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Residue-squaring diagonalisation method and the anharmonic oscillator

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Abstract. A recently-formulated residue-squaring method for perturbation problems is subjected to an exacting test in its application to the problem of diagonalising the Hamiltonian of the nonlinear oscillator with quartic anharmonicity. Unlike other methods, this new iterative diagonalisation method enables several eigenvalues to be calculated simultaneously with little more labour than for a single eigenvalue. Values obtained for the four lowest even-parity levels of the anharmonic oscillator from just two or three iterations are shown to agree well with earlier accurate calculations. An approximate analytical formula for the energy levels is also presented.

Keywords. Residue-squaring method; anharmonic oscillator; diagonalisation.

1. Introduction

In this paper a variant of the iterative method for perturbation problems proposed by one of us (Mathews 1975), is applied to the anharmonic oscillator described by the Hamiltonian $H = \frac{1}{2}x^2 + \frac{1}{2}p^2 + 4\lambda x^4$. The method is basically a prescription for taking a diagonal-dominant matrix to its diagonal form by a series of similarity transformations which reduce the off-diagonal part (of order λ compared to the diagonal part) successively to orders λ^2, λ^4, λ^8.... A study of the anharmonic oscillator by this method is of considerable interest, firstly because of the intrinsic interest of the oscillator itself as a model physical system and secondly because it would provide an exacting test of the power of our iterative method. It is well known that however small the coupling parameter λ may be, the ratio of the off-diagonal to the diagonal elements of the Hamiltonian in the unperturbed representation, *e.g.*, $H_{n,n+2}/H_{nn}$, becomes of order unity for sufficiently large n, so that the anharmonicity is not really a small perturbation. (This is reflected in the behaviour of the Rayleigh-Schrödinger perturbation series which is strongly divergent.) For our purposes what is more pertinent is the ratio $H_{mn}/(H_{mm} - H_{nn})$ which, far from being small, diverges linearly with m for fixed $(m - n)$. Despite this seemingly unpromising initial appearance, a closer inspection of the iterative formula (*see* below) suggests that diagonalisation

of the Hamiltonian might be accomplished by the new method, and the work presented here shows that this conjecture is indeed valid.

The anharmonic oscillator, as a highly interesting physical system, has been studied by a number of authors in recent years. Following the determination of the asymptotic behaviour of the coefficients in the Rayleigh–Schrödinger perturbation series by Bender and Wu (1969), the analyticity properties of the energy eigenvalues in the complex λ-plane have been discussed by Simon (1970), while Loeffel *et al* (1969) have demonstrated the use of Padé approximants in extracting from the Rayleigh–Schrödinger series a converging sequence of approximations for the eigenvalues. Determination of the eigenvalues by a Borel summation method applied to Rayleigh–Schrödinger series has been accomplished by Graffi *et al* (1970). Prior determination of the Rayleigh–Schrödinger series to a very high order is required for accurate calculation using either of these 'improper' summability methods. A more practical calculational method is that of Biswas *et al* (1971) who have reduced the problem to finding the roots of an infinite Hill determinant, and used a recurrence relation existing between truncated determinants of different dimensions to carry the evaluation of the determinant to sufficiently high order till the roots converge. More recently, Graffi and Grecchi (1975) have shown how to reduce the eigenvalue problem for an oscillator with anharmonicity of the type λx^{2m} to the determination of the poles (with respect to the energy parameter) of an $m \times m$ matrix expressed as a continued fraction; successive approximations, with rather fast convergence, being obtained by increasing the number of stages of the continued fraction which are taken into account. Finally we may mention another recursive approach employed by Hioe and Montroll (1975) wherein an iterative scheme is set up for the n-th eigenvalue; the scheme is based on the straightforward expansion of the truncated characteristic determinant of the Hamiltonian matrix (in a suitably chosen harmonic oscillator basis), the truncation being around the (n, n) element. Besides these methods, which in principle can be carried to any accuracy, there is also a formula due to Mathews and Eswaran (1972) for quick estimation of energy eigenvalues (for not too low quantum numbers).

Before presenting the details of our method we mention two of its features which give it a considerable advantage over the others. Firstly, it is relatively easy to extend it to cases of mixed anharmonicities (*e.g.*, when both x^4 and x^6 terms are present); the computational labour involved in mixed cases is not much more than that in the quartic case. Secondly, it gives any number of eigenvalues simultaneously in principle, and in practical evaluation, the computation of a number of eigenvalues costs little additional labour over that of a single eigenvalue.

2. The method

The diagonalisation technique introduced by Mathews (1975) is based on a separation of the matrix H to be diagonalised into purely diagonal and off-diagonal parts D and λR respectively:

$$H = D + \lambda R \tag{1}$$

and the application of a similarity transformation $H' = (1 + \lambda S)^{-1} H(1 + \lambda S)$ with S chosen in such a way as to ensure that the off-diagonal part of H' is $O(\lambda^2)$. Then H' takes the form $H' = D' + \lambda^2 R'$. In the present problem wherein the Hamiltonian H is expressed in terms of operators a, $a\dagger$ with simple commutation properties, it is advantageous to modify the above procedure slightly and define

$$H' = e^{-\lambda A} H e^{\lambda A}$$

$$= H - \lambda[A, H] + \frac{\lambda^2}{2!}[A, [A, H]] - \frac{\lambda^8}{3!}[A, [A, [A, H]]] +$$

$$= D + \lambda\{R - [A, D]\} + \lambda^2\left\{-[A, R] + \frac{1}{2!}[A, [A, D]]\right\} + \ldots \quad (2)$$

If A is chosen such that

$$[A, D] = R, \quad (3)$$

then H' differs from the diagonal part D only by terms of order λ^2 or higher. Hence the diagonal part D' of H' differs from D by terms of $O(\lambda^2)$; and the off-diagonal part R' of H', being also $O(\lambda^2)$ can be written as $\lambda^2 R$:

$$H' = D' + \lambda^2 R'$$

$$= D - \frac{\lambda^2}{2!}[A, R] + \frac{2\lambda^3}{3!}[A, [A, R]] - \frac{3\lambda^4}{4!}[A, [A, [A, R]]] + \ldots$$

that is

$$H' = D - \sum_{\mu=2}^{\infty} \frac{(-1)^{\mu}(\mu - 1)\lambda^{\mu}}{\mu!} R_{\mu} \quad (4)$$

where

$$R_{\mu+1} = [A, R_{\mu}], \mu = 1, 2, \ldots \quad (5)$$

with $R_1 = R$.

It is to be noted that (4) is not a simple power series in λ. This is because R_{μ} itself depends on λ through the λ dependence of A, arising ultimately from the fact that D in eq. (1) includes the diagonal part of the perturbation proportional to λ.

The process which led to H' from H can now be repeated by constructing

$$H'' = e^{-\lambda A'} H' e^{\lambda A'} = D'' + \lambda^4 R''$$

and so on. The last step is ensured by choosing A such that $[A', D'] = R'$. It may be noted that $D'' - D'$ will not involve powers of λ less than λ^4 and similarly $D''' - D''$ will be $O(\lambda^8)$ and so on.

3. Application to the anharmonic oscillator

The anharmonic oscillator Hamiltonian which we seek to diagonalise is

$$H = \tfrac{1}{2}(x^2 + p^2) + 4\lambda x^4$$

$$= \tfrac{1}{2}(2N + 1) + \lambda(a + a\dagger)^4,$$

where $N = a\dagger a$ and a, $a\dagger$ are the annihilation and creation operators obeying the commutation relations

$$[a,\ a\dagger] = 1,\ [N,\ a] = -\ a,\ [N,\ a\dagger] = a\dagger. \tag{7}$$

In the unperturbed representation in which N is diagonal, the diagonal and off-diagonal parts D and λR of H are given by

$$D = \tfrac{1}{2}\,(2N + 1) + 3\lambda\,(2N^2 + 2N + 1) \tag{8 a}$$

$$R = \sum_{l=1}^{2} [a\dagger^{2l}\, R_{1,l}\,(N) + R_{1,l}\,(N)\, a^{2l}] \tag{8 b}$$

with

$$R_{1,1}\,(N) = 4N + 6 \tag{9 a}$$

$$R_{1,2}\,(N) = 1. \tag{9 b}$$

The operator A, determined by the condition (3), is readily seen to be

$$A = \sum_{m=1}^{2} [a\dagger^{2m}\, A_m\,(N) - A_m\,(N)\, a^{2m}] \tag{10}$$

$$A_1\,(N) = -\ \frac{(2N + 3)}{(12\lambda N + 18\lambda + 1)} \tag{11 a}$$

$$A_2\,(N) = -\ \frac{1}{(48\lambda N + 120\lambda + 4)}. \tag{11 b}$$

In view of the forms (8 b) and (10) of R and A it is obvious that

$$R_2 \equiv [A, R],\ R_3 \equiv [A, R_2],\ \ldots,\ R_\mu \equiv [A, R_{\mu-1}] \tag{12}$$

which appear in the expression (4) for H' can be written as

$$R_\mu \equiv \sum_{l=0}^{2\mu} [a\dagger^{2l}\, R_{\mu,l}\,(N) + R_{\mu,l}\,(N)\, a^{2l}] \tag{13}$$

On substituting (13) and (10) in (12) one gets a recursion relation connecting $R_{\mu+1,l}$ to the $R_{\mu,l}$. It can be written in the succinct form

$$R_{\mu+1,l}\,(N) = \sum_{m=-2}^{2} [A_m\,(N + 2l - 2m)\, R_{\mu,l-m}\,(N) - A_m\,(N)\, R_{\mu,l-m}\,(N + 2m)] \tag{14}$$

by introducing the definitions

$$A_{-m}\,(N) = -\ A_m\,(N - 2m) \times \frac{N!}{(N-2m)!} \quad (m > 0) \tag{15 a}$$

$$R_{\mu,-l}\,(N) = R_{\mu,l}\,(N - 2l) \times \frac{N!}{(N - 2l)!} \quad (l > 0). \tag{15 b}$$

The recurrence relation (14) is the basic formula to be employed in evaluating H'. Once the $R_{\mu,l}$ are determined from this relation, starting with (8b) and (10), one has, from (4) and (13),

$$H' = D - \sum_{\mu=2}^{\infty} \frac{(\mu - 1)\ \lambda^\mu}{\mu!} \sum_{l=0}^{2\mu} [a\dagger^{2l}\, R_{\mu,l}\,(N) + R_{\mu,l}\,(N)\, a^{2l}]. \tag{16}$$

The diagonal part, which gives the eigenvalues at this stage of the diagonalisation procedure, is

$$D' = D - 2\sum_{\mu=2}^{\infty} \frac{(\mu-1)\,\lambda^{\mu}}{\mu!}\, R_{\mu,0} \tag{17}$$

The next stage of the iterative process is to start with H' and determine H'' by the same procedure as above. The only difference is that unlike in R and A, where powers higher than a^4 and a^{+4} do not appear, in R' and A' such a limitation does not exist. In practice one finds however that the contribution of off-diagonal elements decreases rapidly with distance from the diagonal, so that one does not have to consider high powers of a and $a\dagger$. Further, for values of λ which have been considered in the literature, we have found that it is not necessary to proceed beyond D'''.

4. Results

As we have noted earlier, in taking D' to be an approximation to the diagonalized form, we are in error only in respect of terms proportional to λ^4 and higher. If such terms are ignored, the eigenvalues are given by D', eq. (17), omitting terms with $\mu > 3$. To this approximation, our calculation gives

$$E_n = \tfrac{1}{2}(2n+1) + 3\lambda(2n^2+2n+1) + F(n) - F(n-4) + G(n) - G(n-2) \tag{18}$$

where

$$F(n) = \frac{(n+4)!}{n!\,(12\lambda n + 30\lambda + 1)}\left[-\frac{\lambda^2}{4} + \frac{\lambda^3}{2}(2n+3)(2n+5)(2n+7)\right] \tag{19 a}$$

and

$$G(n) = \frac{(n+2)!\,(2n+3)^2}{n!\,(12\lambda n + 18\lambda + 1)}\left[-2\lambda^2 - \frac{\lambda^3}{2}(4n^3 + 18n^2 + 74n + 84)\right] \tag{19 b}$$

In particular, for the ground state energy we have

$$E_0 = \tfrac{1}{2} + 3\lambda - \frac{6\lambda^2(7+114\lambda)}{(1+30\lambda)(1+18\lambda)}\,. \tag{20}$$

Curiously, though the procedure of Hioe and Montroll (1975) is quite different from ours, they have also obtained a part of the formula (18) — the part remaining when the terms in λ^3 within the square brackets in eqs (19) are dropped.

As a test of our iterative procedure we have performed numerical calculations for the energies of the lowest four even-parity levels for $\lambda = 0{\cdot}025$ and $\lambda = 0{\cdot}125$. In order to get accuracy to the eighth decimal place in E_0 for $\lambda = 0{\cdot}025$ we found that it was necessary to determine the coefficients up to $\mu = 12$ in the first stage of the calculation, while in the next iteration the $R'_{\mu,l}$ for μ up to 3 only were needed. To get sufficient accuracy in the higher levels also we extended the

above scheme to $\mu = 16$ in the first iteration, $\mu = 8$ in the second iteration and $\mu = 4$ in the third iteration. With this we obtain accuracy to six decimals even for E_6. In all cases and at every stage of the iteration, it was found that terms with $l > 10$ could be ignored as they were too small to make any difference, to the accuracy aimed at. Our results for the lowest four levels are given in table 1. The accuracy indicated is that which is expected from the magnitudes of the off-diagonal elements at the last stage of the calculation and the residue-squaring nature of the procedure. The only other accurate computation for excited levels is that due to Biswas *et al* (1973). Their results are also shown in the table, for comparison. It will be noticed that our expectation regarding accuracy is justified by the agreement between the two sets of results. Incidentally, the analytical formula (18), from which the values given within brackets in table 1 are computed, is seen to yield quite reasonable results for the lower value of λ for low-lying levels.

The rapidity with which the eigenvalues converge as one proceeds through successive stages of the iterative process may be seen from table 2.

Table 1. Energy eigenvalues of the first four even-parity levels of the anharmonic oscillator [Quantities within brackets are calculated using eq. (18)]

	$\lambda = 0{\cdot}025$		$\lambda = 0{\cdot}125$	
	Ours	Biswas	Ours	Biswas
E_0	0·55914632 (0·558936)	0·55914632	0·696176 (0·6860)	0·6961758
E_2	3·13862428 (3·127)	3·1386243	4·32753 (4·264)	4·32752
E_4	6·2203008 (6·162)	6·2203009	9·0288 (9·148)	9·0287
E_6	9·657839 (9·517)	9·657839	14·417 (15·25)	14·4176

Table 2. Approximations to eigenvalues at various stages of the iteration

λ	Stage of iteration	Approximation to		
		E_0	E_2	E_4
0·025	1	0·55914810	3·1388680	6·227620
	2	0·55914632	3·1386251	6·220318
	3	0·55914632	3·1386242	6·220300
0·125	1	0·698177	4·49349	10·0155
	2	0·696258	4·32917	9·0473
	3	0·696176	4·3275	9·0288

Accuracy to the number of figures shown is expected from the magnitudes of the off-diagonal elements remaining at the last stage of iteration; and the agreement with the results of Biswas *et al* (table 1) shows that this expectation is indeed well founded.

5. Discussion

The root cause of the difficulties in devising fast-converging approximation procedures for determination of the eigenvalues of the anharmonic oscillator lies in the fact that the off-diagonal elements $H_{n,n+r}$ grow indefinitely (like n^2) as n increases. This behaviour is responsible for the explosive increase in magnitude of the Rayleigh–Schrödinger coefficients with increasing order in the standard perturbation theory. It is of particular interest to note that in our method, the correction to the diagonal terms which arise at each stage of the iterative procedure is, for large values of the quantum number n, of the order n^2: there is no worsening of the n-dependence as one proceeds with the iterations. Actually this may appear surprising since the off-diagonal matrix A has matrix elements $A_{mn} = -H_{mn}/(H_{mm} - H_{nn})$ which increase linearly with n, and the successive terms in the expression (4) contain increasing number of factors A. What happens is that in evaluating the commutator $[A, R_{\mu-1}]$, the leading power of n gets cancelled between the two terms of the commutator. This may easily be verified, starting from known forms of A and $R_1 \equiv R$. One finds, in fact, that $R_{\mu,l}(N) \propto N^{-(l-2)}$ for large N, so that the matrix of $a\dagger^{2l} R_{\mu,l}(N)$ is $O(n^2)$ for large n, as stated earlier. Having convinced oneself of this result for the multiple commutators occurring in H', one can use similar arguments to extend this result to H'' and so on.

We also note that the method presented here goes through without appreciable increase in complexity if higher powers of x (besides x^4) are also present in the perturbation. While this will produce further off-diagonal terms in R and hence A, this makes a difference only in the first stage of the iterative process (since terms distant from the diagonal are already present, in principle, in H', H'', etc.). However we have already noted that in the multiple commutators appearing in H', H'', etc., off-diagonal elements far removed from the diagonal have little effect. For this reason, the presence of extra terms in the perturbation does not make any great difference to the diagonalisation procedure.

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