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1979 J. Phys. A: Math. Gen. 12 1715

(http://iopscience.iop.org/0305-4470/12/10/018)

J. Phys. A: Math. Gen., Vol. 12, No. 10, 1979. Printed in Great Britain

Schrödinger equation in momentum space

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Received 30 October 1978

Abstract. A differential equation in momentum space is derived for the case of an attractive Coulomb potential. The bound-state energies and the momentum eigenfunctions are shown to arise from this differential equation in a simple fashion. The zero-energy partial-wave momentum eigenfunctions are also derived. The s-wave bound states and their momentum eigenfunctions in a three-dimensional linear potential and an attractive $1/(r+\beta)$ potential are derived by similar techniques. The connection between the quantisation formulae in these potentials and the classical action integral in momentum space is explored.

1. Introduction

In classical mechanics momenta and spatial coordinates are treated on an equal footing in Hamilton's formulation. In quantum mechanics the coordinates and momenta become operators, and the particular form of these operators depends on the choice of representation. Thus the Hamiltonian for a system can be represented in either one of the two equivalent representations: coordinate or momentum. This equivalence is usually illustrated with the example of the one-dimensional harmonic oscillator. The one-dimensional linear potential is another example where the momentum eigenfunctions are particularly simple. But when studying realistic potentials, the coordinate representation is inevitably preferred. Dirac (1958) has argued that the transformation from classical to quantum mechanics should be made by first constructing the classical Hamiltonian in a Cartesian coordinate system and then replacing the coordinates and momenta by their operator equivalents, which are determined by the particular representation that is chosen. The important point, however, is that the transformation should be performed in a Cartesian coordinate system, for it is only in this system that the uncertainty principle between the coordinates and momenta is usually enunciated. Dirac's prescription leads to the proper quantum Hamiltonian in situations that have been encountered without any ambiguity. Most potentials encountered in physics are central potentials and hence the spherical polar coordinate system lends itself as a natural coordinate system for studying the problem. When the potentials are momentum-independent, if the coordinate representation is chosen, only the kinetic energy part of the Hamiltonian contains the momentum operators. Hence the transformation of the kinetic energy term in the classical Hamiltonian to the quantum mechanical operator form can be effected using Dirac's prescription, which leads to a simple form for the kinetic energy operator in the coordinate representation. If, on the other hand, the momentum representation is chosen to study a central potential, $1/r$ for example, the momentum representation of this potential, according to Dirac's rule, would become

$$\frac{1}{(x^2+y^2+z^2)^{1/2}} \rightarrow \mathrm{i}h\left(\frac{\mathrm{d}^2}{\mathrm{d}p_x^2}+\frac{\mathrm{d}^2}{\mathrm{d}p_y^2}+\frac{\mathrm{d}^2}{\mathrm{d}p_z^2}\right)^{-1/2},$$

which is a complicated operator because of the presence of the square root in the denominator. In other words, the representation of the Hamiltonian itself in the momentum representation can be very complicated. This is one good reason for preferring the coordinate representation.

The Schrödinger-type equation for the momentum eigenfunction can be deduced. This equation in momentum space is an integral equation as opposed to the usual differential equation in coordinate space. The reason for studying momentum eigenfunctions is that many physical processes are governed by simple functions of the momentum transfer, and these functional forms are expected to be rational polynomials in the momentum transfer. Momentum eigenfunctions are usually obtained by solving the Schrödinger equation in coordinate space and then Fourier-transforming the coordinate space eigenfunctions. This can be a lengthy process as in the case of Coulomb eigenfunctions in momentum space (Morse and Feshbach 1953). Therefore it is worthwhile to attempt to obtain the momentum eigenfunctions directly. Solutions of the integral equation of the Coulomb problem for bound states are known in the literature on the subject (Bethe and Salpeter 1957). The bound-state momentum space Coulomb eigenfunctions obtained by this procedure and group-theoretical methods (Bechler 1977, Cizek and Paldus 1978, Bayen *et al* 1978) are Geggenbaüer polynomials in a variable which is a simple function of momentum and energy. Since the Geggenbaüer polynomials satisfy a second-order differential equation, it must be possible to derive a differential equation in momentum space directly, at least for the Coulomb potential.

The aim of the present paper is to derive a differential equation in momentum space for the Coulomb potential. In § 2 we derive this equation. Definition of new variables and new functions leads to an extremely simple differential equation. Imposition of simple boundary conditions leads to a trivial quantisation formula. The Coulomb bound states are shown to arise from this equation in a simple fashion. The zero-energy momentum eigenfunctions are also derived. The mathematical procedure developed for the Coulomb potential is then used to derive conditions for bound states in a three-dimensional linear potential and a shifted Coulomb potential in §§ 3 and 4 respectively. In § 5 we study the connection between the new variables used in our description and the action function in momentum space. Section 6 contains a discussion of further implications of this approach. Atomic units will be used throughout.

2. Attractive Coulomb potential

2.1. Bound states

Let us first consider the s-wave Schrödinger equation

$$(-\mathrm{d}^2/\mathrm{d}r^2 - 2b/r + \alpha^2)r\psi = 0, \tag{1}$$

where $-\alpha^2/2$ is the binding energy and b is the Coulomb strength. The momentum eigenfunction is defined by

$$\chi = \int \psi \mathscr{J}_0(pr) r^2 \, \mathrm{d}r, \tag{2}$$

where $\mathscr{J}_0$ is the spherical Bessel function. Henceforth we adopt the notation

$$r\psi = R, \qquad p\chi = f. \tag{3}$$

Equation (1) can be written as

$$(-\mathrm{d}^2/\mathrm{d}r^2 + \alpha^2)R = (2b/r)R. \tag{4}$$

Now we define two different transforms of R. Multiplying both sides of equation (4) by $\sin(pr)$ and integrating over r yields, after imposing the boundary conditions for a bound state R, namely $R \to 0$ as $r \to 0, \infty$,

$$(p^2 + \alpha^2) f^+ = 2b \int_0^\infty \frac{R}{r} \sin(pr) \, \mathrm{d}r, \tag{5}$$

where f^+ is the usual Fourier transform defined by

$$f^+ = \int_0^\infty R \sin(pr) \, \mathrm{d}r. \tag{6}$$

We also define a cosine transform as

$$f^- = \int_0^\infty R \cos(pr) \, \mathrm{d}r. \tag{7}$$

Premultiplying equation (4) by $\cos(pr)$ and integrating over r yields

$$(p^2 + \alpha^2) f^- + \frac{\mathrm{d}R}{\mathrm{d}r}\bigg|_{r=0} = 2b \int_0^\infty \frac{R}{r} \cos(pr) \, \mathrm{d}r. \tag{8}$$

The additional term on the left-hand side of this equation arises because the cosine function does not vanish at the origin; but this surface term is independent of p. From equations (5) and (8) we can deduce that

$$(\mathrm{d}/\mathrm{d}p)(p^2 + \alpha^2) f^+ = 2b f^- \tag{9}$$

and

$$(\mathrm{d}/\mathrm{d}p)(p^2 + \alpha^2) f^- = -2b f^+. \tag{10}$$

Elimination of f^- yields:

$$(\mathrm{d}/\mathrm{d}p)(p^2 + \alpha^2)(\mathrm{d}/\mathrm{d}p)(p^2 + \alpha^2) f^+ = -4b^2 f^+. \tag{11}$$

Thus the s-state momentum eigenfunctions satisfy

$$(1/p)(\mathrm{d}/\mathrm{d}p)(p^2 + \alpha^2)(\mathrm{d}/\mathrm{d}p) p (p^2 + \alpha^2)\chi = -4b^2\chi. \tag{12}$$

To solve this equation in momentum space we define

$$g = (p^2 + \alpha^2) f^+ = (p^2 + \alpha^2) p\chi \tag{13}$$

and an operator

$$[(p^2 + \alpha^2)/2b] \, \mathrm{d}/\mathrm{d}p = \mathrm{d}/\mathrm{d}z. \tag{14}$$

In defining equation (14) we have assumed that such a linear operator in a new variable z can be found. This would be valid provided that

$$\mathrm{d}p/\mathrm{d}z=(p^2+\alpha^2)/2b. \tag{15}$$

Integration of equation (15) provides

$$z=(2b/\alpha)\tan^{-1}(p/\alpha), \qquad p=\tan(\alpha z/2b). \tag{16}$$

Thus the s-wave equation in momentum space becomes

$$\mathrm{d}^2g/\mathrm{d}z^2=-g. \tag{17}$$

We have succeeded in reducing the differential equation in momentum space to a plane-wave equation in a new variable z. The two linearly independent solutions of this equation are $\sin z$ and $\cos z$. If we impose the boundary condition that $g\to 0$ as $p\to 0$, we obtain

$$g=\sin z=\sin[(2b/\alpha)\tan^{-1}(p/\alpha)] \tag{18}$$

and

$$\lim_{p\to\infty} g=\sin(b\pi/\alpha). \tag{19}$$

If we now require g to satisfy the boundary conditions that $g\to 0$ as $p\to\infty$, for g to describe a bound state, we obtain the quantisation condition

$$b\pi/\alpha=n\pi, \tag{20}$$

where n is an integer, i.e.

$$\alpha=b/n. \tag{21}$$

The binding energy is then given by

$$E=-\tfrac{1}{2}\alpha^2=-b^2/2n^2. \tag{22}$$

The wavefunction is given by

$$\chi=\frac{g}{p(p^2+\alpha^2)}=\left[p\left(p^2+\frac{b^2}{n^2}\right)\right]^{-1}\sin\left(2n\tan^{-1}\frac{pn}{b}\right). \tag{23}$$

Thus the requirement that $g\to 0$ as $p\to 0,\infty$ uniquely determines the binding energy and the eigenfunctions. The wavefunction can be normalised using the condition

$$\int \chi^2p^2\,\mathrm{d}p\,\mathrm{d}\Omega=1. \tag{24}$$

The fully normalised eigenfunctions are

$$\chi_n=\left(\frac{n}{2\pi^3b}\right)^{1/2}\frac{1}{p(b^2+p^2n^2)}\sin\left(2n\tan^{-1}\frac{pn}{b}\right). \tag{25}$$

These functions are simply related to the solution in terms of Geggenbaüer polynomials, usually obtained by Fourier-transforming the coordinate space eigenfunctions (Morse and Feshbach 1953).

This successful reduction of the s-wave differential equation in momentum space leads us to consider the operator on the left-hand side of equation (12) to enable the derivation of a differential equation in momentum space for the higher partial waves.

The Schrödinger equation for the radial eigenfunction ψ_l is

$$\left(-\frac{1}{r}\frac{d^2}{dr^2}r+\frac{l(l+1)}{r^2}+\alpha^2\right)\psi_l=2b\frac{\psi_l}{r}. \tag{26}$$

The usual Fourier transform by spherical Bessel function yields

$$(p^2+\alpha^2)\chi_l=2b\int(\psi_l/r)\mathcal{J}_l(pr)r^2\,dr. \tag{27}$$

where

$$\chi_l=\int\psi_l\mathcal{J}_l(pr)r^2\,dr. \tag{28}$$

It is shown in appendix 1 that for bound states χ_l satisfies

$$\frac{1}{p}\frac{d}{dp}(p^2+\alpha^2)\frac{d}{dp}p(p^2+\alpha^2)\chi_l=-4b^2\chi_l+l(l+1)\frac{(p^2+\alpha^2)^2}{p^2}\chi_l. \tag{29}$$

Defining as before

$$g_l=p(p^2+\alpha^2)\chi_l \tag{30}$$

and the variable z by equations (14)–(16), equation (29) can be reduced to the form

$$\frac{d^2g_l}{dz^2}-\frac{\alpha^2l(l+1)}{b^2\sin^2(\alpha z/b)}g_l=-g_l. \tag{31}$$

The technique for solving this equation is similar to that for solving the equation satisfied by spherical Bessel functions (Landau and Lifshitz 1965). The solutions for successive l values are related by

$$g_l=\left(\frac{d}{dz}-\frac{\alpha l}{b}\cot\frac{\alpha z}{b}\right)g_{l-1}. \tag{32}$$

This can be proved by induction (see appendix 2). Equation (32) can also be written in the form

$$g_l=\left(\sin\frac{\alpha z}{b}\right)^l\frac{d}{dz}\frac{1}{[\sin(\alpha z/b)]^l}g_{l-1}. \tag{33}$$

The condition for a bound state of angular momentum l, that $g_l\to 0$ as $p\to\infty$, requires, in view of equation (32),

$$\frac{\lim_{p\to\infty}g_{l-1}}{\lim_{p\to\infty}(dg_{l-1}/dz)}=\lim_{p\to\infty}(\alpha l/b)\tan(\alpha z/b)$$

$$=(\alpha l/b)\lim_{p\to\infty}\tan[2\tan^{-1}(p/\alpha)]=0, \tag{34}$$

i.e.

$$\lim_{p\to\infty}g_{l-1}=0. \tag{35}$$

By recursion, the condition for a bound state of angular momentum l is

$$\lim_{p\to\infty} g_0 = 0. \tag{36}$$

Thus the allowed energy levels are as defined before by equation (21), which determines the bound states for $l = 0$. Equation (33) can also be written by recursion as

$$g_l = \left(\sin\frac{\alpha z}{b}\right)^l \left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\sin(\alpha z/b)}\right)^l g_0. \tag{37}$$

Using equations (18) and (21), we obtain

$$g_l = \left(\sin\frac{z}{n}\right)^l \left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\sin(z/n)}\right)^l \sin z, \tag{38}$$

with

$$z = 2n\tan^{-1}(pn/b). \tag{39}$$

g_l can also be recast as

$$g_l = \left(\sin\frac{z}{n}\right)^{l+1} \left(\frac{1}{\sin(z/n)}\frac{\mathrm{d}}{\mathrm{d}z}\right)^l \frac{\sin z}{\sin(z/n)}. \tag{40}$$

Since

$$\frac{\sin z}{\sin(z/n)} = 2^{n-1}\cos^{n-1}\frac{z}{n} - \frac{(n-2)!}{(n-3)!\,1!}2^{n-3}\cos^{n-3}\frac{z}{n} + \frac{(n-3)!}{(n-5)!\,2!}2^{n-5}\cos^{n-5}\frac{z}{n} - \ldots, \tag{41}$$

$$\frac{1}{\sin(z/n)}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{\sin z}{\sin(z/n)}\right) = -(n-1)2^{n-1}\cos^{n-2}\frac{z}{n} + \frac{(n-2)!}{(n-4)!\,1!}\cos^{n-4}\frac{z}{n} + \ldots. \tag{42}$$

Each successive differentiation in equation (38) reduces the leading power of $\cos(z/n)$ by unity. Since $n-1$ is the leading power of $\cos(z/n)$ in equation (41), the maximum number of possible differentiations (as in equation (38)) that would produce a non-vanishing wavefunction is $n-1$, i.e. the maximum value of l for a given n is $n-1$:

$$l_{\max} = n - 1. \tag{43}$$

The similarity of equation (40) to Rayleigh's formula (Abramowitz and Stegun 1965) for spherical Bessel functions,

$$\mathscr{J}_l(z) = z^l\left(-\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^l \mathscr{J}_0(z), \tag{44}$$

is striking.

2.2. *Zero-energy solutions*

The zero-energy momentum space solutions satisfy equation (29) with $\alpha = 0$:

$$(1/p)(\mathrm{d}/\mathrm{d}p)p^2(\mathrm{d}/\mathrm{d}p)pp^2\chi_l + l(l+1)p^2\chi_l = -4b^2\chi_l. \tag{45}$$

We now define as before

$$g_l = p^2 f_l = pp^2\chi_l \tag{46}$$

and

$$(p^2/2b)(\mathrm{d}/\mathrm{d}p) = \mathrm{d}/\mathrm{d}z. \tag{47}$$

Equation (47) can be solved to give

$$\mathrm{d}p/\mathrm{d}z = p^2/2b, \qquad z = -2b/p. \tag{48}$$

Using equations (46)–(48) in equation (45), we obtain

$$\mathrm{d}^2 g_l/\mathrm{d}z^2 = l(l+1)/z^2 + g_l = 0. \tag{49}$$

This is the equation satisfied by Ricatti–Bessel functions; therefore

$$g_l(z) = z w_l(z) = (-)^{l+1}(2b/p)\mathscr{J}_l(2b/p). \tag{50}$$

Therefore

$$\chi_l = \mathscr{J}_l(2b/p)/p^4. \tag{51}$$

Thus the zero-energy momentum space eigenfunctions have a simple representation. Chen (1978) has arrived at the same answer by group-theoretical considerations.

3. Linear potential

The s-wave radial Schrödinger equation in a three-dimensional linear potential of strength b is

$$(p^2 - k^2)\psi = -2br\psi, \tag{52}$$

where $1/2k^2$ is the energy. As in the Coulomb case we define the sine and cosine transforms f^+ and f^- respectively. In terms of the radial solution

$$r\psi = R \tag{53}$$

we obtain, after premultiplying the Schrödinger equation by $\sin(pr)$ and $\cos(pr)$ and integrating over r, a pair of equations

$$(p^2 - k^2)f^+ = -2b\int_0^\infty rR\sin(pr)\,\mathrm{d}r, \tag{54}$$

$$(p^2 - k^2)f^- + \left.\frac{\mathrm{d}R}{\mathrm{d}r}\right|_{r=0} = -2b\int_0^\infty rR\cos(pr)\,\mathrm{d}r \tag{55}$$

If we let

$$\mathrm{d}R/\mathrm{d}r|_{r=0} = A, \tag{56}$$

we can deduce that

$$(p^2 - k^2)f^+ = +2b(\mathrm{d}/\mathrm{d}p)f^-, \tag{57}$$

$$(p^2 - k^2)f^- = -2b(\mathrm{d}/\mathrm{d}p)f^+ - A. \tag{58}$$

When the inhomogeneous term A is absent, the linearly independent solutions of this pair of equations are $\sin[(p^3/3 - k^2p)/2b]$ and $\cos[(p^3/3 - k^2p)/2b]$. When the inhomogeneous term is present, the solutions f^+ and f^- can be written with the requirement that f^+ vanishes at the origin as

$$f^+=\sin z\Big(B-A\int_0^p \mathrm{d}p'\sin z(p')\Big)-A\cos z\int_0^p \cos z(p')\,\mathrm{d}p', \tag{59}$$

$$f^-=-\cos z\Big(B-A\int_0^p \mathrm{d}p'\sin z(p')\Big)-A\sin z\int_0^p \cos z(p')\mathrm{d}p', \tag{60}$$

where B is a constant and

$$z=(p^3/3-k^2p)/2b. \tag{61}$$

For a bound state we require, as in the Coulomb case, that $(p^2-k^2)f^+$ vanish as $p\to\infty$. This yields the conditions

$$\frac{B}{A}=\int_0^\infty \mathrm{d}p'\sin z(p') \tag{62}$$

and

$$\int_0^\infty \cos z(p')\,\mathrm{d}p'=0. \tag{63}$$

The second condition provides the bound-state energies. The same solution has been derived from coordinate space considerations (Antippa and Phares 1978). Thus f^+ can be written as

$$f^+=A\Big\{\sin\Big[\Big(\frac{p^3}{3}-k^2p\Big)\frac{1}{2b}\Big]\int_p^\infty \sin\Big[\Big(\frac{p'^3}{3}-k^2p'\Big)\frac{1}{2b}\Big]\,\mathrm{d}p'$$
$$-\cos\Big[\Big(\frac{p^3}{3}-k^2p\Big)\frac{1}{2b}\Big]\int_0^\infty \cos\Big[\Big(\frac{p'3}{3}-k^2p'\Big)\frac{1}{2b}\Big]\,\mathrm{d}p'\Big\}. \tag{65}$$

The quantisation condition (63) which we have derived is an exact quantum mechanical quantisation condition. Thus equations (64) and (65) provide the s-wave solution in momentum space directly. It is worth noting that the variable z was obtained from the condition that

$$\mathrm{d}z/\mathrm{d}p=(p^2-k^2)/2b, \tag{66}$$

i.e.

$$z=\frac{1}{2b}\int_0^p (p^2-k^2)\,\mathrm{d}p. \tag{67}$$

4. Shifted Coulomb potential: $v(r)=-b/(r+\beta)$

We now consider the s-wave bound-state solutions in this attractive potential with positive β:

$$(p^2+\alpha^2)\psi=2b\psi/(r+\beta). \tag{68}$$

Defining f^+ and f^- as before, we arrive at the equations

$$(p^2+\alpha^2)f^+=2b\int_0^\infty R\frac{\sin(pr)}{r+\beta}\,\mathrm{d}r, \tag{69}$$

$$(p^2+\alpha^2)f^- + A = 2b\int_0^\infty R\frac{\cos(pr)}{r+\beta}\,\mathrm{d}r, \tag{70}$$

where A is as before the derivative of the radial solution at the origin. Thus

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}p}&(p^2+\alpha^2)f^+ \\
&= 2b\int_0^\infty R\frac{r}{r+\beta}\cos(pr)\,\mathrm{d}r \\
&= 2b\left(\int_0^\infty R\cos(pr)\,\mathrm{d}r - \beta\int_0^\infty \frac{R}{r+\beta}\cos(pr)\,\mathrm{d}r\right) \\
&= [2b-\beta(p^2+\alpha^2)]f^- - \beta A.
\end{aligned} \tag{71}$$

Similarly,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}p}&(p^2+\alpha^2)f^- \\
&= -2b\int_0^\infty R\frac{r}{r+\beta}\sin(pr)\,\mathrm{d}r \\
&= -2b\left(\int_0^\infty R\sin(pr)\,\mathrm{d}r - \beta\int_0^\infty \frac{R\sin(pr)}{r+\beta}\,\mathrm{d}r\right) \\
&= -[2b-\beta(p^2+\alpha^2)]f^+,
\end{aligned} \tag{72}$$

where we have used equations (69) and (70) and the definitions of f^+ and f^-.

If the inhomogeneous term in equation (71) were absent, we would have

$$[2b-\beta(p^2+\alpha^2)]^{-1}(\mathrm{d}/\mathrm{d}p)(p^2+\alpha^2)f^+ = f^-, \tag{73}$$

$$[2b-\beta(p^2+\alpha^2)]^{-1}(\mathrm{d}/\mathrm{d}p)(p^2+\alpha^2)f^- = -f^+ \tag{74}$$

and

$$\left(\frac{p^2+\alpha^2}{2b-\beta(p^2+\alpha^2)}\frac{\mathrm{d}}{\mathrm{d}p}\right)^2(p^2+\alpha^2)f^+ = -(p^2+\alpha^2)f^+. \tag{75}$$

Now we define the operator

$$\frac{\mathrm{d}}{\mathrm{d}z} = \frac{p^2+\alpha^2}{2b-\beta(p^2+\alpha^2)}\frac{\mathrm{d}}{\mathrm{d}p}, \tag{76}$$

which would imply that

$$z = \int\frac{2b-\beta(p^2+\alpha^2)}{p^2+\alpha^2}\,\mathrm{d}p = \frac{2b}{\alpha}\tan^{-1}\left(\frac{p}{\alpha}\right) - \beta p. \tag{77}$$

In terms of z the solutions $(p^2+\alpha^2)f^+$ of equation (75) are $\sin z$ and $\cos z$. We can now solve equations (71) and (72) in terms of these solutions. Requiring that f^+ vanish as $p\to 0$ provides

$$g^+ = (p^2+\alpha^2)f^+ = \sin z\left(B - \beta A\int_0^p \sin z'\,\mathrm{d}p'\right) - \beta A\cos z\int_0^p \cos z'\,\mathrm{d}p' \tag{78}$$

$$g^- = (p^2+\alpha^2)f^- = \cos z\left(B - \beta A\int_0^p \sin z'\,\mathrm{d}p'\right) + \beta A \sin z\int_0^p \cos z'\,\mathrm{d}p'. \tag{79}$$

The requirement that g^+ vanish as $p \to \infty$, for a bound state, yields the conditions

$$B = \beta A\int_0^\infty \sin z'\,\mathrm{d}p', \tag{80}$$

$$\int_0^\infty \cos z'\,\mathrm{d}p' = 0. \tag{81}$$

The second condition can be written in terms of Whittaker functions (Gradshteyn and Ryzik 1965) as

$$\int_0^\infty \cos\left[\frac{2b}{\alpha}\tan^{-1}\left(\frac{p'}{\alpha}\right) - \beta p'\right]\mathrm{d}p' = \frac{\Pi}{\alpha\beta}\frac{1}{\Gamma(b/\alpha)}W_{b/\alpha',1/2}(2\alpha\beta) = 0. \tag{82}$$

The zeros of the Whittaker function provide the true bound states in the potential, in agreement with Mehta and Patil (1978). The momentum eigenfunctions can be obtained from

$$g^+ = \beta A\left(\sin z\int_p^\infty \sin z'\,\mathrm{d}p' - \cos z\int_0^p \cos z'\,\mathrm{d}p'\right]. \tag{83}$$

Thus once again we have been able to show that the bound states are related to an exact quantisation condition (equation (82)). The inhomogeneous terms in the shift Coulomb potential case and the linear potential case are similar. Therefore, in terms of the z variables for the two cases, the solutions and quantisation conditions are similar.

From equations (77), (78) and (83) we can write the zero-energy s-wave solution in the $-b/(r+\beta)$ potential as

$$g^+ = \beta A\left[\sin\left(\frac{2b}{p}+\beta p\right)\int_p^\infty \sin\left(\frac{2b}{p'}+\beta p'\right)\mathrm{d}p' - \cos\left(\frac{2b}{p}+\beta p\right)\int_0^p \cos\left(\frac{2b}{p'}+\beta p'\right)\mathrm{d}p'\right]. \tag{84}$$

In the next section we explore the significance of the variables z which we introduced in each of the three potentials we have considered.

5. Canonical transformations in classical mechanics and action integrals

In classical mechanics, the Hamiltonian is the total energy of the system. For zero angular momentum,

$$H = \tfrac{1}{2}p^2 + v(r) = E = \tfrac{1}{2}k^2, \tag{85}$$

i.e.

$$(p^2 - k^2) = -2v(r). \tag{86}$$

If we now introduce a scaling Q on all radial coordinates such that

$$r \to r/Q, \tag{87}$$

then equation (85) can be solved formally to provide r as a function of Q and p, if we treat Q as a function for the present purpose. Thus r can be expressed as a function of the old momentum p and the new coordinate Q.

To find a new momentum P, conjugate to Q, we consider generating functions of the third kind F_3 (Goldstein 1965), since F_3 is a function of p and Q. In terms of F, the old coordinate r and the new momentum P are given by

$$r = \partial F_3/\partial p, \tag{88}$$

$$P = -\partial F_3/\partial Q. \tag{89}$$

Under the scaling defined by (87), equation (86) becomes

$$(p^2 - k^2) = -2v(r/Q), \tag{90}$$

which can formally be inverted to give

$$r = Qf((p - k^2)/2) \tag{91}$$

where f defines the inverted function. From equations (91) and (88) we obtain

$$\partial F_3/\partial p = -Qf((p^2 - k^2)/2), \tag{92}$$

$$F_3 = -Q \int \mathrm{d}p\, f((p^2 - k^2)/2) + g(Q). \tag{93}$$

If we require the new momenta to be independent of the new coordinate, i.e. if we set $g(Q)$ to be identically zero, then the new momentum is given by

$$P = -\partial F_3/\partial Q = \int \mathrm{d}p\, f((p^2 - k^2)/2). \tag{94}$$

If the new coordinate Q is a constant chosen to be 1 arbitrarily, then

$$P = \int r\, \mathrm{d}p, \tag{95}$$

which is just the action integral in momentum space. The transformation we have referred to above is a point–momentum transformation. Thus the action integral in momentum space is canonically conjugate to a constant function that scales the coordinates.

We now consider the action integrals in momentum space for the three potentials we considered earlier.

A. *Coulomb potential*

$$(p^2 + \alpha^2) = 2b/r, \tag{96}$$

$$P = \int r\, \mathrm{d}p = 2b \int \frac{\mathrm{d}p}{p^2 + \alpha^2}. \tag{97}$$

For negative, zero and positive energies $E = \frac{1}{2}k^2$, the integral can be performed to yield $(2b/\alpha)\tan^{-1}(p/\alpha)$, $-2b/p$ and $(b/k)\ln[(p-k)/(p+k)]$ for the three energy domains respectively. In other words, the action integral is identical to the z variable introduced in the quantum mechanical problem.

B. Linear potential

$$(p^2-k^2)=-2br, \tag{98}$$

$$P=\int r\,\mathrm{d}p=-\frac{1}{2b}\int(p^2-k^2)\,\mathrm{d}p=-\frac{1}{2b}\left(\frac{p^3}{3}-k^2p\right). \tag{99}$$

C. Shifted Coulomb potential

$$(p^2+\alpha^2)\equiv+2b/(r+\beta). \tag{100}$$

Therefore,

$$r=2b/(p^2+\alpha^2)-\beta, \tag{101}$$

$$P=\int r\,\mathrm{d}p=(2b/\alpha)\tan^{-1}(p/\alpha)-\beta p. \tag{102}$$

Thus in each of the three cases the action integral in momentum space is identical to the variable z, which arose in the consideration of the quantum mechanical bound-state eigenvalue problem in the momentum picture. The eigenvalues in the three cases are determined by the conditions

$$A:\qquad \lim_{p\to\infty}\sin P=0 \quad\text{or}\quad \lim_{p\to\infty}P=n\pi, \qquad n=1,2,\ldots, \tag{103}$$

$$B:\qquad \mathrm{Lim}\int_0^\infty \cos P(p)\,\mathrm{d}p=0, \tag{104}$$

$$C:\qquad \int_0^\infty \cos P(p)\,\mathrm{d}p=0. \tag{105}$$

These quantisation conditions are exact as opposed to the approximate semiclassical JWKB-type quantisation conditions which require that the action integral between the classical turning points be equal to $(n+\frac{1}{2})\pi$, n being an integer.

6. Discussion

Review papers by Chen and Chen (1972) and Norcliffe (1974) treat representations of the Coulomb wavefunctions in momentum space and the correspondence identities associated with the Coulomb potentials respectively. The present approach further enriches some of the conclusions reached by these authors. Norcliffe's discussion of the bound states of the Coulomb potentials points out that from the point of view of classical mechanics in momentum space for every physically allowed real value of the momentum there is a physically allowed real value of the coordinates, while the converse does not hold. It is this difference between the coordinate and momentum pictures that indicates why quantum mechanically the bound states are simpler through the momentum picture. The simplicity of the representation of the momentum eigenfunctions in terms of the action integral in momentum space, and the simplicity of the quantisation condition from this point of view, is an interesting aspect that has emerged by the present approach.

The positive-energy Coulomb eigenfunctions in momentum space have been the subject of many investigations. The review papers cited above provide long lists of references. Ford (1964) derived a representation of the s-wave Coulomb half-shell T-matrix. In terms of the action integral in momentum space for positive energies, which has the form $z=(b/k)\ln[(p-k)/(p+k)]$, Ford's expression indeed bears resemblance to a function of the form $\sin z$. The on-shell singularity associated with the Coulomb potential manifests itself simply in terms of z, which contains a factor $\ln(p-k)$. This factor has a logarithmic singularity when $p=k$. This comparison with Ford's expression enables us to identify the function g introduced in equation (13) as the half-shell T-matrix. The simplicity of the recursion relation between different partial-wave solutions g for bound states points in the direction of a similar simple recursion relation between the different positive-energy partial-wave half-shell T-matrix elements, because of the similarity in the structure of the solutions in terms of z for negative, zero and positive energies. These aspects are currently under investigation.

The s-wave differential equation in momentum space for the br and the $-b/(r+\beta)$ potentials contain inhomogeneous terms. For the higher partial waves these inhomogeneous terms are not as simple as for the s-wave. The work of Antippa and Phares (1978) on representing the higher partial-wave solutions in a central linear potential in terms of combinatorial harmonics provides additional incentive towards analysing these solutions from the momentum picture. Further work in this direction is in progress.

Appendix 1

From the Schrödinger equation (equations (26) and (27)) we have

$$
\begin{aligned}
I &= \frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}p}(p^2+\alpha^2)\frac{\mathrm{d}}{\mathrm{d}p}p(p^2+\alpha^2)\chi_l \\
&= \left((p^2+\alpha^2)\frac{1}{p}\frac{\mathrm{d}^2}{\mathrm{d}p^2}p+2\frac{\mathrm{d}}{\mathrm{d}p}p\right)(p^2+\alpha^2)\chi_l \\
&= 2b\left((p^2+\alpha^2)\frac{1}{p}\frac{\mathrm{d}^2}{\mathrm{d}p^2}p+2\frac{\mathrm{d}}{\mathrm{d}p}p\right)\int\frac{\psi_l}{r}\mathcal{J}_l(pr)r^2\,\mathrm{d}r \\
&= 2b\frac{(p^2+\alpha^2)}{p}\int\psi_l\frac{\mathrm{d}^2}{\mathrm{d}p^2}(pr\mathcal{J}_l(pr))\,\mathrm{d}r+4b\int r\psi_l\frac{\mathrm{d}}{\mathrm{d}p}(\mathrm{pr}\mathcal{J}_l(\mathrm{pr}))\,\mathrm{d}r.
\end{aligned}
\tag{A1.1}
$$

But the Ricatti–Bessel functions $w(z)=z\mathcal{J}_l(z)$ satisfy the differential equation

$$\mathrm{d}^2w/\mathrm{d}z^2=[l(l+1)/z^2]w-w. \tag{A1.2}$$

Therefore,

$$I=2b\frac{(p^2+\alpha^2)}{p^2}\left[\int r^2\psi_l\left(\frac{l(l+1)}{pr}\mathcal{J}_l(pr)-pr\mathcal{J}_l(pr)\right)\right]+4b\int r\psi_l\frac{\mathrm{d}}{\mathrm{d}p}(p\mathcal{J}_l(pr))\,\mathrm{d}r. \tag{A1.3}$$

When equation (27) is used to simplify the first term in square brackets we obtain

$$
\begin{aligned}
I &= \frac{(p^2+\alpha^2)}{p^2}l(l+1)(p^2+\alpha^2)\chi_l \\
&\quad -2b\left((p^2+\alpha^2)\int r^2\psi_l r\mathcal{J}_l(pr)\,\mathrm{d}r-2\int r\psi_l\frac{\mathrm{d}}{\mathrm{d}r}(r\mathcal{J}_l(pr)\,\mathrm{d}r\right)
\end{aligned}
\tag{A1.4}
$$

since

$$(\mathrm{d}/\mathrm{d}p)(p\mathcal{J}_l(pr)) = (\mathrm{d}/\mathrm{d}r)(r\mathcal{J}_l(pr)). \tag{A1.5}$$

Therefore

$$J = \frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}p}(p^2+\alpha^2)\frac{\mathrm{d}}{\mathrm{d}p}p(p^2+\alpha^2)\chi_l - l(l+1)\frac{(p^2+\alpha^2)^2}{p^2}\chi_l$$
$$= -2b\left((p^2+\alpha^2)\int r\psi_l r^2\mathcal{J}_l(pr)\,\mathrm{d}r - 2\int r\psi_l\frac{\mathrm{d}}{\mathrm{d}r}(r\mathcal{J}_l(pr))\,\mathrm{d}r\right). \tag{A1.6}$$

But from equations (26) and (28) we also have

$$\int r\mathcal{J}_l(pr)r^2\left(-\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + \frac{l(l+1)}{r^2} + \alpha^2\right)\psi_l\,\mathrm{d}r = 2b\chi_l, \tag{A1.7}$$

i.e.

$$\alpha^2\int r\mathcal{J}_l(pr)r^2\psi_l\,\mathrm{d}r = 2b\chi_l - \int r\mathcal{J}_l(pr)r^2\left(\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + \frac{l(l+1)}{r^2}\right)\psi_l\,\mathrm{d}r. \tag{A1.8}$$

Therefore

$$J = -4b^2\chi_l + 2b\left(\int [l(l+1) - p^2r^2]\mathcal{J}_l(pr)r\psi_l\,\mathrm{d}r - \int r^2\mathcal{J}_l(pr)\frac{\mathrm{d}}{\mathrm{d}r^2}(r\psi_l)\,\mathrm{d}r\right.$$
$$\left. + 2\int r\psi_l\frac{\mathrm{d}}{\mathrm{d}r}(r\mathcal{J}_l(pr))\,\mathrm{d}r\right). \tag{A1.9}$$

Thus

$$\frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}p}(p^2+\alpha^2)\frac{\mathrm{d}}{\mathrm{d}p}(p^2+\alpha^2)\chi_l - l(l+1)\frac{(p^2+\alpha^2)^2}{p^2}\chi_l + 4b^2\chi_l = W, \tag{A1.10}$$

where W includes the terms within the large parentheses. It remains to be shown that W vanishes for bound states.

Since

$$\int_0^\infty r^2\mathcal{J}_l(pr)\frac{\mathrm{d}}{\mathrm{d}r^2}(r\psi_l)\,\mathrm{d}r$$
$$= \int_0^\infty r\psi_l\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r^2\mathcal{J}_l(pr)) + \left(r^2\mathcal{J}_l(pr)\frac{\mathrm{d}}{\mathrm{d}r}(r\psi_l) - r\psi_l\frac{\mathrm{d}}{\mathrm{d}r}r^2\mathcal{J}_l(pr)\right)\Bigg|_0^\infty, \tag{A1.11}$$

$$W = 2b\int r\psi_l\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r^2\mathcal{J}_l(pr) + 2\frac{\mathrm{d}}{\mathrm{d}r}(r\mathcal{J}_l(pr)) + [l(l+1) - p^2r^2]\mathcal{J}_l(pr)\right)$$
$$+ 2b\left(r^2\mathcal{J}_l(pr)\frac{\mathrm{d}}{\mathrm{d}r}r\psi_l - r\psi_l\frac{\mathrm{d}}{\mathrm{d}r}r^2\mathcal{J}_l(pr)\right)\Bigg|_0^\infty. \tag{A1.12}$$

The first term within large parentheses vanishes because of the differential equation satisfied by $\mathcal{J}_l$, i.e.

$$r^2\,\mathrm{d}^2\mathcal{J}_l/\mathrm{d}r^2 + 2r\,\mathrm{d}\mathcal{J}_l/\mathrm{d}r + [p^2r^2 - l(l+1)]\mathcal{J}_l = 0. \tag{A1.13}$$

Thus

$$W = 2br\left(r\mathcal{J}_l(pr)\frac{\mathrm{d}}{\mathrm{d}r}(r\psi_l) - \psi_l\frac{\mathrm{d}}{\mathrm{d}r}(r^2\mathcal{J}_l)\right)\Big|_0^\infty \tag{A1.14}$$

Since the bound-state wavefunction ψ_l vanishes as $r\to 0$ and $r\to\infty$, W is identically zero for bound states.

Appendix 2

To prove that

$$g_l = \left(\frac{\mathrm{d}}{\mathrm{d}z} - \frac{\alpha l}{b}\cot\frac{\alpha z}{b}\right)g_{l-1} \tag{A2.1}$$

let us first assume that g_{l-1} satisfies equation (31):

$$\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} - \frac{\alpha^2}{b^2}l(l-1)\operatorname{cosec}^2\frac{\alpha z}{b}g_{l-1} = -g_{l-1}. \tag{A2.2}$$

From (A2.1)

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}z^2}g_l &= \frac{\mathrm{d}^2}{\mathrm{d}z^2}\frac{\mathrm{d}}{\mathrm{d}z}g_{l-1} - \frac{\alpha l}{b}\bigg[\cot\frac{\alpha z}{b}\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} + 2\frac{\mathrm{d}g_{l-1}}{\mathrm{d}z}\left(-\frac{\alpha}{b}\operatorname{cosec}^2\frac{\alpha z}{b}\right)\\ &\quad + 2\frac{\alpha^2}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}\cot\frac{\alpha z}{b}g_{l-1}\bigg]\\ &= \frac{\mathrm{d}}{\mathrm{d}z}\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} - \frac{\alpha l}{b}\cot\frac{\alpha z}{b}\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} + 2\frac{\alpha^2 l}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}\frac{\mathrm{d}g_{l-1}}{\mathrm{d}z}\\ &\quad - 2\frac{\alpha^3 l}{b^3}\operatorname{cosec}^2\frac{\alpha z}{b}\cot\frac{\alpha z}{b}g_{l-1}.\end{aligned} \tag{A2.3}$$

(A2.3)

Now consider

$$I = \frac{\mathrm{d}^2 g_l}{\mathrm{d}z^2} + g_l - l(l+1)\frac{\alpha^2}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}g_l. \tag{A2.4}$$

Using (A2.1) again in this equation and re-arranging (A2.4) we obtain

$$\begin{aligned}I &= \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} + g_{l-1} - l(l+1)\frac{\alpha^2}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}g_{l-1}\right)\\ &\quad + \frac{2\alpha^2 l}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}g_{l-1} - \frac{\alpha l}{b}\cot\frac{\alpha z}{b}\\ &= \left(\frac{\mathrm{d}^2 g_{l-1}}{\mathrm{d}z^2} + g_{l-1} - l(l+1)\frac{\alpha^2}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}g_{l-1} + \frac{2\alpha^2 l}{b^2}\operatorname{cosec}^2\frac{\alpha z}{b}g_{l-1}\right).\end{aligned} \tag{A2.5}$$

The terms within large parentheses vanish because of (A2.2); therefore

$$I = 0. \tag{A2.6}$$

We have proved that if g_{l-1} satisfies equation (31), then g_l defined by (A2.1) must also satisfy equation (31). Since g_0 satisfies equation (31) with $l=0$, by recursion g_l defined by (A2.1) is the solution of equation (31).

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