{\frac{1}{2}}\,\Gamma(l'-r-\tfrac{1}{2}), \end{aligned} \tag{12}$$

by using the asymptotic expansions of $\Gamma(l'-r)$ and $\Gamma(l'-r-\frac{1}{2})$.

By comparing (11) and (12) it follows that, for large positive r, $R_r = R_{-r-1}$; further (5) is unaltered by changing r into $-r-1$ so that $R_r = R_{-r-1}$ for all values of r.

As regards the convergence of the series $\Sigma\alpha_r R_r(y)$ for large positive r, we have, from (11),

$$\frac{R_r}{R_{r-1}} \sim \frac{2r}{py}\left(1+\frac{l-\frac{1}{2}}{r}\right),$$

and, from the recurrence formula (10),

$$\frac{\alpha_r}{\alpha_{r-1}} \sim \frac{p}{r}\left(1+\frac{m-l-\frac{1}{2}}{r}\right),$$

so that

$$\frac{\alpha_r R_r}{\alpha_{r-1}R_{r-1}} \sim \frac{2}{y}\left(1+\frac{m-1}{r}\right) \quad \text{as } r \to \infty.$$

The series therefore converges for $y > 2$, but as $y \to 2$ it diverges to the order $(y-2)^{-m}$, or $\log(y-2)$ if $m = 0$. Since no change is made by substituting r for $-r-1$ the same results are true for large negative r.

If, however, r is a non-integral number of the form $n \pm s$, where s is a positive integer, and n is so chosen that the positive and negative portions of the series $\sum_{-\infty}^{\infty} \alpha_r R_r(y)$ when $y = 2$ tend to cancel each other, that is, so that

$$\lim_{s\to\infty} \frac{\alpha_{n+s}R_{n+s}(2)}{\alpha_{n-s}R_{n-s}(2)} \to -1, \tag{13}$$

the series will not diverge like $(y-2)^{-m}$ or $\log(y-2)$ when $m = 0$. Since any solution either diverges to this order or is convergent, the series must, when the condition (13) is satisfied, be convergent.

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From (10) we have

$$\frac{\alpha_{n+s}}{\alpha_{n+s-1}} = \frac{2p(n+s+m)(n+s-l')/\{2(n+s)-1\}}{D_{n+s}+\overset{\infty}{\underset{k=s+1}{C}}\left[\frac{E_{n+k}}{D_{n+k}+}\right]},$$

and

$$\frac{\alpha_{n-s}}{\alpha_{n-s+1}} = \frac{-2p(n-s-m+1)(n-s+l'+1)/\{2(n-s)+3\}}{D_{n-s}+\overset{\infty}{\underset{k=s}{C}}\left[\frac{E_{n-k}}{D_{n-k-1}+}\right]}, \tag{14}$$

where, in order to simplify the writing of continued fractions, $\frac{a_n}{b_n+}\frac{a_{n+1}}{b_{n+1}+}\cdots\frac{a_m}{b_m}$ is written as $\overset{m}{\underset{s=n}{C}}\left[\frac{a_s}{b_s+}\right]$, and

$$E_r \equiv \frac{4p^2(r^2-m^2)(r^2-l'^2)}{(2r+1)(2r-1)}, \quad D_r \equiv r(r+1)+A-p^2.$$

From (14) it follows that

$$\frac{\alpha_{n+s}}{\alpha_n} = \prod_{t=1}^{s}\frac{2p(n+t+m)(n+t-l')}{(2n+2t-1)(n+t)(n+t+1)}\frac{1}{B_t}, \tag{14a}$$

where

$$B_t \equiv 1+\frac{A-p^2}{(n+t)(n+t+1)}+\frac{\overset{\infty}{\underset{k=t+1}{C}}\left[\frac{E_{n+k}}{D_{n+k}+}\right]}{(n+t)(n+t+1)},$$

and

$$\frac{\alpha_{n-s}}{\alpha_n} = \prod_{t=1}^{s}\frac{2p(t+m-n-1)(t-n-l'-1)}{(2t-2n-3)(t-n)(t-n+1)}\frac{1}{B'_t}, \tag{14b}$$

where

$$B'_t \equiv 1+\frac{A-p^2}{(t-n)(t-n-1)}+\frac{\overset{\infty}{\underset{k=t}{C}}\left[\frac{E_{n-k}}{D_{n-k-1}+}\right]}{(t-n)(t-n-1)};$$

also from (11) and (12) it follows that

$$\frac{R_{n+s}(2)}{R_{n-s}(2)} = \frac{2^{n+s+1}p^{-n-s}2^{-n-s-m-1}\Gamma(n+s+l'+\frac{1}{2})}{2^{s-n}p^{n-s+1}2^{s-n-m}\Gamma(l'-n+s-\frac{1}{2})} = \frac{1}{p^{2n+1}}\frac{\Gamma(s+n+l'+\frac{1}{2})}{\Gamma(s-n+l'-\frac{1}{2})}. \tag{15}$$

By expressing the linear factors in α_{n+s}/α_n and α_{n-s}/α_n which involve t in terms of Γ functions and using the asymptotic expansion of $\Gamma(x)$ for large positive x it can be shown that the condition (13) reduces to

$$-1 = \frac{\Gamma(n+\frac{1}{2})\Gamma(n+2)\Gamma(n+1)\Gamma(m-n)\Gamma(-n-l')}{p^{2n+1}\Gamma(-n-\frac{1}{2})\Gamma(-n+1)\Gamma(-n)\Gamma(m+n+1)\Gamma(n-l'+1)}\prod_{1}^{\infty}\left(\frac{B'_t}{B_t}\right). \tag{16}$$

Finally, the equation for the determination of A is, from (10),

$$0 = D_n+\overset{\infty}{\underset{k=1}{C}}\left[\frac{E_{n+k}}{D_{n+k}+}\right]+\overset{\infty}{\underset{k=0}{C}}\left[\frac{E_{n-k}}{D_{n-k-1}+}\right]. \tag{17}$$

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3. In the particular case when $m = 0$ we can obtain a solution of (1) in the form $\Sigma\alpha_r R_r(\lambda)$. From (7) we have

$$\lambda^2\frac{d^2R_r}{d\lambda^2}+2\lambda\frac{dR_r}{d\lambda}+\{-p^2\lambda^2+2l'p\lambda-r(r+1)\}R_r=0, \tag{18}$$

and since (1) is now

$$(\lambda^2-1)\frac{d^2f}{d\lambda^2}+2\lambda\frac{df}{d\lambda}+\{-p^2\lambda^2+2l'p\lambda+A\}f=0$$

we have, assuming $f=\Sigma\alpha_r R_r(\lambda)$ and using (18),

$$0=\Sigma\alpha_r\left\{-\frac{d^2R_r}{d\lambda^2}+[A+r(r+1)]R_r\right\}. \tag{19}$$

From (6), which reduces to two terms on the right-hand side, we have

$$\frac{d^2R_r}{d\lambda^2}=-p\frac{r+1-l'}{2r+1}\frac{dR_{r+1}}{d\lambda}-p\frac{r+l'}{2r+1}\frac{dR_{r-1}}{d\lambda}$$

and, by using (6) again, this is equal to

$$p^2\left\{\frac{(r+1-l')(r+2-l')}{(2r+1)(2r+3)}R_{r+2}+\frac{R_r}{2r+1}\left[\frac{\overline{r+1}^2-l'^2}{2r+3}+\frac{r^2-l'^2}{2r-1}\right]+\frac{(r+l')(r-1+l')}{(2r+1)(2r-1)}R_{r-2}\right\},$$

whence (19) is satisfied if

$$\Sigma\alpha_r\left\{p^2\frac{(r+1-l')(r+2-l')}{(2r+1)(2r+3)}R_{r+2}+p^2\frac{(r+l')(r-1+l')}{(2r+1)(2r-1)}R_{r-2}\right.$$
$$\left.-R_r\left[A+r(r+1)-\tfrac{1}{2}p^2\left(1+\frac{1-4l'^2}{(2r-1)(2r+3)}\right)\right]\right\}=0,$$

which leads to the recurrence relation

$$p^2\frac{(r+2+l')(r+1+l')}{(2r+3)(2r+5)}\alpha_{r+2}-\alpha_r\left[A+r(r+1)-\tfrac{1}{2}p^2\left(1+\frac{1-4l'^2}{(2r-1)(2r+3)}\right)\right]$$
$$+p^2\frac{(r-1-l')(r-l')}{(2r-3)(2r-1)}\alpha_{r-2}=0. \tag{20}$$

The contour in the definition of R_r in (3) is, as in § 2, taken from $+\infty$ round $z=p$ and back to $+\infty$; the same difficulty arises as regards convergence at $\lambda=1$ and is met in the same way by taking r to be a non-integral number and making the positive and negative portions of the series $\sum_{-\infty}^{\infty}\alpha_r R_r(\lambda)$ cancel each other as $r\to\infty$. In (20) r must therefore be a non-integral number equal to $n\pm 2s$, where s is an integer and n must be chosen so that

$$\lim_{s\to\infty}\frac{\alpha_{n+2s}R_{n+2s}}{\alpha_{n-2s}R_{n-2s}}=-1.$$

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As in § 2 we have the equations

$$\frac{\alpha_{n+2s}}{\alpha_{n+2s-2}} = \frac{p^2(n+2s-l')(n+2s-l'-1)/\{(2n+4s-1)(2n+4s-3)\}}{F_{n+2s} - \underset{k=s}{\overset{\infty}{C}}\left[\frac{G_{n+2k+2}}{F_{n+2k+2}-}\right]} \tag{20a}$$

and $$\frac{\alpha_{n-2s}}{\alpha_{n-2s+2}} = \frac{p^2(n-2s+1+l')(n-2s+2+l')/\{(2n-4s+3)(2n-4s+5)\}}{F_{n-2s} - \underset{k=s}{\overset{\infty}{C}}\left[\frac{G_{n-2k}}{F_{n-2k-2}-}\right]},$$

where $$F_r \equiv A + r(r+1) - \tfrac{1}{2}p^2\left[1 + \frac{1-4l'^2}{(2r-1)(2r+3)}\right],$$

$$G_r \equiv p^4 \frac{(r^2-l'^2)\{(r-1)^2-l'^2\}}{(2r-3)(2r-1)^2(2r+1)}.$$

The equation from which A is to be determined is

$$F_n = \underset{k=0}{\overset{\infty}{C}}\left[\frac{G_{n+2k+2}}{F_{n+2k+2}-}\right] + \underset{k=0}{\overset{\infty}{C}}\left[\frac{G_{n-2k}}{F_{n-2k-2}-}\right], \tag{21}$$

and the condition for the cancelling of the negative and positive portions of the series $\sum_{-\infty}^{\infty} \alpha_{2r} R_{2r}(1)$ as $r \to \infty$ leads to the result

$$-1 = \frac{2^{2n+1}\Gamma(n+\frac{1}{2})\Gamma(n+2)\Gamma(-n-l')}{p^{2n+1}\Gamma(-n-\frac{1}{2})\Gamma(-n+1)\Gamma(n-l'+1)} \prod_{t=1}^{\infty}\left(\frac{J_t'}{J_t}\right) \tag{22}$$

by using the asymptotic expansion of $\Gamma(x)$ and the duplication formula

$$\pi^{\frac{1}{2}}\Gamma(2x) = 2^{2x-1}\Gamma(x)\Gamma(x+\tfrac{1}{2}),$$

where

$$J_t \equiv 1 + \frac{1}{(n+2t)(n+2t+1)} \times \left\{A - \tfrac{1}{2}p^2\left[1 + \frac{1-4l'^2}{(2n+4t+3)(2n+4t-1)}\right] - \underset{k=t}{\overset{\infty}{C}}\left[\frac{G_{n+2k+2}}{F_{n+2k+2}-}\right]\right\},$$

and $$J_t' \equiv 1 + \frac{1}{(n-2t)(n-2t+1)} \times \left\{A - \tfrac{1}{2}p^2\left[1 + \frac{1-4l'^2}{(2n-4t+3)(2n-4t-1)}\right] - \underset{k=t}{\overset{\infty}{C}}\left[\frac{G_{n-2k}}{F_{n-2k-2}-}\right]\right\}.$$

The presence of the term in p^4 in G_r shows that this solution is more rapidly convergent for small values of p than any previously obtained, but it is of necessity more cumbersome owing to the fact that n has to be determined to satisfy (22).

4. We now turn to equation (2), where the range of value of μ is $-1 \leqslant \mu \leqslant 1$, which differs from (1) only in the substitution of l for l'. This equation can be satisfied by a series of the type $\Sigma \alpha_r R_r(y)$, where $y = \mu + 1$, and we have to choose the contour so that $R_r(y)$ is finite when $\mu = -1$, that is, when $y = 0$. This contour,

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for general values of r, l and m, consists of a circuit in the form of a figure of eight enclosing the two poles $\mu = \pm 1$ followed by a similar circuit in the opposite direction, so that, after completing both circuits, the integrand returns to its original value.

But equation (7), with l' changed into l, can readily be seen to be satisfied by

$$R'_r(y) = e^{py} \sum_{s=r-m}^{\infty} \frac{(-2py)^s \Gamma(s+m+l+1)}{\Gamma(s+r+m+2)\,\Gamma(s-r+m+1)}, \tag{23}$$

which, if $r \geqslant m$, is finite when $y = 0$. Since the solution must be single-valued when $y = 0$, r, as well as m, must be integral and the contour takes the simpler form of a loop enclosing both $\mu = -1$ and $\mu = +1$. It can be verified that (5) and (6) are satisfied by $R'_r(y)$, whence we have, as before (cf. (10)), the result that a solution of (2) is $\Sigma \alpha_r R'_r(y)$, where $y = \mu + 1$, if

$$2p\frac{(r+1+l)(r+1-m)}{2r+3}\alpha_{r+1} + [A - p^2 + r(r+1)]\alpha_r - 2p\frac{(r-l)(r+m)}{2r-1}\alpha_{r-1} = 0, \tag{24}$$

where r is integral and not less than m.

For large values of r, $R'_r(y)$ reduces to its first term

$$e^{py}(-2py)^{r-m}\Gamma(r+l+1)/\Gamma(2r+2),$$

so that

$$R'_r/R'_{r-1} \sim -(r+l)\,2py/\{(2r+1)\,(2r)\},$$

and since $\dfrac{\alpha_r}{\alpha_{r-1}} \sim \dfrac{p}{r}\left(1 + \dfrac{m-l-\frac{1}{2}}{r}\right)$, it follows that $\lim\limits_{r\to\infty} \dfrac{\alpha_r R'_r}{\alpha_{r-1} R'_{r-1}} = 0$, so that the series $\sum\limits_{m}^{\infty} \alpha_r R'_r(y)$ is convergent for all finite values of y.

The equation for determining A is then the same as (17) if n is zero and all values of $k < m$ are omitted; this gives

$$D_m + \overset{\infty}{C}_{k=m+1} \left[\frac{E_k}{D_k +}\right] = 0. \tag{25}$$

This equation is essentially the same as that given by Baber and Hassé [loc. cit. equation (31)], so that it gives no new method for finding the values of A; but the solution itself is of a different type and would be suitable for numerical calculation for values of μ near -1 in terms of the function $R'_r(\mu + 1)$ defined by (23). Since (2) is unchanged by changing the signs of μ and l there is a similar solution which would be suitable for calculations for values of μ near $+1$.

5. In the case of $m = 0$ we have, by an argument similar to that given in § 3, a solution of the form $\sum\limits_{-\infty}^{\infty} \alpha_{2r} R'_{2r}(\mu)$, where r is an integer and $R'_r(\mu)$ is defined by (23) for both positive and negative values of r. From this definition it can be shown that, r being a positive integer, $R'_{-r-1}(\mu) = R'_r(\mu)$ since the terms in $R'_{-r-1}(\mu)$ which involve negative powers of μ all vanish, and this result is the one

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required to prove, by using the results given in § 4, that the doubly infinite series $\sum_{-\infty}^{\infty} \alpha_{2r} R'_{2r}(\mu)$ is convergent for all finite values of μ since both the positive and negative portions of the series are separately convergent.

The equation giving A is then

$$F_0 + \overset{\infty}{\underset{k=0}{C}} \left[\frac{G_{2k+2}}{F_{2k+2}-}\right] + \overset{\infty}{\underset{k=0}{C}} \left[\frac{G_{-2k}}{F_{-2k-2}-}\right] = 0, \tag{26}$$

where
$$F_r \equiv A + r(r+1) - \tfrac{1}{2}p^2\left\{1 + \frac{1-4l^2}{(2r-1)(2r+3)}\right\}$$

and
$$G_r \equiv \frac{p^4(r^2-l^2)\{(r-1)^2-l^2\}}{(2r-3)(2r-1)^2(2r+1)}.$$

Further
$$\frac{\alpha_{2r}}{\alpha_{2r-2}} = \frac{p^2(2r-l)(2r-l-1)/\{(4r-3)(4r-1)\}}{F_{2r} - \overset{\infty}{\underset{k=r}{C}} \left[\frac{G_{2k+2}}{F_{2k+2}-}\right]}$$

and
$$\frac{\alpha_{-2r}}{\alpha_{-2r+2}} = \frac{p^2(2r-1-l)(2r-2-l)/\{(4r-5)(4r-3)\}}{F_{-2r} - \overset{\infty}{\underset{k=r}{C}} \left[\frac{G_{-2k}}{F_{-2k-2}-}\right]}.$$

These results are identical with those given in § 3 except that in this case $n = 0$ and l' is replaced by l.

The expression in equation (26) is more rapidly convergent for small values of p than any hitherto given since if inverted r times it gives as the first approximation $F_r = 0$, so that

$$A + r(r+1) - \tfrac{1}{2}p^2\left\{1 + \frac{1-4l^2}{(2r-1)(2r+3)}\right\} = 0,$$

which is obtained as the second approximation from equation (31) of Baber and Hassé.

6. It was pointed out by Baber and Hassé that it would be a difficult matter to obtain from Hylleraas' or Jaffé's solutions of equation (1) the general value of A for small values of p, and the expression for the energy for small values of R [equation (41) in their paper] was derived by a perturbation method; it can now be shown that this result follows from § 2.

Equation (17) gives as a first approximation $D_n = 0$ or $A = -n(n+1)$, and as a second approximation

$$0 = n(n+1) + A - p^2 + \frac{4p^2\{(n+1)^2-m^2\}\{(n+1)^2-l'^2\}}{(2n+1)(2n+3)\,2(n+1)} + \frac{4p^2(n^2-m^2)(n^2-l'^2)}{(2n+1)(2n-1)(-2n)}$$

or
$$A = -n(n+1) + \tfrac{1}{2}p^2\left\{1 + \frac{1-4l'^2-4m^2+12l'^2m^2/\{n(n+1)\}}{(2n+3)(2n-1)}\right\}. \tag{27}$$

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The corresponding result for equation (2) is given by (25) when inverted r times, which means that there are r nodes in μ, so that it reads

$$0 = D_{m+r} + \overset{\infty}{C}_{k=m+r+1}\left[\frac{E_k}{D_k+}\right] + \overset{m+1}{C}_{k=m+r}\left[\frac{E_k}{D_{k-1}+}\right],$$

and, taking the second approximation and writing $q = m+r$, we obtain a form similar to (27), namely

$$A = -q(q+1) + \tfrac{1}{2}p^2\left\{1 + \frac{1-4l^2-4m^2+12l^2m^2/\{q(q+1)\}}{(2q+3)(2q-1)}\right\}. \tag{28}$$

Equating these two values of A we have $n = q$ as a first approximation and, as a second approximation,

$$n = q + \frac{2p^2(l^2-l'^2)[1-3m^2/\{q(q+1)\}]}{(2q-1)(2q+1)(2q+3)}. \tag{29}$$

Equation (16) has still to be satisfied. For this purpose it is more convenient to put it into a different form which, though more complicated, can be dealt with more easily. We put $A = -q(q+1)+\alpha p^2$ and $n = q+\beta p^2$, where α and β are given by (28) and (29) respectively and, since we know that, when p vanishes, l' becomes an integer N which is the total quantum number of the combined atom, we put $l' = N+\gamma$ and we require to prove that $\gamma = \beta p^2$ to $O(p^2)$. Writing (14a) in the form

$$\frac{\alpha_{n+s}}{\alpha_n} = \prod_{t=1}^{s}\left[\frac{2p(n+t+m)(n+t-l')/(2n+2t-1)}{(n+t)(n+t+1)+A-p^2+\overset{\infty}{C}_{k=t+1}\left[\frac{E_{n+k}}{D_{n+k}+}\right]}\right]$$

and putting $A = -q(q+1)+\alpha p^2$, we find that

$$\frac{\alpha_{n+s}}{\alpha_n} = \prod_{t=1}^{s}\left[\frac{2p(n+t+m)(n+t-l')}{(2n+2t-1)(t+n-q)(t+n+q+1)H_t}\right],$$

where
$$H_t \equiv 1 + \frac{(\alpha-1)p^2}{(t+n-q)(t+n+q+1)} + \frac{\overset{\infty}{C}_{k=t+1}\left[\frac{E_{n+k}}{D_{n+k}+}\right]}{(t+n-q)(t+n+q+1)}.$$

Similarly
$$\frac{\alpha_{n-s}}{\alpha_n} = \prod_{t=1}^{s}\left[\frac{2p(t+m-n-1)(t-n-l'-1)}{(2t-2n-3)(t-q-n-1)(t+q-n)H'_t}\right],$$

where
$$H'_t = 1 + \frac{(\alpha-1)p^2}{(t-q-n-1)(t+q-n)} + \frac{\overset{\infty}{C}_{k=t}\left[\frac{E_{n-k}}{D_{n-k-1}+}\right]}{(t-q-n-1)(t+q-n)}.$$

The condition (16) then reduces, by the same process as used in § 2, to

$$-1 = \frac{\Gamma(n+\frac{1}{2})\Gamma(n+q+2)\Gamma(n-q+1)\Gamma(m-n)\Gamma(-n-l')}{p^{2n+1}\Gamma(-n-\frac{1}{2})\Gamma(-n+q+1)\Gamma(-n-q)\Gamma(m+n+1)\Gamma(n-l'+1)}\prod_{1}^{\infty}\left(\frac{H'_t}{H_t}\right). \tag{30}$$

To $O(p^2)$ all the quantities H_t are for large t of the form $1+Kp^2/t^2$, so that as a first approximation the product converges to unity. The same result is true for

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the quantities H'_l, with the exception of H'_{2q+1} and H'_{2q} which to a first approximation are

$$1-\frac{(\alpha-1)}{\beta(2q+1)}-\frac{4\{(q+1)^2-m^2\}\{(q+1)^2-N^2\}}{\beta(2q+1)^2(2q+3)(2q+2)},$$

and

$$1-\cfrac{4p^2(q^2-m^2)(q^2-N^2)/\{(2q-1)(2q+1)2q\}}{D_{-q-1}+\cfrac{E_{-q-1}}{D_{-q-2}+}\cdots}$$

respectively, of which the latter is equal to

$$1+\frac{2(q^2-m^2)(q^2-N^2)/\{(2q-1)(2q+1)q\}}{(2q+1)\beta H'_{2q+1}},$$

so that

$$H'_{2q}H'_{2q+1}=1-\frac{(\alpha-1)}{\beta(2q+1)}-\frac{2(q^2-m^2)(q^2-N^2)}{\beta(2q+1)^2(2q-1)q}-\frac{4\{(q+1)^2-m^2\}\{(q+1)^2-N^2\}}{\beta(2q+1)^2(2q+2)(2q+3)}.$$

If we use values of the Γ functions in (30) which are correct to a first approximation, of which the important ones for our purpose are

$$\Gamma(m-n)=\frac{(-)^{q-m+1}}{\beta p^2(q-m)!},\quad \Gamma(-n-l')=\frac{(-)^{N+q+1}}{(\gamma+\beta p^2)(N+q)!},$$

$$\Gamma(-n-q)=(-)^{2q+1}/\{\beta p^2(2q)!\},$$

and

$$\Gamma(n-l'+1)=(-)^{N-q}/\{(\gamma-\beta p^2)(N-q+1)!\},$$

(30) becomes

$$p^{2N+1}(-)^{q-m}=\frac{\Gamma(q+\frac{1}{2})(2q+1)!(2q)!(N-q+1)!(\gamma-\beta p^2)}{\Gamma(-q-\frac{1}{2})(q-m)!(N+q)!(m+q)!(\gamma+\beta p^2)}H'_{2q}H'_{2q+1}$$

and, since $2N+1\geqslant 3$ and $H'_{2q}H'_{2q+1}$ is finite, it follows that $\gamma=\beta p^2$ to $O(p^2)$. Hence

$$l'=N+\frac{2p^2(l^2-l'^2)[q(q+1)-3m^2]}{q(q+1)(2q-1)(2q+1)(2q+3)}. \tag{31}$$

Since

$$2lp=R(N_1-N_2),\quad 2l'p=R(N_1+N_2),\quad R^2E'=-4p^2,$$

we find from (31) that

$$\frac{R(N_1+N_2)}{2p}=N-\frac{2R^2N_1N_2[q(q+1)-3m^2]}{q(q+1)(2q-1)(2q+1)(2q+3)},$$

and finally that

$$E'=-\frac{(N_1+N_2)^2}{N^2}-\frac{4N_1N_2(N_1+N_2)^2R^2[q(q+1)-3m^2]}{N^3q(q+1)(2q-1)(2q+1)(2q+3)}, \tag{32}$$

which is equation (41) of the paper referred to above, since $q=m+r$. When $q=0$ and therefore $m=0$ (and $r=0$) we take the limiting value of the second term in (32) as $q\to 0$.

7. The utility of this method of solving the λ-equation is severely restricted by a difficulty which arises so soon as n reaches the value $q+\frac{1}{2}$, which it does for

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quite small values of p. The difficulty arises from the fact that the equations are unchanged if instead of n we write $2q+1-n$, so that they can be regarded as equations in $(n-q-\frac{1}{2})^2$. This can be seen from the fact that equation (10) is unaltered if we replace n by $2q+1-n$ and s by $-s-2q-2$; the quantity α_s in the unaltered equation is the coefficient of R_{n+s} and in the altered equation it is the coefficient of $R_{2q+1-n-s-2q-2}$, that is, of R_{-n-s-1} which is equal to R_{n+s}, so that the entire problem remains unchanged by the transformation. Thus the expression $(n-q-\frac{1}{2})^2$, after decreasing to zero as p increases, becomes negative so that, if p exceeds a small value (about $\frac{1}{2}$ in the ground state), n becomes complex. The equations can be arranged so that their solution is possible without prohibitive labour but it seems that, except for small values of p, this method can never be as useful as those based on the solutions given by Hylleraas and Jaffé respectively.

SUMMARY

The paper deals with new solutions of the differential equations of the two-centre problem which are expressed in terms of the confluent hypergeometric function. By means of this function a solution of the λ-equation (1) is obtained which enables the separation constant A to be found for small values of the parameter p in a rapidly convergent series, which for the special case of $m = 0$ is still more rapidly convergent. The solution for the μ-equation (2) in the general case is of the same character as regards rapidity of convergence as solutions previously obtained, but when $m = 0$ it again possesses a higher rate of convergence as compared with solutions given by other investigators.

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