Comments on a paper concerning the analytic continued fraction technique for bound states

1982 J. Phys. A: Math. Gen. 15 L1

(http://iopscience.iop.org/0305-4470/15/1/001)

J. Phys. A: Math. Gen. 15 (1982) L1–L5. Printed in Great Britain

LETTER TO THE EDITOR

Comments on a paper concerning the analytic continued fraction technique for bound states

George P Flessas
Department of Natural Philosophy, University of Glasgow, Glasgow G12 8QQ, Scotland

Received 19 October 1981

Abstract. We show that the treatment of bound and confined states for a class of confinement potentials by application of the analytic continued fraction method, as presented in a recent paper published here, is erroneous and may lead to wrong results for the eigenvalues of the relevant Schrödinger equation.

Recently Datta and Mukherjee (1980) considered a confining potential of the form

$$V(r) = -a/r + br + cr^2 \qquad c > 0. \tag{1}$$

The corresponding radial Schrödinger equation reads

$$R''(r) + [(2\mu/h^2)(E + a/r - br - cr^2) - l(l+1)/r^2]R(r) = 0. \tag{2}$$

E = energy, l = relative orbital angular momentum. Making the standard transformation

$$R(r) = r^{l+1} \exp(-\tfrac{1}{2}r^2\alpha - \beta r)g(r) \tag{3}$$

we get for $g(r)$ the differential equation

$$g'' + 2[(l+1)/r - \alpha r - \beta]g' + \{\varepsilon - (2l+3)\alpha + [a - 2\beta(l+1)]/r\}g = 0 \tag{4}$$

with

$$\alpha = [(2\mu/h^2)c]^{1/2} \qquad \beta = (2\mu/h^2)^{1/2}(b/c^{1/2}) \tag{5}$$

$$\varepsilon = \beta^2 + e \qquad e = (2\mu/h^2)E. \tag{6}$$

Equation (4) is solved by

$$g(r) = \sum_{n=0}^{\infty} p_n r^n \tag{7}$$

where the p satisfy, with $p_{-1} = 0$,

$$(n+2)(n+2l+3)p_{n+2} + [a - 2\beta(n+l+2)]p_{n+1} + [\varepsilon - (2n+2l+3)\alpha]p_n = 0. \tag{8}$$

Equation (8) can be written as

$$\frac{p_{n+1}}{p_n} = \frac{-[\varepsilon - (2n+2l+3)\alpha]}{-2\beta(n+l+2) + a + (n+2)(n+2l+3)p_{n+2}/p_{n+1}}. \tag{9}$$

Repeated application of equation (9) for $n = 0, 1, 2, 3, \ldots$ gives

$$\frac{p_1}{p_0} = \cfrac{-[\varepsilon-(2l+3)\alpha]}{-2\beta(l+2)+a-\cfrac{2(2l+3)[\varepsilon-(2l+5)\alpha]}{-2\beta(l+3)+a-\cfrac{3(2l+4)[\varepsilon-(2l+7)\alpha]}{-2\beta(l+4)+a-\ddots}}} \tag{10}$$

Finally, using equation (8) we obtain for $n = -1$

$$p_1/p_0 = -[2\beta(l+1)+a]/(2l+2) \tag{11}$$

and consequently equation (10) yields

$$-2\beta(l+1)+a = \cfrac{(2l+2)[\varepsilon-(2l+3)\alpha]}{-2\beta(l+2)+a-\cfrac{2(2l+3)[\varepsilon-(2l+5)\alpha]}{-2\beta(l+3)+a-\ddots}} \tag{12}$$

Equations (11)–(12) can be found also in Datta and Mukherjee's paper but we have repeated them here in order to point out the error in the argument they use regarding equation (12). These authors claim that equation (12) is the 'consistency condition' for the existence of the solution for the system of equations (8), the solutions of (12) in ε or, equivalently, E being the energy eigenvalues for the problem. This is, however, a false statement and totally confusing with respect to the correct eigenvalues, as we shall verify below.

(i) The differential equation (4) can be written as

$$g'' + 2\frac{(l+1-\alpha r^2-\beta r)}{r}g' + \frac{\{[\varepsilon-(2l+3)\alpha]r+a-2\beta(l+1)\}r}{r^2}g = 0. \tag{13}$$

Hence, according to the general theory of linear differential equations (Morse and Feshbach 1953) equation (13) has at $r = 0$ a *regular* singular point and at $r = \infty$ an irregular singular point. The indicial equation of (13) has the roots 0 and $-(2l+1)$. Obviously, owing to equation (3), we must discard $-(2l+1)$. Thus we get equations (7)–(8). Now, from equation (8) we can calculate *recursively any* p_n (cf any textbook on differential equations) and there is no need whatsoever to take account of any 'consistency condition'. What Datta and Mukherjee actually do is using a method described by Morse and Feshbach (1953) in connection with the Mathieu equation. This method is applicable when one has the solution of a differential equation in the form (7) and wishes to prove that the series converges for every r. Then (cf Morse and Feshbach, pp 556–9) in the case of a three-term recurrence relation for the coefficients of the series in question we obtain the equivalent formulae to equations (9)–(12) and the value of the relevant parameter (denoted with s in the case of the Mathieu equation), for which the series is convergent for *all* r, can be calculated from an equation of the type (12). But such a procedure is *absolutely* superfluous here because the series (7), as the differential equation (13), i.e. (4), has no other singularities between 0 and ∞, converges (Morse and Feshbach 1953) for all $r \in [0, \infty)$. Thus the phrase 'consistency condition' used by Datta and Mukherjee in respect of equation (8) is meaningless and the p exist for any E. Moreover, since the series in equation (7) converges for *all* $r \geqslant 0$, we obtain $p_n \to 0$ for $n \to \infty$. It is recalled that the Mathieu equation has an *irregular* singular point at $r = 0$

and so the convergence of the solving series cannot be ascertained otherwise than as described by Morse and Feshbach.

(ii) The statement made in the paper of Datta and Mukherjee that 'equation (3) gives the appropriate asymptotic behaviour of the solution of equation (2)' is wrong. One must investigate the behaviour of $g(r)$ for $r \to \infty$ and examine if it compensates $\exp(-\frac{1}{2}r^2\alpha - \beta r)$ in equation (3), because if this happens, then $\lim_{r\to\infty} R(r) \nrightarrow 0$ which means that such an $R(r)$ is physically unacceptable. This is precisely the well known method adopted in the case of the harmonic oscillator ($a = b = 0$ in equations (1)–(2)) which leads to the familiar Laguerre polynomials. In the case of the potential (1) the correct eigenvalues will be obtained solely from the requirement that $g(r)$ as $r \to \infty$ does *not* compensate $\exp(-\frac{1}{2}r^2\alpha - \beta r)$.

(iii) Equation (12) gives those E values for which the representation of p_1/p_0 by means of the continued fraction (10) is valid. In the case of the Mathieu equation the representation of the corresponding p_1/p_0 as a continued fraction is a sufficient condition, as shown in Morse and Feshbach (1953, pp 557–8), for the convergence of the series solving the Mathieu differential equation, whereas in our case such a condition is completely irrelevant. In no case need the E values calculated from equation (12) be those that ensure that $R(r)$ remains normalisable. Equation (12) gives the correct eigenvalues only in the case of the harmonic oscillator ($a = b = 0$), simply because we get a two-term recursion relation then ($a = b = 0$ in equation (8)) for the p and equation (12) is fulfilled for those E values, for which the series satisfying equation (4) (for $a = b = 0$) terminates. Such a termination, however, of the series in equation (4) in the general case $a \neq 0, b \neq 0$ and for E values derived from equation (12) is not possible. Indeed, by using equation (8) we obtain

$$p_n = \frac{(-1)^n p_0}{n!(2+2l)(3+2l)\dots(n+1+2l)} D_n \qquad D_1 = a - 2\beta(l+1) \qquad n \geqslant 1 \tag{14}$$

$$D_n = \begin{vmatrix} a-2\beta(l+1) & 1(2+2l) & 0 & & \\ \varepsilon-(2.2-1+2l)\alpha & a-2\beta(l+2) & 2(3+2l) & & \\ 0 & \varepsilon-(2.3-1+2l)\alpha & a-2\beta(l+3) & & \\ 0 & 0 & \ddots & \varepsilon-(2n-1+2l)\alpha & a-2\beta(l+n) \\ \vdots & & \ddots & & \end{vmatrix}$$

and consequently the series in equation (7) terminates, say $p_n = 0$ for $n \geqslant N+1$, if and only if, as follows from equations (8) and (14),

$$\varepsilon = (2n + 2l + 3)\alpha \tag{15}$$

$$D_{n+1} = 0. \tag{16}$$

Equations (15)–(16), which are equivalent to those that one obtains for the one-dimensional doubly anharmonic oscillator (Singh *et al* 1980) and for the one-dimensional Schrödinger equation with the potential $x^2 + \lambda x^2/(1+gx^2)$ (Flessas 1981, Whitehead *et al* 1982), show that terminating solutions of equation (4) are possible only if a relation between l, a, b and c holds. This condition is obtained by inserting equation (15) into equation (16) and implies that at least one of the parameters a, b, c becomes l-dependent, a result which contrasts with that of the one-dimensional cases mentioned above. The eigenvalues are given by equation (15).

(iv) From equations (8)–(9) we deduce that for large n, p_{n+1}/p_n behaves like $\pm(2\alpha/n)^{1/2}$. This shows that, as of course is expected from the convergence of

$g(r)$, $(p_{n+1}/p_n)\to 0$ as $n\to\infty$ and that $g(r)$ for large r behaves like either of the series

$$G(r)=\sum_{n=0}^{\infty}\frac{(2\alpha)^{n/2}}{(n!)^{1/2}}r^n \qquad \text{or} \qquad G_1(r)=\sum_{n=0}^{\infty}\frac{(-1)^n(2\alpha)^{n/2}}{(n!)^{1/2}}r^n \tag{17}$$

which converge for $r\in[0,\infty)$. We consider now the first alternative in equation (17). This possibility is realised if all p are positive. Let us for simplicity take the harmonium potential, where $b=0$ in equation (1). Then equation (8) shows that for $a<0$ and $0<\varepsilon<(2l+3)\alpha$ we have $p_n>0$ if $p_0>0$. Further, we compare $G(r)$ with

$$\exp(\tfrac{1}{2}r^2\alpha)=\sum_{n=0}^{\infty}\frac{(\frac{1}{2}\alpha)^n}{n!}r^{2n} \tag{18}$$

by comparing the coefficients of even r powers in $G(r)$ with those of equation (18). Thus it is easily verified that for sufficiently large but *finite n*, say N, the inequality

$$\frac{(2\alpha)^{2n/2}}{((2n)!)^{1/2}}>\frac{(\frac{1}{2}\alpha)^n}{n!} \qquad n\geqslant N \tag{19}$$

is satisfied. Since

$$\exp(\tfrac{1}{2}r^2\alpha)=r^{2N-2}\frac{(\frac{1}{2}\alpha)^{N-1}}{(N-1)!}[1+O(1/r)]+\sum_{n\geqslant N}^{\infty}\frac{(\frac{1}{2}\alpha)^n}{n!}r^{2n} \tag{20}$$

and

$$G(r)=r^{2N-1}\frac{(2\alpha)^{(2N-1)/2}}{[(2N-1)!]^{1/2}}[1+O(1/r)]+\sum_{n\geqslant 2N}^{\infty}\frac{(2\alpha)^{n/2}}{(n!)^{1/2}}r^n \tag{21}$$

equations (19)–(21) verify, as a little thought reveals, that $G(r)$ and, hence, also $g(r)$ compensates $\exp(-\frac{1}{2}r^2\alpha)$ for $r\to\infty$. Therefore if ε fulfils $0<\varepsilon<(2l+3)\alpha$ and $a<0$ then (cf equations (5)–(6)) e with $0<e<(2l+3)\alpha$ cannot be an eigenvalue of equation (2). This important result is totally missed by Datta and Mukherjee (1980) in their treatment of the harmonium potential. One can give other examples with $b\gtreqless 0$, which verify the inadequacy of equation (12) for the calculation of the eigenvalues of equation (2). This was to be expected in view of (i)–(iii).

(v) The method used by Datta and Mukherjee (1980) has been first applied to the study of the $ax^2+bx^4+cx^6$ potential by Singh *et al* (1978). In the paper of Singh *et al* (1978) the relation equivalent to equation (12) is utilised for the calculation of the eigenvalues which are obtained as poles of a 'Green function' constructed from that relation. Datta and Mukherjee's paper proceeds along exactly the same lines. Nowhere in both papers is the basic requirement, that the wavefunction remains normalisable, incorporated into the method. Of course some eigenvalues may still be solutions of equation (12) but in no case need *all* the eigenvalues be *the* solutions of that equation.

To sum up we have verified that the method of Datta and Mukherjee (1980) for the calculation of eigenvalues is based on a mathematically meaningless relation and may thus lead to wrong results for the eigenvalues in question. That procedure should not be used without a proper incorporation into it of the physically important requirement that $R(r)\to 0$ as $r\to\infty$. Thus one may obtain further eigenvalues in addition to those for which the series in equation (7) terminates.

References

Datta D P and Mukherjee S 1980 *J. Phys. A: Math. Gen.* **13** 3161–70
Flessas G P 1981 *Phys. Lett.* **83A** 121–2
Morse P M and Feshbach H 1953 *Methods of Mathematical Physics* (London: McGraw-Hill) p 532
Singh V, Biswas S N and Datta K 1978 *Phys. Rev.* D **18** 1901–8
Singh V, Rampal A, Biswas S N and Datta K 1980 *Lett. Math. Phys.* **4** 131–4
Whitehead R R, Watt A, Flessas G P and Nagarajan M A 1982 *J. Phys. A: Math. Gen.* **15** to be published