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1987 J. Phys. A: Math. Gen. 20 839

(http://iopscience.iop.org/0305-4470/20/4/019)

J. Phys. A: Math. Gen. **20** (1987) 839-845. Printed in the UK

JWKB method and quasilinearisation

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Received 1 April 1986

Abstract. The eikonal solution of the radial Schrödinger equation for spherically symmetric potentials is treated by the quasilinearisation technique. The first iteration contains all the terms of the full expansion of the eikonal series obtained by Fröman and Fröman but with different coefficients. The strength of the centrifugal potential appropriately modified in each order of approximation is obtained stipulating the proper behaviour of the wavefunction at the origin. It leads to an iterative map which converges very fast due to quadratic convergence of quasilinearisation. The energy eigenvalues for the Coulomb potential are obtained by this technique.

1. Introduction

The radial Schrödinger equation with spherically symmetric potentials can be treated as a one-dimensional problem and JWKB solutions of different orders can be obtained by the method of Fröman and Fröman [1]. The behaviour at the origin of the JWKB wavefunction for different orders when the centrifugal barrier potential is taken to be of the form L^2/r^2 has been fully discussed in the literature [2-4]. It has been found earlier by Langer and Kemble that the first-order solution requires the modification of L^2 being replaced by $(l+\frac{1}{2})^2$ and not by $l(l+1)$. Recently it has been shown [5] that the effective modified value of L^2 can be determined in any order using the Fröman and Fröman series for the logarithmic derivative of the wavefunction and that the effective value of L^2 when all orders are summed is the actual value $l(l+1)$. Their prescription for the determination of L^2 also leads to the correct spectrum of eigenvalues in any order.

Our approach differs from the usual Fröman-Fröman series solution for the logarithmic derivative y of the wavefunction though we start with the usual Riccati equation [1]. We use the quasilinearisation approach to solve the Riccati equation for y. The merit of this method is its quadratic convergence as shown by Bellman and Kalaba [8]. This is explained in a later section. The initial choice of $y_0 = ik$ leads, even in the first order of approximation, to an infinite series of Fröman-Fröman type terms [9] but with different coefficients. For this first iterate, the appropriate value of L^2 is already close to $l(l+1)$. The second stage of iteration leads to an iterative map for which $(l+1)$ becomes the fixed point when proper behaviour of the wavefunction at the origin is imposed. The correct value of $l(l+1)$ for L^2 is obtained immediately. Calculation of the eigenspectrum can also be achieved by this iterative procedure.

Section 2 deals with the quasilinearisation technique for solving Riccati equations [8]. In § 3 we use this methodology for the case of the Coulomb potential to arrive at the iterative map for the determination of L^2. We derive in § 4 the energy spectra and summarise our discussion in § 5.

0305-4470/87/040839+07$02.50

2. The method of quasilinearisation

In this section we describe the method of quasilinearisation of Bellman and Kalaba [8]. This may also be called the Newton-Raphson-Kantorovich approximation scheme for solving non-linear differential equations.

If we start with the Riccati equation of the type

$$v' + v^2 + p(t)v + q(t) = 0 \tag{2.1}$$

with initial value $v(0) = c$ we can write this equation using the maximum operation procedure as

$$v' = -\max_{v_0}(2vv_0 - v_0^2) - p(t)v - q(t) \tag{2.2}$$

with $v_0(0) = v(0) = c$.

Let us take the auxiliary linear equation

$$w' = v_0^2 - 2v_0 w - p(t)w - q(t) \qquad \text{with } w(0) = c. \tag{2.3}$$

It can be easily shown that $v \leqslant w$. Having obtained the solution of (2.3) as w, we can use w as the initial assumed value v_0 in equation (2.2) to obtain the next successive approximation. Hence for the nth approximation we obtain the recurrence equation

$$v_n' = v_{n-1}^2 - 2v_n v_{n-1} - p(t)v_n - q(t) \tag{2.4}$$

with $v_n(0) = c$.

It has been shown [11] that the sequence $\{v_n\}$ of approximations possesses monotonicity and quadratic convergence. Hence if our initial guess for v_0 is close enough we can get convergence to the actual value very quickly within two or three iterations as seen from many applications such as 'identification problems' and other types of boundary value problems with non-linearities (as shown in [8]). This method can also be applied with ease for matrix Ricatti equations [13] to find the bounds for the solutions. We apply this method to obtain convergent solutions for the logarithmic derivatives of the radial Schrödinger equation in the following section.

3. Application to radial Schrödinger equations

In this section we treat the reduced radial Schrödinger equation for spherically symmetric potentials by a quasilinearisation technique and investigate the nature of the centrifugal barrier term given the behaviour of the solution near the origin. Corresponding analysis for various orders of JWKB approximation can be found in the literature [2-7].

The radial Schrödinger equation for a spherically symmetric potential is

$$U'' + \lambda^2 k^2 U = 0 \tag{3.1}$$

with

$$\lambda^2 = 2m/\hbar^2 \qquad k^2 = (E - V_{\text{eff}})$$

where

$$V_{\text{eff}} = V(r) + L^2\hbar^2/2mr^2. \tag{3.2}$$

The correct value of L^2 corresponding to the stipulated behaviour of $U \sim r^{l+1}$ near the origin is the main theme of different investigations. We consider potentials which satisfy the requirement $r^2V(r) \to 0$ as $r \to 0$ and k^2 has a single minimum with two turning points.

For solutions of the eikonal form

$$U = A \exp(\lambda S(r)) = A \exp\left(\lambda \int^r y(r')\, dr'\right) \tag{3.3}$$

we find y to satisfy the Riccati equation

$$y' = -\lambda(y^2 + k^2). \tag{3.4}$$

Expanding $y = \sum_{n=0}^{\infty} y_n/\lambda^n$, we get from (3.4) the following recursion relation:

$$\frac{dy_{\nu-1}}{dr} = -\sum_{\mu=0}^{\nu} y_\mu y_{\nu-\mu} \tag{3.5}$$

with $y_0 = \pm ik$. $y_1, y_2, \ldots$, can be easily obtained as

$$y_0 = \pm ik \qquad y_1 = -\frac{k'}{2k} \qquad y_2 = \pm\frac{1}{2ik}\left(\frac{k''}{2k} - \frac{3k'^2}{4k^2}\right) \qquad \text{etc.} \tag{3.6}$$

We stipulate that $U \sim r^{l+1}$ as $r \to 0$ and U vanishes as $r \to \infty$. For the familiar JWKB solution, i.e. $y = y_0 + y_1 = (ik - k'/2k)$, r^{l+1} behaviour of the solution results if $L^2 = (l+\frac{1}{2})^2$. A similar analysis for series summed up to a finite number of higher-order terms [2-4] has been carried out. It was recently demonstrated [5] that if all orders are summed the proper value of $L^2 = l(l+1)$ is recovered. To apply the quasilinearisation technique we first rewrite (3.4) after the transformation $dx = \lambda\, dr$ as

$$y' + y^2 + k^2 = 0 \tag{3.7}$$

with the initial condition $y(x_0) = ik(x_0)$. This is the same type of Riccati equation as (2.1) with $p = 0$ and $q = k^2$. Hence using the quasilinearisation technique we obtain the set of recurrence differential equations

$$y'_{p+1} = y_p^2 - 2y_p y_{p+1} - k^2 \qquad \text{with } y_{p+1}(x_0) = ik(x_0). \tag{3.8}$$

Starting with the initial approximation $y_0(x) = ik(x)$, we obtain for $p = 1$, $y'_1 = y_0^2 - 2y_0y_1 - k^2$ with $y_1(x_0) = y_0(x_0) = ik(x_0)$, a constant, i.e.

$$y'_1 = -2k^2 - 2 iky_1. \tag{3.9}$$

We can easily integrate (3.9) and obtain y_1 as

$$y_1(x) = y_1(x_0) \exp\left(-2i\int_{x_0}^{x} k(x')\, dx'\right) - 2\int_{x_0}^{x} ds\, k^2(s) \exp\left(-2i\int_s^x k(t)\, dt\right). \tag{3.10}$$

Integrating the second term in (3.10) by parts leads to

$$y_1(x) = ik(x) - i\int_{x_0}^{x} ds\, k'(s) \exp\left(-2i\int_s^x k(t)\, dt\right). \tag{3.11}$$

Successive integrated parts of (3.11) lead to the series

$$y_1(x) = ik(x) - \frac{k'}{2k} + \frac{1}{2ik}\left(\frac{k''}{2k} - \frac{k'^2}{k^2}\right) + \frac{1}{8k}\left(\frac{k'''}{k^2} - \frac{4k''k'}{k^3} + \frac{3k'^2}{k^4}\right) + \ldots$$

$$= \sum_{n=0}^{\infty} \mathscr{L}_n^{(1)}. \tag{3.12}$$

The terms $\mathscr{L}_n^{(1)}$ satisfy [9]

$$\mathscr{L}_n^{(1)} = \frac{1}{2ik}\frac{d}{dx}(-\mathscr{L}_{n-1}^{(1)}) \qquad \text{with } \mathscr{L}_0^{(1)} = ik. \tag{3.13}$$

It is important to note that the first iterate y_1 itself is an infinite series similar to the usual WKB series [1] though not identical. Besides being a better approximation, the first iterate y_1 is also expressible in a closed integral form. For iterate of any order p, we can write

$$y_p = \sum_{n=0}^{\infty} \mathscr{L}_n^{(p)} \tag{3.14}$$

and $\mathscr{L}_n^{(p)}$ can be obtained recursively since

$$\mathscr{L}_n^{(p)} = \frac{1}{2y_{p-1}}\frac{d}{dx}(-\mathscr{L}_{n-1}^{(p)}) \qquad \text{with } \mathscr{L}_0^{(p)} = \frac{y_{p-1}^2 - k^2}{2y_{p-1}}. \tag{3.15}$$

In the integral form

$$y_p(x) = \frac{y_{p-1}^2(x) - k^2(x)}{2y_{p-1}(x)} - \int_{x_0}^{x} ds \frac{d}{ds}\left(\frac{y_{p-1}^2(s) - k^2(s)}{2y_{p-1}(s)}\right) \exp\left(-2\int_s^x y_{p-1}(t)\,dt\right). \tag{3.16}$$

Equation (3.14) and hence (3.16) is equivalent to summing a certain class of diagrams for the given potential. For $p = 1$ the first few terms of the series (3.12) can be computed explicitly for the Coulomb potential as

$$\begin{aligned} \mathscr{L}_0^{(1)} &= \frac{iP}{x} \qquad \mathscr{L}_1^{(1)} = \frac{1}{2P^2}\left(\frac{\lambda e^2}{2} - \frac{L^2}{x}\right) \\ \mathscr{L}_2^{(1)} &= \frac{1}{4iP^5}\left[E\lambda e^2 x^2 - \left(3EL^2 + \frac{\lambda^2 e^4}{2}\right)x - 2L^2\lambda e^2 + \frac{L^4}{x}\right] \end{aligned} \tag{3.17}$$

where $P = (Ex^2 + \lambda e^2 x - L^2)^{1/2}$.

In general for an arbitrary n we can write

$$\mathscr{L}_n^{(1)} = i^n 2^{1-n} P^{(4-3n)}\left(\frac{A_{n,-1}}{x} + \sum_{k=0}^{2(n-2)} A_{n,k} x^k\right) \qquad \text{with } A_{n,-1} = L^{2(n-1)}. \tag{3.18}$$

It is to be noted that $y_1 = \Sigma\, \mathscr{L}_n^{(1)}$ has no zero even though each $\mathscr{L}_n^{(1)}$ may have zeros. However, y_1 has branch points and/or singularities at zeros of P corresponding to the classical turning points and a simple pole at $x = 0$. All higher iterates y_p also have the same structure.

4. Determination of the appropriate values of L^2 in every order

In this section we analyse the nature of iterates y_p obtained by quasilinearisation and determine the appropriate value of L^2 of the centrifugal barrier that would guarantee the stipulated behaviour of y_p at the origin, namely $y_p \sim (l+1)/x$ as $x \to 0$ for every p.

From equation (3.17) it is easy to see that

$$\mathscr{L}_n^{(1)} \underset{x\to 0}{\sim} \frac{A_{n,-1}}{x} i^n 2^{1-n}(-L^2)^{(4-3n)/2} \tag{4.1}$$

where $A_{n,-1} = L^{2(n-1)}$. Hence

$$y_1 \underset{x\to 0}{\sim} \frac{1}{x} 2L^2 \sum_{n=1}^{\infty} (-1)^n \left(\frac{1}{2L}\right)^n. \tag{4.2}$$

Summing the series, (4.2) predicts the behaviour of y_1 as

$$y_1 \sim f_1/x \qquad \text{where } f_1 = -2L^2/(2L+1). \tag{4.3}$$

Successively iterating (4.3) by substitution in (3.15) we can obtain the behaviour of the pth-order iterate y_p near the origin. If y_{p-1} behaves as f_{p-1}/x then from (3.15) and (3.14) it can be seen that y_p behaves as

$$y_p \sim \frac{f_p}{x} = \left(\frac{f_{p-1}^2 + L^2}{2f_{p-1} - 1}\right)\frac{1}{x}. \tag{4.4}$$

The same result can also be obtained rather easily (as shown in the appendix) by carrying out the integral (3.16) after substituting $y_{p-1} \sim f_{p-1}/x$. Hence the coefficient of $1/x$ in successive orders is given by the functional equation

$$f_p = \frac{f_{p-1}^2 + L^2}{2f_{p-1} - 1} \tag{4.5}$$

(with the initial value $f_0 = -L$). This is an iterative map and for high iterates we can replace (4.5) by

$$F = \frac{F^2 + L^2}{2F - 1} \qquad \text{or} \qquad F(F-1) = L^2. \tag{4.6}$$

Since $F = l+1$ is a fixed point of the iterative map we obtain the value of L^2 as

$$L^2 = l(l+1). \tag{4.7}$$

It is worth noting that we need not consider high iterates to obtain the value of $L^2 = l(l+1)$. Even f_2 given by

$$f_2 = \frac{f_1^2 + L^2}{2f_1 - 1}$$

leads to the solution $L^2 = l(l+1)$ if we recognise that both f_1 and f_2 should have the value $l+1$ in order to have the stipulated behaviour near the origin. Thus quasilinearisation leads elegantly to the correct solution even at the second stage of iteration. Also from (4.6), the straightforward solution for F is

$$F = \tfrac{1}{2} + L(1 + 1/4L^2)^{1/2}$$

as was obtained by Seetharaman and Vasan.

5. Energy eigenvalues

It will be our aim in this section to compute the energy of the bound states using the usual Sommerfeld quantisation condition. Corresponding to our solution of U in (3.3) the quantisation condition is

$$\oint y(x)\, \mathrm{d}x = 2\pi \mathrm{i} n_r = I \tag{5.1}$$

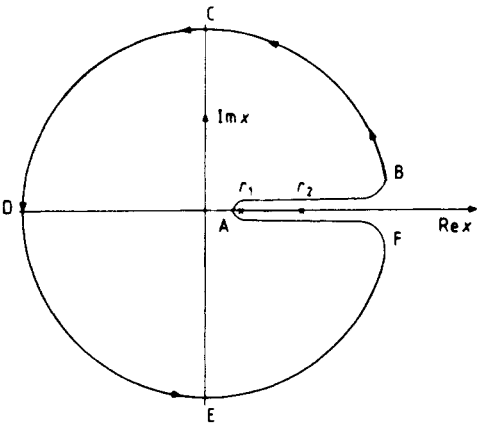

Figure 1.

n_r being the radial quantum number and the contour is going round the branch cut connecting the two turning points at $x = r_1$ and r_2 which are the zeros of k^2 in the complex x plane. The singularity structure of y as was discussed in § 3 consists of a simple pole at the origin and two branch points on the real axis. To evaluate the integral in (5.1) we adopt the familiar technique of integration in the complex x plane along the contour ABCDEFA shown in figure 1. Hence

$$I = -2\pi i \text{ residue at } x = 0 + \oint_\Gamma y(x)\,dx \tag{5.2}$$

where Γ is a circle of very large radius R. The residue of y_p at $x = 0$ is just f_p (i.e. the coefficient of the $1/x$ term). For large x, y behaves as ik for the Coulomb case as can be seen either from the series $\Sigma\, \mathscr{L}_n^{(p)}$ in which the dominant term is ik or from the differential equation itself. Hence, we have for large x, $y_p \sim i\sqrt{E}(1+\lambda e^2/2Ex)$ which contributes $-\pi e^2\lambda/\sqrt{E}$ to the integral over Γ. Hence from (5.2)

$$2\pi i n_r + 2\pi i f_p = -\pi\lambda e^2/\sqrt{E}. \tag{5.3}$$

Since in every order f_p is $l+1$ we have for E (using $\lambda^2 = 2m/\hbar^2$)

$$E = -\frac{2me^4\pi^2}{h^2(n_r+l+1)} \tag{5.4}$$

as bound-state eigenvalues of the energy. Equation (5.4) also remains valid for $l = 0$ [12].

6. Conclusion

The method of quasilinearisation used in this work to obtain the eikonal solution to the Schrödinger equation is seen to be very different from the Fröman series approach, and produces infinite series like the Fröman series even at the first stage of iteration. The usefulness of the method is enhanced because an integral form is also available in addition to a series representation for various iterates. We have shown in the

appendix how the powerful integral form can be used to bypass the series method to obtain the iterated map for f_p. For the Coulomb potential the iterated map leads to the actual value of L^2 at the second stage of iteration itself. The results obtained with regard to the appropriate value of L^2 are valid for any spherically symmetric potential, such as an isotropic quartic oscillator for instance, so long as the potential satisfies the condition $r^2v(r)\to 0$ as $r\to 0$. Energy eigenvalues for the Coulomb potential could easily be obtained from the semiclassical quantisation condition. For the quartic oscillator also energy eigenvalues can be calculated using well known methods [6, 7] either from the series (3.12) or its integral represenation (3.16). Application of the method of quasilinearisation to other potentials is in progress.

Appendix

In this appendix we will illustrate the usefulness of the integral form (3.16). The iterated map (4.5) can be easily obtained using (3.16). Substituting $y_{p-1}\sim f_{p-1}/x$ and $k^2\sim -L^2/x$ (for $x\to 0$) in (3.16) we obtain

$$y_p(x) \underset{x\to 0}{\sim} \frac{f_{p-1}^2+L^2}{2f_{p-1}}\left[\frac{1}{x}-\int_{x_0}^{x} \mathrm{d}s \frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{1}{s}\right)\left(\frac{s}{x}\right)^{2f_{p-1}}\right] \tag{A1}$$

where we have used

$$\exp\left(-2\int_s^x y_{p-1}(t)\,\mathrm{d}t\right)=\left(\frac{s}{x}\right)^{2f_{p-1}}$$

i.e.

$$y_p(x)\sim\frac{f_{p-1}^2+L^2}{2f_{p-1}}\left(\frac{1}{x}+\frac{1}{x^{2f_{p-1}}}\int_{x_0}^{x} \mathrm{d}s\, s^{2f_{p-1}-2}\right). \tag{A2}$$

Evaluating the integral and setting the lower limit $x_0=0$, we obtain

$$y_p(x)=\frac{f_{p-1}^2+L^2}{2f_{p-1}}\left(\frac{1}{x}+\frac{1}{2f_{p-1}-1}\frac{1}{x}\right)=\frac{f_{p-1}^2+L^2}{2f_{p-1}-1}\frac{1}{x}=\frac{f_p}{x}. \tag{A3}$$

Hence the iterated map (4.5) holds as found by this integral representation and yields the correct result for L^2.

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