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The Hill determinant method in application to the sextic oscillator: limitations and improvement

M Tater

Institute of Nuclear Physics, Czechoslovak Academy of Sciences, CS 250 68 Řež, Czechoslovakia

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Abstract. Using the sextic anharmonic oscillator $ax^2+bx^4+cx^6$ as a testing ground it is shown why the Hill determinant method has a limited range of applicability. A possible improvement is suggested and discussed.

1. Introduction

The Hill method is a non-perturbative approach to the eigenvalue problem which gained certain popularity in numerical calculations of the energies of various potentials, e.g. the quartic anharmonic oscillator (Biswas *et al* 1971, 1973), the confinement potentials (Chaudhuri *et al* 1987), the rotating harmonic oscillator (Singh *et al* 1982) and the $\lambda x^2/(1+gx^2)$ potential (Hautot 1981, Chaudhuri and Mukherjee 1983). On the other hand, it has been pointed out that this method has a limited domain of applicability in the plane of couplings (Znojil 1982, Chaudhuri and Mukherjee 1984) and doubt has been expressed as to whether the boundary condition $\psi_n(x)\to 0$ as $|x|\to\infty$ is incorporated into the method or not (Flessas 1982, Chaudhuri 1983, Masson 1983). Recently, Chaudhuri and Mukherjee (1984) and Chaudhuri (1983) found an explicit example (employing a so-called terminated solution) when the Hill method fails to produce the correct eigenvalues. From this fact we can draw the conclusion that the results of the Hill method should be checked to see whether or not the normalisation condition is violated, and whether an upper bound on ψ_n has been derived to this end. This, however, leaves the problem unsolved, at least from the point of view of practical evaluation of the eigenvalues, because imposing this condition may eliminate spurious levels but says nothing about how to find the correct ones. Naturally, such objections rather limit the appeal of this method.

The aim of this paper is to reveal the underlying grounds and to attempt a remedy. We do not tackle the problem in its full complexity, but choose the sextic anharmonic oscillator as an illustrative example. We believe that it displays all of the salient features of the more general problem.

The sextic anharmonic oscillator, i.e. the system described by the Hamiltonian

$$H=p^2/2\mu+ax^2+bx^4+cx^6 \qquad c>0 \tag{1.1}$$

can serve as a useful model in certain situations of physical interest, or simply as a test for various methods. It has been used in calculations of the vibrational spectra of molecules (Lister *et al* 1978) and in a description of the behaviour of a ^{3}He-^{4}He mixture and so-called metamagnets near the tricritical point (Aragão de Carvalho

1977). Reviews of the physical background can be found in Kincaid and Cohen (1975) and Stryjewski and Giordano (1977). Eigenvalues of (1.1) were also compared with the results of resummation of perturbation series in field theory (Caswell 1979, Sobelman 1979).

In the following section it is shown that the Hill method is not equivalent to the eigenvalue problem

$$H\psi = E\psi \qquad \|\psi\| < \infty \tag{1.2}$$

because the eigenvectors need not have finite form. This basic fact ensures that the method can either converge to the correct value, converge to an incorrect value or need not converge at all. It is demonstrated in § 3 that the accuracy of the eigenvectors is not properly assessed or, to put it another way, the convergence of eigenvectors is not checked. This drawback provides a starting point for an improvement that ensures the convergence *a priori* and thus enlarges the range of applicability, which is the second objective of this paper. Comparison with other methods can be found in § 4. The Hill method and its modification is finally presented in a more general context in § 5.

2. Discussion of the Hill method

The problem (equation (1.2)) has been attacked by several authors using different methods. It was probably Singh *et al* (1978) who first drew attention to the controversial features of the Hill method. They applied the continued fraction technique to represent the Green function of (1.2). In this approach, eigenvalues are obtained as poles of the Green function. It can, however, be shown that the continued fraction technique is equivalent to the Hill method. they also found conditions for the existence of terminated solutions, i.e. relations $f_n(a, b, c, E) = 0$ under which ψ_n can be written as (polynomial) $\times \exp(-\alpha x^4/4 + \beta x^2/2)$. The corresponding eigenvalues occur as the nodes of the determinant of an $n \times n$ tridiagonal matrix.

Following Singh *et al*, ψ is written as

$$\psi(x) = \exp(-\alpha x^4/4 + \beta x^2/2) \sum_{N=0}^{\infty} a_N x^{2N+v} \tag{2.1}$$

$v = 0, 1$ according to the parity, and a new set of coupling constants is introduced:

$$\alpha = \left(\frac{2\mu c}{\hbar^2}\right)^{1/2} \qquad \beta = -\frac{b}{2}\left(\frac{2\mu}{\hbar^2 c}\right)^{1/2} \qquad \gamma = \left(\frac{2\mu}{\hbar^2 c}\right)^{1/2}\left(\frac{b^2}{4c} - a\right). \tag{2.2}$$

We convert the Schrödinger equation (1.2) to the recurrence relation

$$A_N a_{N+1} + B_N a_N + C_N a_{N-1} = 0 \tag{2.3}$$

with $a_{-1} = 0$ and

$$\begin{aligned} A_N &= (2N+v+2)(2N+v+1) \qquad & B_N &= \varepsilon + \beta(4N+2v+1) \\ C_N &= \alpha(\gamma - 4N - 2v + 1) \qquad & \varepsilon &= 2\mu E/\hbar^2. \end{aligned} \tag{2.4}$$

Now, it is usually required that the infinite determinant

$$\begin{vmatrix} B_0, & A_0, & & \\ C_1, & B_1, & A_1, & \\ & C_2, & B_2, & A_2, \\ & & \vdots & \vdots & \vdots \end{vmatrix} \tag{2.5}$$

vanishes in order 'to ensure a non-trivial solution' and it is claimed that this condition can be fulfilled for specific values of the parameter ε. This is, however, a misunderstanding, because non-trivial solutions exist for all values of ε, as was pointed out by Znojil (1982). The problem lies in confusing two different norms.

The above-mentioned requirement must be interpreted in the algebraic sense

$$\begin{pmatrix} B_0, & A_0, & & & \\ C_1, & B_1, & A_1, & & \\ & C_2, & B_2, & A_2, & \\ & \vdots & \vdots & & \vdots \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{2.6}$$

and it implies that the norm $\Sigma_{N=0}^{\infty} |a_N|^2$ must be used, and not the physically relevant norm $\int |\psi_n|^2 \, dx$ as is tacitly assumed. But the former norm imposes no additional restriction on ε. From this point of view the vanishing of the Hill determinant (2.5) is not well founded and one should not be surprised if it admits a non-physical result.

The standard technique for evaluation of roots of (2.5) is based on the belief that roots of successive minors of (2.5) tend toward the energy eigenvalues of (1.2). We introduce the following example that shows that this belief is not justified.

Drawing on investigations by Singh *et al* (1978), Znojil (1982) and Chaudhuri and Mukherjee (1984), we infer that the applicability of the method is limited to positive values of the subdominant coupling constant b. On the other hand, a continuous change of b to $-b$ must produce a smooth change in energy $E_n = E_n(b)$. For the sake of simplicity the harmonic term is dropped in our example, i.e. $a = 0$. Figure 1(a) shows the convergence of the Hill method at a point where it works well. Halving b (figure 1(b)) the first inconvenience is encountered, namely the first few even approximants have no real roots. This absence of real roots is not surprising in view of the non-symmetry of the matrix (2.5). Now, as b approaches 0 the number of even approximants without real roots increases rapidly and the method becomes inefficient, because besides this the convergence of the odd approximants also slows down conspicuously. In the case of $b = 0$ the even approximants have no real roots, while the odd ones have only one real root, which remains identically zero. Going to negative values of b (figure 1(c)) one can observe behaviour similar to that in figure 1(b): the first few even approximants are without real roots and since $N \geqslant N_{\min}(b)$, there is convergence to a certain value, which, however, is not the correct eigenvalue. $N_{\min}$ decreases with decreasing b (cf figures 1(c) and 1(d)).

This investigation revealed two facts which are worthy of mention. First, we note the symmetry relation that holds between approximants:

$$D_N(a, -b, c, -E) = (-1)^N D_N(a, b, c, E) \qquad N = 1, 2, \ldots \tag{2.7}$$

where D_N denotes the $N \times N$ minor of (2.5). It can be easily proved using the recurrence relation

$$D_N = B_{N-1} D_{N-1} - A_{N-2} C_{N-1} D_{N-2}. \tag{2.8}$$

Indeed, because $b \to -b$, $E \to -E$ implies $A_N \to A_N$, $B_N \to -B_N$, $C_N \to C_N$, and $D_1 \to -D_1$, $D_2 \to D_2$, one immediately arrives at (2.7). This symmetry causes that the approximants with $b < 0$ converge to $-E_n$ ($|b|$) instead of to $E_n(b)$.

Second, we note the dependence of the number of real roots on b. This dependence is plotted in figure 2. If we choose an N, e.g. $N = 4$, then $D_4(b)$ has no real root provided that $|b| < b_{02}$, has two real roots only if $b_{02} < |b| < b_{24}$ and has four real roots

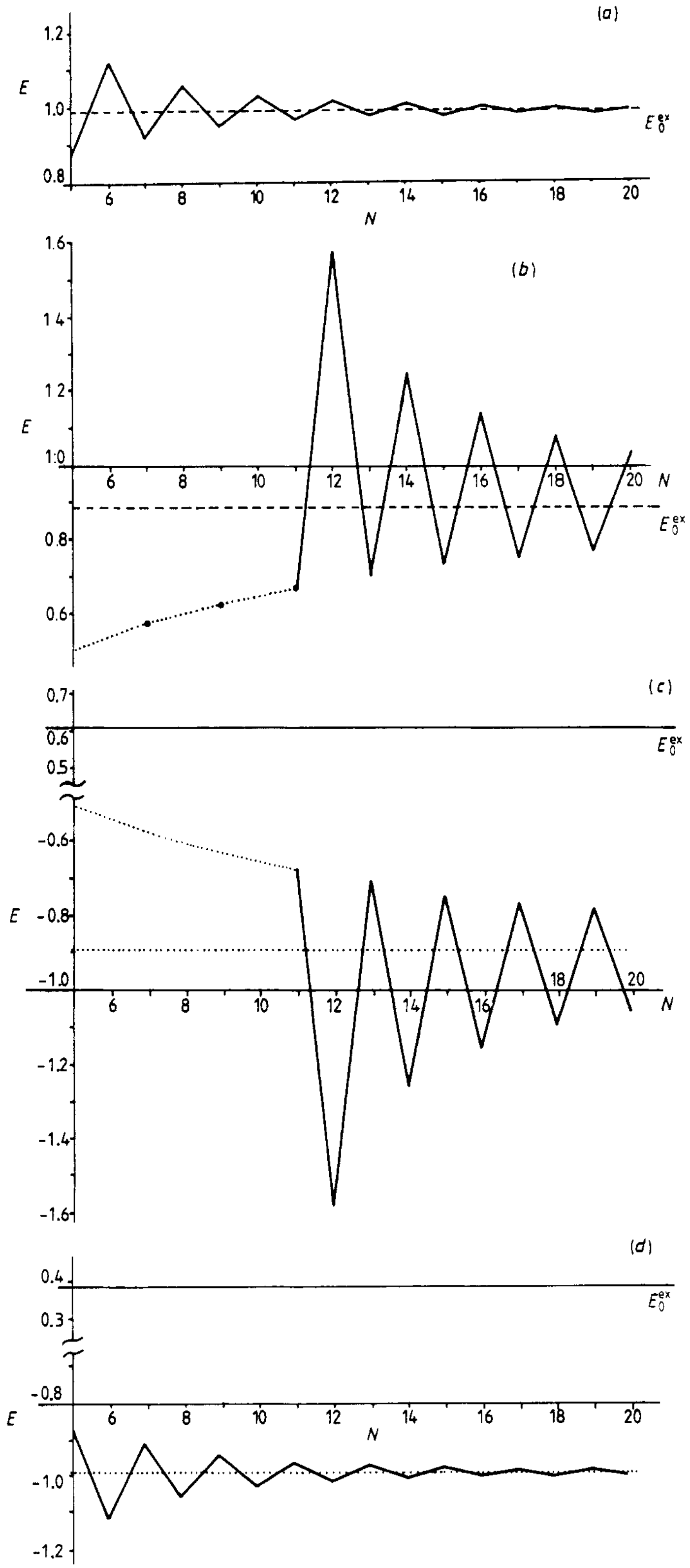

Figure 1. The convergence of the Hill method for $V(x) = bx^4 + x^6/5$. Figures (*a*), (*b*), (*c*), (*d*) show the convergence for different values of b, i.e. $b = 0.5$, 0.25, -0.25 and -0.5, respectively. Figures (*c*) and (*d*) demonstrate that the Hill method can converge to an incorrect value.

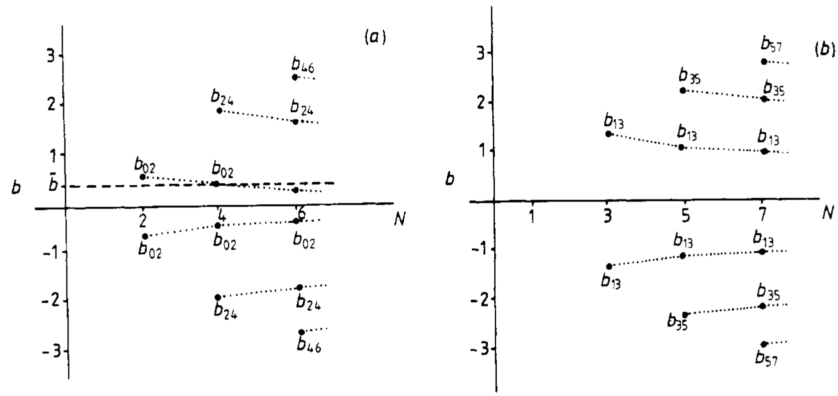

Figure 2. The dependence of the number of roots of Hill approximants on the subdominant coupling constant b. (a) shows the dependence of even approximants, and (b) the same for odd approximants for $V(x) = bx^4 + x^6/5$ and even parity.

if $|b| > b_{24}$. Alternatively, choosing some $\tilde{b}$, we can find the corresponding N which ensures that $D_M(\tilde{b})$, $M > N$, has the required number of real roots. The even approximants (figure 2(a)) and the odd approximants (figure 2(b)) are plotted separately. One should only keep in mind that the odd determinants are polynomials of odd degree in energy and thus they have always at least one real root. This fact also explains the asymmetry between the even and odd approximants in figures 1(b), (c). This asymmetry disappears when computing an excited state of the same parity. According to this author's experience it is always the greatest roots that cease to be real as $|b|$ increases (N being kept fixed), while the lower ones remain real and stable.

The above-mentioned behaviour in the case when $b = 0$ is now obvious in view of (2.8) and figure 2. More precisely, $B_{N-1} = \varepsilon$, $A_{N-2}C_{N-1} < 0$ ($N = 3, 4, \ldots$), $D_1 = \varepsilon$, $D_2 = \varepsilon^2 + 6\alpha(1 + 4v) > 0$, and hence

$$\begin{aligned} &D_N > 0 && \text{if } \varepsilon > 0 \\ &D_{2m} > 0 \text{ and } D_{2m+1} < 0 && \text{if } \varepsilon < 0 \\ &D_{2m} > 0 \text{ and } D_{2m+1} = 0 && \text{if } \varepsilon = 0. \end{aligned}$$

If we do not insist on the choice $\beta = -b(2\mu/\hbar^2 c)^{1/2}/2$ and let β be a free parameter, the relation (2.7) is still valid and now becomes

$$D_N(a, -b, c, -\beta, -E) = (-1)^N D_N(a, b, c, \beta, E) \tag{2.9}$$

(cf Znojil 1986). In this case we have a four-term recurrence instead of (2.3). Killingbeck (1986) showed that this recurrence relation produces the true and false energies as well, when one varies the parameter β. He was also able to find values of $\langle x^2 \rangle$ with minimal additional effort (see Killingbeck 1985) and thus to distinguish between the two cases, because spurious energies yield negative values for $\langle x^2 \rangle$.

Naturally, the question that now arises is whether we can discover a criterion (different from evaluating $\langle x^2 \rangle$) that can distinguish between spurious and correct eigenvalues. Previous investigations (Flessas 1982, Chaudhuri 1983) suggest that we should analyse the convergence of the corresponding eigenvectors.

3. Improvement of the method

It is a common experience that the divergent solution is always present to some degree in a numerical solution of an eigenvector when solving (1.2) in the differential equation formulation. The quality of a given result depends on the degree to which this component is suppressed. The Hill method shows similar behaviour, i.e. deterioration of convergence, as may be seen from table 1.

Table 1. The deterioration of the convergence of eigenvectors evaluated using the Hill method. The left column shows the correct results, while the right one the results for an energy very close to the exact one. The potential used is $V(x) = 2x^4 + x^6/5$.

N	$a_N/a_{N-1}(E_0 = 1.384\,633\,338\,37)$	$a_N/a_{N-1}(E = 1.384\,633\,3408)$
1	0.4257	0.4257
2	0.1002	0.1002
3	0.0027	0.0027
4	−0.0404	−0.0404
5	−0.0629	−0.0629
6	−0.0758	−0.0760
7	−0.0836	−0.0825
8	−0.0883	−0.0930
9	−0.0913	−0.0749
10	−0.0930	−0.1603
11	−0.0941	0.0275
12	−0.0941	1.1187

From this observation it follows that we have to carry out a more thorough analysis in order to obtain additional information about the ratio a_N/a_{N-1}. The determinantal formula of Singh *et al* (1978)

$$a_N = \frac{(-1)^N a_0}{A_0 \ldots A_{N-1}} \begin{vmatrix} B_0, & A_0, & & \\ C_1, & B_1, & A_1, & \\ & \cdots & & . \\ & & C_{N-1}, & B_{N-1} \end{vmatrix} \tag{3.1}$$

makes it possible to estimate the asymptotic behaviour of a_N and indicates that a_N/a_{N-1} must be negative in order to fulfil the physical requirement $\|\psi_n\| < \infty$. Alternating signs of a_N is a necessary condition, which allows for cancellation of exponents in (2.1). It would be desirable to know the asymptotic form of this ratio. In particular, it would enable us to check the convergence at each step. To this end a_N/a_{N-1} is expressed in a more convenient form

$$a_N = \frac{(-1)^N a_0}{A_0 \ldots A_{N-1}} \begin{vmatrix} 1, & & \\ \delta_0, & 1, & \\ & \cdots & \\ & \delta_{N-2}, & 1 \end{vmatrix} \begin{vmatrix} d_0, & \eta_0, & & \\ & d_1, & \eta_1, & \\ & & \cdots & \\ & & & d_{N-1} \end{vmatrix}. \tag{3.2}$$

The determinant on the RHS of (3.1) then equals the product $d_0 \ldots d_{N-1}$ and

$$\frac{a_N}{a_{N-1}} = -\frac{d_{N-1}}{A_{N-1}}. \tag{3.3}$$

The quantities d_N and d_{N-1} are related by the recurrence

$$d_N = B_N - A_{N-1}C_N/d_{N-1} \qquad d_0 = B_0. \tag{3.4}$$

It is only a matter of convenience to substitute $C_N f_N A_{N-1}$ for d_{N-1} and write

$$a_N/a_{N-1} = -C_N f_N \tag{3.5}$$

and

$$1/f_N + A_N C_{N+1} f_{N+1} = B_N. \tag{3.6}$$

Now, it is supposed that the mappings $f_N \to f_{N+1}$ are almost N independent in the asymptotic region and their fixed points are searched for. Keeping only leading-order terms, the dominant part of the dependence $f = f(N)$ is obtained. Proceeding this way $A_N C_{N+1} = -16\alpha N^3 + O(N^2)$, $B_N \approx O(N)$ and can therefore be omitted in this step. We assume

$$f_N = \varphi_0/N^\nu \tag{3.7}$$

where φ_0 and ν are to be adjusted, and substitute it into (3.6). Two possible solutions are obtained:

$$\nu = \tfrac{3}{2} \qquad \varphi_0 = \iota/4\alpha^{1/2} \qquad \text{where } \iota = \pm 1. \tag{3.8}$$

Going one step further, the first correction

$$f_N = (\varphi_0 + \varphi_1/N^{\nu'})/N^{3/2} \tag{3.9}$$

is found to be

$$\nu' = \tfrac{1}{2} \qquad \varphi_1 = -\beta/8\alpha. \tag{3.10}$$

This suggests that the general ansatz should be of the form

$$f_N = \frac{1}{N^{3/2}} \sum_{i=0}^{\infty} \frac{\varphi_i}{N^{i/2}}. \tag{3.11}$$

Inserting it into (3.6) and carrying out the comparison of the independent powers of N yields

$$\begin{aligned}
\varphi_2 &= \iota(\beta^2/\alpha + \gamma - 3 - 6v)/32\alpha^{1/2} \\
\varphi_3 &= -[\varepsilon + \beta^3/2\alpha + 4\beta^2 + \beta(\gamma - 3 - 4v)]/32\alpha \\
\varphi_4 &= \iota[3\beta^4/16\alpha^2 + 2\beta^3/\alpha + \beta^2(3\gamma - 5 - 10v)/8\alpha \\
&\qquad + (3\gamma^2 - 10\gamma - 20\gamma v + 120v - 5)/16]/32\alpha^{1/2} \\
\varphi_5 &= -[\beta^3(\gamma - 6v + 2)/8\alpha + (\beta^2 + \varepsilon/4)(\gamma - 6v) \\
&\qquad + \beta(\gamma^2 - 3\gamma - 6\gamma v + 30v + 43)/4]/32\alpha
\end{aligned} \tag{3.12}$$

and so on.

The sign ambiguity must be treated in conjunction with the already mentioned requirement $\|\psi_n\| < \infty$. Because $C_N < 0$ for sufficiently large N, (3.5) implies that f_N must be negative in the asymptotic region. It fixes ι to be -1; the second fixed point (i.e. $\iota = 1$) is not physically acceptable.

The transcendental equation (3.5) with (3.11) and (3.12) thus replaces the algebraic prescription $a_N = 0$ of the Hill method. Solving it, one gets not only eigenvalues but also physically acceptable eigenvectors with the same level of precision. Let us now turn our attention to tests of practicability.

4. Discussion of results

We begin with a comparison of the standard Hill method and the modified version (3.5) in the region where the former works. The precision of results found by means of (3.5) obviously depends on the number of terms in (3.11) taken into account. This is indicated by the superscript k:

$$f_N^{(k)} = \frac{1}{N^{3/2}} \sum_{i=0}^{k} \frac{\varphi_i}{N^{i/2}}. \tag{4.1}$$

From table 2 it is clearly seen that (3.5) is better than the Hill method and that the convergence improves with increasing k. The picture looks similar for the case of excited states (table 3). Figure 3 demonstrates that the new version gives correct results in the vicinity of $b=0$, which was the stumbling block of the original method. Table 4 repeats results of Caswell (1979) for the potential $V(x) = -x^2/2 + cx^6$. Comparison confirms the loss of precision for small values of c in the results obtained by resummation of the perturbation series (his results are measured with respect to the minimum of the potential well and the energies of table 4 are twice his energies).

Besides this, the modification proposed substantially extends the region of couplings in which a required precision of eigenenergies and eigenvectors may be achieved. It treats the corresponding wavefunction on the same level of accuracy as the energy. It practically removes the threat of overflow ($|D_N/D_{N-1}| \approx N^{3/2}$) because it needs only the ratio $a_N/a_{N-1} \approx d_{N-1}$, which is evaluated recursively.

The validity of the fixed point approximation is not limited to the sextic anharmonic oscillator. It provides, at least in principle, a quite general tool for finding the accumulation points of $f_N \to f_{N+1}$ mappings and the dependence on N in the physically acceptable one. It can be done for a given type of potential once and forever (if a greater number of terms in (3.11) is desired, symbolic language manipulations are advisable).

Table 2. The dependence of the ground-state energy obtained by the improved Hill method on N and k (see (4.1)) for $V(x) = 2x^4 + x^6/5$.

N	Hill	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$
5	1.384 638 724	1.384 629 676	1.384 636 021	1.384 631 682	1.384 632 982	1.384 631 896	1.384 633 499
7	1.384 633 565	1.384 633 222	1.384 633 412	1.384 633 299	1.384 633 328	1.384 633 308	1.384 633 333
8	1.384 633 280	1.384 633 365	1.384 633 322	1.384 633 346	1.384 633 341	1.384 633 344	1.384 633 340
10	1.384 633 333	1.384 633 340	1.348 633 337	1.384 633 339	1.384 633 339	1.384 633 339	1.384 633 339
11	1.384 633 340	1.384 633 338	1.384 633 339	1.384 633 338	1.384 633 338	1.384 633 338	1.384 633 338

Table 3. The dependence of E_6 obtained by the improved Hill method on N and k (see (4.1)) for $V(x) = 2x^4 + x^6/5$.

N	Hill	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$
15	36.547 158 03	36.525 255 11	36.532 098 26	36.529 229 01	36.527 912 60	36.528 447 24	36.528 306 70
20	36.527 934 48	36.528 757 47	36.528 542 48	36.528 620 07	36.528 651 03	36.528 640 63	36.528 643 17
25	36.528 668 09	36.528 628 47	36.528 637 46	36.528 634 56	36.528 633 49	36.528 633 84	36.528 633 77
30	36.528 632 07	36.528 634 41	36.528 633 94	36.528 634 08	36.528 634 13	36.528 634 11	36.528 634 11
31	36.528 635 28	36.528 633 92	36.528 634 19	36.528 634 11	36.528 634 08	36.528 634 09	36.528 634 09

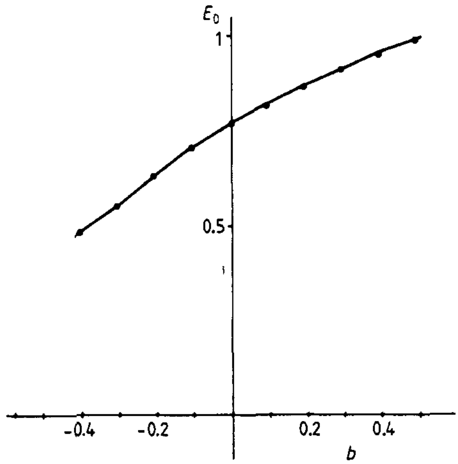

Figure 3. The smooth dependence $E_0 = E_0(b)$ in the vicinity of $b = 0$ for $V(x) = bx^4 + x^6/5$. The energy is evaluated using the improved Hill method (3.5).

Table 4. Energies E_0 and E_1 for $V(x) = -x^2/2 + cx^6$.

c	E_0	E_1
100	4.222 916 4	16.124 304
10	2.273 357 8	8.832 790 6
1	1.090 758 9	4.540 610 0
0.1	0.229 084 04	1.737 951 9
0.05	−0.044 241 316	1.006 303 7
0.02	−0.515 877 88	0.000 000 0
0.01	−1.090 331 6	−0.884 562 51
0.007	−1.525 984 3	−1.423 602 0
0.005	−2.055 248 9	−2.011 235 6

The method is, however, not fully devoid of unpleasant features. First, there is a question of the optimal cut-off k. It is always possible to find a minimal cut-off $k_{\min}$ such that the equation (3.5) has a root in the vicinity of the correct value, while for $k < k_{\min}$ it need not have any root. For given values of couplings a, b, c it is difficult to guess $k_{\min}$ in advance. Alternatively, we can find combinations of a, b, c such that more than the first few corrections (i.e. five or so) are necessary.

Second, in the domain of applicability of the Hill method, the correct value lies between two successive roots $E_n^{(N-1)}$ and $E_n^{(N)}$, where $D_M(E_n^{(M)}) = 0$, $M = N-1, N$. The ratio a_N/a_{N-1} is negative only in this interval, which may be very small for sufficiently large N and therefore the root could not be easily detectable by purely numerical means. In that case it is probably better to find $E_n^{(N-1)}$ and $E_n^{(N)}$ for a small N in order to estimate the value roughly, and then to switch to the new algorithm (3.5). In particular, terminated solutions, which represent the ultimate case in this respect, must be dealt with separately. These two points, however, do not represent very serious impediments.

The values in tables 2–4 were checked by two other methods. The first one has a variational character, namely the successive approximants provide upper bounds on eigenenergies. It is nothing but the prescription

$$\det(\mathcal{H}_{mn}) = 0 \tag{4.2}$$

where $(\mathcal{H}_{mn})$ is $H - E$ in the harmonic oscillator basis. This method is rather straightforward, but its convergence is slow. It is worth noting that this method can be modified in the same way (Znojil and Tater 1986) as the Hill method is modified in this paper, but the series analogous to (3.11) is in integral powers of $N^{-1/4}$.

The second method represents a natural generalisation of the method described in Znojil *et al* (1985), i.e. backward-run seven-term recurrences, which arise from (1.2) by writing ψ in the harmonic oscillator basis.

We have also done tests in order to compare the energies reported by other authors (Biswas *et al* 1971, 1973, Hioe *et al* 1976) and no difference has been found. On the other hand, the method proposed by Ginsburg (1982) leads to the same results as the Hill method when the correct asymptotics are used, i.e. $\exp(-\alpha x^4/4 + \beta x^2/2)$ is used as his weight function. This is not surprising, because one then gets the same recurrence relation (2.3), and requiring $a_N(E) = 0$ and choosing $a_{N-1} = \kappa$, where κ is a scaling constant, a_0 can be written as

$$a_0 = \frac{(-1)^N \kappa}{A_1 \ldots A_{N-1}} \begin{vmatrix} B_1, & A_1, & & \\ C_2, & B_2, & A_2, & \\ & & \ldots & \\ & & C_{N-1}, & B_{N-1} \end{vmatrix}. \tag{4.3}$$

It remains now to fulfil $A_0 a_1 + B_0 a_0 = 0$, i.e. the condition that determines the energy. Insertion of (4.3) and a similar expression for a_1 into it yields

$$\frac{(-1)^N D_N}{A_0 \ldots A_{N-1}} = 0 \tag{4.4}$$

which proves the above-mentioned assertion.

5. The Hill method revisited

Having investigated the Hill method and its improvement, it is now desirable to draw some general features that would be useful in other cases, i.e. to have an indication whether they are susceptible to an analogous modification. First, we are going to demonstrate that the Hill method corresponds to a particular choice of free parameter, which has no physical background.

To this end we re-express the coefficients a_N in a different form. This will be done in three steps. First of all we split the matrix in (2.6) into three factors

$$\begin{pmatrix} B_0, & A_0, & \\ C_1, & B_1, & A_1, \\ & & \ldots \end{pmatrix} = \begin{pmatrix} 1, & A_0 f_1, & \\ & 1, & A_1 f_2, \\ & & \ldots \end{pmatrix} \begin{pmatrix} 1/f_0 & & \\ & 1/f_1 & \\ & & \ldots \end{pmatrix} \begin{pmatrix} 1, & & \\ C_1 f_1, & 1, & \\ & & \ldots \end{pmatrix}. \tag{5.1}$$

Again, the quantities are related by the recurrence

$$1/f_N = B_N - C_{N+1} A_N f_{N+1}. \tag{5.2}$$

It is important to realise now that the splitting (5.1) is not unique. Indeed, we have a whole one-parametric family, because $f_0(\varepsilon)$ can be chosen arbitrarily, regardless of whether ε has a physical value or not.

The next step consists in substituting a new auxiliary vector $(w_0, w_1, \ldots)$ for $(a_0, a_1, \ldots)$:

$$w_0 = a_0/f_0 \qquad C_N a_{N-1} + A_N/f_N = w_N \qquad N = 1, 2, \ldots . \tag{5.3}$$

This reduces the three-term recurrences (2.3) to

$$w_0 = a_0/f_0 \qquad w_{N-1} + A_{N-1} f_N w_N = 0 \qquad N = 1, 2, \ldots \tag{5.4}$$

fully equivalent to (2.3). The coefficient w_N can be expressed as

$$w_N = (-1)^N w_0 / A_0 \ldots A_{N-1} f_1 \ldots f_N. \tag{5.5}$$

In the final step we complete the re-expression of a_N as a function of $f_0, \ldots, f_N$ and a_0. Combining (5.3) and (5.5) repeatedly we have

$$a_N = a_0 \sum_{j=0}^{N} \left[\left(\prod_{i=j+1}^{N} C_i f_i \right) \left(\prod_{i=0}^{j-1} A_i f_i \right)^{-1} \right] \tag{5.6}$$

where $\Pi_{i=m}^{n} = 1$ for $m > n$.

After these preparatory manipulations we are ready to discuss the Hill method. The requirement $a_N = 0$ can be fulfilled only by the choice $1/f_0 = 0$, as follows from (5.6). Once we start with some f_0, all f_N $(N > 0)$ are determined by (5.2), but there is no guarantee that we arrive at the accumulation point that ensures correct asymptotic behaviour of the wavefunction (cf § 2). Paralleling Znojil (1983) we see that we should start with f_N where $N \approx \infty$ in the physical fixed point and go backward to f_0.

It is worth noting here that Masson (1983) showed in the continued fraction formulation that the Hill method applied to the rotating harmonic oscillator can give physical results, but the continued fractions must be analytically continued onto the second sheet. This is carried out by replacing the tail of the continued fraction by an approximately correct tail. Such a modification, though theoretically illuminating, is of practical interest only under certain conditions that are generally hard to fulfil. Masson actually used the fixed point argumentation, but stayed with the forward-running implementation.

Hautot (1986) showed explicitly what happens in the case of the sextic anharmonic oscillator when we change $b \to -b$. If $b > 0$, the solution of recurrences (2.3) represents a dominated solution, while for $b < 0$ the solution becomes dominant and the corresponding wavefunction is not square integrable. His modification of the algorithm consists in letting α and β be free parameters (similar to Killingbeck), applying the generalised Miller algorithm to the recurrences for various values of α and β and then selecting the optimal values $\alpha_{\text{opt}}, \beta_{\text{opt}}$. This ensures that one arrives at a true eigenvalue, but the preparatory procedure need not be convenient for automatic computation. Our approach avoids this procedure, though the convergence need not be the optimal one.

Our improvement goes further. We do not start with f_∞, but with a finite N (depending on the number of terms in (3.11) taken into account, i.e. on k in (4.1)) thus making use of the knowledge of the asymptotic behaviour of f_N. It fixes the free parameter f_0 due to (5.2), obviously in a way different from the Hill method.

Finally, the last question that remains to be answered is whether there is a quantity sensitive to the applicability of the Hill method. To answer this question positively it is necessary to distinguish between two results. We leave the symbol a_N/a_{N-1} for the Hill approach and denote by T_N the same ratio obtained from the backward-run recurrences (equivalent to (2.3))

$$C_N/T_N + B_N + A_N T_{N+1} = 0 \qquad N = 1, 2, \ldots \tag{5.7}$$

initialised at infinity. These two quantities have a non-vanishing difference

$$t_N = a_N/a_{N-1} - T_N. \tag{5.8}$$

Indeed, expressing B_N from (2.3) and from (5.7) and comparing them we have

$$t_{N+1} = \frac{C_N}{A_N T_N} \frac{a_{N-1}}{a_N} t_N. \tag{5.9}$$

Extending (5.7) to $N = 0$ in a natural way we can write

$$-C_0/T_0 = B_0 + A_0 T_1 \tag{5.10}$$

and thus

$$t_1 = C_0/A_0 T_0. \tag{5.11}$$

Combining (5.9) and (5.11) yields

$$t_N = \frac{a_0}{a_{N-1}} \prod_{j=0}^{N-1} \frac{C_j}{A_j T_j} \tag{5.12}$$

which is a quantity accessible to more thorough analysis (cf Znojil 1982). If t_N vanishes the Hill method gives correct results. Otherwise it can be used for testing in a similar way as that in which the oscillation theorem is used.

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