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COMMENT

Continued fractions and the potential models of confinement—reply to a comment

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Abstract. The analytic continued-fractional formula for energies of the bound states in the harmonium potential $V(r) = a\,r^{-1} + br + cr^2$, as suggested by Singh *et al* and criticised by Flessas, is correct if and only if $b > 0$. This is the special case of the more general result. We extend here the analytic construction of the Green function and the rigorous specification of its validity to the whole class of potentials with $r^2 V(r) =$ polynomial in r^α, $\alpha =$ positive rational number.

1. Introduction

In a recent letter (1982, referred to as 'Comments' in what follows), George Flessas considers the harmonium potential

$$V(r) = gr^{-2} + ar^{-1} + br + cr^2, \qquad c > 0, \tag{1}$$

and claims that the analytic representation of the related binding energies E by Datta and Mukherjee (1980) is 'based on a ... mathematically meaningless relation' (equation (12) of 'Comments'). We disagree with such a statement. The main purpose of the present paper is to clarify the essence of the method and to show that Datta and Mukherjee's basic relation is in fact related directly to the asymptotic behaviour of the wavefunctions and, when complemented by the 'applicability condition'

$$b > 0, \tag{2}$$

it gives indeed the complete spectrum of the physical bound-state energies. Moreover, we intend to show that equation (1) is just a special case of the fractionally anharmonic oscillator potentials

$$\begin{gathered} V(r) = \sum_{i=1}^{I} g_i r^{\alpha_i}, \\ \alpha_i = \text{rational}, \alpha_i \geqslant -2, \lim_{r\to 0} r^2 V(r) > -\tfrac{1}{4}, I < \infty, \lim_{r\to\infty} V(r) > -\infty, \end{gathered} \tag{3}$$

all of which admit the similar and compact construction of the Green function $G(E)$ in terms of the so-called 'extended' (Znojil 1976, 1983) and convergent continued fractions. Again, an adequate generalisation of the 'applicability' condition (2) (see equation (23) below) must be satisfied.

The material is organised as follows. In the preparatory §2 we reduce the general non-relativistic power-law confinement problem to its canonical form and characterise

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any force (3) by the integers p ('fractionality'), q ('anharmonicity') and t ('subharmonicity')—equation (1)+(2) corresponds to $p=1$, $q=1$ and $t=2$. All the potentials with the same q may be considered equivalent from the formal point of view.

In § 3, we consider any $q \geqslant 1$ and transform the canonical differential Schrödinger equation to the algebraic recurrences by the standard power-series method. In a constructive way we show that this linear system of equations for the expansion (Taylor) coefficients admits the various 'non-Hill-determinant' interpretations of the eigenvalue problem, the 'Hill-determinant' formalism being only the one specified by the simplest choice of an auxiliary sequence F_k. For $q=1$ in particular, this formulation enables us to simplify our earlier proof (Znojil 1982) of the correct asymptotic behaviour of the $q=1$ wavefunctions in the harmonium potential (1)+(2). In § 4 we show how this result may be extended to cover all q but defer the rather complicated details to a separate publication (Znojil 1983).

2. Classification of the power-law potentials

Let us consider first the Coulomb-type forces (3) in the Schrödinger equation

$$[-\mathrm{d}^2/\mathrm{d}r^2 + l(l+1)/r^2 + V(r)]\psi(r) = E\psi(r), \qquad l=0,1,\ldots, \tag{4}$$

i.e. assume that $V(\infty)=0$ and $\max \alpha_i < 0$, $i=1,2,\ldots,I$, in (3). We restrict our attention to the discrete spectrum only, $E<0$, and put $\alpha_i = -2n_i/M$, where n_i are integers, $0<n_i \leqslant M$, and M is the corresponding minimal common denominator. Next, we put $p = M\times T = 2q+2$ ($T=1$ for $M=$ even and $T=2$ for $M=$ odd), introduce the new variables in (4) (cf Quigg and Rosner 1979)

$$r = x^p, \qquad \psi(r) = r^{(1-1/p)/2}\chi(x) \tag{5}$$

and get the new form of the Schrödinger equation

$$[-\mathrm{d}^2/\mathrm{d}x^2 + L(L+1)/x^2 + W(x)]\chi(x) = \varepsilon\chi(x) \tag{6}$$

with the particular (canonical, even) 'polynomially anharmonic' type of potential (3)

$$W(x) = \sum_{j=1}^{2q+1} G_j x^{2j}, \tag{7}$$

$$G_{p-1} = -p^2 E, \qquad G_{p-1-n_iT} = p^2 g_i, \qquad i=1,2,\ldots,I,$$

and with the 'modified' angular momenta L

$$(L+\tfrac{1}{2})^2 = p^2(l+\tfrac{1}{2})^2 + p^2 g_{i_0}, \qquad n_{i_0} = M \tag{8}$$

and reinterpreted couplings ($E \to G_{p-1}$, $G_0 \to$ 'new' energy $\varepsilon = -G_0$).

Let us now remove the restriction $\max \alpha_i < 0$. Provided that some of the n_i are negative, $\min n_i = -N_I < 0$, and that $g_I > 0$, i.e. $V(\infty) = +\infty$, the whole energy spectrum becomes discrete (also in equation (6) where $G_{2q+1} = p^2 g_I > 0$ and $q > (p-2)/2$).

Since the transformation (5) is sufficiently smooth, it preserves the character (regularity in the origin and asymptotic behaviour) of the solutions. Hence, we need not distinguish between different p for the same q—the potentials with $p \leqslant 2q+2$ are all equivalent. Thus, any power-law potential (3) may be classified by the pair of integers q (degree of the polynomial $W(x)$ or 'anharmonicity') and p (exponent in (5) or 'fractionality' of V). For irrational α in (3), we may put $p=q=\infty$. For the superpositions of powers we may introduce also another auxiliary parameter $t \geqslant 0$ such that

$$G_{2q-t} \neq 0, \qquad G_{2q-t+1} = \ldots = G_{2q} = 0. \tag{9}$$

This reflects the asymptotic behaviour of the Coulomb-type V ($p = 2q+2$) and will prove to be useful also for $p < 2q+2$—see below.

A small sample of the 'simplest' potentials is displayed in table 1. Let us notice that the harmonium potential (1) (with $q = 1$ and $p = 2$) appears to be equivalent to the sextic anharmonic oscillator ($q = p = 1$). In connection with the point (i) of 'Comments', we may therefore recall the $q = 1$ results of Singh *et al* (1978, cf also 1979) and Znojil (1982) giving both the compact solution to equation (6) and a rigorous foundation of the 'Hill-determinant' eigenvalue method.

Table 1. The simplest fractionally anharmonic potentials.

q	p	Potential ($a > -1/4$)	Comment
0	1	$ar^{-2} + cr^2$	$c > 0$
	2	$ar^{-2} + br^{-1}$	$E < 0$
1	1	$ar^{-2} + cr^2 + dr^4 + er^6$	$e > 0$
	2	$ar^{-2} + br^{-1} + dr + er^2$	$e > 0$
	3	$ar^{-2} + br^{-4/3} + cr^{-2/3} + er^{2/3}$	$e > 0$
	4	$ar^{-2} + br^{-3/2} + cr^{-1} + dr^{-1/2}$	$E < 0$
2	1	$\ldots + er^6 + fr^8 + gr^{10}$	$g > 0$
	2	$\ldots + er^2 + fr^3 + gr^4$	$g > 0$
	3	$\ldots + er^{2/3} + fr^{4/3} + gr^2$	$g > 0$
	4	$\ldots + fr^{1/2} + gr$	$g > 0$
	5	$\ldots + er^{-2/5} + gr^{2/5}$	$g > 0$
	6	$\ldots + er^{-2/3} + fr^{-1/3}$	$E < 0$

3. Recurrence relations

In accord with the standard textbooks and recent results (Znojil 1981) we may easily verify that an ansatz

$$\chi(x) = x^{L+1} \, \mathrm{e}^{-f(x)} \varphi(x), \tag{10}$$

$$f(x) = \sum_{j=1}^{q+1} \beta_j x^{2j}/2j, \qquad \beta_{q+1} = G_{2q+1}^{1/2},$$

$$\beta_k = (2\beta_{q+1})^{-1}\left(G_{q+k} - \sum_{j=k+1}^{q} \beta_j \beta_{q+k+1-j}\right), \qquad k = q, q-1, \ldots, 1,$$

$$\varphi(x) = \sum_{n=0}^{\infty} h_{n+1} x^{2n},$$

inserted into (6) leads to the $(q+2)$-term recurrences

$$\sum_{j=\max(1,i-q)}^{i+1} Q_{ij} h_j = 0, \qquad i = 1, 2, \ldots, \tag{11}$$

where

$$Q_{jj+1} = B_j = -4j(j+L+1/2),$$

$$Q_{j+kj} = C^{(k)}_{j+k} = 4\beta_{k+1}(j+L/2-\tfrac{1}{2}) + G_k - \sum_{i=1}^{k} \beta_i\beta_{k+1-i} + (2k+1)\beta_{k+1},$$

$$k = 0, 1, \ldots, q, \qquad j = 1, 2, \ldots.$$

Proposition 1. Equation (11) is not an eigenvalue problem.

Proof. Choosing a normalisation $h_1 = 1$, we obtain the non-trivial solution to (11)

$$h_{n+1} = \frac{\Gamma(L+\frac{3}{2})}{4^n n!\Gamma(n+L+\frac{3}{2})} \det\begin{pmatrix} Q_{11} \ldots Q_{1n} \\ Q_{n1} \ldots Q_{nn} \end{pmatrix} \tag{12}$$

(cf also Znojil 1981) for each energy E or ε.

Proposition 2. We may rewrite recurrences (11) in the shortened $(q+1)$-term form.

Proof. When we introduce the various sequences F_k, $k = 1, 2, \ldots$ defined from *arbitrary* initialisations by the recurrence

$$F_k = -1 \Big/ \left(C^{(0)}_k + \sum_{j=1}^{q} C^{(j)}_{k+j} \prod_{m=0}^{j-1} B_{k+m} F_{k+m+1} \right) \tag{13}$$

the purely algebraic manipulations give from (11) (with $w_1 = h_1/F_1$)

$$h_k/F_k = w_k + \sum_{i=1}^{\min(q,k-1)} U^{(i)}_k h_{k-i}, \tag{14}$$

$$w_k = w_1 \Big/ \prod_{j=2}^{k} B_{j-1}F_j, \qquad U^{(q)}_{q+k} = C^{(q)}_{q+k},$$

$$U^{(m)}_{m+k} = C^{(m)}_{m+k} + B_{m+k}F_{m+k+1}U^{(m+1)}_{m+k+1}, \qquad m = q, q-1, \ldots, 1, \qquad k = 1, 2, \ldots.$$

Obviously, the requirement $w_k = 0$ is equivalent to the particular though fully admissible choice of

$$1/F_1 = 0. \tag{15}$$

Let us now choose $q = 1$ and return to 'Comments'. Since the method of Singh *et al* (1978) and of Datta and Mukherjee (1980) is based on equation (15) (i.e. equation (12) of 'Comments'), it specifies uniquely the *physical* sequences F_2, $F_3, \ldots$ and h_2 $h_3, \ldots$ (cf (13) and (14), respectively). In this 'reverted' formulation, the energies must be determined independently, from the physical boundary conditions imposed on the wavefunctions (cf also point (ii) of 'Comments'). We may formulate the corresponding result as follows.

Proposition 3. For the $q = 1$ potential (1)+(2), all physical binding energies may be formally defined by the condition

$$F_k C^{(1)}_k < 0, \qquad k > k_0, \tag{16}$$

in the limit $k_0 \to \infty$.

Proof. For $k \gg 1$ and $b > 0$, the mappings $F_k \to F_{k+1}$ and $F_{k+1} \to F_k$ have positive and negative points of accumulation, respectively. This follows from figure 1 with $x = F_k C_k^{(1)}$ and $y = F_{k+1} C_{k+1}^{(1)}$ and from the inequalities

$$\mathrm{d}y(x_{(\pm)})/\mathrm{d}x = -(1+\beta_1 y(x_{(\pm)})/\beta_2)^{-1} < 0, \tag{17}$$

$$|\mathrm{d}y(x_{(+)})/\mathrm{d}x| < 1, \qquad |\mathrm{d}y(x_{(-)})/\mathrm{d}x| > 1.$$

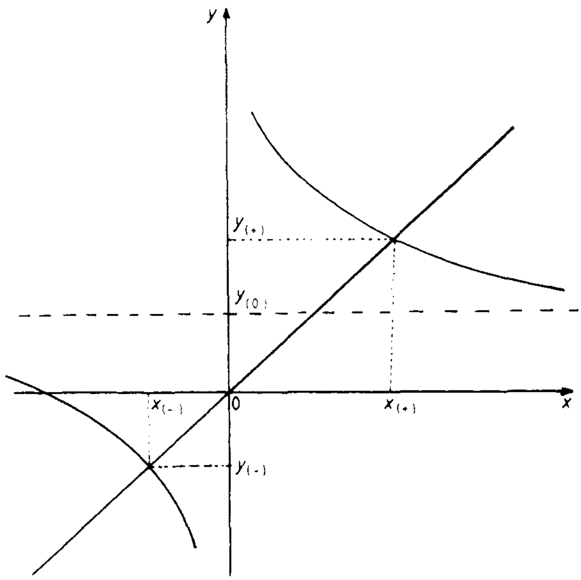

Figure 1. Mapping of the ratio $h_k/h_{k-1} = x$ onto $y = h_{k+1}/h_k$ with $q = 1$, $b > 0$, $k \gg 1$, $y_{(0)} = \beta_1/k = b/2k\sqrt{c} > 0$ and $y_{(\pm)} = \pm(\beta_2/k + y^2_{(0)})^{1/2} + y_{(0)} = x_{(\pm)}$.

As a consequence, the n dependence of $F_{2n}C_{2n}^{(1)}$ or $F_{2n+1}C_{2n+1}^{(1)}$ may be characterised by a smooth interpolation curve of the type displayed in figure 2. Hence (in accord with equation (17) of 'Comments' and Stirling's formula), the $q = 1$ wavefunction regular in the origin behaves in the asymptotic region as a superposition of the two increasing exponentials given by the two separate summations over the even and odd indices n in (10). For almost all energies, these two exponentials cannot cancel because of the positivity of their relative sign,

$$h_k/h_{k-1} = F_k C_k^{(1)} \sim x_{(+)} > 0, \qquad k \gg 1, \tag{18}$$

cf the counterexample (iv) in 'Comments'. *Vice versa*, the two exponentials may cancel and meet the physical asymptotic requirements provided that the forward-running recurrence $F_k \to F_{k+1}$ becomes unstable. This is reflected by equation (16). In the light of the oscillation theorem ($\operatorname{sgn} \varphi(x) = \pm \operatorname{sgn} \Delta E$ whenever $x \gg 1$ is sufficiently large and $\Delta E = E - E_{\text{phys}} \neq 0$ is sufficiently small), we may conclude that no physical energy will be lost.

Obviously the numerical use of equation (16) will be hindered by the loss of precision. Nevertheless, the stable algorithm may be obtained simply by a reinterpretation of the whole construction.

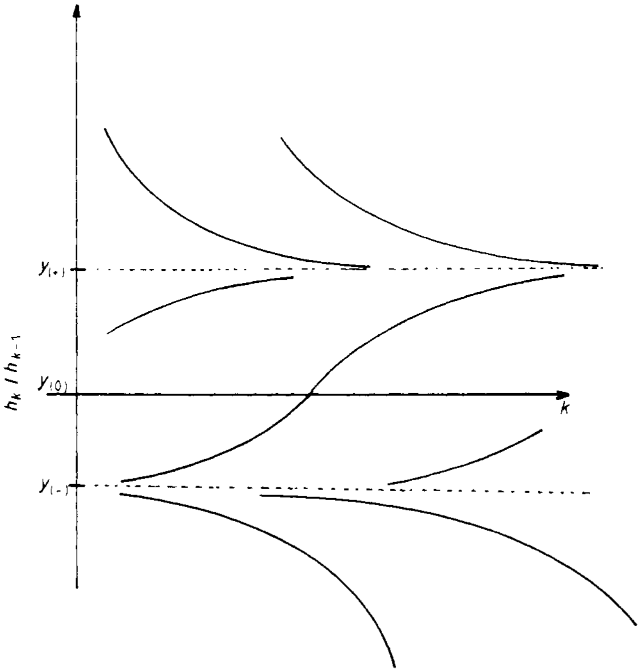

Figure 2. Behaviour of the sequences h/h_{k-1} with the fixed parity of k in the $k \gg 1$ asymptotic region ($q = 1$).

Proposition 4. For $q = 1$, let us pick up an arbitrary initialisation $F_N = a \in (-\infty, \infty)$ of the sequence $F_k = F_k^{(N,a)}$. Then equation (15) ($1/F_1{}^{(N,a)} = 0$) gives the physical spectrum in the limit $N \to \infty$ if and only if the condition (2) is satisfied.

Proof. This is a simplification of that given elsewhere (Znojil 1982). For each physical energy (but $b > 0$ only), the sequence of the backward-generated $F_k^{(N,a)}$, $k \ll N$, almost (or exactly, for $N = \infty$) coincides with the physical F_k. This follows from equation (16) and figure 2 where $y_{(-)}$ becomes a point of accumulation. For the smaller k, this coincidence survives if and only if the energies are physical—otherwise, we would get a contradiction with proposition 3.

4. Binding energies

From the asymptotic form of the differential Schrödinger equation, we obtain that $\chi(x) \sim \exp[+f(x)]$ for $E \neq E_{\text{phys}}$ so that $d\chi/df \sim \chi$ for $f \gg 1$. Inserting this estimate into equation (10), we get, rather formally,

$$h_{n+1} = [(\rho\beta_{q+1})^{\rho n}/\Gamma(\rho n + 1)]b_{n+1}, \qquad \rho = (q+1)^{-1}, \tag{19}$$

with the new expansion coefficients b. With any $q \geq 1$, this enables us to generalise proposition 3 and to decompose the wavefunction into the $q + 1$ asymptotically growing exponentials cancelling at the physical energies.

Proposition 5. If the values F_k lie close to a negative fixed point of the mappings $F_{k+i} \to F_k$, $i = 1, 2, \ldots, q$, for all $k \gg 1$, then equation (15) defines the binding energies.

Proof. When we ignore the $O(1/k)$ corrections in the $k \gg 1$ asymptotic region, the recurrences (13) with $L_k = B_{k-1}F_k$ acquire a simple form

$$L_n = n/(\beta_1 + \beta_2 L_{n+1} + \cdots + \beta_{q+1} L_{n+1} L_{n+2} \cdots L_{n+q}) \tag{20}$$

possessing only one or two common real fixed points $P_k (= L_k = \ldots = L_{k+q}$ in (20)),

$$P_n \sim \varepsilon (n/\beta_{q+1})^{\rho}, \qquad n \gg 1, \qquad \varepsilon = \pm 1, \tag{21}$$

for $q =$ even or odd, respectively. Since $B_n = -4n^2(1 + O(1/n))$ and $C_n^{(i)} = 4n\beta_{i+1}$, $i = 0, 1, \ldots, q$, the insertion of (19) and $L_n \sim P_n$ into (14) gives

$$\sum_{j=0}^{q} \varepsilon^j b_{n+j} = (\text{constant } (n)/F_1)(1 + O(1/n)^{\rho}), \qquad \varepsilon = \operatorname{sgn} P_n. \tag{22}$$

With $\varepsilon = +1$, this implies that near a root E_0 of $1/F_1$, the superposition of the $q+1$ b's changes sign. The asymptotic n-dependence of $b_{(q+1)n+j}$, $j = 0, 1, \ldots, q$, becomes fairly smooth, in full analogy with the $q = 1$ example of § 3. For sufficiently large n, the change of sign of the superposition of the $q+1$ neighbouring b's corresponds therefore to the change of sign of the $q+1$ partial summations over $n \equiv$ constant (mod $q+1$) in equation (10), i.e. to the change of sign of $\chi(x)$ in the asymptotic region. Now, similarly to the oscillation-theorem argument of proposition 3, the latter change of sign (mutual cancellation of the growing exponentials in $\chi(x)$) specifies precisely the complete spectrum of the binding energies. In the light of equation (22), it occurs if and only if the transcendental equation (15) is satisfied. Due to the strength of the assumptions, no restriction similar to equation (2) is needed.

In a way similar to proposition 4 it is possible to satisfy the assumptions of proposition 5 by starting the recurrences (13) in infinity. Deferring the detailed discussion of the rather complicated technical questions to Znojil (1983), let us formulate this possibility as the final

Conjecture. When we consider the particular subclass of the potentials $W(x)$ in equation (6) with

$$G_{2q-t} > 0, \qquad G_{2q-t+1} = \ldots = G_{2q} = 0, \qquad 0 \leq t < q, \tag{23}$$

and introduce the 'extended continued fractions' $F_k^{(\infty,0)} = \lim_{N\to\infty} f_k^{(N,0)}$ defined by the recurrences (13) and initialisation $F_{N+i}^{(N,0)} = 0$, $i = 1, 2, \ldots, q$, then the physical binding energies become roots of the transcendental equation

$$1/F_1^{(\infty,0)} = 0. \tag{24}$$

Concerning the proof, it is probably rather complicated—its $q = 2$ version was given by Znojil (1981) for a particular type of W. The proof of a weaker version of the conjecture will be given elsewhere (Znojil 1983). The $q \geq 1$ 'applicability condition' (23) coincides with equation (2) at $q = 1$ and seems to be a restriction immanent in the present continued-fractional formalism and not easily removable without a use of the forward-running recurrences.

5. Summary

Although our arguments concern the general potential (3) rather than its special case (1) only, we may parallel 'Comments', with the same numbering of topics, showing the following.

(i) The $q = 1$ 'consistency condition' of Datta and Mukherjee (1980) represents a correct eigenvalue method if and only if equation (2) holds. Its generalisation to $q > 1$ is possible and it has been described here in detail, omitting only some of the more extensive proofs.

(ii) The correct physical asymptotic behaviour of the wavefunctions is guaranteed by the formalism since the wavefunction may be written as a superposition of $q+1$ growing exponentials which do not cancel off the physical energy.

(iii) The formalism gives the terminating solutions as special cases, of course.

(iv) The counterexamples of 'Comments' are correct but violate either the applicability condition (2) or correspond simply to $E \neq E_{\text{phys}}$.

(v) We may summarise that for $b > 0$ (or equation (23) in general), the Green function $F_1^{(\infty,0)}$ represents an analytic resummation of the perturbation series and its singularities define the complete discrete spectrum. As a continued-fractional algorithm, this may be used even in the numerical computations after some amendments (Znojil 1981), contrary to the original expectations of Singh *et al* (1978).

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