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LETTER TO THE EDITOR

On the applicability of the Hill determinant and the analytic continued fraction method to anharmonic oscillators

George P Flessas† and G S Anagnostatos‡

† Department of Natural Philosophy, The University, Glasgow G12 8QQ, UK
‡ Tandem Acceleration Laboratory, NRC Demokritos, Aghia Paraskevi Attiki, Athens, Greece

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Abstract. We finish a line of argument started in an earlier paper and show that the application of the Hill determinant and the associated analytic continued fraction method for the calculation of eigenvalues of anharmonic oscillators is of dubious validity and may thus lead to erroneous results. In this context some theorems concerning the eigenvalues of the λx^4 and the doubly anharmonic oscillators are proved.

The Hill determinant method has been used (Biswas *et al* 1971, 1973) for the calculation of the ground-state eigenvalues of the λx^{2m} anharmonic oscillator. Along these lines and by application of the analytic continued fraction method, which is mathematically equivalent to the Hill determinant approach, Singh *et al* (1978) treated the doubly anharmonic oscillator $ax^2+bx^4+cx^6$. Recently Datta and Mukherjee (1980) have applied exactly the same procedure to the interaction $V(r)=-a/r+br+cr^2$.

In a previous paper (Flessas 1982) we discussed the aforementioned method and verified its inadequacy for the calculation of the energy spectrum of the Datta and Mukherjee (1980) potential. In this Letter we show the Hill determinant technique to be wanting also in the case of the oscillator with either quartic or quartic and sextic anharmonicity. These findings prove, therefore, that the above technique should *not* be used without a proper incorporation into it of the main physical requirement that the wavefunction of the relevant Schrödinger equation is normalisable.

We begin by considering the oscillator with quartic anharmonicity. Regarding this model we have the Schrödinger equation

$$y''(x)+(E-x^2-\lambda x^4)y(x)=0 \qquad \lambda>0. \tag{1}$$

Biswas *et al* (1971) make the ansatz

$$y(x)=\exp(-\tfrac{1}{2}x^2)f(x) \tag{2}$$

and obtain for $f(x)$ the differential equation

$$f''(x)-2xf'(x)+(E-1-\lambda x^4)f(x)=0. \tag{3}$$

They set

$$f(x)=\sum_{n=0}^{\infty} c_n x^{2n} \tag{4}$$

and get from equation (3) the difference equation

$$2(n+1)(2n+1)c_{n+1}+(E-4n-1)c_n-\lambda c_{n-2}=0. \tag{4a}$$

At this point these authors claim that we have to ensure that non-trivial c_n exist. Thus, they conclude, we must require that the infinite determinant of the coefficients of the homogeneous simultaneous equations ($4a$) vanish, i.e., with

$$D_n=\begin{vmatrix} E-1 & 2 & 0 & 0 & . & . & & \\ 0 & E-5 & 12 & 0 & . & . & & \\ -\lambda & 0 & E-9 & 30 & 0 & 0 & & \\ 0 & -\lambda & 0 & E-13 & 56 & & & \\ \vdots & & \ddots & & \ddots & & & \\ & & & & & & E-4(n-2)-1 & 2(n-1)(2n-3) \\ & & & & & -\lambda & 0 & E-4(n-1)-1 \end{vmatrix} \tag{5a}$$

they get

$$\lim_{n\to\infty} D_n=0. \tag{5b}$$

Equation ($5b$), according to Biswas *et al* (1971), considered as an equation in E, is the eigenvalue condition for equation (1). This is, however, a false statement and completely confusing with respect to the correct eigenvalues, as we will show below.

The c_n exist for *all* finite E and λ, and they can be calculated recursively from equation ($4a$) (cf any textbook on differential equations). No additional constraint needs to be imposed. What Biswas *et al* actually do is simply to apply the Hill determinant method used in the context of the Mathieu differential equation. As described in detail by Morse and Feshbach (1953) in the case of the Mathieu equation the solution is practically written in the form of equation (4), while the corresponding coefficients, denoted here by $c_n^{(M)}$, satisfy a recursion relation analogous to equation ($4a$). Owing to the fact that 0 and ∞ are *irregular* singular points of the Mathieu equation, we can establish the convergence of the series solution for $0<x<\infty$ only by ensuring that the $c_n^{(M)}$, when calculated recursively from the three-term difference equation they fulfil, no longer increase. In other words we require that $c_n^{(M)}\to 0$ as $n\to\pm\infty$ and thus we get from the $c_n^{(M)}$ recursion formula, since $c_n^{(M)}$ can be written in the form of a determinant, the equivalent relation to equation ($5b$), i.e. the Hill determinant which we equate with zero. Put another way, we first truncate the infinite system of equations for the $c_n^{(M)}$, say with $n=\pm N$ and assume $c_i^{(M)}\approx 0$ for $|i|>N$. Then we have a *finite* system of homogeneous simultaneous equations for the $c_n^{(M)}$ and so the determinant of the coefficients must be zero. Finally we let $N\to\infty$ and arrive, of course, at the same Hill determinant. In this way the characteristic quantity of the Mathieu equation, denoted by s, can be calculated. In the case of equation (3), however, the series (4) converges for $-\infty<x<\infty$ according to the general theory on differential equations and so we deduce $(c_n x^{2n})\xrightarrow[n\to\infty]{} 0$ for $x\in(-\infty,\infty)$ whence

$c_n \to 0$ as $n \to \infty$ for *every* finite E, λ. Now it can be easily checked that

$$c_n = \frac{(-1)^n}{2\times 12\times 30\times \ldots \times[2n(2n-1)]} D_n \qquad n \geq 2. \tag{6}$$

A glance at equations (5*b*) and (6) reveals that Biswas *et al* constrain E such that $\lim_{n\to\infty} c_n = 0$. But this is absolutely superfluous here since as indicated prior to equation (6), we have $c_n \to 0$ as $n \to \infty$ for arbitrary E, λ. The correct eigenvalues can be calculated *only* from the requirement that the series in equation (4) for $|x| \to \infty$ does not compensate $\exp(-\frac{1}{2}x^2)$ in equation (2) so that $y(x)$ remains normalisable. Condition (5*b*) alone is incapable of ensuring that $f(x)$ for $|x| \to \infty$ is sufficiently well behaved that $y(x) \to 0$ as $|x| \to \infty$, since it is taken from an entirely different context, i.e. that of the Mathieu equation.

Using equation (4*a*) it can be verified (cf also equation (9) of Biswas *et al* (1971)) that

$$\left.\frac{c_{n+1}}{c_n}\right|_{n\to\infty} \approx \left(\frac{\lambda}{4n^2}\right)^{1/3}. \tag{7}$$

Equation (7), which demonstrates the convergence of $\Sigma\, c_n x^{2n}$ for $x \in (-\infty, \infty)$ known already, implies that $f(x)$ in equation (4) behaves for large $|x|$ like

$$F(t) = \sum_{n=0}^{\infty} [(\lambda/4)^{1/3}]^n t^n (n!)^{-2/3} \qquad t = x^2. \tag{8}$$

Evidently the series in equation (8) converges for $t \in [0, \infty)$. Now it is readily seen that

$$F(t) > \sum_{n=0}^{\infty} [(\lambda/4)^{1/3}]^n t^n (n!)^{-1} = \exp[(\lambda/4)^{1/3} x^2]. \tag{9}$$

Equation (9) exhibits the important result that $f(x)$ behaves *stronger* than $\exp[(\lambda/4)^{1/3}x^2]$ for $|x| \to \infty$. This, in conjunction with equation (2), establishes the fact that for $\lambda > 0.5$ the solution (2) for equation (1) definitely becomes *unphysical* for any finite E. In view of this result the bounds given for $y(x)$ by Biswas *et al* are wrong (equation (10) of that paper).

Moreover, in the numerical application of equation (5*b*) Biswas *et al* truncate the infinite determinant and consider the $(n+1)\times(n+1)$ approximant, D_{n+1}, to D, i.e. $D_{n+1} = 0$. This implies (cf equation (6)) that we require $c_{n+1} = 0$ and *assume* $c_i \approx 0$ for $i \geq n+2$. Such an assumption entails the approximation of the physically acceptable solution to equation (1) by $\exp(-\frac{1}{2}x^2)\times$polynomial. This is plausible because $\exp(-\frac{1}{2}x^2)\times$polynomial is an exact solution of the harmonic oscillator equation $\lambda = 0$ in equation (1). However, the physical wavefunction of equation (1) cannot in this way be approximated to any degree of accuracy since the limit $n \to \infty$ will yield an unphysical solution as noted after equation (9), although some finite E values may be obtained from equation (5*b*).

To summarise, the method of Biswas *et al* (1971) has nothing to do with the actual Hill determinant procedure and all it does is to verify the possibility of approximating the correct wavefunction of equation (1) by $\exp(-\frac{1}{2}x^2)\times$polynomial, the polynomial being derived from a series which renders, at any rate for $\lambda > 0.5$, the $y(x)$ in equation (2) *unphysical.* Some eigenvalues may, of course, be solutions of equation (5*b*), but in general the set of eigenvalues of equation (1) need not coincide with the set of E solutions of equation (5*b*). The same comments can be made regarding the case of the $(x^2 + \lambda x^{2m})$ oscillator (Biswas *et al* 1973).

We now turn our attention to the doubly anharmonic oscillator as investigated by Singh *et al* (1978). The corresponding Schrödinger equation is

$$-(\hbar^2/2m)y''(x)+(ax^2+bx^4+cx^6)y(x)=Ey(x) \qquad a, c>0. \tag{10}$$

The ansatz (Singh *et al* 1978)

$$y(x)=\exp(-\tfrac{1}{4}x^4\alpha+\tfrac{1}{2}x^2\beta)f(x) \tag{11}$$

$$\alpha=(2mc/\hbar^2)^{1/2} \qquad \beta=-\tfrac{1}{2}b(2m/\hbar^2c)^{1/2} \tag{11a}$$

yields

$$f''(x)+2(-\alpha x^3+\beta x)f'(x)+[(\beta^2-3\alpha-2ma/\hbar^2)x^2+2mE/\hbar^2+\beta]f(x)=0. \tag{12}$$

Singh *et al* solve equation (12) by setting

$$f(x)=x^v\sum_{n=0}^{\infty}a_nx^{2n} \tag{13}$$

where $v=0, 1$ for the even and odd parity states, respectively, and

$$(2n+2+v)(2n+1+v)a_{n+1}+[\varepsilon+\beta(4n+1+2v)]a_n+\alpha[\gamma-(4n-1+2v)]a_{n-1}=0 \tag{14}$$

$$\varepsilon=2mE/\hbar^2 \qquad \gamma=[2m/(\hbar^2c)]^{1/2}(-a+b^2/4c). \tag{14a}$$

From equation (14) one can easily obtain

$$\frac{a_n}{a_{n-1}}=\cfrac{-C_n}{B_n-\cfrac{A_nC_{n+1}}{B_{n+1}-\cfrac{A_{n+1}C_{n+2}}{B_{n+2}-\ddots}}} \tag{15}$$

where

$$A_n=(2n+1+2v)(2n+2+v) \qquad B_n=\beta(4n+1+2v)+\varepsilon$$

$$C_n=-\alpha(4n+2v-\gamma-1) \tag{15a}$$

and since

$$\frac{a_1}{a_0}=-\frac{\varepsilon+\beta(2v+1)}{(v+1)(v+2)} \tag{15b}$$

one gets from equation (15)

$$-[\varepsilon+\beta(2v+1)]=\cfrac{\alpha(v+1)(v+2)(3+2v-\gamma)}{\varepsilon+\beta(2v+5)+\cfrac{\alpha(7+2v-\gamma)(v+3)(v+4)}{\varepsilon+\beta(2v+9)+\ddots}} \tag{16}$$

Singh *et al* (1978) claim that equation (16), considered as an equation in E, gives the energy eigenvalues of equation (10). This is, however, an unsubstantiated conclusion and the relation of condition (16) to the correct eigenvalues is not at all clear.

(i) Singh *et al* in writing down equation (16) actually utilise the second alternative available, the first being the Hill determinant, for ensuring the convergence for $0<x<\infty$ of the series solving the Mathieu differential equation. In such a way the characteristic quantity, s, of the Mathieu equation can be determined. Indeed, as set out by Morse and Feshbach (1953), the equivalent relation to equation (16), derived from the recursion relation analogous to equation (14), is sufficient for the convergence of the series in question. In the case of equation (12), however, condition (16) is completely meaningless, since the series in equation (13) is convergent for $x \in (-\infty, \infty)$. Equation (16) in no case ensures that $y(x)$ in equation (11) remains normalisable (and we cannot expect it to do so since its origin lies in the Mathieu equation).

(ii) From equation (14) we observe that for large n

$$a_{n+1}/a_n \approx \pm(\alpha/n)^{1/2} \tag{17}$$

The positive sign in equation (17) is realised if, for example, as an inspection of equation (14) reveals,

$$b>0 \qquad 0<\varepsilon<\tfrac{1}{2}b(2m/\hbar^2c)^{1/2}(2v+1) \qquad \gamma<2v+3 \tag{18}$$

as then the choice $a_0>0$ necessarily implies $a_n>0$. Consequently the series in equation (13) for $|x|\to\infty$ behaves like the series

$$F(t)=\sum_{n=0}^{\infty}\frac{\alpha^{n/2}}{(n!)^{1/2}}t^n \qquad t=x^2 \tag{19}$$

which is convergent for $t \geqslant 0$. We proceed to compare $F(t)$ with

$$\exp(\tfrac{1}{4}t^2\alpha)=\sum_{n=0}^{\infty}\frac{(\alpha/4)^n}{n!}t^{2n} \qquad t=x^2 \tag{20}$$

by comparing the coefficients of equal even powers in $F(t)$ and $\exp(\frac{1}{4}t^2\alpha)$. It is straightforward to prove that from a sufficiently large but *finite n*, say N, we get

$$\frac{\alpha^{2n/2}}{[(2n)!]^{1/2}}>\frac{(\alpha/4)^n}{n!} \qquad n \geqslant N. \tag{21}$$

Now

$$\exp(\tfrac{1}{4}t^2\alpha)=t^{2N-2}\frac{(\alpha/4)^{N-1}}{(N-1)!}(1+\mathrm{O}(t^{-1}))+\sum_{n\geqslant N}^{\infty}\frac{(\alpha/4)^n}{n!}t^{2n} \tag{22}$$

$$F(t)=t^{2N-1}\frac{\alpha^{(2N-1)/2}}{[(2N-1)!]^{1/2}}(1+\mathrm{O}(t^{-1}))+\sum_{n\geqslant 2N}^{\infty}\frac{\alpha^{n/2}}{(n!)^{1/2}}t^n. \tag{23}$$

Equations (21)–(23) show that $F(t)$, and thus also $f(x)$, compensates $\exp(-\frac{1}{4}x^4\alpha)$ for $|x|\to\infty$. Hence, according to equation (18), if $b>0$ and $\gamma<2v+3$, any E satisfying the inequality $0<E<\frac{1}{2}b[\hbar^2/(2mc)]^{1/2}(2v+1)$ *cannot* be an eigenvalue for equation (10). This physically important result is completely missed in the relevant theorem I of Singh *et al.* In view of the comments in (i) this is not at all surprising. Further, the above result casts serious doubt on the assertion that equation (16) yields all the eigenvalues of equation (10).

In summary, we have verified that the methods used in the context of the Mathieu (or more generally the Hill) differential equation are *not*, nor should they be, directly applicable to the equations obtained in relation to various anharmonic oscillators. In these procedures the requirement that the wavefunction remain normalisable has to be incorporated so as to ensure that the values we obtain for E are the physically correct ones. No general method for doing this seems to exist (Znojil 1982a and private communication) and thus one is forced to carry out rather extensive investigations for every potential under consideration. To our knowledge the only known exact solutions for anharmonic oscillators can be written as either (exponentials) × (polynomials) (Flessas 1979, Flessas and Das 1980, Znojil 1982b) or as definite integrals (Flessas 1981a, b). In both cases the actual notion of the Hill determinant or the analytic continued fraction method is irrelevant since we obtain the above solutions either by rigorously truncating infinite series, whose behaviour for $|x| \to \infty$ may generate an unphysical wavefunction, or by representing the wavefunction $y(x)$ as an integral with $y(x) \to 0$ for $|x| \to \infty$.

Note added in proof. As observed in our previous work (Flessas 1982) and elsewhere, equation (15) simply gives the *terminating* solutions, i.e. $C_N = 0$ and $\alpha_n = 0$ for $n \geq N$, to equation (10). But these solutions are obtainable directly from equation (14) and one does not actually need to write down equation (15).

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