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Sextic-oscillator puzzle and its solution

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The construction of sextic oscillators using Hill determinants [V. Singh, S. N. Biswas, and K. Datta, Phys. Rev. D **18**, 1901 (1978)] fails for certain couplings [cf., e.g., R. N. Chaudhuri, Phys. Rev. D **31**, 2687 (1985)]. A simple explanation and a cure are found: The better choice of the underlying ansatz is proved to give all the energy levels for any couplings.

I. INTRODUCTION

An interest in anharmonic oscillators is currently motivated by their phenomenological[1] as well as methodological[2] use. In the latter context, Singh, Biswas, and Datta[3] have conjectured an analytic resummation of the divergent perturbation series for the particular example

$$\left[-\frac{d}{dr^2}+\frac{l(l+1)}{r^2}+ar^2+br^4+cr^6-E\right]\psi(r)=0 \; . \quad (1.1)$$

Unfortunately, as a number of authors have pointed out,[4-6] the construction ceases to be physical for $b\le 0$. Such an anomaly is rather puzzling for a number of reasons.

(i) The construction proceeds in full analogy with the exactly solvable harmonic oscillator. In the wave function $\psi(r)$ specified by an infinite series

$$\psi(r)=r^{l+1}\exp[-(\tfrac{1}{2}\alpha r^2)^2-\tfrac{1}{2}\beta r^2]\sum_{n=0}^{\infty}p_0 r^{2n} \; ,$$
$$c=\alpha^4,\ \beta=b/(2\alpha^2) \; , \quad (1.2)$$

the physical threshold and asymptotic behavior are factored out.

(ii) Formula (1.2) characterizes the sextic anharmonicity as one of the simplest "next-to-solvable" interactions. Indeed, an insertion of Eq. (1.2) makes the differential radial Schrödinger equation equivalent to the algebraic three-term recurrences:

$$\begin{aligned}
&B_n p_{n+1}-A_n p_n-C_n p_{n-1}=0 \; ,\\
&B_n=(2n+2l+3)(2n+2) \; ,\\
&A_n=(4n+2l+3)\beta-E \; , \qquad (1.3)\\
&C_n=(4n+2l+1)\alpha^2+a-\beta^2 \; ,\\
&n=0,1,\ldots,\ p_{-1}=0 \; .
\end{aligned}$$

For any other polynomial anharmonicity (including the quartic one), a similar procedure always leads to at least four-term recurrences.[7]

(iii) With respect to an explicit solvability of Eq. (1.3),

$$p_{n+1}=\left[\prod_{k=0}^{n}B_k\right]^{-1}\det\mathcal{H}_n \; , \quad (1.4)$$

$$\mathcal{H}_n=\begin{pmatrix} A_0 & -B_0 & & \\ \cdots & & & \\ C_k & A_k & -B_k & \\ & \cdots & & \\ & & C_n & A_n \end{pmatrix},\ n=0,1,\ldots \; ,$$

the Hill-determinant requirement[8] $p_{N+1}=0$ or

$$\det\mathcal{H}_N=0,\ N\gg 1 \quad (1.5)$$

represents an extremely plausible secular equation. Computationally, its reliability has been confirmed for a number of interactions.[8]

(iv) The roots of Eq. (1.5) are physical for $b>0$ (Ref. 6) and manifestly unphysical for $b\le 0$.[5] It is difficult to understand the reasons for such an asymmetry.[9]

An immediate motivation of this paper lies in the recent construction of explicit $b\le 0$ counterexamples.[5] Indeed these are the very interactions that are interesting from the purely phenomenological point of view: The shape of potentials varies between the single- and triple-well structure [for $b\ge -(3ac)^{1/2}$ and $b<-(3ac)^{1/2}$, respectively], while the double-well form appears for the negative values of coupling a.

In essence, my comment has two parts. In the first one (Secs. II and III), a short reevaluation of the solution of Singh *et al.* employs the standard theory of difference equations.[10] For $b>0$, I reconfirm the reliability of Eq. (1.5) and for $b\le 0$ one finds that the Hill-determinant prescription leaves the binding energies entirely indeterminate in the limit $N\to\infty$.

In the second part of the paper (Sec. IV), the idea of removing the indeterminacy of energies is developed in detail. Because of the introduction of a free parameter in (1.2), I am able to derive Eq. (1.5) as a physical boundary condition pertaining to a modified form of recurrences (1.3). In the summary (Sec. V), I then emphasize that the standard "derivation" of the Hill determinants as reflecting some "truncation of recurrences" is misleading and unable to specify a domain of validity of the eigenvalue condition (1.5).

II. THE METHOD OF SINGH *et al.*, AND TAYLOR COEFFICIENTS AS SOLUTIONS OF A DIFFERENCE EQUATION

The solution (1.2)-(1.4) of the differential Schrödinger equation (1.1) is physical at the origin: $\psi(r)\sim r^{l+1}$, $r\sim 0$. Its asymptotic behavior is in general unphysical:

$$\psi(r)\sim d_1\exp(\tfrac{1}{4}a^2r^4)+d_2\exp(-\tfrac{1}{4}a^2r^4),\quad r\gg 1\ . \tag{2.1}$$

At the physical energies $E=E_{\rm phys}$, the dominant component disappears and changes sign.[11] Thus, we have $d_1=d_1(E_{\rm phys})=0$, i.e.,

$$\psi(r)\sim\exp(-\tfrac{1}{4}a^2r^4),\quad E=E_{\rm phys},\ r\gg 1\ . \tag{2.2}$$

An explicit use of this change of sign is the main idea.

Formula (1.2) converts the differential equation (1.1) into the difference equation (1.3) and, formally, we may treat p_n as a new representation of the wave function. Indeed, we may choose $p_0=1$ as normalization and understand $p_{-1}=0$ as a boundary condition "at the origin." Let us now complement it by an appropriate reinterpretation of the asymptotic boundary conditions.

The analysis may be significantly simplified by changing variables $p_n\to q_n$:

$$p_n=q_n\frac{\alpha^n2^{-n/2}\Gamma(v+\frac{1}{2}n)}{\Gamma(1+\frac{1}{2}n)\Gamma(t+\frac{1}{2}n)},\quad n=0,1,\ldots,\quad t=\tfrac{1}{2}l+\tfrac{5}{4}\ ,$$
$$v=\tfrac{1}{2}t+\frac{1}{8\alpha^2}(a-\beta^2)\ . \tag{2.3}$$

Here, for the time being, the sign of α will be kept free, $\alpha=\pm\sqrt{\alpha^2}$. Then, we may rewrite Eq. (1.3) in the two possible nonequivalent forms:

$$q_{n+1}-q_{n-1}=Q_nq_n\ ,$$
$$Q_n=Q_n^{(\pm)}=\frac{\Gamma(v+\frac{1}{2}n)\Gamma(\frac{1}{2}+\frac{1}{2}n)\Gamma(t-\frac{1}{2}+\frac{1}{2}n)}{\Gamma(v+\frac{1}{2}+\frac{1}{2}n)\Gamma(1+\frac{1}{2}n)\Gamma(t+\frac{1}{2}n)}\frac{A_n}{8\alpha\sqrt{2}}\ ,$$
$$n=0,1,\ldots,\quad \mathrm{sgn}\alpha=\pm 1\ . \tag{2.4}$$

In both these cases, an estimate $Q_n=O(1/\sqrt{n})$ is valid and implies that

$$|q_{n+1}-q_{n-1}|\ll|q_n|,\quad n\gg 1\ .$$

Such a "smoothness property" motivates approximations of the type

$$q_{n+m}=q_n+m\frac{d}{dn}q_n+\cdots,\quad n\gg|m|\ . \tag{2.5}$$

Combined with the asymptotic representations[12]

$$\frac{\Gamma(x+\gamma)}{\Gamma(x+\delta)}=x^{\gamma-\delta}\left[1+\frac{(\gamma-\delta)(\gamma+\delta-1)}{2x}+\cdots\right],\quad x\gg 1\ , \tag{2.6}$$

and

$$\sqrt{n}Q_n=\frac{\beta}{\alpha}-\frac{1}{8\alpha n}\left[\left(3+2l+\frac{a-\beta^2}{\alpha^2}\right)\beta+2E\right]+O\left(\frac{1}{n^2}\right)\ ,\quad n\gg 1\ , \tag{2.7}$$

the truncated Taylor series (2.5) gives

$$\frac{d}{d_n}q_n=\frac{\beta}{2\alpha\sqrt{n}}q_n,\quad n\gg 1,\ \beta\neq 0\ . \tag{2.8}$$

After simple integration, we get an asymptotic estimate

$$q_n=\exp\left(\frac{\beta}{\alpha}\sqrt{n}\right),\quad n\gg 1,\ \beta\neq 0\ , \tag{2.9}$$

compatible to Eq. (2.5). For $\beta=0$, a similar procedure leads to the similar result

$$q_n=\exp\left(\frac{E}{4\alpha\sqrt{n}}\right),\quad n\gg 1,\ \beta=0\ . \tag{2.10}$$

One may conclude that in the $n\to\infty$ asymptotic region, the general solution of the difference equation for the Taylor coefficients p_n is a superposition of the two linearly independent exponential components:

$$p_n=\frac{\Gamma(\frac{1}{2}n+v)}{\Gamma(\frac{1}{2}n+1)\Gamma(\frac{1}{2}n+t)}\left(\frac{|\alpha|}{\sqrt{2}}\right)^n\times\left[c_1\exp\left(\frac{\beta}{|\alpha|}\sqrt{n}\right)+(-1)^nc_2\exp\left(-\frac{\beta}{|\alpha|}\sqrt{n}\right)\right]\ ,\quad n\gg 1\ . \tag{2.11}$$

At the point $b=0$, the symbol β is formally to be replaced by the value of $E/(4n)$.

III. AN ANALYSIS OF THE PHYSICAL ASYMPTOTICS

In accord with the preceding comment[6] on Ref. 3, one may visualize $\psi(r)$ as a superposition of the two functions $\chi^{(+)}(r)$ and $\chi^{(-)}(r)$ defined as summations (1.2) over the even and odd indices, respectively. Their mutual asymptotic cancellation may characterize the physical behavior (2.2).

In the present setting, we may employ the formula (2.11) and write the general form of $\psi(r)$ as a superposition of four terms

$$\psi(r)=c_1\chi^{(+,+)}(r)+c_2\chi^{(+,-)}(r)+c_1\chi^{(-,+)}(r)-c_2\chi^{(-,-)}(r),\quad r\gg 1,\ \chi^{(\pm,\pm)}(r)>0\ , \tag{3.1}$$

where the new superscript denotes the sign of α in the formulas (2.3) and (2.9). Obviously, because of the respective definitions, we may derive estimates of the type

$$\chi_{(r)}^{(+,\varepsilon)} \sim \sum_{n=\text{even}} p_n r^{2n+l+1} \exp(-\tfrac{1}{4}\alpha^2 r^4 - \tfrac{1}{2}\beta r^2)$$
$$\sim \exp(\cdots) \sum_{m=0}^{\infty} r^{4m+l+1} (\tfrac{1}{2}\alpha^2)^m \frac{m^{v-t} \exp[(\beta/\alpha)\sqrt{2m}\,]}{\Gamma(m+1)} \left[1 + O\left(\frac{1}{\sqrt{m}}\right)\right]$$
$$\sim \exp(\cdots) \sum_m [(\tfrac{1}{2}\alpha^2 r^4)^m/m! + \text{corrections}] \sim \exp(\tfrac{1}{4}\alpha^2 r^4 + \cdots),\ r \gg 1\ . \tag{3.2}$$

This is compatible with the form (2.1).

At the physical energies, the mutual cancellation of exponentials must be discussed separately in the following two situations.

A. $b > 0$

On an arbitrary level of precision $1+O(n^{-\text{const}})$, we may notice that Eq. (2.11), i.e.,

$$q_n \sim c_1 \exp\left(\frac{\beta}{|\alpha|}\sqrt{n}\right) + (-1)^n c_2 \exp\left(-\frac{\beta}{|\alpha|}\sqrt{n}\right),\quad n \gg 1,\ \beta > 0\ , \tag{3.3}$$

represents in effect a single exponential. Indeed, the second (sign-changing) term in (3.3) is exponentially smaller than the first one. Without any loss of precision, it may (and must) be incorporated in an error estimate ($c_2 \equiv 0$).

In the light of Eq. (3.2), one may conclude that the $c_2 = 0$ general solution of recurrences (1.3) always specifies an exponentially increasing function $\psi(r)$. The only possibility for $\psi(r)$ to change sign at $E = E_{\text{phys}}$ lies just in the coefficient $c_1 = c_1(E)$ in (3.3). Obviously, the zeros of $\psi(\infty)$ and $c_1(E)$ coincide—the wave function has an asymptotic node if and only if the energy satisfies the condition $c_1(E) = 0$.

For sufficiently large index n, the zeros of $c_1(E)$ also coincide with the zeros of $p_n = p_n(E)$—this is obvious immediately, e.g., for formula (2.3). Thus, one may conclude that $E = E_{\text{phys}}$ if and only if Eq. (1.5) holds, at least in the limit $N \to \infty$. Obviously, a use of a sufficiently large but finite index N introduces a small error. Unfortunately, in practice, we are doing the computations far from the "real" asymptotic domain $n \gg 1$ [e.g., we do not have $n^{-\text{const}} \gg \exp(-\text{const}\sqrt{n})$, etc.]. Nevertheless, in practical applications the convergence of Eq. (1.5) is usually fairly good.[9]

B. $b \le 0$.

Proceeding in full analogy with the preceding case, we may write

$$q_n \sim c_1 \left(1 + \frac{E}{4|\alpha|\sqrt{n}}\right) + (-1)^n c_2 \left(1 - \frac{E}{4|\alpha|\sqrt{n}}\right),\quad n \gg 1 \tag{3.4}$$

for $b = 0$. In such a case, an estimate of the type

$$\psi(r) \sim \exp(+\tfrac{1}{4}\alpha^2 r^4)[c_1 O(r^{\text{const}}) + c_2 O(r^{\text{const}})]$$
$$\sim \exp(\tfrac{1}{4}\alpha^2 r^4) O(r^{\text{const}}),\ r \gg 1 \tag{3.5}$$

shows that the sign of $\psi(\infty)$ becomes indeterminate. From Eq. (1.5), we would get merely $c_1 = (-1)^{N+1} c_2 = +c_2$ or $-c_2$, so that one of the exponentials in $\psi(r)$ remains unsuppressed for $r \to \infty$. The wave function becomes manifestly unphysical in this case.

For $b < 0$ and $n \gg 1$, the exponential suppression will now "swallow up" the coefficient c_1 in Eq. (2.11). Unfortunately, the two dominant exponentials compensate each other in the remaining part of asymptotic form (3.1). For $r \to \infty$, the difference between the physical and unphysical asymptotic behaviors disappears.

In analogy with the similar results obtained in a slightly different problem by Masson,[4] we may try to replace Eq. (1.5) by another condition obtainable, e.g., by an analytic continuation or fixed-point expansion.[9] This lies beyond the scope of the present paper.

IV. THE MODIFIED EXPONENTIAL FACTOR

A. The choice of wave functions

We may notice that the indeterminate character of the $b \le 0$ asymptotics of Sec. III B is in fact related merely to the sign of β in (2.11). Vice versa, whenever we choose β as a parameter independent of the coupling b, we may hope for an improved behavior of the corresponding wave functions.

Technically, the above-mentioned modification is extremely easy. When one denotes $\bar{\beta} = b/(2\alpha^2)$ and assumes that $\beta \ne \bar{\beta}$ in general, an insertion of (1.2) in (1.1) leads merely to a slightly modified form of the recurrences (1.3):

$$B_n p_{n+1} - A_n p_n - C_n p_{n-1} - D_n p_{n-2} = 0,\ n = 0,1,\ldots\ . \tag{4.1}$$

Here, $D_n = D_0 = 2\alpha^2(\bar{\beta} - \beta)$ is nonzero and the difference equation (4.1) is in general of the third order.[10]

Of course, a transition to four-term recurrences does not alter the general form of their solution (1.4). Indeed, the initial conditions $p_{-1} = p_{-2} = 0$ make this solution unique, with the explicit determinantal form

$$p_{n+1} = \frac{\Gamma(l+\frac{3}{2}) p_0}{4^{n+1}(n+1)!\,\Gamma(n+l+\frac{5}{2})} \det \begin{pmatrix} A_0 & -B_0 & & \\ \cdots & & & \\ D_k & C_k & A_k & -B_k \\ & \cdots & & \\ & D_n & C_n & A_n \end{pmatrix},\ n = 0,1,\ldots\ . \tag{4.2}$$

In the $n\to\infty$ asymptotic region, we may proceed in an almost complete analogy with Sec. II. Indeed, (unchanged) parametrization (2.3) gives the difference equations

$$q_{n+1}-q_{n-1}=Q_nq_n+R_nq_{n-2}\ , \tag{4.3}$$

$$R_n=\frac{(\bar\beta-\beta)\Gamma(n/2+v-1)\Gamma((n+1)/2)\Gamma((n-1)/2+t)}{2\alpha\sqrt{2}\Gamma((n+1)/2+v)\Gamma(n/2)\Gamma(n/2+t-1)}$$

$$\approx\frac{\bar\beta-\beta}{2\alpha\sqrt{n}}+O(n^{-3/2}),\ q_{-1}=q_{-2}=0,\ n=0,1,\dots,$$

containing Eq. (2.4) as a special case with $\beta=\bar\beta$. Along the same lines, we may also obtain the extension of Eq. (2.9),

$$q_n=\exp\left[\frac{\beta+\bar\beta}{2\alpha}\sqrt{n}\right],\ n\gg1,\ \mathrm{sgn}\alpha=\pm1\ . \tag{4.4}$$

Now, the first nontrivial problem may be formulated as a necessity to find the third independent solution to the four-term recurrences (4.1).

Without going into detail,[10] we may notice that the missing solutions of Eq. (4.1) may be parametrized via a formula complementing Eq. (2.3):

$$p_n=\left[\frac{\beta-\bar\beta}{2}\right]^n\frac{q_n}{n!},\ n=0,1,\dots\ . \tag{4.5}$$

The third independent reformulation of Eq. (4.1) is then obtained:

$$q_n-q_{n-1}=\frac{1}{n}\left[\frac{\bar\beta^2-\beta^2}{4\alpha^2}q_n+\text{corrections}\right],\ n\gg1\ . \tag{4.6}$$

Its asymptotic solution

$$q_n=n^{(\bar\beta^2-\beta^2)/(4\alpha^2)},\ n\gg1 \tag{4.7}$$

represents the third independent asymptotic component of the general solution of Eq. (4.1):

$$p_n=\left[c_1\exp\left[\frac{\gamma}{|\alpha|}\sqrt{n}\right]+(-1)^nc_2\exp\left[-\frac{\gamma}{|\alpha|}\sqrt{n}\right]\right]\times\frac{\Gamma(v+\frac12n)}{p(1+\frac12n)\Gamma(t+\frac12n)}\left[\frac{|\alpha|}{\sqrt2}\right]^n+c_3\frac{(\beta-\bar\beta)^n}{2^nn!}n^{(\bar\beta^2-\beta^2)/(4\alpha^2)},\ n\gg1,\ \gamma=\tfrac12(\beta+\bar\beta)\ . \tag{4.8}$$

Fortunately, the third component becomes asymptotically negligible compared to the preceding two terms. Thus, it may be omitted from all the forthcoming formulas. We may conclude that Eq. (2.11) remains valid in the present case as well. The only difference lies in the modified interpretation of the parameter β.

B. Formulation and proof of the new Hill-determinant prescription

In our ansatz (1.2) with the free parameter $\beta\neq\bar\beta$, let us choose β such that $\gamma>0$:

$$\beta>-\bar\beta\ . \tag{4.9}$$

Then, the asymptotic formula (4.8) will become analogous to Eq. (3.3):

$$p_n\sim c_1\frac{\Gamma(v+\frac12n)}{\Gamma(1+\frac12n)\Gamma(t+\frac12n)}\left[\frac{|\alpha|}{\sqrt2}\right]^n\exp\left[\frac{\gamma}{|\alpha|}\sqrt{n}\right]+\text{corrections},\ n\gg1\ . \tag{4.10}$$

As a consequence, the oscillation theorem for $\psi(r)$, $r\to\infty$ becomes again equivalent to the eigenvalue condition $c_1(E)=0$, i.e., up to a nonzero factor in (4.10), to the old Hill-determinant condition $p_{N+1}=0$, $N\gg1$. With the new form of the corresponding matrix $\mathcal{H}_n$, we have

$$\det\begin{pmatrix}A_0 & -B_0 & & & & \\ \dots & & & & & \\ D_k & C_k & A_k & -B_k & & \\ & \dots & & & & \\ & & & D_N & C_N & A_N\end{pmatrix}=0,\ N\gg1\ . \tag{4.11}$$

This is our final equation—it defines the physical spectrum of energies (exactly in the limit $N\to\infty$).

Whenever $b>0$, we may return to the old prescription and, choosing $\beta=\bar\beta>0$, reproduce precisely the algorithm of Singh *et al.*[3] Even in that case, a variation of $\beta\neq\bar\beta$ may be employed for an acceleration of convergence. For the "dangerous" couplings $b\leq0$, the condition (4.9) excludes the former choice: The four-term recurrences cannot be shortened to the three-term form within the framework of the method of Hill determinants.

V. SUMMARY

We have found for the potential $V(r)=ar^2+br^4+cr^6$ and its bound states, that the compact form of recurrences,[3] for $b\leq0$, leads to an indeterminate character of the asymptotic behavior of the wave functions $\psi(r)$ at $r\to\infty$. The Hill determinants may be used in the $b>0$ cases only.

We have also found that a less compact form of the Hill-determinant recurrences corresponds to a variable form of the asymptotics. As a consequence, an introduction of a free parameter in the basic ansatz for $\psi(r)$ may restore the validity of the Hill-determinant secular equation. This result may probably be extended to the various further potentials. In the present case, the condition of applicability of the Hill-determinant method is simple and has a form of inequality (4.9).

In a broader methodical context, the transformation of ordinary differential equation (1.1) into (a triplet of) an equivalent difference equation [cf., e.g., Eqs. (4.3) and (4.4)] proved to be a useful technical trick which simplifies understanding the underlying mathematics. In this setting, the essence of the method is almost trivial—we solve the difference Schrödinger equation and impose the physical "Hill-determinant" boundary conditions on p_n for $n\to\infty$.

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