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Application of continued fractions to bound state and scattering problems

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Abstract. The logarithmic derivative of the wavefunction has been put in the form of an infinite continued fraction by the repeated use of successive differentiations of the Schrödinger equation. The eigenvalues and eigenfunctions for bound states have been obtained either by terminating or by a suitable procedure of summing the infinite continued fraction. Various examples have been considered. For scattering problems the relevant Jost function has been calculated from the various convergents of the continued fraction. The resemblance of the procedure to the Padé approximants has been noted. Our results on phase-shift calculation have been compared with those obtained by other means.

1. Introduction

Various approximation techniques to solve the Schrödinger equation for quantum-mechanical problems have been developed. The perturbation method was the first to be used and is now well known. This method is equally suitable for the study of both bound state and scattering problems. In addition to this, the Fredholm solution (Jost and Pais 1951) to the equivalent Schrödinger equation in an integral form is sometimes found useful. This method is essentially an analytic continuation of the usual Born perturbation series. Recently there have been many attempts to improve upon the standard perturbation method. The main concern in all these approaches has been to obtain a quicker and more convergent summation procedure. Of these, mention must be made of the determinantal techniques used by Baker (1958) and Blankenbecler *et al* (1960) in connection with the solution of the integral equation of the D function of the N/D method of solution of the dispersion integral relations. Among the other existing methods we must emphasize the factorization technique (Infeld and Hull 1951, Morse and Feshback 1953) originally due to Schrödinger. The method essentially consists of constructing a series of ladder operators similar to those of the creation and annihilation operators of quantum mechanics for the harmonic oscillator case. It is also significant because it generates a group structure satisfying a suitable algebra for the ladder operators. In fact the list of the approximation techniques so far developed is quite an inexhaustive one. To complete this brief summary, we would like to mention a recent nonperturbative method proposed in the literature by Biswas *et al* (1971) based on the infinite Hill determinant. The efficiency of this method is amply justified by applying the method to calculate the eigenvalue of the one dimensional λx^{2m} anharmonic oscillator problem. The most interesting part of the work lies in the fact that the various Padé approximants of the perturbation series for the energy eigenvalue problem of the λx^{2m} oscillator do sum closely to the exact values obtained by the Hill determinant technique.

It is well known that the relevant perturbation series mentioned above is a divergent one and various Padé approximants are just the approximation of the series by rational fractions (Baker 1965). In this connection we would like to point out how a continued fraction technique can be developed directly on the Schrödinger differential equation itself to determine the energy eigenvalues and scattering phase shifts in a given problem. The similarity of the present method with the Padé approximants is obvious. The various successive convergents to the infinite continued fraction closely resemble the various Padé approximants to the relevant problem. To illustrate our method, let us consider the normal harmonic oscillator eigenvalue problem.

The Hamiltonian for the problem is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad (1.1)$$

leading to the following differential equation $H\psi = E\psi$ for the energy spectra. This reduces, with the definitions

$$\psi = \exp(-\frac{1}{2}x^2)f, \quad \xi = \left(\frac{m\omega}{\hbar}\right)^{1/2}, \quad \epsilon = \frac{2E}{\hbar\omega},$$

to

$$f'' - 2\xi f' + (\epsilon - 1)f = 0. \quad (1.2)$$

Equation (1.2) can be written as

$$\frac{f'}{f} = \frac{1 - \epsilon}{-2\xi + f''/f'} \quad (1.3)$$

on differentiating (1.2) we have

$$\frac{f''}{f'} = \frac{3 - \epsilon}{-2\xi + f'''/f''} \quad (1.4)$$

continuing this process and finally substituting these back in (1.3), we have the following infinite continued fraction as the solution:

$$\frac{f'}{f} = \frac{1 - \epsilon}{-2\xi + \frac{3 - \epsilon}{-2\xi + \dots}} \quad (1.5)$$

It is interesting to note that the continued fraction (1.5) terminates when $\epsilon = 2n + 1$, $n = 0, 1, 2, \dots$, and then the corresponding wavefunctions are easily found to be

$$f_0 = 1, \quad f_1 = 2\xi, \quad f_2 = 2\xi^2 - 1, \dots$$

It is trivial to recognize that these are the usual Hermite polynomial solutions to the harmonic oscillator problem with the accepted energy eigenvalues. To see rigorously that the n th eigenfunction is

$$\psi_n(\xi) = H_n(\xi) \exp(-\frac{1}{2}\xi^2),$$

we note from (1.5) that for the n th eigenvalue we must have

$$\frac{f'_n}{f_n} = \frac{-2n}{-2\xi + \frac{-2n+2}{-2\xi + \dots}} = \frac{F'}{F} \quad (\text{say}).$$

Hence for $n + 1$, we have

$$\frac{f'_{n+1}}{f_{n+1}} = \frac{-2n-2}{-2\xi + \frac{2n}{-2\xi + \dots}} = \frac{-2n-2}{-2\xi + F'/F}$$

Thus the consistency requirement suggests that

$$\frac{d}{d\xi}(-2\xi F + F') = (-2n-2)F$$

or

$$F'' - 2\xi F' + 2nF = 0$$

which is just the equation for the n th Hermite polynomial.

In the next section we illustrate further our method to discuss the hydrogen atom problem and bound state eigenvalues for an S wave exponential case. In § 3 we generalize our method to the determination of the phase shift in the scattering problem. The efficiency of our method has been shown by comparing our calculations of a few convergents to the exact results already available. For the purpose of comparison of the phase shifts, we have chosen the exactly solvable potential model of Bhattacharjie and Sudarshan (1962).

2. Hydrogen atom and other solvable potentials

In this section we continue our discussion on the use of the continued fraction technique by applying the method to a few solvable problems. In the last section we only mentioned the case of a one-dimensional harmonic oscillator. Below, we consider the hydrogen atom problem, the exponential and Hulthen's potential and finally the three-dimensional isotropic harmonic oscillator problem (Schiff 1968). The equation to be solved is,

$$(\nabla^2 + V)\psi = E\psi \quad (2.1)$$

where V is the central potential, and $\hbar = 2m = 1$. Writing $\psi = U(r)Y_{lm}(\theta, \phi)/r$, we have the equation for U as

$$U'' + \left(E - V - \frac{l(l+1)}{r^2}\right)U = 0. \quad (2.2)$$

Introducing the variable $\rho = \chi r$, $\chi = \sqrt{-E}$ and

$$U(r) = \rho^{l+1} e^{-\rho} v(\rho),$$

we have

$$v'' + 2\left(\frac{l+1}{\rho} - 1\right)v' + \left(\frac{V}{E} - \frac{2(l+1)}{\rho}\right)v = 0. \quad (2.3)$$

2.1. Hydrogen atom problem

$$V(r) = -\frac{Ze^2}{r} \quad (2.4)$$

then equation (2.3) becomes

$$\rho' \frac{d^2 v}{d\rho'^2} + (2l+2-\rho') \frac{dv}{d\rho'} + \{n-(l+1)\}v = 0$$

where

$$n = \frac{Ze^2}{2\chi}, \quad \rho' = 2\rho. \quad (2.5)$$

The solution of equation (2.5) is given by

$$\frac{v'}{v} = \frac{-n+l+1}{(2l+2-\rho') + \frac{\rho'(-n+l+2)}{(2l+3-\rho') + \dots}}. \quad (2.6)$$

The continued fraction (2.6) terminates when

$$n = l + n_r + 1, \quad n_r = 0, 1, 2, \dots$$

This gives

$$E = -\frac{Z^2 e^4}{4(n_r + l + 1)^2}. \quad (2.7)$$

The corresponding wavefunctions are

$$v_0 = 1, \quad v_1 = 2l+2-\rho', \quad v_2 = \rho'^2 - 2\rho'(2l+3) + (2l+3)(2l+2), \dots$$

or in general,

$$v_{n_r} = \frac{1}{(2l+1)} {}_1F_1(-n_r, 2l+2, \rho') \prod_{m=0}^{n_r} (2l+m+1), \quad (2.8)$$

where ${}_1F_1$ is the confluent hypergeometric function and it is connected with the associated Laguerre polynomial $L_{n_r-1}^{2l+1}(\rho')$. Hence we have completely solved the hydrogen atom problem.

2.2. Exponential potential

$$V(r) = -A \exp(-r/a). \quad (2.9)$$

The radial Schrödinger equation for $l = 0$ for the potential (2.9) is

$$\frac{d^2 U}{dr^2} + \{E + A \exp(-r/a)\}U = 0. \quad (2.10)$$

Putting

$$U = e^{-\rho} v(\rho), \quad \rho = \chi r, \quad \chi = \sqrt{-E}$$

and introducing the variable $\xi = \exp(-\rho/2\chi a)$, we obtain

$$\frac{d^2 v}{d\xi^2} + \frac{b}{\xi} \frac{dv}{d\xi} + c^2 v = 0 \quad (2.11)$$

where $b = 1 + 4\chi a$, $c^2 = 4a^2 A$. To solve (2.11), we put

$$v(\xi) = \exp(-ic\xi)X(\xi), \quad \xi = \frac{x}{2ic}.$$

Then we get

$$x \frac{d^2 X}{dx^2} + (b-x) \frac{dX}{dx} - \frac{b}{2} X = 0. \tag{2.12}$$

The solution is

$$\frac{X'}{X} = \frac{\frac{1}{2}b}{(b-x) + \frac{x(\frac{1}{2}b+1)}{(b-x+1) + \dots}}. \tag{2.13}$$

The above continued fraction terminates when

$$\frac{1}{2}b = -n, \quad n = 0, 1, 2, \dots$$

This gives the energy eigenvalues

$$E = -\frac{(2n+1)^2}{16a^2}.$$

To show that the wavefunction is the Bessel function, we rewrite equation (2.13) as

$$\frac{X'_n}{X_n} = \frac{-n}{(b-x) + \frac{(-n+1)}{(b-x-1) + \dots}}.$$

This gives,

$$X_n = \frac{(b+n-1)!}{(b-1)!} {}_1F_1(-n, b; x)$$

collecting all these, we find that

$$U \sim e^{-xr} e^{-ic\xi} {}_1F_1(-n, -2n; 2ic\xi)$$

where

$$\xi = \exp(-r/2a).$$

Using Kummer's relation (see, eg Watson 1944)

$$e^{-cz} {}_1F_1(-p, -2p, 2cz) = {}_0F_1(\frac{1}{2}-p, \frac{1}{4}c^2 z^2),$$

and the result

$$J_\nu(z) = \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} {}_0F_1(\nu+1, -\frac{1}{4}z^2)$$

it is easy to see that

$$U \sim J_k(c\xi) = J_k(2a\sqrt{A} \exp(-r/2a))$$

where

$$k^2 = -4a^2 E > 0 \quad \text{for } E < 0. \tag{2.14}$$

2.3. Hulthen's potential ($l = 0$)

$$V(r) = \frac{-\lambda\mu e^{-\mu r}}{1 - e^{-\mu r}}. \quad (2.15)$$

The equation to be solved is

$$\frac{d^2U}{dr^2} + \left(k^2 + \frac{\lambda\mu e^{-\mu r}}{1 - e^{-\mu r}} \right) U = 0 \quad (2.16)$$

for this, we make the transformation,

$$U = e^{-ikr}g(r), \quad z = e^{-\mu r}$$

and get the equation

$$z(1-z)g'' + \{c - (a+b+1)z\}g' - abg = 0 \quad (2.17)$$

where a, b, c are given by

$$\begin{aligned} a &= \frac{ik}{\mu} + \frac{\sqrt{(-k^2 + \lambda\mu)}}{\mu} \\ b &= \frac{ik}{\mu} - \frac{\sqrt{(-k^2 + \lambda\mu)}}{\mu} \\ c &= 1 + \frac{2ki}{\mu}. \end{aligned} \quad (2.18)$$

The solution of (2.17) in the form of a continued fraction is given by

$$\frac{g'}{g} = \frac{ab}{\{c - (a+b+1)z\} + \frac{z(1-z)\{ab + (a+b+1)\}}{\{c+1 - (a+b+3)z\} + \dots}}. \quad (2.19)$$

The continued fraction (2.19) terminates when a or b is a negative integer, that is,

$$n = -a, -b \quad n = 0, 1, 2, \dots$$

and, therefore, the energy eigenvalues are given by

$$E = k^2 = -\frac{1}{4n^2}(\lambda - n^2\mu)^2.$$

To show that the solution of (2.19) is a hypergeometric function, we rewrite (2.19) as,

$$\frac{g'_n}{g_n} = \frac{-n(a+b+n)}{\{c - (a+b+1)z\} + \frac{z(1-z)\{-n(a+b+n) + (a+b+1)\}}{\{c+1 - (a+b+3)z\} + \dots}} \quad (2.20)$$

then it is easy to see that

$$g_n = \frac{(c+n-1)!}{(c-1)!} {}_2F_1(a, b, c; z).$$

2.4. Three-dimensional isotropic harmonic oscillator

$$V(r) = \frac{1}{2}\mu\omega^2 r^2.$$

The radial part of the Schrödinger equation for the three-dimensional isotropic harmonic oscillator is

$$U'' + \left(k^2 - \lambda^2 r^2 - \frac{l(l+1)}{r^2} \right) U = 0 \quad (2.21)$$

where

$$U = Rr, \quad \lambda = \mu\omega, \quad k^2 = 2\mu E; \quad \hbar = 1.$$

Putting $U = r^{l+1} \exp(-\frac{1}{2}\lambda r^2)W(r)$ and introducing the variable $\xi = \lambda r^2$, we obtain

$$\xi W'' + \left\{ \left(l + \frac{3}{2} \right) - \xi \right\} W' - \left\{ \frac{1}{2} \left(l + \frac{3}{2} \right) - \frac{1}{2} s \right\} W = 0 \quad (2.22)$$

where $s = k^2/2\lambda = E/\omega$.

The continued fraction development for the above equation gives,

$$\frac{W'}{W} = \frac{\left\{ \frac{1}{2} \left(l + \frac{3}{2} \right) - \frac{1}{2} s \right\}}{\left(l + \frac{3}{2} - \xi \right) + \frac{\xi \left\{ \frac{1}{2} \left(l + \frac{3}{2} \right) + 1 - \frac{1}{2} s \right\}}{\left\{ \left(l + \frac{3}{2} + 1 \right) - \xi \right\} + \dots}} \quad (2.23)$$

This gives the energy spectrum for the three-dimensional harmonic oscillator as,

$$E = \omega \left(l + \frac{3}{2} + 2n_r \right), \quad n_r = 0, 1, 2, \dots$$

and the wavefunction is

$$\psi_{n_r, l, m} = C_{n_r, l, m} r^l \exp(-\frac{1}{2}\lambda r^2) {}_1F_1(-n_r, l + \frac{3}{2}, \lambda r^2) Y_{lm}(\theta, \phi).$$

3. Scattering problem

To apply our method to calculate the phase shift for potential scattering, we follow Bargmann (1949). Accordingly we put $g(k, r) = e^{ikr}f(k, r)$ where $f(\pm k, r)$ are two independent solutions of the usual radial Schrödinger equation (for S wave) which are defined by their asymptotic behaviour for large r , namely,

$$\lim_{r \rightarrow \infty} e^{\pm ikr} f(\pm k, r) = i.$$

The equation for $g(k, r)$ is then given by

$$g'' - 2kig' = V(r)g \quad (3.1)$$

where

$$\lim_{r \rightarrow \infty} g(k, r) \rightarrow 1$$

for every real nonvanishing k . It is now easy to connect the phase shift through the expression

$$S(k) = e^{2i\delta(k)} = \frac{f(k)}{f(-k)} \quad (3.2)$$

where

$$f(k) \equiv f(k, r = 0).$$

To find $f(k)$ we use the continued fraction development for $g'(k, r)/g(k, r)$. Writing $X = g'(k, r)/g(k, r)$, we have (Ince 1956)

$$X = \frac{1}{Q_0 + \frac{P_1}{Q_1 + \frac{P_2}{Q_2 + \dots}}} \quad (3.3)$$

where

$$Q_0 = -\frac{2ki}{V(r)}, \quad P_1 = \frac{1}{V(r)}$$

and

$$Q_n = \frac{Q_{n-1} + P'_n}{1 - Q'_{n-1}}, \quad P_{n+1} = \frac{P_n}{1 - Q'_{n-1}}.$$

Rewriting (3.3) in the form

$$X = a_1 + \frac{b_2}{a_2 + \frac{b_3}{a_3 + \dots + \frac{b_n}{a_n}}} \quad (3.4)$$

We find that $a_1 = 0$, $a_2 = Q_0, \dots, a_n = Q_{n-2}$, $b_2 = 1$, $b_3 = P_1, \dots, b_n = P_{n-2}$. If $p_n/q_n, p_{n-1}/q_{n-1}, p_{n-2}/q_{n-2}$ are the n th, $(n-1)$ th and $(n-2)$ th convergents of the infinite continued fraction X . Then

$$X = \frac{p_n}{q_n} = \frac{a_n p_{n-1} + b_n p_{n-2}}{a_n q_{n-1} + b_n q_{n-2}} \quad (3.5)$$

We can then write

$$\begin{pmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{pmatrix} = \begin{pmatrix} p_{n-1} & p_{n-2} \\ q_{n-1} & q_{n-2} \end{pmatrix} \begin{pmatrix} a_n & 1 \\ b_n & 0 \end{pmatrix}$$

using the matrix recurrence relation we easily find that

$$\begin{aligned} \begin{pmatrix} p_n & p_{n-1} \\ q_n & q_{n-1} \end{pmatrix} &= \begin{pmatrix} a_1 & 1 \\ b_1 & 0 \end{pmatrix} \begin{pmatrix} a_2 & 1 \\ b_2 & 0 \end{pmatrix} \dots \begin{pmatrix} a_n & 1 \\ b_n & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} Q_0 & 1 \\ 1 & 0 \end{pmatrix} \dots \begin{pmatrix} Q_{n-2} & 1 \\ P_{n-2} & 0 \end{pmatrix}. \end{aligned} \quad (3.6)$$

The equation (3.6) is a crucial formula for our further numerical analysis.

To obtain the phase shifts we need the following recurrence relations:

$$\begin{aligned} Q_s^n &= \frac{Q_{s-1}^n + P_s^{n+1} + \sum_{j=0}^{n-1} {}^n C_j Q_{s-1}^{n+1-j} Q_s^j}{1 - Q'_{s-1}} \\ P_{s+1}^n &= \frac{P_s^n + \sum_{j=0}^{n-1} {}^n C_j Q_{s-1}^{n+1-j} P_{s+1}^j}{1 - Q'_{s-1}} \end{aligned}$$

where $Q_s^n = d^n Q_s / dr^n$ etc. Then using all these results we can easily obtain the phase

shifts. From equations (3.4), (3.5) and (3.6) we have for $f(k, r = 0)$ in the n th convergent

$$f(k) = \exp \left\{ - \int_0^\infty \left(\frac{p_n}{q_n} \right)_{k,r} dr \right\}. \tag{3.7}$$

We notice from equation (3.7) that various convergents for $f(k)$ are rational fractions, which closely resemble various Padé approximants.

If the continued fraction is convergent, then in the limit $n \rightarrow \infty$ we get the exact answer for our phase shift. The necessary and sufficient condition for the convergence of the continued fraction is given by a theorem due to Perron (see eg Ince 1956, Wall 1948) which states that the continued fraction converges and has the value f'/f if $f \neq 0$ and (i) $P_n \rightarrow P, Q_n \rightarrow Q$ as $n \rightarrow \infty$, (ii) the roots ρ_1 and ρ_2 of the equation $\rho^2 = Q\rho + P$ are of unequal modulus and (iii) if $|\rho_2| < |\rho_1|$ then

$$\lim |f^{(n)}|^{1/n} < |\rho_2|^{-1}$$

provided that $|\rho_2| \neq 0$. When $|\rho_2| = 0$ the last condition is replaced by the condition that the limit is finite.

To see the efficiency of our method, we first discuss a few solvable cases. For the exponential potential and some other solvable potentials proposed by Bhattacharjie and Sudarshan (1962), we find that the first few convergents almost lead to the exact answers. We tabulate below the calculations of the phase shifts for a few cases of known solvable potentials. The convergence of our calculations is remarkable.

Table 1. The phase shift of scattering from the exponential potential $V(r) = -\lambda e^{-r}$. δ_s represents the phase shift calculated by the Sasakawa (1963) model. The numbers in brackets denote the approximations of the continued fraction method.

$k \backslash \lambda$		0.5	1.0	1.5	2.0	2.5
1.0	δ_{CF}	0.201(10)	0.434(10)	0.638(10)	0.804(10)	0.981(10)
	δ_s	0.200	0.399	0.593	0.782	0.962
1.5	δ_{CF}	0.149(9)	0.295(8)	0.439(9)	0.579(9)	0.715(9)
	δ_s	0.144	0.277	0.398	0.509	0.614
2.0	δ_{CF}	0.117(6)	0.231(7)	0.344(7)	0.455(8)	0.564(8)
	δ_s	0.113	0.213	0.302	0.381	0.448
2.5	δ_{CF}	0.096(6)	0.190(5)	0.283(5)	0.375(5)	0.465(5)
	δ_s	0.092	0.174	0.247	0.312	0.362
3.0	δ_{CF}	0.081(5)	0.160(4)	0.239(4)	0.318(5)	0.395(5)
	δ_s	0.078	0.147	0.209	0.266	0.308

Table 2. The phase shift of scattering from the potential $V(r) = -2\alpha^2/\cosh^2 \alpha r$ with $\alpha = 1.0$.

k	$\tan \delta_{CF}$	Exact value (Bhattacharjie and Sudarshan 1962)
1.0	1.032(10)	1.000
1.5	0.668(7)	0.667
2.0	0.500(7)	0.500
2.5	0.400(5)	0.400

Consideration of the present method to various other physical phenomena including the application to the Bethe–Salpeter equation and the Regge trajectory calculation will be reported elsewhere.

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