# Comment on the anharmonic oscillator and the analytic theory of continued fractions

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It is shown that the analytic-continued-fraction method may lead to wrong results for the eigenvalues of the anharmonic oscillators of the type $ax^2+bx^4+cx^6$ with $c>0$.

Anharmonic oscillators of the type $ax^2+bx^4+cx^6$ with $c>0$ have been studied extensively by Singh, Biswas, and Datta[1] using the theory of continued fractions[2] and the method of the Hill determinant.[3] They have considered the eigenvalue equation

$$\left[-\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x) \tag{1}$$

with the potential energy given by

$$V(x)=ax^2+bx^4+cx^6,\quad c>0\ . \tag{2}$$

It is well known[4] that there are an infinite number of discrete energy levels if the potential energy $V(x)$ increases to infinity as $|x|\rightarrow\infty$, and there cannot be any energy level smaller than the least value of $V(x)$. The potential (2) is always bounded from below for all values of $a$ and $b$, and therefore all the energy eigenvalues cannot be negative for this problem. The WKB approximation gives positive-energy excited states for this potential. It is shown here that for some values of the parameters $a$ and $b$, the Hill determinant method of Singh *et al.*[1] fails to produce positive eigenvalues for the potential (2). It is necessary that along with the eigenvalue condition the condition of normalization of the wave function should also be imposed. The implication of the boundary condition $\psi(x)\rightarrow 0$ *as* $|x|\rightarrow\infty$ is discussed here.

The Schrödinger equation (1) is transformed to the form

$$\frac{d^2\phi}{dx^2}+2(-\alpha x^3+\beta x)\frac{d\phi}{dx}+[(\beta^2-a-3\alpha)x^2+E+\beta]\phi=0 \tag{3}$$

by making the substitution

$$\psi(x)=\exp(-\tfrac{1}{4}\alpha x^4+\tfrac{1}{2}\beta x^2)\phi(x)\ , \tag{4}$$

where $\alpha=c^{1/2}>0$ and $\beta=-\frac{1}{2}bc^{-1/2}$. It is clear from the differential Eq. (3) that $x=0$ is an ordinary point and $x=\infty$ is an irregular singular point of the differential equation. Therefore in the region $|x|<\infty$ Eq. (3) admits convergent series solution

$$\phi(x)=\sum_{n=0}^{\infty}a_n x^{2n+\nu}\ , \tag{5}$$

where $\nu=0$ for the even-parity solution and $\nu=1$ for that of odd parity. The coefficients $a_n$ satisfy the difference equation

$$(2n+2+\nu)(2n+1+\nu)a_{n+1}+[E+\beta(4n+1+2\nu)]a_n+[\beta^2-a-(4n-1+2\nu)\alpha]a_{n-1}=0 \tag{6}$$

with $n=0,1,2,\ldots$, and $a_{-1}=0$.

The necessary and sufficient condition that nontrivial $a_n$ exist is that the infinite Hill determinant vanishes:

$$\begin{vmatrix} b_{11} & b_{12} & 0 & \cdots \\ b_{21} & b_{22} & b_{23} & \cdots \\ 0 & b_{32} & b_{33} & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix}=0\ , \tag{7}$$

where the nonzero tridiagonal matrix elements $b_{ij}$ are given by

$$b_{ii}=E+(4i-3+2\nu)\beta\ , \tag{8a}$$

$$b_{i\,i+1}=(2i+\nu)(2i-1+\nu)\ , \tag{8b}$$

$$b_{i\,i-1}=\beta^2-a-(4i-5+2\nu)\alpha\ . \tag{8c}$$

If $D_n$ denotes the first $n\times n$ determinant then

$$D_n=b_{nn}D_{n-1}-b_{n-1\,n}b_{n\,n-1}D_{n-2}\ . \tag{9}$$

By repeated application of Eq. (6) we can express all the coefficients in terms of $a_0$:

$$a_n=(-1)^n a_0 D_n/(2n+\nu)!\ .$$

According to Singh *et al.*[1] the zeros of $D_n$ in the energy parameter $E$ will determine the energy eigenvalues of the problem when $n\rightarrow\infty$. It has been pointed out[5-7] that all the eigenvalues should not be allowed since the boundary conditions $\psi(x)\rightarrow 0$ as $x\rightarrow\pm\infty$ are not incorporated into the method. Since $x=\infty$ is an irregular singular point of the differential Eq. (3) the series (5) may not be valid at $x=\pm\infty$. The boundary conditions are satisfied when the series (5) terminates.

When

$$b_{n+1\,n}=\beta^2-a-(4n-1+2\nu)\alpha=0 \tag{10}$$

the infinite Hill determinant (7) reduces to the form

$$\begin{vmatrix} A & C \\ 0 & B \end{vmatrix}=|A|\,|B|\ , \tag{11}$$

where $|A|=D_n$ is an $n\times n$ determinant and $|B|$ is a determinant of infinite order:

$$|B| = \begin{vmatrix} b_{n+1,n+1} & b_{n+1,n+2} & 0 & \cdots \\ b_{n+2,n+1} & b_{n+2,n+2} & b_{n+2,n+3} & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix} . \tag{12}$$

Now the vanishing of the Hill determinant means either (i) $|A|=0$ or (ii) $|B|=0$.

*(i)* $|A| = 0$. The $n$ number of roots will appear from the vanishing of $D_n$ whence $a_n=0$ follows. It is clear from the recurrence relation (6) that if $a_n=b_{n+1n}=0$, then $a_{n+1}=a_{n+2}=\cdots=0$ and $\phi(x)$ reduces to a polynomial in $x$. This feature immediately raises the question as to what happens to the remaining eigenvalues as we must have infinity of solutions. Singh *et al.*[1] conjectured that the remaining infinity of solutions are obtained from the zeros of the infinite determinant $B$. We would like to show that this conjecture may lead to wrong results.

*(ii)* $|B| = 0$. The zeros of $|B|$ given by Eq. (12) should be examined with respect to the constrained values of the couplings which satisfy (10). Let us take the simplest case in which $b_{21}=0$ or

$$\beta^2 - a - (3+2\nu)\alpha = 0 \ . \tag{13}$$

$|A|$ is then a $1\times 1$ determinant which produces the eigenvalue $E=-(1+2\nu)\beta$. The corresponding unnormalized eigenfunction (apart from the exponential $x$ factor) is $\phi(x)=a_0x^\nu$. If $B_n$ denotes the first $n\times n$ determinant of $B$ we have the following difference equation satisfied by $B_n$:

$$B_n = [E + (4n+1+2\nu)\beta]B_{n-1} + 4(n-1)(2n+\nu)(2n-1+\nu)\alpha B_{n-2} \ , \tag{14}$$

with $B_0=1$ and $B_1=E+(5+2\nu)\beta$. If we expand $B_n$ in terms of the parameter $E$, we find that $B_n$ is a polynomial of degree $n$,

$$B_n = \sum_{r=0}^{n} p_r(\beta)E^r \ , \tag{15}$$

with $p_n(\beta)=1$. It can be easily checked that for $\beta<0$ the coefficients of successive powers of $E$ alternate in sign, showing that there are no real negative zeros of $B_n$. When $\beta\geqslant 0$ all the coefficients $p_r(\beta)$ are non-negative indicating that $B_n$ will never vanish for any real positive values of $E$. But we already know[4] that all the eigenenergies cannot be negative for this problem. Thus, the Hill determinant method may be applicable for $\beta<0$ and the method fails to produce all the correct eigenvalues for $\beta\geqslant 0$, which is consistent with the earlier observation made by Znojil.[8] By constructing the auxiliary continued fraction in terms of $T_n=a_n/a_{n-1}$, $n=1,2,\ldots$, Znojil[8] has shown that the Green's function $G(E)$ of Singh *et al.*[1] is unphysical for $\beta>0$. He has further shown that for $\beta<0$ the poles of $G(E)$ coincide with the anharmonic binding energies. Our method is completely different from that of Znojil in the sense that we have examined here the zeros of the Hill determinant directly and have shown that the method may fail when $\beta\geqslant 0$. It is also true, in general, when $b_{n+1n}=0$ and $\beta\geqslant 0$. The correct eigenvalues may be obtained by an analytic continuation of the continued fraction accomplished with the aid of modified approximants.[7]

For the even-parity solutions we choose $a=-2$, $b=-2$, and $c=1$ so that the condition (13) is satisfied and at the same time $\beta>0$. We compute the first two even-parity eigenvalues by solving the Schrödinger equation (1) numerically and obtain the results $-1.000$ and $3.628$, which clearly show that the conjecture of Singh *et al.*[1] is not correct.

We have examined here the vanishing of the determinant $B_n$ and have shown that $B_n$ for any finite value of $n$ will never vanish for any real positive value of $E$ when $\beta\geqslant 0$. From the difference equation (14) we find that if $B_n$ and $B_{n-1}$ are positive for $E>0$ and $\beta\geqslant 0$ then $B_{n+1}$ is also positive for $E>0$ and $\beta\geqslant 0$. In this way we assume that the proof constructed here is applicable to the determinant $B_n$ as $n\to\infty$. It is further assumed that the zeros of finite truncations of an infinite determinant in the energy parameter converge to those of the infinite determinant.

Along with the eigenvalue condition (7) the condition for the normalizability of the wave function should also be imposed. We consider the absolute series for $\phi(x)$. From (4) we find that $\psi(x)$ is normalizable when

$$\phi(x) \leqslant M \exp(\tfrac{1}{4}\alpha x^4 - \tfrac{1}{2}\beta x^2)/x^{2-\nu} \ \text{as } x\to\infty \ , \tag{16}$$

where $M$ is a constant. By making the series expansion and comparing the coefficients of $x^{2K+\nu}$ we get the following bounds on $a_K$:

$$|a_K| \leqslant \sum_{p=0}^{L} \frac{M(\alpha/4)^p(-\beta/2)^{K+1-2p}}{p!(K+1-2p)!} \ , \tag{17}$$

where $L=K/2$ or $(K+1)/2$ whichever is an integer. The corresponding bound on $D_K$ is

$$|D_K| \leqslant \sum_{p=0}^{L} \frac{M}{a_0} \frac{(2K+\nu)!(\alpha/4)^p(-\beta/2)^{K+1-2p}}{p!(K+1-2p)!} \ . \tag{18}$$

For each eigenvalue as determined by the vanishing of the Hill determinant the normalization condition (17) or (18) should be checked.

It should be mentioned that our proof of nonapplicability of the method of the Hill determinant applies only to those values of the couplings for which $\beta>0$ $(b<0)$ *and* which satisfy the conditions of constraint such as to cause the appropriate Hill determinant to factor and *not* for all $\beta>0$. However, the bounds on $a_K$ and $D_K$ as given by (17) and (18) are true for all values of the couplings. When the Hill determinant is factored into two determinants, the zeros of the determinant of finite order give the correct eigenvalues and well-behaved eigenfunctions, whereas the zeros of the determinant of infinite order may give rise to spurious eigenvalues. A particular feature of the eigenvalues of the potential $ax^2+bx^4+cx^6$ is that Rayleigh-Schrödinger perturbation theory may not be applicable for negative $b$. This potential has been discussed by a number of authors[9,10] in the context of negative $b$. Recently, Banerjee and Bhattacharjee[11] have developed a scaled Hill-determinant technique and equivalent harmonic-oscillator model for the potential $V(x)=\pm x^2+\lambda x^4$ for all values of the coupling parameter $\lambda$. The Hill-determinant method also works extremely well for the $x^2+\lambda x^{2m}$ anharmonic oscillators.[3] One should be cautious in applying the method of the Hill determinant for the doubly anharmonic oscillator of type given by (2) particularly when some of the couplings of the potential are negative.[8,12]

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