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1982 J. Phys. A: Math. Gen. 15 2801

(http://iopscience.iop.org/0305-4470/15/9/029)

J. Phys. A: Math. Gen. 15 (1982) 2801–2808. Printed in Great Britain

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Received 16 December 1981

Abstract. The analytical solution of the Schrödinger equation is presented in the case $m=0$ for the angular equation of the dipolar potential.

1. Introduction

The problem of dipolar field (Turner 1966, Turner and Fox 1966, 1965, Lévy-Leblond 1967, Dugan and Maggee 1966, Altschuler 1957, Mittelman and von Holdt 1965, Cross and Herschbach 1965, Cross 1967, Itikawa 1967), in non-relativistic quantum mechanics, leads to the Schrödinger equation (with the usual well known boundary conditions)

$$\left(-\frac{\hbar^2}{2m}\nabla^2+\frac{\boldsymbol{p}\cdot\boldsymbol{r}}{r^3}\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r}) \tag{1}$$

where m is the particle mass, $\boldsymbol{p}$ the dipolar momentum (conventional) and E the total energy.

In spherical coordinates (reference frame as in figure 1) equation (1) is separable

$$\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+g\frac{\cos\theta}{r^2}+K^2\right)\psi(r,\theta,\varphi)=0 \tag{2}$$

where

$$g=-(2m/\hbar^2)p \qquad K^2=(2m/\hbar^2)E. \tag{3}$$

In fact, putting

$$\psi(\boldsymbol{r})=R(r)\Theta(\theta)\Phi(\varphi) \tag{4}$$

we have

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r}+K^2r^2-\lambda\right)R(r)=0 \tag{5}$$

$$\left(\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}+g\cos\theta+\frac{\mu^2}{\sin^2\theta}+\lambda\right)\Theta(\theta)=0 \tag{6}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}+\mu^2\right)\Phi(\varphi)=0 \tag{7}$$

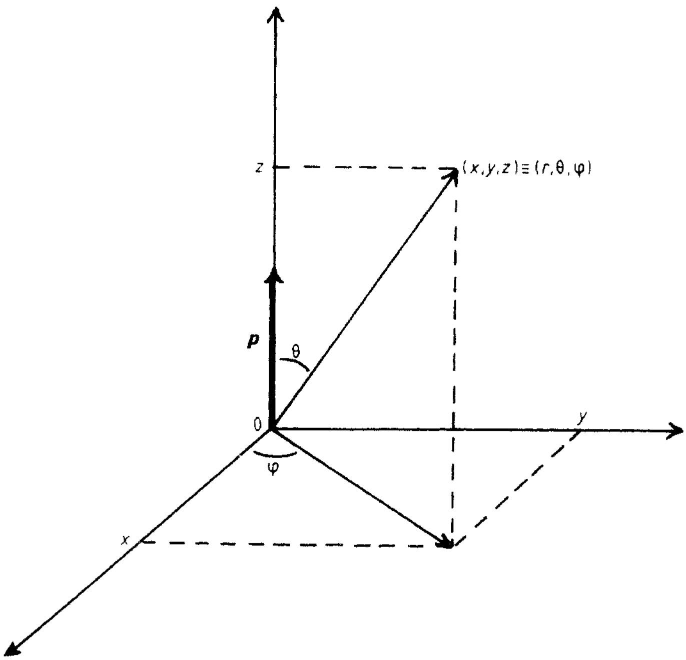

Figure 1.

for λ and μ^2 arbitrary separation constants. Under the conditions

$$\Phi(\varphi+2\pi)=\Phi(\varphi) \qquad \int_0^{2\pi} \mathrm{d}\varphi|\Phi|^2=1 \tag{8}$$

equation (7) gives the solutions

$$\Phi(\varphi)=(2\pi)^{-1/2}\,\mathrm{e}^{\mathrm{i}m\varphi} \qquad \mu^2=m^2 \qquad m=0,\pm1,\pm2,\ldots. \tag{9}$$

Equation (5) reduces to Bessel's equation showing a typical problem of singular potential, however completely solved in literature (Case 1950, Meetz 1964, Behncke 1968, Nelson 1964, Landau and Lifshitz 1966).

Solving equation (6) is the true problem. The solutions are not known to the best knowledge of the author, at least in the sense of analytic solutions and not perturbative or numerical ones (Hunziker and Günther 1980).

In the following we present the analytic solution of equation (6) for the case $m=0$.

2. Physical solutions

Equation (6) reduces to non-angular form by substitution

$$z=\cos\theta \tag{10}$$

from where

$$\left((1-z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2}-2z\frac{\mathrm{d}}{\mathrm{d}z}+gz-\frac{m^2}{1-z^2}+\lambda\right)y(z)=0. \tag{11}$$

Let us observe that, for $g=0$, (11) is the Legendre associated equation. Just for physical reasons we must seek a solution such that

$$y(z) \xrightarrow[g\to 0]{} P_l^m(z) \tag{12}$$

where $P_l^m(z)$ are Legendre associated polynomials.

Particularly, for $m=0$, all reduces to

$$\left((1-z^2)\frac{\mathrm{d}^2}{\mathrm{d}z^2}-2z\frac{\mathrm{d}}{\mathrm{d}z}+gz+\lambda\right)y(z)=0 \tag{13}$$

$$y(z) \xrightarrow[g\to 0]{} P_l(z) \tag{14}$$

to which we shall pay exclusive attention in the following.

Let us define

$$z=2t+1; \tag{15}$$

then we have

$$\left(t(t+1)\frac{\mathrm{d}^2}{\mathrm{d}t^2}+(2t+1)\frac{\mathrm{d}}{\mathrm{d}t}+at+b\right)y(t)=0 \tag{16}$$

where

$$a=-2g \qquad b=-(g+\lambda). \tag{17}$$

The singular points of (16) are $-1, 0, +\infty$; the first two are regular singular points, the last is an irregular one.

The characteristic equation at the origin gives

$$\alpha^2=0$$

from where we deduce the existence of an analytical solution at 0 (actually it can be analytically continued on all the real line). That is just the physical solution we are seeking for.

Let us put

$$L(s)=\int_0^\infty \mathrm{d}t\ \mathrm{e}^{-st}y(t); \tag{18}$$

then we have the Laplace transform of (16) (Ditkin and Prudnikov 1965):

$$s^2\frac{\mathrm{d}^2L}{\mathrm{d}s^2}+(-s^2+2s-a)\frac{\mathrm{d}L}{\mathrm{d}s}+(-s+b)L(s)=0. \tag{19}$$

By factorisation

$$L(s)=\frac{\exp[\frac{1}{2}(s-a/s)]}{\sqrt{s}}\mathscr{L}(s) \tag{20}$$

and changing the independent variable by

$$s=\sqrt{a}\,\xi \tag{21}$$

(19) reduces to

$$\left(\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}+\xi\frac{\mathrm{d}}{\mathrm{d}\xi}-\frac{a}{4}\left(\xi^2+\frac{1}{\xi^2}\right)+b-\frac{a}{2}-\frac{1}{4}\right)\mathscr{L}(\xi)=0$$

or

$$\left(\xi^2\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}+\xi\frac{\mathrm{d}}{\mathrm{d}\xi}+\frac{1}{2}g\left(\xi^2+\frac{1}{\xi^2}\right)-\lambda-\frac{1}{4}\right)\mathscr{L}(\xi)\doteq 0 \tag{22}$$

whence by changing again the independent variable

$$\xi=\mathrm{e}^{\eta} \tag{23}$$

we have the Mathieu equation (Campbell 1955, MacLachlan 1947)

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}-(\lambda+\tfrac{1}{4})+g\cosh 2\eta\right)\mathscr{L}(\eta)=0. \tag{24}$$

On the other hand, since (Gradsteyn and Ryzhik 1980)

$$\int_0^\infty \mathrm{d}t\,\mathrm{e}^{-st}P_l(1+2t)=\frac{\mathrm{e}^{s/2}}{\sqrt{\pi s}}K_{l+\frac{1}{2}}(\tfrac{1}{2}s) \tag{25}$$

it follows that the initial problem transforms in solving the Mathieu equation (22) under the condition

$$\mathscr{L}(\eta)\xrightarrow[g\to 0]{}\frac{1}{\sqrt{\pi}}K_{l+\frac{1}{2}}(\tfrac{1}{2}s). \tag{26}$$

3. Dougall's method

The evident similarity of the Mathieu equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}-p+q\,\mathrm{e}^{2\eta}+q\,\mathrm{e}^{-2\eta}\right)y(\eta)=0 \tag{27}$$

with Bessel's equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}-\nu^2+q\,\mathrm{e}^{\pm 2\eta}\right)y(\eta)=0 \tag{28}$$

suggested to Dougall (1923, 1926) a new method of solving (27). Unfortunately Dougall's results, though of great interest, have had scant diffusion.

Here let us draw the principles of the method, with some minor changes in order to use it in solving the particular problem at hand.

If we write Bessel's equation for two arbitrary cylindrical functions $Z_\nu^{(1)}$ and $Z_\mu^{(2)}$ (not necessarily of the same type)

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}-\nu^2+q\,\mathrm{e}^{-2\eta}\right)Z_\nu^{(1)}(\sqrt{q}\,\mathrm{e}^{-\eta})=0 \qquad \left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}-\mu^2+q\,\mathrm{e}^{2\eta}\right)Z_\mu^{(2)}(\sqrt{q}\,\mathrm{e}^{\eta})=0 \tag{29}$$

by cross multiplication and addition, we have

$$Z_\mu^{(2)}(\sqrt{q}\,e^\eta)\frac{d^2}{d\eta^2}Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})+Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})\frac{d^2}{d\eta^2}Z_\mu^{(2)}(\sqrt{q}\,e^\eta)$$
$$+(-\nu^2-\mu^2+2\cosh 2\eta)Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})Z_\mu^{(2)}(\sqrt{q}\,e^\eta)=0.$$

Now, observing that

$$Z_\mu^{(2)}(\sqrt{q}\,e^\eta)\frac{d^2}{d\eta^2}Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})+Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})\frac{d^2}{d\eta^2}Z_\mu^{(2)}(\sqrt{q}\,e^\eta)$$
$$=\frac{d^2}{d\eta^2}(Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})Z_\mu^{(2)}(\sqrt{q}\,e^\eta)-2q\dot{Z}_\nu^{(1)}(\sqrt{q}\,e^{-\eta})\dot{Z}_\mu^{(2)}(\sqrt{q}\,e^\eta))$$

(where $\dot{Z}$ denotes the first derivative) and remembering the well known functional relations

$$2\frac{d}{dt}Z_\lambda(t)=Z_{\lambda-1}(t)-Z_{\lambda+1}(t) \qquad t(Z_{\lambda-1}(t)+Z_{\lambda+1}(t))=2\lambda Z_\lambda(t)$$

it follows that

$$2q\dot{Z}_\nu^{(1)}(\sqrt{q}\,e^{-\eta})\dot{Z}_\mu^{(2)}(\sqrt{q}\,e^\eta)$$
$$=-2\nu\mu Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})Z_\mu^{(2)}(\sqrt{q}\,e^\eta)$$
$$+q(Z_{\nu-1}^{(1)}(\sqrt{q}\,e^{-\eta})Z_{\mu-1}^{(2)}(\sqrt{q}\,e^\eta)+Z_{\nu+1}^{(1)}(\sqrt{q}\,e^{-\eta})Z_{\mu+1}^{(2)}(\sqrt{q}\,e^\eta)).$$

Therefore

$$\left(\frac{d^2}{d\eta^2}-(\nu+\mu)^2+2q\cosh 2\eta\right)Z_\nu^{(1)}(\sqrt{q}\,e^{-\eta})Z_\mu^{(2)}(\sqrt{q}\,e^\eta)$$
$$=q(Z_{\nu-1}^{(1)}(\sqrt{q}\,e^{-\eta})Z_{\mu-1}^{(2)}(\sqrt{q}\,e^\eta)+Z_{\nu+1}^{(1)}(\sqrt{q}\,e^{-\eta})Z_{\mu+1}^{(2)}(\sqrt{q}\,e^\eta)). \tag{30}$$

This functional relation among products of Bessel functions is the basis of Dougall's series solution.

Actually if we write

$$y(\eta)=\sum_{-\infty}^{+\infty}D_n^{(\rho)}Z_n^{(1)}(\sqrt{q}\,e^{-\eta})Z_{n+\rho}^{(2)}(\sqrt{q}\,e^\eta) \tag{31}$$

in (27), we obtain the Dougall coefficients $D_n^{(\rho)}$ from

$$((2n+\rho)^2-p)D_n^{(\rho)}=q(D_{n-1}^{(\rho)}+D_{n+1}^{(\rho)}) \tag{32}$$

which is the characteristic recurrent relation for Mathieu's equation.

Incidentally, notice that changing η to $-\eta$ in (31) we obtain generally two linearly independent solutions.

Of course, in specific cases, the convergence of the series (31) must be proven so that solution makes sense.

4. The transform of the physical solution

Let us choose

$$\mathscr{L}(\eta)=\sum_{-\infty}^{+\infty} D_n^{(\rho)} J_n(\tfrac{1}{2}\sqrt{g}\,\mathrm{e}^{+\eta}) H^{(1)}_{n+\rho}(\tfrac{1}{2}\sqrt{g}\,\mathrm{e}^{-\eta})$$

whence

$$\mathscr{L}(s)=\sum_{0}^{+\infty} J_n\left(\frac{\mathrm{i}g}{s}\right)(D_n^{(\rho)} H^{(1)}_{n+\rho}(\tfrac{1}{2}\mathrm{i}s)+(-1)^n D^{(\rho)}_{-n+\rho} H^{(1)}_{-n+\rho}(\tfrac{1}{2}\mathrm{i}s)). \tag{33}$$

It is important to prove that the series (33) is uniformly and absolutely convergent. Since (Horn 1899)

$$J_\nu(z)\sim\frac{1}{\Gamma(\nu+1)}\left(\frac{z}{2}\right)^{\nu} \qquad \nu\to\infty$$

$$H^{(1)}_\mu(z)=\frac{J_{-\mu}(z)-\mathrm{e}^{\mu\pi\mathrm{i}}J_\mu(z)}{\mathrm{i}\sin\mu\pi}$$

$$\sim-\frac{\mathrm{e}^{\mu\pi\mathrm{i}}}{\mathrm{i}\sin\mu\pi\,\Gamma(1+\mu)}\left(\frac{z}{2}\right)^{\mu} \qquad \mu\to\infty$$

we have for large n

$$\frac{J_{n+1}(\mathrm{i}g/s)H^{(1)}_{n+1+\rho}(\mathrm{i}s/2)}{J_n(\mathrm{i}g/s)H^{(1)}_{n+\rho}(\mathrm{i}s/2)}\sim\frac{g}{4}\,\frac{1}{(n+1)(n+\rho+1)}$$

which secures the convergence of the series.

On the other hand, from (32), for $q\sim 0$ we have

$$D_n^{(\rho)}\sim\frac{q^n}{\Gamma(-\sqrt{p}+\rho+2n)\Gamma(\sqrt{p}+\rho+2n)}, \tag{34}$$

therefore, in our case, it must be

$$\rho=l+\tfrac{1}{2} \qquad D_n^{(\rho)}=0 \qquad n=-1,-2,\ldots \tag{35}$$

in order that the confluence condition (26) be satisfied.

Finally we have

$$\mathscr{L}(s)=\sum_{n=0}^{\infty} D_n^{(l+\frac{1}{2})} J_n(\mathrm{i}g1/s) H^{(1)}_{n+l+\frac{1}{2}}(\mathrm{i}s/2) \tag{36}$$

or

$$\mathscr{L}(s)=\frac{2}{\pi\mathrm{i}}\sum_{n=0}^{\infty} \mathrm{e}^{\mathrm{i}\pi(l+\frac{1}{2})/2} D_n^{(l+\frac{1}{2})} I_n(g/s) K_{n+l+\frac{1}{2}}(s/2) \tag{37}$$

whence the physical solution transform

$$L(s)=\frac{\exp(s/2+g/s)}{\sqrt{\pi s}}\sum_{r=0}^{\infty} D_n^{(l+\frac{1}{2})} I_n(g/s) K_{n+l+\frac{1}{2}}(s/2) \tag{38}$$

redefining Dougall's coefficients as follows

$$
\begin{aligned}
&D_0^{(l+\frac{1}{2})}=1\\
&[l(l+1)-\lambda]D_0^{(l+\frac{1}{2})}=\tfrac{1}{2}gD_1^{(l+\frac{1}{2})}\\
&[(2n+l)(2n+l+1)-\lambda]D_n^{(l+\frac{1}{2})}=\tfrac{1}{2}g(D_{n-1}^{(l+\frac{1}{2})}+D_{n+1}^{(l+\frac{1}{2})}).
\end{aligned}
\tag{39}
$$

5. The inverse transform

If we call $\mathscr{P}_l(g;z)$ the physical solutions (eigenfunctions), from (18) and (38) follows

$$
\mathscr{P}_l(g;z)=\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\mathrm{d}s\,\frac{\exp(\frac{1}{2}sz+g/s)}{\sqrt{\pi s}}\sum_{n=0}^{\infty}D_n^{(l+\frac{1}{2})}I_n(g/s)K_{n+l+\frac{1}{2}}(s/2)\qquad c\in\mathbb{R}_+^*
\tag{40}
$$

or, since it is legitimate to reverse the order of sum and integration,

$$
\mathscr{P}_l(g;z)=\sum_{n=0}^{\infty}D_n^{(l+\frac{1}{2})}\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\mathrm{d}s\,\frac{\exp(\frac{1}{2}sz+g/s)}{\sqrt{\pi s}}I_n(g/s)K_{n+l+\frac{1}{2}}(s/2)\qquad c\in\mathbb{R}_+^*.
\tag{41}
$$

It must be noted that, though the Bessel function $K_{n+l+\frac{1}{2}}(s/2)$ has a branch point at the origin, nevertheless $K_{n+l+\frac{1}{2}}(s/2)/\sqrt{s}$ has there only a pole of order $n+l+1$; while $I_n(g/s)$ gives an essential singularity.

Since the origin is the sole singularity (not at infinity), it follows that the convergence abscissa of the Laplace integrals (41) is 0.

Unfortunately the integrals (41) do not have a closed form explicit expression. However, it is not difficult to read the analytical properties of the solution directly from the integral representation.

It is useful to define the new class of functions

$$
\mathscr{P}_{n,l}(g;z)=\frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\mathrm{d}s\,\frac{\exp(\frac{1}{2}sz+g/s)}{\sqrt{\pi s}}I_n(g/s)K_{n+l+\frac{1}{2}}(s/2)\qquad\forall n\ l\in\mathbb{N}\qquad c\in\mathbb{R}_+^*
\tag{42}
$$

so the physical solution can be written

$$
\mathscr{P}_l(g;z)=\sum_{n=0}^{\infty}D_n^{(l+\frac{1}{2})}\mathscr{P}_{n,l}(g;z)
\tag{43}
$$

which seems the more appropriate expression for the problem at hand.

Let us point out the recurrence functional relations

$$
\frac{\mathrm{d}}{\mathrm{d}z}\mathscr{P}_{n,l+1}(g;z)=\frac{n+l+\frac{1}{2}}{2}\mathscr{P}_{n,l}(g;z)+\frac{\mathrm{d}}{\mathrm{d}z}\mathscr{P}_{n,l-1}(g;z)
\tag{44}
$$

$$
\mathscr{P}_{n+1,l}(g;z)=\mathscr{P}_{n,l+1}(g;z)-\frac{n}{g}\frac{\mathrm{d}}{\mathrm{d}z}\mathscr{P}_{n,l+1}(g;z)
\tag{45}
$$

which follow trivially from the analogous ones for the cylindrical functions.

6. The eigenvalues

The eigenvalues are completely determined from (39). In fact from

$$\frac{D_1^{(l+\frac{1}{2})}}{D_0^{(l+\frac{1}{2})}}=\frac{l(l+1)-\lambda}{\frac{1}{2}g}$$

$$\frac{D_1^{(l+\frac{1}{2})}}{D_0^{(l+\frac{1}{2})}}=\frac{\frac{1}{2}g}{(l+2)(l+3)-\lambda-\frac{1}{2}g\dfrac{D_2^{(l+\frac{1}{2})}}{D_1^{(l+\frac{1}{2})}}}=\sum_{n=1}^{\infty}{}_{\downarrow}\;-\frac{\frac{1}{2}g}{(l+2n)(l+1+2n)-\lambda}$$

where $\sum_{\downarrow}$ is the continued fraction symbol, we obtain the implicit eigenvalue equation

$$l(l+1)-\lambda=\tfrac{1}{2}g\sum_{n=1}^{\infty}{}_{\downarrow}\;-\frac{\frac{1}{2}g}{(l+2n)(l+1+2n)-\lambda} \tag{46}$$

from where we can obtain very accurate numerical values.

7. Concluding remarks

In conclusion we must point out that while the case $m=0$ can be considered, analysed and resolved in its full generality, the case $m\neq 0$, though slightly different, does not seem resolvable by these methods.

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