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LETTER TO THE EDITOR

Hill determinants and $1/N$ theory

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Abstract. A computationally efficient form of the Hill determinant method is devised, giving both E and $\langle x^2 \rangle$ values, and is used to test the accuracy of that method in the light of recent criticisms. l^{-1} and N^{-1} asymptotic theories are used to check the numerical results.

The Hill determinant method for the calculation of the energy eigenvalues of the Schrödinger equation has recently been the subject of some controversy. Biswas *et al* (1971, 1973) used the method to calculate energy levels for the perturbed harmonic oscillator, but Flessas and Anagnostatos (1982) criticised their work on mathematical grounds, claiming that the Hill determinant approach can lead to erroneous eigenvalues. In fact the energy values of Biswas *et al* (1971, 1973) can be checked by finite difference or other techniques and are of high accuracy, any small errors being attributable to the use of a fixed convergence factor $\exp(-\frac{1}{2}x^2)$ in their postulated form of the wavefunction. The use of a factor $\exp(-\frac{1}{2}\beta x^2)$, with β variable, removes this difficulty (Banerjee 1978). Hautot and Nicolas (1983) examined the arguments of Flessas and Anagnostatos (1982) and concluded that they were based on a wrong estimate of the asymptotic amplitude of the wavefunction associated with the Hill determinant eigenvalue. They concluded that the Hill determinant approach is fully justified on mathematical grounds. Killingbeck (1985a) commented on the controversy, taking the view that the most effective approach for the opponents of the method would be to produce an example which explicitly showed its failure. Chaudhuri (1985) has recently claimed to produce such an example. He treated a harmonic oscillator perturbed by a potential of form $bx^4 + cx^6$, with $b < 0$ and $c > 0$, and with a particular choice of the convergence factor $\exp(-\alpha x^4 + \beta x^2)$ in the postulated wavefunction. He showed that, for a special choice of the various parameters, it is possible to force the Hill determinant to have no positive eigenvalues while the Schrödinger equation has one negative eigenvalue (-1) and an infinite number of positive eigenvalues. We have verified by computation that truncating Chaudhuri's special case Hill determinant at any order gives the fixed eigenvalue -1 and no other real positive eigenvalues. Chaudhuri's convergence factor forces the matrix to be tridiagonal but leads to the production of wrong real eigenvalues. Firstly, we establish some useful mathematical properties of the Hill determinant approach and show how they are relevant to the points made by previous authors. Then we set out a very simple version of the Hill determinant approach and show that it leads to energy and $\langle x^2 \rangle$ values for a perturbed oscillator in any number of dimensions. Finally, we show both N^{-1} and l^{-1} type perturbation approaches for a perturbed oscillator, using the results to verify that the Hill determinant method can indeed give accurate eigenvalues for the perturbed oscillator problem.

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The most commonly used form for the wavefunction in the Hill determinant approach to perturbed one-dimensional oscillators is

$$\psi(x) = \exp(-\tfrac{1}{2}\beta x^2) \sum A_n x^{2n+p} \tag{1}$$

where p is the parity index (0 or 1) and β is varied to improve the rate of convergence of the resulting computations. When the ansatz (1) is used in a Schrödinger equation of the type

$$-D^2\psi + \sum_1^M V_m x^{2m}\psi = E\psi \tag{2}$$

the result is a recurrence relation for the A_n. For the case $M = 2$, for example, the recurrence relation has the matrix form

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 & 0 & \cdot \\ c_2 & d_2 & e_2 & 0 & 0 & \cdot \\ b_3 & c_3 & d_3 & e_3 & 0 & \cdot \\ 0 & b_4 & c_4 & d_4 & e_4 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \cdot \\ \cdot \end{bmatrix} = 0 \tag{3}$$

where E appears explicitly only in the diagonal d_n terms. If the assumption $A_N = 0$ is inserted into the recurrence relation, then the first $N+1$ equations of the set (3) are uncoupled from the rest and yield what looks like an $(N+1)\times(N+1)$ matrix eigenvalue problem. We denote by D_N the determinant of the upper left square matrix which is isolated when e_N is set equal to zero; inspection of (3) yields the recurrence relation

$$D_N = d_N D_{N-1} - e_{N-1}c_N D_{N-2} + e_{N-2}e_{N-1}b_N D_{N-3} \tag{4}$$

and also shows that the recurrence relation for the A_N is

$$e_N A_N = -d_N A_{N-1} - c_N A_{N-2} - b_N A_{N-2}. \tag{5}$$

Multiplying (5) by the product $(-1)^n e_1 e_2 \ldots e_{N-1}$ reveals that the quantities $(-1)^n e_1 e_2 \ldots e_N A_N$ and D_N obey the same recurrence relation and so may be taken to be proportional or equal, because of the arbitrary scaling factor which can be applied to the A_n. The relationship between the A_N and the D_N has been used by several of the authors whose work has already been cited, to transfer attention from the determinants D_N to the sequence A_N and the wavefunction $\psi(x)$ which it produces. Flessas and Anagnostatos (1982) pointed out that the A_N must tend to zero for any value of E as N tends to infinity, with the implication that no particular E values should be favoured by the requirement $A_N(E) = 0$. We wish to make two points about this part of their argument. Firstly, it is indubitably true that the $A_N(E)$ tend to zero for any real E, but this simply means that for any finite x the function $\psi(x)$ of equation (1) converges to a definite value; the power series approach (Killingbeck 1985b) uses this to obtain accurate energies by varying E to make $\psi(x)$ zero on a boundary at $x = L$. Secondly, the Hill determinant approach actually finds E values $E_n(N)$ such that $A_N(E) = 0$ for a fixed N and then checks whether the $E_n(N)$ attain limiting values as N is increased; this leads to definite energy values even though the $A_N(E)$ for any fixed E tend to zero as N is increased. With regard to the problem of how $\psi(x)$ depends on x and E, the published literature contains conflicting views. Biswas *et al* (1971) quoted formulae which appear to show that $\psi(x)$ is square integrable for any E, whereas Flessas and Anagnostatos (1982) claimed to establish that $\psi(x)$ is not

square integrable for any E if the potential in (2) takes the form $x^2+\lambda x^4$ with $\beta=1$ and $\lambda>\frac{1}{2}$. We might say that these two views represent opposite ends of the spectrum; Hautot and Nicolas (1983) took the view that the test $A_N(E)=0$ yields definite E values, together with A_n sequences which simulate the subdominant solutions of the recurrence relation (5); these subdominant solutions correspond to square integrable solutions of the Schrödinger equation (2). Hautot and Nicolas (1983) would thus regard as superfluous the suggestions of Flessas and Anagnostatos (1982) and of Chaudhuri (1985), that the E values for which $A_N(E)=0$ have to be further filtered by a special test which imposes square integrability conditions on the resulting $\psi(x)$. The mathematical arguments of Hautot and Nicolas (1983) appear sound to us and also agree with our computational experience using simple convergence factors. Before setting out our computational procedure and results, we make a few comments about the way in which the present work differs from previous work. Firstly, we do not attempt to force the square matrix in (3) to be tridiagonal; the relationship between the D_N and the A_N remains valid, as our discussion showed, even when the b_n or previous elements are non-zero. All that matters is that the only non-zero elements above the diagonal are the e_n, i.e. we have an upper Hessenberg matrix. Secondly, since the A_N recurrence relation is usually more simple than the D_N one it is preferable to use it, varying E to make $A_N(E)$ zero. Thirdly, by using the technique introduced by Killingbeck (1985a, b) it is possible to find the expectation values such as $\langle x^2\rangle$, $\langle x^4\rangle$, etc without reconstructing the A_n sequence associated with an eigenvalue. The accurate computation of the A_n, after E had been found, caused some difficulty for Biswas *et al* (1973); Hautot and Nicolas (1983) formulated a modified Miller algorithm to overcome the problem. We manage to bypass the difficulty by using the following approach.

We start from the form of the Schrödinger equation when an angular spherical harmonic factor Y_l^m has been factored out of the wavefunction. In three dimensions the equation is

$$-D^2\phi-2r^{-1}D\phi+l(l+1)\phi+V\phi=E\phi \tag{6}$$

where we take the radial potential $V(r)$ to have the form

$$V(r)=\sum V(m)r^m. \tag{7}$$

The regular solution to (6) will behave as r^l near the origin, so we postulate ϕ of the form

$$\phi(r)=\exp(-\tfrac{1}{2}\beta r^2)\sum_0^\infty A_n r^{n+l}. \tag{8}$$

This yields the recurrence relation

$$(n+2)(n+2l+3)A_{n+2}=[(2n+2l+3)\beta-E]A_n-\beta^2A_{n-2}+\sum V_mA_{n-m}. \tag{9}$$

By differentiating (9) with respect to E and V_m we can also obtain the recurrence relations for the quantities

$$B_N=\partial A_N/\partial E, \qquad C_N=\partial A_N/\partial V_m. \tag{10}$$

Since most of the coefficients are common to the three recurrence relations, it is computationally efficient to use them simultaneously. The calculation starts at $N=0$ with $A_0=1$ and all other A, B and C coefficients zero for $0>N>-M$. As each set

A_N, B_N, C_N is computed, the ratios

$$\Delta E_N = -A_N/B_N, \qquad \langle r^m\rangle_N = -C_N/B_N \tag{11}$$

are formed. These give the energy correction and the $\langle r^m\rangle$ estimate, and as N increases they settle down to fairly stable values, the degree of stability increasing as the energy estimate nears an eigenvalue. When the first few digits of E have stabilised the run is repeated using the corrected energy $E+\Delta E$; after a few iterations, accurate stable values of E and $\langle r^m\rangle$ result. The calculation is simply an application to the Hill determinant method of the techniques recently explained in detail by Killingbeck (1985a, b) with reference to power series and finite difference methods. The computation works well on an interactive microcomputer, since the operator can judge when the ΔE value has converged sufficiently to start the next run; starting from a very rough E estimate it is possible to obtain accurate E and $\langle r^2\rangle$ values in less than a minute for each state.

By studying the form of the Schrödinger equation in one and two dimensions, we found that the algorithm described above can be used in one, two or three dimensions by making the appropriate choice of l. In three dimensions l is the usual angular momentum value $(0, 1, 2, \ldots)$. In two dimensions l is set equal to $|m|-\frac{1}{2}$, where m is the magnetic quantum number. In one dimension, with only even powers of r (i.e. x) in the potential, $l=-1$ gives an even parity state and $l=0$ gives odd parity states. By comparison with the equations of Hikami and Brezin (1979) we also found that states of spherical symmetry in N dimensions can be treated by setting $l=\frac{1}{2}(N-3)$.

We now consider the N^{-1} and l^{-1} type perturbation approaches where the Schrödinger equation,

$$-D^2\psi + (Ar^{-2}+Br^4)\psi = E\psi, \tag{12}$$

is used, A and B being very large positive numbers. Physically this represents a situation in which a particle of large mass vibrates at the bottom of the deep potential well in the potential. The potential minimum is at a position given by $r^6=(A/2B)$ and the potential, expressed with respect to that minimum as origin, takes the form

$$V = \tfrac{3}{2}(2BA^2)^{1/3} + 6(4AB^2)^{1/3}x^2 + \ldots. \tag{13}$$

The harmonic oscillator approximation for the energy levels is thus

$$E_n = \tfrac{3}{2}(2BA^2)^{1/3} + 6^{1/2}(4AB^2)^{1/6}(2n+1) + \ldots. \tag{14}$$

Higher order terms could be calculated in principle, but the result (14) already suffices to give the first two terms in the N^{-1} and l^{-1} series which we require.

As a test case we looked at the Schrödinger equation (6) in three dimensions with $V(r)=\lambda l^{-1}r^4$, i.e. an l dependent potential. By setting $\phi = r^{-1}\psi$ in (6) and then using the change of variable $r=Rl^{1/2}$ we obtain the Schrödinger equation (12) with $A=l(l+1)$, $B=l^2\lambda$ but with the eigenvalue lE instead of E on the right. Setting these A and B values into (14) and expanding in powers of l gives a series for the eigenvalue of (6) when $V(r)=\lambda l^{-1}r^4$,

$$E_n(l) = \tfrac{3}{2}(2\lambda)^{1/3}l + (2\lambda)^{1/3}[1+6^{1/2}(2n+1)] + O(l^{-1}). \tag{15}$$

For spherically symmetric states in N dimensions the Schrödinger equation (6) generalises to the form

$$-D^2\phi - (N-1)r^{-1}D\phi + V(r)\phi = E\phi. \tag{16}$$

The function $r^{(N+1)/2}\phi$ is found to obey the equation (6) for the case $l=\frac{1}{2}(N-3)$, which leads to the rule already quoted. We can proceed as for the l^{-1} theory, except that we use the potential $V(r)=\lambda N^{-1}r^4$. The change of variable $r=RN^{1/2}$ leads to equation (12) with $A=\frac{1}{4}(N-1)(N-3)$, $B=\lambda N^2$. The use of (14) then gives the result

$$E_n(N)=\tfrac{3}{4}N\lambda^{1/3}+\lambda^{1/3}[(2n+1)6^{1/2}-2]+O(N^{-1}). \tag{17}$$

Table 1. Lowest eigenvalue of equation (6) for selected l ($V=l^{-1}r^4$).

l	E	$\langle r^2\rangle$
1	7.108 4442	1.333 4087
2	8.605 6487	2.153 8224
3	10.347 316	2.956 6586
4	12.159 017	3.754 6576
5	14.000 561	4.550 7492
10	23.349 854	8.523 2960
20	42.196 812	16.461 747
40	79.968 051	32.336 271
80	155.550 00	64.064 486
160	306.733 84	127.580 62
320	609.111 54	254.572 78

Table 2. Lowest s state energy in N dimensions ($V=N^{-1}r^4$).

N	E	$\langle r^2\rangle$
1	1.060 3621	0.362 022 65
2	1.861 0921	0.820 810 56
3	2.634 5461	1.300 3407
4	3.398 1502	1.788 1539
5	4.157 0434	2.280 0967
10	7.926 7576	4.762 1131
20	15.437 713	9.752 1488
40	30.443 495	19.746 934
80	60.446 466	39.744 274
160	120.447 97	79.742 938
320	240.448 73	159.742 30

Table 1 shows the ground-state energy for several l values in three dimensions and table 2 shows the lowest s state energy as a function of the number of dimensions. All numbers were calculated by the rapid Hill determinant method, a β value of 2 being adequate to give a good convergence rate throughout. The λ value was set equal to 1.

Numerical analysis of the results of table 1 gave for the first two coefficients in the series

$$E_0(l)=\sum_{1}^{-\infty}\varepsilon(n)l^n \tag{18}$$

the values $\varepsilon(0)=1.889\,88$, $\varepsilon(1)=4.346$. Using $n=0$ in (15) gives $\varepsilon(0)=1.889\,8816$, $\varepsilon(1)=4.346\,0847$, which confirms the accuracy of the Hill determinant eigenvalues.

For the N^{-1} series, we extracted from table 2 the coefficients $\varepsilon(0) = 0.750\ 000$, $\varepsilon(1) = 0.499\ 490$, $\varepsilon(2) = -0.2441$. Use of $n = 0$ in (17) gives $\varepsilon(0) = \frac{3}{4}$, $\varepsilon(1) = 0.499\ 4897$. From the analytic results quoted by Yaffe (1983), we deduce an $\varepsilon(2)$ value of $-0.244\ 1043$, which again indicates the accuracy of the numerical energies. Furthermore, the ratios $\langle r^2 \rangle l^{-1}$ and $\langle r^2 \rangle N^{-1}$ tend to the correct limiting values $(A/2B)^{1/3}$ given by the theory; at large l or N, the particle is localised at the bottom of the potential well.

Further calculations were performed to check the Hill determinant method. First, it was checked that the $(2n+1)$ factors in (15) and (17) do correctly describe the variation of the $\varepsilon(1)$ coefficient for the first few excited states. Second, the method was used for the potential x^2. For a wide range of β values (2-10) the correct energies and $\langle x^2 \rangle$ values of the harmonic oscillator were obtained. For $\beta \neq 1$, the exact wavefunction must be an infinite series, yet our results contradict the comment of Flessas and Anagnostatos (1982) that, for such a case, the Hill determinant approach would be unreliable. Third, we treated the special case potential $-2x^2 - 2x^4 + x^6$ which Chaudhuri (1985) used in his work. We quickly found the two lowest even parity energies -1 and 3.629 8265. The latter value correct Chaudhuri's value of 3.628 and shows that with the simple factor $\exp(-\frac{1}{2}\beta x^2)$ in the wavefunction, the anomalous behaviour specially contrived by Chaudhuri can be avoided; higher energy levels are also calculated easily.

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