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Failure of the Hill determinant method for the sextic anharmonic oscillator

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Abstract. An extended analysis of eigenvalues and wavefunctions resulting from the Hill determinant method is carried out for the one-dimensional sextic anharmonic oscillator. It is shown that, in spite of a seemingly natural ansatz of the method, irrelevant wavefunctions may appear, leading to incorrect eigenvalues. The domain of applicability of the method is limited and its practical use demands *a priori* investigation before concrete calculations of spectral characteristics. Effective variational calculations based on adequate trial functions are performed and comparison of the results of both approaches is presented.

1. Introduction

Polynomial potentials in non-relativistic quantum mechanics still attract attention in many areas of physics. Motivation comes from different problems, where the anharmonic character of the interaction plays an important role. Solution of most of these problems requires finding the corresponding energy spectrum, frequently only a part of it and, explicitly or implicitly, the wavefunctions. The possibility of writing down the solution in a compact form is unlikely [1] and thus it is necessary to tackle this task from the numerical point of view. Generally, many approaches have been developed, whose character ranges from perturbational, variational or recursive techniques to methods tailored to particular cases. Nevertheless, a common feature is observed, namely that evaluating eigenvalues are considerably faster and easier than reaching a comparable degree of precision of wavefunctions [2]. In consequence, this experience drew attention to the quality of wavefunctions or their approximants and to the proper assessment of their accuracy.

The present paper is not an attempt to add another algorithm to the list of the existing ones. Our objective is to demonstrate that analysing the wavefunctions first can avoid a lot of trouble that one may meet in evaluating energies. To show this in its full complexity is definitely beyond the scope of one paper. Instead, we shall discuss the so-called Hill determinant method applied to the one-dimensional sextic anharmonic oscillator (see e.g. [3] and references therein). We have chosen this specific combination for the following reasons. First, the Hill procedure proved to be deceitful as already shown in [4], because, while it may converge to the correct value,

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it need not converge at all and, worst of all, it may converge to the wrong value. It is worth noting that this method is currently used [5] in application to various potentials and having been properly adapted it gives correct results [6]. Simplicity and transparency of the algorithm together with its rate of convergence might account for its popularity. Second, the sextic anharmonic oscillator is a favourite object of investigation due to the relative diversity of physical situations it can model (one, two or three minima). This oscillator ranks among the so-called quasi-exactly-solvable problems (see [1] and historical references therein) and provides us with the richest variety of so-called terminated solutions of all polynomial potentials, so far as it is known. These solutions, having a form of a polynomial multiplied by an exponential function, serve as welcome reference points in our discussion and, in addition, it turns out that they divide the space of coupling constants into areas of similar behaviour. It is worth noting that these particular solutions also turned out to be of practical use in solving the quartic anharmonic oscillator [6].

The paper is organized in the following way. The next section reminds the reader of the construction of the Hill approximants and exposes the limited range of their applicability to energy level evaluation. Section 3 is devoted to comparison of the Hill approximants and the exact wavefunctions in different domains of the coupling constants and manifestation of their unfit structure. For the exact wavefunctions we employ the specially adapted variational functions that we regard as the most suitable trial functions for polynomial potentials because of the reliability and fast convergence of the procedure. We consider it useful to share our experience, which is presented in section 4.

2. Hill method

As already mentioned the sextic anharmonic oscillator

$$V(x) = \lambda_2 x^2 + \lambda_4 x^4 + \lambda_6 x^6 \qquad \lambda_6 > 0 \tag{1}$$

covers fairly diverse physical situations with one, two and three minima (a classification which can easily be seen from figure 1). If we scale off the leading coupling constant (i.e. $\lambda_6 = 1$), we are left with the two remaining ones, λ_2, λ_4. Into the addition, if the condition

$$(\tfrac{1}{4}\lambda_4^2 - \lambda_2) = 4n + 2\nu - 1 \qquad n = 1, 2, \ldots \tag{2}$$

is fulfilled, where $\nu = 0, 1$ according to the parity, the Schrödinger equation admits the first n solutions of a given parity of a form

$$\psi(x) = P_{n-1}(x) \mathrm{e}^{-x^4/4 - \lambda_4 x^2/4} \tag{3}$$

where P_n is a polynomial of the nth degree. They are sometimes called terminated solutions. In fact, potential (1) with condition (2) corresponds to one of the quasi-exactly-solvable problems and has a hidden $\mathrm{sl}_2(\mathbb{R})$ symmetry [1]. This explains the origin of the terminated solutions as a reflection of the existence of finite-dimensional representations of $\mathrm{sl}_2(\mathbb{R})$. Conditions (2) are represented as the broken curves in

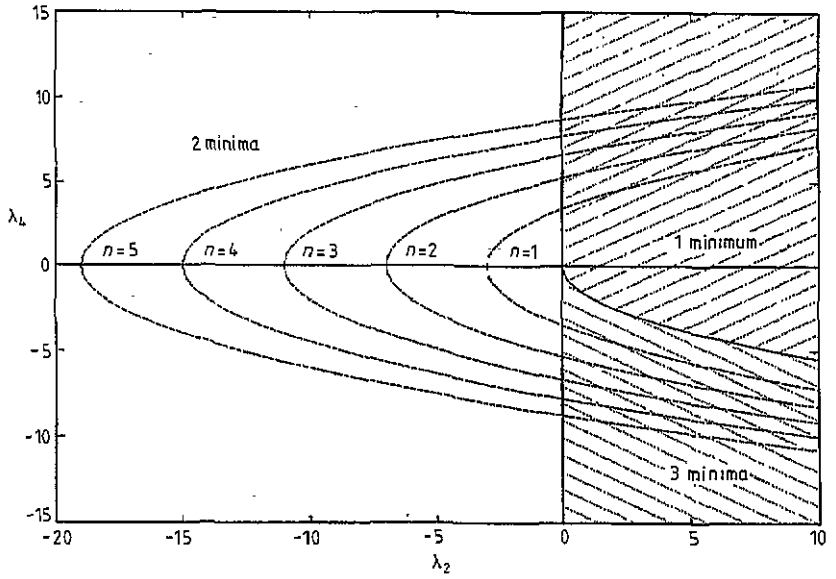

Figure 1. Areas in (λ_2, λ_4)-plane ($\lambda_6 = 1$), where the potential (1) has one, two or three minima. The broken parabolas indicate the terminated solutions (2) ($\nu = 0$).

figure 1 and they divide the (λ_2, λ_4) plane into a set of curved strips. For the sake of clarity, two salient cases, namely $\lambda_4 = 0$ and $\lambda_2 = 0$, will be dealt with separately.

Thus, we start with the potential

$$V(x) = x^6 + \lambda_2 x^2. \tag{4}$$

It is a natural tendency to factor out as much of the wavefunction in a compact form as we are able to. The asymptotic behaviour of wavefunctions at $|\, x \,| \longrightarrow \infty$ is given by

$$\psi(x) \longrightarrow \mathrm{e}^{-x^4/4} \tag{5}$$

and it is therefore quite natural to parametrize wavefunctions in the form

$$\psi(x) = f(x)\mathrm{e}^{-x^4/4}. \tag{6}$$

Now, we come to the Hill method considering, for example, eigenstates with positive parity, i.e. $\nu = 0$. The Hill method assumes that the wavefunctions are in the form (6) and looks for the factor f in the form of a power series†

$$f(x) = \sum a_i x^{2i}. \tag{7}$$

† Let us emphasize that the extraction of the exponential factor which controls the leading asymptotic behaviour of an eigenfunction, looks relevant, if one looks at this procedure from the point of view of perturbation theory of the 'nonlinearization' method [2]. Basically, if we wanted to find the factor f in this perturbation theory, it should lead to a convergent perturbation series.

Let us insert this ansatz into the Schrödinger equation with the potential (4). This converts the Schrödinger equation into a three-term recurrence relation for a_i and it is straightforward to express a_i in the form

$$a_i = \frac{(-1)^i}{(2i)!} H_i a_0 \tag{8}$$

where H_i is a determinant of a three-diagonal matrix

$$H_i = \begin{vmatrix} E & 2 & & & & \\ -\lambda_2 - 3 & E & 12 & & & \\ & -\lambda_2 - 7 & E & 30 & & \\ & & \ddots & \ddots & \ddots & \\ & & -\lambda_2 - 4i - 5 & & E & \end{vmatrix}. \tag{9}$$

The stumbling block lies in the following idea of the method. One assumes that the series (8) converges in the sense, that $a_i \to 0$ as $i \to \infty$. To check this assumption, one tentatively puts

$$a_N = 0 \tag{10}$$

and then finds those values of E for which this condition is fulfilled. This calculation is then repeated for successive values of N. These roots, $E^{(N)}$, should represent an approximation to the eigenvalues and the smallest real roots for each N should correspond to the ground-state energy. Let us compare the lowest real roots $E_{\min}^{(N)}, E_{\min}^{(N+1)}, E_{\min}^{(N+2)} \ldots$ first. If they do not change substantially, one hopes that convergent results have been reached. Then one repeats the same procedure for the next lowest roots (which should represent the second excited state energies) and so on. This is a crucial point of the method because it is not always so, namely the roots need not be real or need not converge, which makes the method ill defined [4, 8], although this is not obvious at first sight.

In order to demonstrate this, we have plotted, in figure 2, the dependence of the first five Hill approximants on the parameter λ_2 and compared them with the exact results for the ground-state energy (E_0), the second excited (E_2), and the fourth excited state (E_4). By exact results we refer to eigenenergies that can be obtained by several different methods producing identical results, however with different amounts of labour. It is a matter of personal preference in this instance that we have employed methods of a variational character to get these numbers in the simple case of (1). The procedure described later ranks among them too and seems to be optimal from many points of view.

The overall view of figure 2 shows that the Hill approximants we obtain are symmetric with respect to the λ_2 axis, i.e. $E \to -E$. This is so due to the symmetry of Hill determinants

$$H_i(\lambda_6, -\lambda_4, \lambda_2) = (-1)^i H_i(\lambda_6, \lambda_4, \lambda_2) \tag{11}$$

discussed in [4, 9].

Generally, the nth determinant provides us with n roots, which should approximate the first n eigenvalues of positive parity, E_0, E_2, ..., E_{2n-2}. The

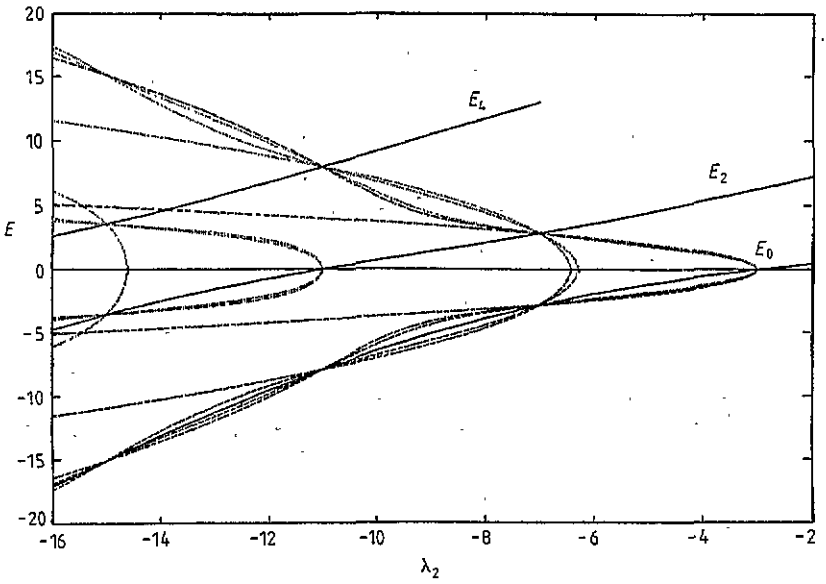

Figure 2. The dependence of the first five Hill approximants on λ_2. The first approximant remains identically zero. We tried to distinguish approximants to the ground state, E_0 (broken curve), the second excited state, E_2 (chain curve), and the fourth excited state, E_4 (dotted), but the correspondence makes sense only for the ground state. The full curves show the exact solutions.

first deficiency that we find is striking: *these energies are real only in certain intervals of* λ_2—all even determinants (9), (10) have only complex roots for $\lambda_2 > -3$—we thus have no real approximants to the energy in this interval (!). $\lambda_2 = -3$ is the rightmost point where all even approximants have at least two real roots. Points $\lambda_2 = -11, -19, \ldots$ represent a sequence of values of λ_2, where more roots become real, i.e. for $\lambda_2 < -11$ the approximants H_4, H_6, $H_8, \ldots$ have four real roots, for $\lambda_2 < -19$ the approximants H_6, $H_8, \ldots$ have six real roots etc.

Odd determinants behave in a slightly different way. There is always at least one real root, which remains identically zero due to symmetry (11). This root clearly has no physical significance in spite of the fact that it coincides with the exact solutions in points $\lambda_2 = -3, -11, -19, \ldots$. Similarly to the behaviour of the even approximations, new real roots start to appear at certain points. This time they do not form at one common point but at points forming a sequence that moves to the right with increasing n. Table 1 illustrates this situation by listing the points where new pairs of real roots appear.

Another remarkable feature is the coincidence of the exact and certain Hill solutions at points $\lambda_2 = -3, -7, -11, \ldots$. Indeed, all approximants intersect at these points with the exact energies and the wavefunctions also coinciding. This is not so surprising since this coincidence is present from the very beginning, cf (10) and (3).

Now, convergence is determined by this setting. We refer the reader to [4], which shows graphic representations of selected typical examples. Here we confine ourselves to commenting on convergence from a general point of view. The previously mentioned sequence $\lambda_2 = -3, -7, -11, \ldots$ separates areas of similar behaviour.

Table 1. The values of λ_2, where new pairs of roots of odd Hill approximants appear.

n	1st pair	2nd pair	3rd pair	4th pair	etc.
3	−6.4286				
5	−6.2924	−14.6081			
7	−6.2245	−14.4826	−22.6894		
9	−6.1824	−14.4125	−22.5766	−30.7374	
11	−6.1530	−14.3660	−22.5094	−30.6353	—
19	−6.0883	−14.2683	−22.3802	−30.4566	—
51	−6.0115	—	—	—	—
101	−5.9776	—	—	—	—

First, let us examine the interval $(-3,-7)$. Taking for example $\lambda_2 = -6$ and considering the ground state, we find the even approximants converge to the exact energy from below, while the odd determinants have no real roots up to $n < 65$ (!). Then they start to appear and approach the limit from above. As to the energy of the second excited state E_2, we encounter an example of a convergence to an unphysical value. Owing to the previously discussed symmetry (11), the values obtained for both even and odd approximants are the same as those for the ground state but with opposite sign. This implies that they converge in the way we have just depicted to $-E_0$. Figure 2, however, demonstrates that all roots (both even and odd) clearly lie below the exact value. On the other hand, if we do not go far from $\lambda_2 = -7$ to the right, the difference between the exact eigenenergy and $-E_0$ is small and our physical intuition does not give a reliable guarantee, which we find particularly vexing. We go through this result once more in section 3, examining the corresponding wavefunctions.

If we go to the interval $(-11,-7)$, the picture changes slightly. All approximants to the ground-state energy have real roots converging to the correct value; the even ones from above, the odd ones from below. Keeping the symmetry (11) in mind, it is clear that we have roots placed symmetrically with respect to the λ_2 axis. These roots converge at each point of the interval $(-11,-7)$, however, to $-E_0$. This curve 'interpolates' between exact values of E_2 and E_4 in the endpoints of this interval, but bears no relevance either to E_2 or to E_4. Notwithstanding this we always end up with convergent results that could be mistaken for the right answer, at least in close vicinity to the endpoints.

Instead of continuing this discussion (no basically new phenomenon is met—the main features repeat and become more involved and sophisticated) we look at another particular case of the original potential (1):

$$V(x) = x^6 + \lambda_4 x^4. \tag{12}$$

In figure 3 we plotted the energies of the first three levels and corresponding Hill approximants against λ_4. This potential displays another type of symmetry (cf (11)) which we are going to inspect: figure 3 is symmetric with respect to simultaneous change of sign of both axes, $\lambda_4 \to -\lambda_4$ and $E \to -E$. Let us note that the coincidence of the Hill approximants and the exact solutions are also present, now for $\lambda_4 = \pm 2\sqrt{3}, \pm 2\sqrt{7}, \pm 2\sqrt{11}, \ldots$, where this potential becomes quasi-exactly-solvable.

It is the point $\lambda_4 = 0$ which seems to be the most suitable starting point of our discussion. It is evident that the Hill approach fails completely in this case. Only odd determinants have a real root, which remains identically zero, while all eigenvalues are positive (!).

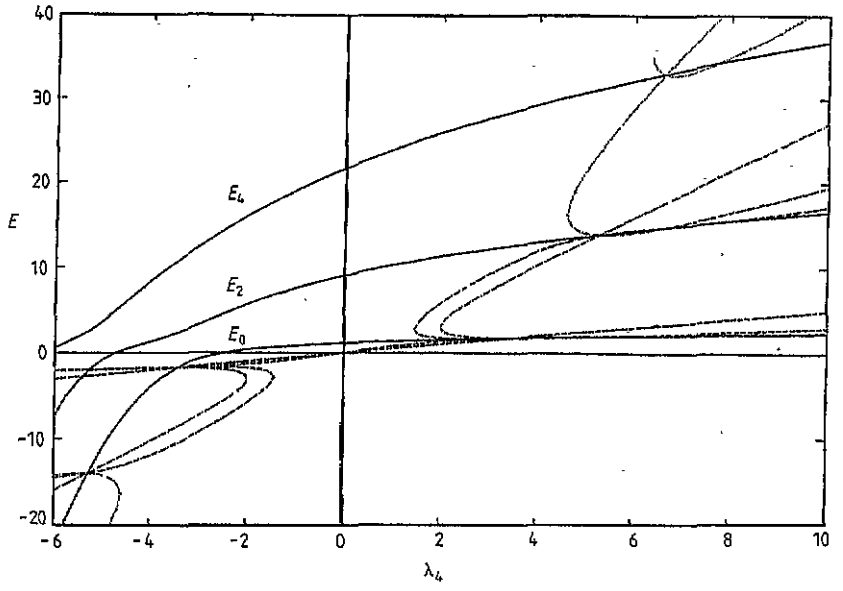

Figure 3. The dependence of the first five Hill approximants on λ_4. The curves have the same meaning as in figure 2.

In the direction of positive values the quality of approximation improves considerably. In the interval $(0, 2\sqrt{3})$ we obtain real roots for all odd determinants lying below the exact value. The even ones behave in an analogous manner as the odd approximants in figure 2, namely they have real roots beginning at some points, and these points form a sequence moving to the left. As already stated, the Hill method does not reproduce the physical result in the beginning, but succeeds for $\lambda_4 = 2\sqrt{3}$. This implies that the algorithm is inefficient near the beginning and gets better for higher λ_4. Be this as it may, if we reach a limit, it is the correct result. The second excited state is approximated correctly by even determinants from below. The closer to the point $2\sqrt{7}$, the sooner (with increasing n) odd approximants produce relevant values which converge to the correct answer from above. The picture develops according to the same pattern, only higher levels start to be involved.

The situation for negative λ_4 is quite different. As a consequence of the symmetry, we get convergence to the same results as for positive λ_4 but with the opposite sign. Thus, we have again found a case of convergence to an unphysical value; e.g., for λ_4 from the interval $(-2\sqrt{3}, 0)$ all physical energies lie above the Hill value. If we look further to the left the situation does not become any better. The symmetry of the Hill determinants does not reflect the descent of the physical levels, except for the terminated solutions.

The dependence of energy levels on the coupling constants we have just described is not encouraging. Therefore it is important to reveal the reason and to understand where this trouble occurs and why.

3. Analysis of wavefunctions

From the discussion of energy convergence it is not clear why we get such a peculiar

dependence on coupling constants when the original ansatz (7), (8), (10) seems to be so 'natural' and acceptable. This is, however, not so if we look at the corresponding wavefunctions. The condition $a_N = 0$ proves not to be 'natural' and imposes a severe restriction on the coefficients (8) of the pre-exponential factor (7). The wavefunctions resulting from the Hill procedure sometimes do not fit not only because of the wrong position of nodes, but also because their number is at variance with the oscillation (Sturm) theorem. An instance demonstrating it is listed in table 2.

Table 2. Number of nodes of the Hill wavefunctions ($\lambda_2 = 0$); n is the order of the Hill approximant and roots E_i are numbered in ascending order, i.e. they need not be in accordance with the oscillation theorem. Energies and wavefunctions are complex in the intervals of λ_4 not listed in this table.

	Intervals of λ_4			
$n = 2$				
	$(-\infty, -2\sqrt{3})$	$(-2\sqrt{3}, -2)$	$(2, 2\sqrt{3})$	$(2\sqrt{3}, +\infty)$
E_0	0	0	2	0
E_2	2	0	2	2
$n = 3$				
	$(-\infty, 2\sqrt{3})$	$(2\sqrt{3}, 5.110)$	$(5.110, +\infty)$	
E_0	0	2	0	
	$(-\infty, -5.383)$	$(-5.383, -2\sqrt{3})$	$(2\sqrt{3}, 5.383)$	$(5.383, +\infty)$
E_2	2	0	4	2
	$(-\infty, -6.907)$	$(-6.907, -6.163)$	$(-6.163, -2\sqrt{3})$	$(2\sqrt{3}, +\infty)$
E_4	0	4	2	4

It is also instructive to compare the coefficients of f in (8) obtained from the Hill procedure with those of the exact solutions. There is a disputable point: how to find the exact wavefunctions in this form. We propose a variational procedure whose details are left to section 4. A prescription for choosing adequate trial functions is given in [2] (for details cf [10]). Loosely speaking it leads to a variational procedure which is of non-linear Ritz character, optimizing the previously mentioned coefficients in the pre-exponential factor f and/or in the exponential factor in (3), preserving the correct asymptotics at large distances. Comparison of these coefficients with the Hill ones reveals how far from the physical situation these solutions are, cf table 3.

Table 3. The deviation of the Hill from exact wavefunctions for $V(x) = x^6 - 3x^4$ expressed via the coefficients of the pre-exponential factor (7).

	a_1	a_2	a_3	a_4	a_5	E_0
Exact	0.204 30	0.196 74	0.001 00	0.000 63	0.002 20	−0.6605
Hill	0.089 87	0.018 91	0.006 78	0.000 80	0.000 75	−1.6723

We should add a remark here. The wavefunction has been investigated since an early stage of the discussion. It has been explicitly demonstrated that the pre-exponential factor (7) with the coefficients (8) may lead to compensation for the exponential behaviour for $|x| \to \infty$, if E has a non-physical value and, furthermore, thus lead to deterioration of the square integrability of the wavefunction [8]. Another

interesting discussion of this point has been made by Hautot [3]. However, a detailed investigation of structure of wavefunction approximants has not yet been done as far as we know.

4. Variational calculations

Let us discuss this variational procedure. The quality of variational calculations depends heavily on trial functions. We start with the wavefunction with the correct asymptotical behaviour ($\lambda_6 = 1$) in the form

$$\psi(x) = g(x)\exp(-x^4/4 - \lambda_4 x^2/4) \tag{13}$$

The function $g(x)$ has no singularities at finite, real x (only zeros in the case of excited states) and grows no faster than a power of x at large x. Therefore let us represent g by the partial sum of the Taylor expansion (even parity)

$$g(x) = 1 + \sum_{n=1}^{N} a_n x^{2n}. \tag{14}$$

Now we will treat the coefficients a_n as variational parameters. In order to avoid unnecessary complexity we shall investigate the potential (4) first. At this point it is fitting to keep in mind the form of the terminated solutions (condition (2)). As already mentioned these solutions occur only for $\lambda_2 = -3, -7, -11, \ldots$; this sequence plays the role of reference points (see section 2). We listed the eigenfunctions explicitly for the first five points in table 4. Evidently, our procedure must reproduce them.

Let us now discuss the ground state. The first point we choose is $\lambda_2 = -3$, which reduces to $E_0 = 0$ and a mere exponential

$$\psi_1(x) = \mathrm{e}^{-x^4/4}. \tag{15}$$

It requires no variational parameter; direct evaluation confirms it. If we allow for one variational parameter, a_1, we get the results presented in table 5. It really reproduces the exact solutions in $\lambda_2 = -3$ and -7, gives two-digit agreement in energy with the exact solutions in the interval $(-7, -3)$. It gradually deteriorates at points distant from the endpoints in both directions. Reaching $\lambda_2 \simeq -12.857\,56$, the whole picture collapses, because the value of a_1 goes to infinity. It could also be demonstrated by explicit evaluation of the optimal a_1. Although the variational results for energy are fairly good, at least in certain areas, the trial wavefunctions for $\lambda_2 > -3$ are less adequate, because they have one node. We shall indicate later how to put it right.

Considering the second variational parameter a_2 enlarges the range of applicability on both sides (see table 5). The solution in $\lambda_2 = -11$ is reproduced exactly and the precision of energy is increased up to three digits in the interval $(-11, -3)$. However, the new wavefunctions are not devoid of the undesirable feature of having one node for $\lambda_2 > -3$. Inclusion of more coefficients a_n in the pre-exponential factor of the trial function (14) proceeds in this line; we get excellent agreement of variational and exact energies, fairly good wavefunctions in the interval specified roughly by points $\lambda_2 = -3$ and $\lambda_2 = -4n + 1$, if n variational parameters are taken into account and physically wrong behaviour outside this interval, which

Table 4. The first five sets of the terminated solutions of even parity of the quasi-exactly-solvable problem (i.e. $n = 1, \ldots, 5$ and $\nu = 0$) for $V(x) = x^6 + \lambda_2 x^2$.

n	λ_2	E_i	$\psi_i(x)\exp(-x^4/4)$
1	−3	$E_0 = 0$	1
2	−7	$E_0 = -2\sqrt{2}$	$1 + \sqrt{2}x^2$
		$E_2 = 2\sqrt{2}$	$1 - \sqrt{2}x^2$
3	−11	$E_0 = -8$	$1 + 4x^2 + 2x^4$
		$E_2 = 0$	$1 - \frac{2}{3}x^4$
		$E_4 = 8$	$1 - 4x^2 + 2x^4$
4	−15	$E_0 = -\sqrt{120 + 48\sqrt{5}}$	$1 + \sqrt{30 + 12\sqrt{5}}x^2 + (4 + 2\sqrt{5})x^4 + \frac{2}{15}\sqrt{150 + 60\sqrt{5}}x^6$
		$E_2 = -\sqrt{120 - 48\sqrt{5}}$	$1 + \sqrt{30 - 12\sqrt{5}}x^2 + (4 - 2\sqrt{5})x^4 - \frac{2}{15}\sqrt{150 - 60\sqrt{5}}x^6$
		$E_4 = \sqrt{120 - 48\sqrt{5}}$	$1 - \sqrt{30 - 12\sqrt{5}}x^2 + (4 - 2\sqrt{5})x^4 + \frac{2}{15}\sqrt{150 - 60\sqrt{5}}x^6$
		$E_4 = \sqrt{120 + 48\sqrt{5}}$	$1 - \sqrt{30 + 12\sqrt{5}}x^2 + (4 + 2\sqrt{5})x^4 - \frac{2}{15}\sqrt{150 + 60\sqrt{5}}x^6$
5	−19	$E_0 = -\sqrt{320 + 96\sqrt{6}}$	$1 + \sqrt{80 + 24\sqrt{6}}x^2 + (12 + 4\sqrt{6})x^4 + \left(\frac{1}{5} + \frac{2}{15}\sqrt{6}\right)\sqrt{320 + 96\sqrt{6}}x^6 + \left(\frac{4}{5} + \frac{8}{15}\sqrt{6}\right)x^8$
		$E_2 = -\sqrt{320 - 96\sqrt{6}}$	$1 + \sqrt{80 - 24\sqrt{6}}x^2 + (12 - 4\sqrt{6})x^4 + \left(\frac{1}{5} - \frac{2}{15}\sqrt{6}\right)\sqrt{320 - 96\sqrt{6}}x^6 + \left(\frac{4}{5} - \frac{8}{15}\sqrt{6}\right)x^8$
		$E_4 = 0$	$1 - \frac{4}{3}x^4 + \frac{4}{21}x^8$
		$E_6 = \sqrt{320 - 96\sqrt{6}}$	$1 - \sqrt{80 - 24\sqrt{6}}x^2 + (12 - 4\sqrt{6})x^4 + \left(-\frac{1}{5} + \frac{2}{15}\sqrt{6}\right)\sqrt{320 - 96\sqrt{6}}x^6 + \left(\frac{4}{5} - \frac{8}{15}\sqrt{6}\right)x^8$
		$E_8 = -\sqrt{320 + 96\sqrt{6}}$	$1 - \sqrt{80 + 24\sqrt{6}}x^2 + (12 + 4\sqrt{6})x^4 - \left(\frac{1}{5} + \frac{2}{15}\sqrt{6}\right)\sqrt{320 + 96\sqrt{6}}x^6 + \left(\frac{4}{5} + \frac{8}{15}\sqrt{6}\right)x^8$

Table 5. Values of energies $E_{\rm var}^{(0)}$, $E_{\rm var}^{(1)}$, $E_{\rm var}^{(2)}$, $E_{\rm var}^{(3)}$, $E_{\rm var}^{(4)}$ compared with the parameter λ_2 from the variational procedure with the trial function (13)–(14) having none, one, two, three and four variational parameters, $\beta = 0$. $E_{\rm ex}$ is the exact energy (see text).

λ_2	$E_{\rm var}^{(0)}$	$E_{\rm var}^{(1)}$	$E_{\rm var}^{(2)}$	$E_{\rm var}^{(3)}$	$E_{\rm var}^{(4)}$	$E_{\rm ex}$
3	2.8679	2.0947	1.961 45	1.939 34	1.936 02	1.935 48
2	2.3899	1.8071	1.713 89	1.699 54	1.697 52	1.697 21
1	1.9120	1.5047	1.445 27	1.436 88	1.435 78	1.435 62
0	1.4340	1.1822	1.149 55	1.145 38	1.144 87	1.144 80
−1	0.9560	0.832 19	0.818 41	0.816 84	0.816 67	0.816 65
−2	0.4780	0.443 53	0.440 41	0.440 10	0.440 07	0.440 06
−3	0.0000	0.000 00	0.000 00	0.000 00	0.000 00	0.000 00
−4	−0.4780	−0.521 22	−0.523 13	−0.523 26	−0.523 26	−0.523 26
−5	−0.9560	−1.1490	−1.153 30	−1.153 52	−1.153 53	−1.153 54
−6	−1.4340	−1.9125	−1.915 35	−1.915 46	−1.915 46	−1.915 46
−7	−1.9120	−2.8284	−2.828 43	−2.828 43	−2.828 43	−2.828 41
−8	−2.3899	−3.8914	−3.900 48	−3.900 63	−3.900 63	−3.900 64

is especially annoying for positive λ_2. Summarizing this part, we can say that the method works principally well, but we would appreciate even higher efficiency and last but not least a wider range of applicability.

In order to achieve this we should somehow simulate the inclusion of more variational parameters in a reasonable way. To this end let us modify the exponential factor in (13) by a quadratic term with an additional variational parameter β:

$$\psi(x) = g(x)\exp(-x^4/4 - \beta x^2/2). \tag{16}$$

Clearly, such a term should influence all coefficients of $g(x)$ leaving the leading asymptotical behaviour unchanged. As the results show this simple trick does improve the quality of the trial function considerably. For instance, even putting $g(x) = 1$ and minimizing with respect to the parameter β increases the relative accuracy in energy by one order, giving, for example, two correct digits for such a distant point as $\lambda_2 = 10$. Adding another free parameter, namely a_1, we find an interesting picture, cf table 6. We reach three-digit agreement in energy in the interval $(-15, -3)$ and high accuracy (two digits) for $\lambda_2 > -3$. Evidently, the exact solutions and our variational results coincide for $\lambda_2 = -3$ and $\lambda_2 = -7$ (at $\beta = 0$). For $\lambda_2 = -15$ the trial wavefunction is incapable of describing the true answer. However, if $\lambda_2 \geqslant -3$, $a_1 = 0$ exactly; i.e. all the change is modelled by the quadratic term in the exponential in (16). It can be confirmed by analysing the solution of the corresponding equations

$$\frac{\partial E(\beta, a_1)}{\partial \beta} = 0 \qquad \frac{\partial E(\beta, a_1)}{\partial a_1} = 0. \tag{17}$$

The point $\lambda_2 = -3$ is important, because (17) has only one solution in the region $\lambda_2 \geqslant -3$ while two solutions for $\lambda_2 > -3$, one of them being the absolute minimum.

Table 6. Values of the ground-state energies $E^{(2)}_{0,\mathrm{var}}$, $E^{(3)}_{0,\mathrm{var}}$, $E^{(4)}_{0,\mathrm{var}}$, $E^{(5)}_{0,\mathrm{var}}$ $E^{(6)}_{0,\mathrm{var}}$ compared with the parameter λ_2 from the variational procedure with the trial function (13) and (14) having two, three, four, five and six variational parameters. E_{ex} is the exact energy (see text).

λ_2	$E^{(2)}_{0,\mathrm{var}}$	$E^{(3)}_{0,\mathrm{var}}$	$E^{(4)}_{0,\mathrm{var}}$	$E^{(5)}_{0,\mathrm{var}}$	$E^{(6)}_{0,\mathrm{var}}$	E_{ex}
3	1.946 212	1.935 517	1.935 517	1.935 482	1.935 482	1.935 483
2	1.707 632	1.697 241	1.697 241	1.697 208	1.697 208	1.697 208
1	1.445 160	1.435 654	1.435 654	1.435 625	1.435 625	1.435 625
0	1.152 624	1.144 825	1.144 825	1.144 803	1.144 803	1.144 802
−1	0.821 799	0.816 662	0.816 662	0.816 649	0.816 649	0.816 649
−2	0.441 990	0.440 073	0.440 073	0.440 068	0.440 068	0.440 068
−3	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
−4	−0.523 200	−0.523 200	−0.523 268	−0.523 268	−0.523 269	−0.523 269
−5	−1.153 410	−1.153 410	−1.153 538	−1.153 538	−1.153 538	−1.153 538
−6	−1.915 384	−1.915 384	−1.915 464	−1.915 464	−1.915 464	−1.915 464
−7	−2.828 427	−2.828 427	−2.828 427	−2.828 427	−2.828 427	−2.828 427
−8	−3.900 373	−3.900 632	−3.900 632	−3.900 635	−3.900 635	−3.900 635

Such a feature is also present if a_2 is included. We can reproduce the solution in $\lambda_2 = -11$ with this trial function (together with $\lambda_2 = -3$ and $\lambda_2 = -7$) and the optimal a_2 is exactly zero in $(-7, -3)$. Relatively high accuracy (four digits) is achieved in a fairly wide area of λ_2 and the corresponding wavefunctions have no nodes as expected (indicating thus that we proceed in the proper way). Taking a_3 into consideration shifts the interval in which $a_3 = 0$ to $(-11, -7)$ and so on. The

vanishing a_is manifest themselves in table 6 in repeated values of energy (i.e. including another variational parameter improves neither energy nor the wavefunction).

The corresponding variational calculations of the energies of the second excited states are shown in table 7. Products of the exponential function (16) and pre-exponential factors (14) have been used as trial fuctions. First, the calculation of the ground state has been performed and the resultant trial function was exploited as an approximate expression for the ground-state eigenfuction. Trial functions of the second excited state have also been chosen in the form (14), (16), orthogonal to the approximate ground-state functions already obtained. Tables 6 and 7 demonstrate the high quality of our choice of the trial functions yielding fairly accurate results.

Table 7. Values of energies $E^{(2)}_{2,\mathrm{var}}$, $E^{(3)}_{2,\mathrm{var}}$, $E^{(4)}_{2,\mathrm{var}}$, $E^{(5)}_{2,\mathrm{var}}$ of the second excited state compared with the parameter λ_2 from the variational procedure with the trial function (13)-(14) having two, three, four and five variational parameters. E_{ex} is the exact energy (see text).

λ_2	$E^{(2)}_{2,\mathrm{var}}$	$E^{(3)}_{2,\mathrm{var}}$	$E^{(4)}_{2,\mathrm{var}}$	$E^{(5)}_{2,\mathrm{var}}$	E_{ex}
3	11.735 082	11.735 082	11.681 219	11.681 219	11.680 971
2	10.887 343	10.887 343	10.836 685	10.836 685	10.836 460
1	10.013 347	10.013 347	9.966 820	9.966 820	9.966 622
0	9.114 685	9.114 685	9.073 251	9.073 251	9.073 085
−1	8.194 807	8.194 807	8.159 398	8.159 398	8.159 265
−2	7.259 881	7.259 881	7.231 300	7.231 300	7.231 201
−3	6.319 788	6.319 788	6.298 562	6.298 562	6.298 349
−4	5.388 823	5.388 823	5.375 008	5.375 008	5.374 970
−5	4.485 127	4.485 127	4.478 051	4.478 051	4.478 031
−6	3.627 373	3.627 373	3.625 342	3.625 342	3.625 331
−7	2.828 427	2.828 427	2.828 427	2.828 427	2.828 427
−8	2.089 236	2.086 570	2.086 570	2.086 528	2.086 528

Let us turn our attention to the following fact. Independent of the value of the parameter λ_2, the coefficients a_i in the pre-exponential factor (14) decrease quickly with growing i. In the case of the second excited state, this reflects the bifurcatory nature of the node position equation $g(x) = 0$ (see (14)). Apart from this it signals the non-algebraic nature of this equation for the values of λ_2 different from those corresponding to the quasi-exactly-solvable cases (see (2)). A similar phenomenon has already been observed for the multi-dimensional anharmonic asymmetric oscillator [11] and the Zeeman effect at hydrogen [10].

Table 8 illustrates the same from another point of view, namely it shows how fast (or slowly) a_1 reaches the correct value in different intervals of λ_2. The terminated solutions mark intervals in which we must allow for as many variational parameters as non-vanishing coefficients in the pre-exponential factor of the corresponding terminated wavefunctions. Higher as behave in the same way, only the number of variational parameters taken into account must be increased accordingly.

It is important to note here the following. If we know the exact eigenenergy (it is not important for the moment where or how we got it) and plug it in the Hill expressions for the coefficients a_is, we get reasonable (generically, non-vanishing) values of these coefficients. It destroys the original, stumbling assumption (10) of the Hill method. In other words, the Hill method is not suitable for finding the eigenvalues, but provides a good representation of the eigenfunctions, if the energy

Table 8. The convergence of the coefficient a_1 for the ground state with increasing the number of variational parameters $a_i, i = 1, 2, 3, 4, 5$. The quadratic term in x in the exponential factor of the trial function is included (see (16), $\beta \neq 0$ is admitted); the correct form of the pre-exponential factor (see (6), (7)) is reconstructed by expanding the exponential $e^{-\beta x^2}$ into the Taylor series and rearranging the powers of x. The exact values of terminated solutions of the quasi-exactly-solvable problem are marked by asterisks.

λ_2	1 par.	2 par.	3 par.	4 par.	5 par.
3	1.589 24	1.615 78	1.615 36	1.814 81	1.814 81
2	1.356 57	1.450 68	1.450 61	1.685 36	1.685 36
1	1.109 06	1.283 85	1.283 60	1.556 41	1.556 41
0	0.846 63	1.114 29	1.114 27	1.427 49	1.427 49
−1	0.570 93	0.940 07	0.940 07	1.294 91	1.294 91
−2	0.286 27	0.745 22	0.745 22	1.139 68	1.139 68
−3	0.000 00*	0.000 00*	0.000 00*	0.000 00*	0.000 00*
−4	0.604 86	0.604 86	1.050 46	1.050 47	1.132 27
−5	0.845 44	0.845 44	1.276 55	1.276 55	1.272 10
−6	1.094 89	1.094 89	1.484 70	1.484 70	1.494 51
−7	1.414 21*	1.414 21*	1.414 21*	1.414 21*	1.414 21*
−8	1.851 32	2.152 52	2.152 53	2.447 79	2.447 79

is already known. Comparing them with our variational wavefunctions we found that β is an indicator of the difference between variational and Hill coefficients a_i. If β is small, these two methods do not differ drastically. For λ_2 positive, however, we have large β, if the number of variational parameters is limited to five or six, and the corresponding coefficients differ substantially from the Hill ones. This demonstrates that we need many more Hill terms in order to achieve convergent results. The variational procedure produces more effective representation of the wavefunction in this case.

What happens if a non-zero λ_4 is admitted?—as a matter of fact, not much. In doing so we have, in fact, picked out a point in the (λ_2, λ_4) plane (see figure 1) belonging to one of those curved strips. And what was said in the case of $\lambda_4 = 0$ remains valid.

5. Conclusions

The Hill method was investigated from different standpoints. It has also been improved into more reliable forms that could be applicable in evaluating eigenenergies of various potentials. To our knowledge, nobody has analysed the corresponding wavefunctions in the same way as we have, which is the most reliable and most complex indication. We found that the Hill procedure is incorrect from this point of view. This might be surprising, because this method takes into account the proper asymptotic behaviour. Nevertheless the choice of coefficients in (8) means that their values are far from the true answer in many areas of coupling constants, as the comparison with our variational results shows.

One of the main aims of the paper was to find out the reason why wrong results emerge in such a simple and well established method. First, we showed that two types of problems can occur: the complexity of the eigenvalues and/or the breaking down the normal properties of eigenfunctions such as the number of nodes etc. We have explained that these problems are the consequences of the approximation of the

infinite-dimensional matrix by a sequence of finite-dimensional ones (see equation (8)). According to this, the exact coefficients in the pre-factor of a wavefunction (6) can have no concern at all to those calculated through the Hill method. Our results show that the convergence of Hill method calculations can be very slow and, even worse, can converge to the wrong values (see table 8 and figure 2). We localized the main reason for this phenomenon explicitly, demonstrating that in intermediate steps, the Jacobi matrices may not satisfy the condition of existence of real eigenvalues (see e.g. [12]). This means that the original Hill method possesses a non-obvious, intrinsic drawback: *the method does not contain a property which ensures the existence of only real eigenvalues at each intermediate step. However, making some modifications to the original Hill method and somehow removing this drawback, we are not guaranteed that there are no more hidden drawbacks, connected in such a way of approximation of the infinite-dimensional matrix by finite-dimensional ones.*

The struggle for some reliable reference data led us to a very effective and conceptually easy variational procedure, which is interesting in itself. The efficiency of these trial functions is not so surprising. If one treats them as inputs to the perturbation theory of the 'non-linearization' method [2, 10], they lead to a rapidly convergent iterative procedure. Such an analysis has been carried out in detail for the quarkonium potential [2].

Owing to the fact that our trial functions have the same form as the Hill functions we find a very rapid convergence in energy (the true asymptotic tail) and a controllable convergence rate for the wavefunctions. The procedure is linked to the terminated solutions in a natural way and thus provides us with the possibility of estimating the number of necessary variational parameters (determined by neighbouring terminated solutions). These features make our method a recommendable and well performing algorithm applicable to other polynomial potentials.

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