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On the applicability of the Hill determinant method

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Abstract. We show that, contrarily to what Flessas and Anagnostatos claim in a recent Letter to the Editor of this Journal, the so-called Hill determinant method is perfectly suited to the numerical resolution of Schrödinger's equation.

1. Introduction

Recently Flessas and Anagnostatos (1982) claimed that the Hill determinant (HD) method was unable to furnish the correct spectrum of Schrödinger's equation. We intend to show that their argument is based on an inaccurate analysis of the problem so that their conclusions appear as completely misleading. It must be pointed out that two papers (Flessas 1979, 1981) dealing with the rotating harmonic oscillator have been similarly criticised by Fröman *et al* (1980) and Karlsson *et al* (1982).

2. The HD method

In order to clarify our argument we shall concentrate on the example treated by Flessas and Anagnostatos (1982), i.e. the calculation of the eigenvalues of the anharmonic oscillator:

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

We try the solution by setting

$$\psi = \exp(-\omega x^2) \sum_{k=0}^{\infty} C_k x^{2k} \tag{2}$$

(even states only; the odd states are treated similarly). It immediately follows that the C_k obey the third-order recurrence relation

$$(2k+1)(2k+2)C_{k+1} + (E - 2\omega - 8\omega k)C_k + (4\omega^2 - 1)C_{k-1} - \lambda C_{k-2} = 0 \tag{3}$$

with $C_{-1} = C_{-2} = C_{-3} = \ldots = 0$ and $k = 0, 1, 2, \ldots$. The role played by the parameter

ω will be mentioned later. The HD method as presented by Biswas *et al* (1971, 1973) consists of rewriting the recurrence in the form of an infinite linear homogeneous system with the unknowns $C_0, C_1, C_2, \ldots$ and then equating to zero the determinant D of the corresponding infinite matrix. That equation may be written as

$$D = \begin{vmatrix} E-2\omega & 2 & & & & \\ 4\omega^2-1 & E-10\omega & 12 & & & \\ -\lambda & 4\omega^2-1 & E-18\omega & 30 & & \\ & -\lambda & 4\omega^2-1 & E-26\omega & 56 & \\ & & \cdot & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \cdot \\ & & & & \cdot & \cdot \end{vmatrix} = 0.$$

The numerical calculation of the roots of D is performed by truncating D to its kth-order approximant $D^{(k)}$ and calculating the limit of the roots of $D^{(k)}$ when k tends to infinity. Banerjee (1978, 1979) first observed that the numerical value given to the dummy parameter ω has a great influence on the rapidity of the convergence process. It immediately appeared that the value $\omega = \frac{1}{2}$ chosen by Biswas *et al* (1971, 1973) was far from optimal. Hautot and Magnus (1979) explained that phenomenon and presented accurate theoretical estimates for the best ω values. Flessas and Anagnostatos (1982) contest the validity of the method: they claim that the calculated C_k do not necessarily lead to a square integrable function $\psi = \exp(-\omega x^2)\,\Sigma\, C_k x^{2k}$. However, we now proceed to show that they really do. A simple examination of recurrence (3) led Flessas and Anagnostatos to the conclusion that

$$C_{k+1}/C_k \sim (\lambda/4k^2)^{1/3}$$

(equation (7) of their paper (1982) where $\omega = \frac{1}{2}$ for the sake of simplicity). Then they crudely summed that asymptotic formula between 1 and k to obtain the following (wrong) asymptotic expression for C_k:

$$C_k \sim (\lambda/4)^{k/3}/k!^{2/3}.$$

Then introducing those C_k in (2) they arrived at the conclusion that the resulting ψ became unphysical when $\lambda > 0.5$. They therefore concluded the invalidity of the whole method described by Biswas *et al* (1971, 1973). That line of argument is erroneous because the correct asymptotic behaviour of C_k is quite different. The correct approach to the problem is as follows: recurrences like (3) have been studied by Birkhoff (1930) and Birkhoff and Trjitzinsky (1933) who showed that their solutions are asymptotic to expressions of the type $k^w a^k \exp(\alpha k^m + \beta k^n + \ldots)(\ln k)^r$. Denef and Piessens (1974) have shown how to calculate the coefficients $a, w, \alpha, \beta, \ldots$ which are present in these asymptotic scales and Hautot and Ploumhans (1979) have published extended tables of coefficients which are useful in practical examples. If we apply that procedure to our recurrence (3) we find that three independent solutions are asymptotic to

$$C_k^{(l)} \sim \frac{[\exp(2i\pi l/3)\lambda^{1/3}/9^{1/3}]^k}{\Gamma(2k/3)}\, k^{-4/3} \exp[\omega 2^{2/3}\lambda^{-1/3}\, e^{4i\pi l/3} k^{2/3} - \tfrac{1}{6}2^{1/3}(4\omega^2-3)\lambda^{-2/3}\, e^{2i\pi l/3} k^{1/3}], \qquad l = 0, 1, 2. \tag{4}$$

It is easily shown that $C_k^{(0)}$ is dominant when k is large and that both $C_k^{(1)}$ and $C_k^{(2)}$ are dominated: $|C_k^{(0)}| > |C_k^{(1)}| \sim |C_k^{(2)}|$. The general solution of recurrence (3) is therefore asymptotic to a linear combination of the $C_k^{(l)}$:

$$C_k \sim \alpha C_k^{(0)} + \beta C_k^{(1)} + \gamma C_k^{(2)}$$

where α, β and γ depend on E and on the initial conditions. We note that C_k is generally asymptotic to $C_k^{(0)}$ except if $\alpha = 0$.

A simple inspection of recurrence (3) shows that the limiting conditions $C_{-n} = 0$ $(n = 1, 2, \ldots)$ are automatically fulfilled if one chooses $C_{-1} = C_{-2} = 0$ so that α, β and γ are defined as functions of E except for an unimportant multiplicative constant. When E is taken at an arbitrary value α does not generally vanish and the corresponding C_k are dominant; when E is equal to well chosen values then $\alpha(E)$ vanishes and the corresponding C_k are subdominant. Now let us recall that Schrödinger's equation (1) has two linearly independant solutions which are asymptotic to

$$\psi_{\text{div}} \sim |x|^{-1} \exp(\lambda^{1/2}|x|^3/3),$$
$$\psi_{\text{conv}} \sim |x|^{-1} \exp(-\lambda^{1/2}|x|^3/3)$$

in each sector of the complex plane (Sibuya 1975).

When E is chosen arbitrarily the ψ function which vanishes at $x = +\infty$ generally diverges at $x = -\infty$. However, for well selected E values the same function is well behaved at $x = +\infty$ and $x = -\infty$: these are the eigenvalues of the problem. If we recall the starting expansion set for ψ, i.e. $\psi = \exp(-\omega x^2) \sum C_k x^{2k}$, it appears that ψ_{conv} and ψ_{div} are respectively generated by subdominant and dominant C_k sequences (a direct proof is reported in the appendix). From that viewpoint the quantised values of the energy parameter E are those for which a subdominant sequence C_k exists which is characterised by the initial conditions $C_{-n} = 0$: the resulting generated ψ function will behave like ψ_{conv} at $x = +\infty$ and also at $x = -\infty$ because of the even parity of the expression which defines ψ in terms of the C_k. We may express this in other words: the minimal (distinguished) solution of the recurrence generates the minimal (distinguished) solution of the associated differential equation. Because we need to determine a subdominant solution of the starting recurrence we now turn to its practical calculation through the generalised Miller algorithm.

Let us consider a linear homogeneous recurrence of order n written as

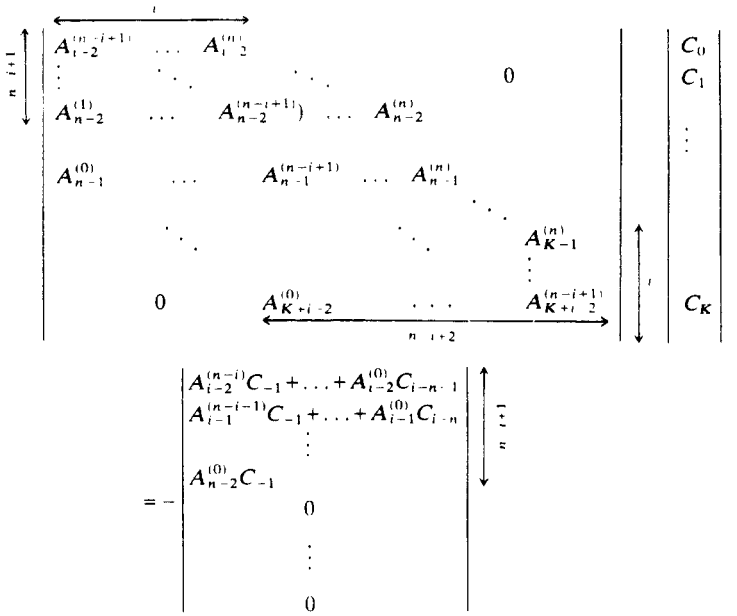
$$A_k^{(n)} C_{k+1} + A_k^{(n-1)} C_k + \ldots + A_k^{(0)} C_{k-n+1} = 0.$$

Let us consider a fundamental system of n independent solutions whose asymptotic behaviours are contrasted with the maximum. For k sufficiently large one has

$$|C_k^{(1)}| \geqslant |C_k^{(2)}| \geqslant \ldots \geqslant |C_k^{(n)}|.$$

It is well known (see e.g. Gautschi 1967) that the forward recursion is convenient for the stable numerical calculation of the dominant solution $C_k^{(1)}$ while the backward recursion stably calculates the dominated $C_k^{(n)}$. That procedure is known as Miller's algorithm (Miller 1952). The stable calculation of the intermediate solutions $C_k^{(2)} \ldots C_k^{(n-1)}$ is only possible through a generalised algorithm which has been studied by Oliver (1968). To calculate $C_k^{(i)}$ $(i \in (1, \ldots, n))$ one has to solve the following

linear system:



The value of K must be chosen large enough to ensure the required number nb of significant figures in $C_1^{(i)} \ldots C_k^{(i)}$:

$$nb \sim \log_{10}|C_K^{(i-1)} C_k^{(i)} / C_K^{(i)} C_k^{(i-1)}|. \tag{5}$$

A good estimate of K is generally obtained if $C_k^{(i)}$ is replaced by its asymptotic behaviour in (5).

Applying that algorithm to our problem in the case $i = 2$ (since we are only interested in a subdominant solution), we obtain the linear system

$$\begin{vmatrix} E-2\omega & 2 & & & & \\ 4\omega^2-1 & E-10\omega & 12 & & & \\ -\lambda & 4\omega^2-1 & E-18\omega & 30 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & & & & 2K(2K-1) \\ & & -\lambda & (4\omega^2-1) & E-2\omega-8\omega K & \end{vmatrix} \begin{vmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \\ C_K \end{vmatrix} = - \begin{vmatrix} (4\omega^2-1)C_{-1} - \lambda C_{-2} \\ -\lambda C_{-1} \\ 0 \\ \vdots \\ 0 \end{vmatrix}.$$

If we now impose the initial conditions $C_{-1} = C_{-2} = 0$ we retrieve a linear homogeneous system. Its nontrivial solution exists if and only if we require the vanishing of its determinant which is nothing other than the HD of the problem.

In summary, we have shown that equating the HD to zero is equivalent to searching for the subdominant solution of the associated recurrence compatible with $C_{-n} = 0$ ($n = 1, 2, \ldots$). That minimal solution is precisely the one which generates the minimal solution of the corresponding Schrödinger equation.

3. Discussion and conclusion

It is interesting to try to understand how HDM works. First of all we notice that Schrödinger's equation (1) is of order two while the associated recurrence (3) is of

order three, so there is no one-to-one correspondence between the solutions of (1) and (3). In fact, simple algebraical calculations indicate that the ψ function defined by (2) with the C_k solutions of recurrence (3) obeys the following non-homogeneous differential equation:

$$\psi''+(E-x^2-\lambda x^4)\psi=[\lambda C_{-2}+\lambda C_{-1}x^2-(4\omega^2-1)C_{-1}]\exp(-\omega x^2).$$

This equation coincides with the starting equation (1) if and only if we impose $C_{-1}=C_{-2}=0$. However, if we impose three initial conditions $C_{-2}=C_{-1}=0$ and $C_0=1$ (this last value being inessential) on the solution of a third-order recurrence like (3), we generate a dominant sequence C_k unless E takes one of those well selected values for which a subdominant solution of (3) exists characterised by $C_{-2}=C_{-1}=0$. Those values are precisely the eigenvalues of the problem since a dominant solution of (3) is unable to generate the required minimal solution of (1). In other words, recurrence (3) possesses a subdominant solution, for any E, but with non-vanishing starting values C_{-2} and C_{-1}. The eigenvalues are precisely found when the extra conditions $C_{-2}=C_{-1}=0$ are fulfilled. The correct interpretation to be given to HDM is therefore not to express a consistency condition on the infinite linear homogeneous system (3) as initially thought by Biswas *et al* (1971), but to get a finite approximation to a subdominant solution of the recurrence relation (3) which is consistent with the initialisation $C_{-1}=C_{-2}=0$.

Once the eigenvalues E have been determined the sequence C_k may be computed through the recursive scheme (3). However, great care must be taken not to use the simple forward recursion which is unstable for subdominant solutions (Gautschi 1967). Table 1 clearly illustrates that point where the correct values are given by the generalised Miller algorithm.

In conclusion, there is no reason to doubt that HDM leads to the correct eigenvalue spectrum in the case of anharmonic oscillators. We have tested many of them (Hautot and Magnus 1979) up to $x^2+\lambda x^{12}$ without encountering any difficulties; the calculated wavefunctions always exhibit the expected asymptotic behaviour at large x. The eigenvalues coincide with those which can be obtained by a simple method due to Killingbeck (1981) which discusses the changes of sign of $\psi(E,x)$ (for x large) when E increases and passes through an eigenvalue. It is remarkable that the same eigenvalues are obtained when the same discussion is made on $C_n(E)$ (for n large).

Appendix

Here we use a direct method to demonstrate that the dominant (subdominant) solution of recurrence (3) generates a ψ_{div} (ψ_{conv}) function.

Using the asymptotic behaviour of the C_k we may write ($l=0,1,2$)

$$\psi^{(l)}=\sum_{k=0}^{\infty}C_k^{(l)}\exp(-\omega x^2)x^{2k}\sim\sum\exp(-\omega x^2)a^k k^{-4/3}x^{2k}\exp(bk^{2/3}-ck^{1/3})/\Gamma(2k/3)$$

where we have set for the sake of brevity

$$a=\exp(2i\pi l/3)\lambda^{1/3}/9^{1/3},\qquad b=\omega 2^{1/3}\lambda^{-1/3}\exp(4i\pi l/3),$$
$$c=2^{1/3}\lambda^{-2/3}(4\omega^2-3)\exp(2i\pi l/3)/6.$$

Table 1. (a) Wrong C_k-values calculated (with six significant figures) through the simple forward recursion (3). The initial error ($\sim 10^{-6}$) is dramatically amplified so that for $k > 25$ the C_k become dominant, i.e. of unique sign. The number 25 is unimportant: it depends on the number of significant figures used in the calculation. (b) Correct C_k-values calculated through the generalised Miller algorithm. Note the expected alternation of signs. We have chosen $C_0 = 1$ in both cases.

k	$C_k^{(a)}$	$C_k^{(b)}$	k	$C_k^{(a)}$	$C_k^{(b)}$
1	−1.209E−01	−1.209E−01	21	−3.310E−23	−5.820E−23
2	−3.787E−02	−3.787E−02	22	−4.764E−24	−6.791E−24
3	6.873E−03	6.873E−03	23	5.738E−25	4.154E−25
4	3.634E−04	3.634E−04	24	1.600E−26	3.996E−27
5	−1.468E−04	−1.468E−04	25	−3.469E−28	−1.230E−27
6	4.066E−06	4.063E−06	26	9.513E−29	3.205E−29
7	1.529E−06	1.529E−06	27	6.244E−30	1.860E−30
8	−1.289E−07	−1.290E−07	28	1.622E−31	−1.346E−31
9	−6.735E−09	−6.747E−09	29	1.987E−32	2.992E−34
10	1.378E−09	1.377E−09	30	1.532E−33	2.725E−34
11	−2.090E−11	−2.113E−11	31	6.994E−35	−9.159E−36
12	−7.757E−12	−7.786E−12	32	4.611E−36	−2.440E−37
13	4.903E−13	4.868E−13	33	3.158E−37	2.449E−38
14	1.974E−14	1.936E−14	34	1.681E−38	−2.968E−40
15	−3.193E−15	−3.234E−15	35	9.498E−40	−3.360E−41
16	5.479E−17	5.057E−17	36	5.686E−41	1.477E−42
17	1.191E−17	1.150E−17	37	3.069E−42	1.184E−44
18	−6.263E−19	−6.649E−19	38	1.629E−43	−2.641E−45
19	−1.248E−20	−1.595E−20	39	8.849E−45	5.623E−47
20	3.212E−21	2.912E−21			

That series for $\psi^{(l)}$ is asymptotic to the following integral (x large):

$$\psi^{(l)} \sim \int a^z z^{-4/3} x^{2z} \exp(-\omega x^2 + bz^{2/3} - cz^{1/3}) \frac{dz}{\Gamma(2z/3)}.$$

Such an integral can be evaluated by the saddle point method:

$$\int \exp f(z)\, dz \sim (-2\pi/f''(z^*))^{1/2} \exp f(z^*)$$

where the saddle point z^* is defined by the equation $f'(z^*) = 0$. In our case we have used Stirling's formula:

$$f(z) \simeq -\omega x^2 + 2z \ln x + \{\tfrac{2}{3} + \ln[a(\tfrac{2}{3})^{2/3}]\}z - \tfrac{5}{6} \ln z - \tfrac{2}{3} z \ln z + bz^{2/3} - cz^{1/3}.$$

The unique saddle point of f is easily deduced asymptotic to

$$z^* \sim \tfrac{3}{2} a^{3/2} x^3.$$

Then we obtain the final result:

$$\psi^{(l)} \sim (-2\pi/f''(z^*))^{1/2} \exp f(z^*)$$
$$\sim x^{-1} \exp(\pm \lambda^{1/2} x^3/3) \qquad (x \sim +\infty)$$

where the + sign corresponds to the case $l = 0$ (dominant C_k: $\psi^{(l)} \sim \psi_{\text{div}}$) and the − sign corresponds to both cases $l = 1, 2$ (subdominant C_k: $\psi^{(l)} \sim \psi_{\text{conv}}$).

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