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# Inner product methods for eigenvalue calculations

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**Abstract.** An inner product method of calculating eigenvalues is developed in both numerical and perturbation theoretic forms, and shown to be applicable to bound state and resonant state problems. The method is used to treat a problem in which the perturbed energy is a non-analytic function of a perturbation parameter.

## 1. Introduction

Many techniques can be used to obtain the energy eigenvalues for the one-dimensional Schrödinger equation in the special case where the potential is a finite polynomial. Killingbeck (1983) gave a survey of several available methods which are suitable for microcomputers, including methods based on diagonal hypervirial relations. Such relations involve the expectation values $\langle\psi|x^N|\psi\rangle$, where $\psi$ is the unknown eigenfunction. They can be used in direct numerical calculations (Richardson and Blankenbecler 1979) or in perturbation theoretic calculations using renormalised series (Killingbeck 1981a). However, Blankenbecler *et al* (1980) pointed out that it is also possible to construct a formalism based on the inner product $\langle\phi|x^N|\psi\rangle$, where $\phi$ is some convenient reference function. They gave a few numerical examples for perturbed oscillator problems.

The present work reports a more detailed analysis and numerical evaluation of the inner product approach, and presents several new results. Section 2 derives the fundamental recurrence relations used by the inner product approach and points out that the energy formula used has close links with that for the renormalised series approach. Section 3 presents a version of the recurrence relations suitable for numerical calculations, and demonstrates that the approach used by Blankenbecler *et al* (1980) can be considerably simplified. The energy eigenvalues appear in our work and in that of Blankenbecler as the zeros of a function $E-E_c$; § 3 reports for a first time the presence of singularities in this function. Section 4 gives a modification of the basic recurrence relations which permits them to be used in the calculation of Rayleigh-Schrödinger perturbation series for the energy. Sections 3 and 4 thus set out two alternative versions of the inner product approach. Sections 5 and 6 apply these two versions together, first to a resonant state problem and second to a special test problem which involves an eigenvalue which is a non-analytic function of a perturbation parameter. Section 6 also comments that perturbation theory can cope fairly well with this non-analytic energy if it is used in a manner akin to that of the renormalised series approach (Killingbeck 1981a). Section 7 briefly points out that the ideas which work for perturbed oscillator problems can be used also for perturbed Coulomb potential

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problems. Section 8 comments on some double precision tests which were carried out and § 9 points out some problems which have arisen out of the results of the present work.

We should perhaps emphasise again a point which adds extra interest to the study of methods which calculate energies without yielding wavefunctions (Killingbeck 1979, 1983). Once an accurate energy calculation is available it is possible to get expectation values such as $\langle\psi|x^2|\psi\rangle$ by adding a small term $\varepsilon x^2$ to the potential and noting that the energy change should be $\varepsilon\langle\psi|x^2|\psi\rangle$. This eigenvalue differencing approach reduces the problem to that of calculating energies, which are usually the quantities most easy to obtain.

## 2. The basic recurrence relations

We start from a Schrödinger equation with a monomial potential function of even parity,

$$H\psi = -D^2\psi + C_M x^M \psi = E\psi \tag{1}$$

(with $M$ an even positive integer) and introduce a reference function

$$\phi = x^P \exp(-bx^2/2) \tag{2}$$

where $b$ is a variable real positive parameter and $P$ (the parity indicator) is either 0 or 1. We define the inner product quantities

$$S_N = \langle\phi|x^N|\psi\rangle \tag{3}$$

and work out $\langle\phi|x^N H|\psi\rangle$ by operating first to the right and then to the left with $H$. The choice (2) for $\phi$ simplifies the algebra. Equating the two results gives

$$[E-(2N+2P+1)b]S_N = C_M S_{N+M} - b^2 S_{N+2} - N(N+2P-1)S_{N-2}. \tag{4}$$

For the special case $N=0$ the recurrence relation takes the form

$$[E-(2P+1)b]S_0 = C_M S_M - b^2 S_2. \tag{5}$$

Equation (5) is directly related to the usual energy shift formula of Rayleigh-Schrödinger perturbation theory. If the Hamiltonian in equation (1) is expressed in the form

$$-D^2 + b^2x^2 + [C_M x^M - b^2x^2] \tag{6}$$

then the reference function $\phi$ is an eigenfunction of $-D^2+b^2x^2$ with eigenvalue $(2P+1)b$. The energy shift due to the perturbation $V$ in square brackets is given by the equation

$$\Delta E\langle\phi|\psi\rangle = \langle\phi|V|\psi\rangle \tag{7}$$

of perturbation theory. This is equivalent to equation (5), and shows that the inner product approach with reference function (2) is implicitly based on a partitioning of the Hamiltonian similar to that used in the renormalised series approach (Killingbeck 1981a), except that the perturbation parameter is set equal to 1. The inner product method can be used either in a direct numerical calculation of $E$ (§ 3) or in a perturbation series approach (§ 4). When the potential in equation (1) is a polynomial, it is clear that an appropriate sum of terms with varying $M$ must be used in equations (4) and (5). The computations described in § 3 show the rather surprising feature that excited state energies can be obtained, even though the energy shift formula is based on a nodeless function $\phi$ which is a scaled harmonic oscillator ground state wavefunction.

## 3. The numerical version of the method

The perturbed oscillator Hamiltonian

$$H = -D^2 + \mu x^2 + \lambda x^4 = H(\mu, \lambda) \tag{8}$$

will be used as an example to show how the equations of § 2 lead to numerical results for eigenvalues. To proceed we write down the appropriate version of equation (4), divide it by $S_N$, and then introduce the quantities $R_N$ such that

$$S_{N+2} = R_N S_N. \tag{9}$$

After a little rearrangement we obtain a 'downhill' recurrence relation,

$$R_{N-2} = N(N+2P-1)/T_N \tag{10}$$

where

$$T_N = (2N+2P+1)b - E + (\mu - b^2)R_N + \lambda R_N R_{N+2}. \tag{11}$$

If the perturbing potential is changed to $\lambda x^6$, then the last term in (11) adds an extra factor $R_{N+3}$ (and so on for higher powers). The energy formula associated with (11) is obtained by using the appropriate sum of terms in (5) and is written in the form

$$E_c = (2P+1)b + (\mu - b^2)R_0 + \lambda R_0 R_2 \tag{12}$$

with the symbol $E_c$ (calculated energy) being used instead of $E$. The computational procedure is simple: all the $R_N$ for $N > N_0$ are set equal to zero, the recurrence relation is used to calculate the lower $R_N$ down to $R_0$ for some trial $E$, and then $E_c$ is calculated from equation (12). The idea is to make $E_c$ equal to $E$. This is most efficiently achieved by regarding $(E_c - E)$ as a function of $E$ and employing any convenient root finding algorithm (Killingbeck 1985) to locate the roots. These roots are then the approximate eigenvalues. The procedure used here is well suited to modern microcomputers, which will automatically assign zero values to all the $R_N$ array elements as soon as an array dimension is declared. Blankenbecler *et al* (1980) undertook a lengthy analysis of the asymptotic form of the $S_N$ and the $R_N$, to get starting values for the downhill recurrence, and also used a more complicated reference function $\phi$ when studying the octic perturbed oscillator. Our empirical microcomputer investigation showed that neither of these complications is necessary. It also revealed an extra feature of the method which was not apparent in the ground state calculations of Blankenbecler *et al* (1980), and which we discuss below. Table 1 shows how the estimated ground state energy for the Hamiltonian $H(1, 1)$ varies with $b$ and $N_0$. The true energy should be independent of $b$, of course, and for a fixed $N_0$ the use of the 'plateau criterion' (Killingbeck 1981a) that $|\partial E/\partial b|$ shall be a minimum might be used to pick out a 'best' $E$ value. However, the most simple procedure is to increase $N_0$; this dramatically decreases the $b$ dependence of the calculated energy and so simplifies the calculation.

A detailed computation of the quantity $(E_c - E)$ as a function of $E$ shows that each zero of the function (except for the lowest of each parity) has a neighbouring singularity just below it. The function varies as $(E - E_s)^{-1}$ in the neighbourhood of a

**Table 1.** Energy estimates for the $H(1, 1)$ ground state. (Only the trailing digits are shown; the starting digits 1.39 are common to all the entries.)

| $b$ \ $N_0$ | 20 | 30 | 40 | 50 |
|---|---|---|---|---|
| 2 | 21 624 | 23 617 | 23 513 | 23 516 |
| 3 | 23 519 | 23 519 | 23 516 | 23 516 |
| 4 | 23 662 | 23 517 | 23 516 | 23 516 |
| 5 | 25 214 | 23 516 | 23 516 | 23 516 |
| 6 | 70 566 | 23 765 | 23 516 | 23 516 |

singularity at $E = E_s$, and the gap between each zero and its partner singularity becomes smaller for the higher eigenvalues. Table 2 shows some typical results for the even parity states. To find the singularities the slight change $(E_c - E) \rightarrow (E_c - E)^{-1}$ was made in the root finder program; this interchanges the zeros and singularities in the function. The results show that the gap between a zero and its corresponding singularity increases with $b$, so that it is not very difficult to find several excited state energies even with a simple root finding algorithm. The algorithm used was a Newton's method algorithm with an attenuator built in to avoid instability (Killingbeck 1984, 1985). Any method which locates the 'roots' of a function $f(E)$ by finding boundaries between regions of positive and negative $f(E)$ would suffice to locate the singularities as well as the zeros. For example, the microcomputer method of Kantaris and Howden (1983) would be applicable as a root finder in conjunction with the inner product method.

**Table 2.** $E$ values at which the function $E - E_c$ has a zero or a singularity. Results are shown for the even parity states, with $P = 0$ and $N_0 = 100$ throughout.

| Zeros | Singularities | | |
|---|---|---|---|
| $b = 3, 5, 7$ | $b = 3$ | $b = 5$ | $b = 7$ |
| 1.392 3516 | — | — | — |
| 8.655 0500 | 7.540 7938 | 6.836 2395 | 6.464 2938 |
| 18.057 557 | 17.685 259 | 17.045 286 | 16.549 630 |
| 28.835 338 | 28.739 366 | 28.356 130 | 27.909 557 |
| 40.690 386 | 40.669 757 | 40.494 553 | 40.175 213 |
| 53.449 102 | 53.445 358 | 53.378 964 | 53.187 932 |

## 4. A perturbation-theoretic version

If the monomial term in the Schrödinger equation (1) is written as $\lambda^I V_M x^M$, then we may postulate the series expansions

$$S_N = \sum S_N^M \lambda^M \tag{13}$$

$$E = \sum E_M \lambda^M. \tag{14}$$

Substituting these expansions into (4) and taking coefficients of the $\lambda^K$ terms on each side leads after some rearrangement, to an 'uphill' recurrence relation for the coefficients:

$$2NbS_N^K = N(N+2P-1)S_{N-2}^K - V_M S_{N+M}^{K-I} + S \tag{15}$$

where

$$S = \sum_{1}^{K} E_J S_N^{K-J}. \tag{16}$$

The energy equation (5) produces the perturbation equations

$$E_J = V_M S_M^{J-I} \qquad (J > I) \tag{17}$$

$$E_0 = (2P+1)b \tag{18}$$

if the traditional intermediate normalisation $S_0 = 1$ is used. This is achieved in the computation by setting $S_0$ equal to 1 and all other $S_N$ equal to zero (the latter step being accomplished automatically on a modern microcomputer). From the equations above and the discussion of § 2 it is clear that the perturbation theory derived here refers to the even and odd parity ground states of the Schrödinger equation

$$-D^2\psi + b^2x^2\psi + \lambda^I V_M x^M \psi = E\psi \tag{19}$$

and perturbations involving various powers of $\lambda$ as well as $x$ can be handled by adding appropriate terms into equations (15) and (17). The series for the energy will be a divergent alternating series, but can be made to yield reasonable numerical results by using the renormalising approach which was originally used for hypervirial series (Killingbeck 1981a, b). The inner product and hypervirial algorithms produce identical energy series, so the perturbed oscillator results of Killingbeck (1981a, b) are reproduced by the inner product approach.

## 5. Quasi-bound state energies

If the numerical calculation of § 3 is carried out with the perturbation parameter $\lambda$ set equal to a small negative number (typically between 0 and $-0.05$) then the resulting energies for low-lying states are obtained just as easily as the corresponding energies for $\lambda > 0$. However, the Hamiltonian (8) should not have true bound states for $\lambda < 0$ and so the calculated energies are presumably to be interpreted as the real parts of the complex energies associated with narrow resonances. The inner product approach thus gives a speedy method for calculating such quantities. For a true bound state the calculated energy reaches a limit and then remains constant as $N_0$ is increased. For the resonant states, however, the calculated energy fluctuates as $N_0$ is increased, so that only a limited number of stable decimal digits can be quoted. Table 3 shows some results for the ground state of the perturbed oscillator. The energies quoted agree to the number of digits given with those obtained by two other calculations. The first of these used the approach of § 4, summing the Rayleigh–Schrödinger energy series to its smallest term for each $\lambda$. The second calculation involved using the Dirichlet conditions $\psi(\pm X) = 0$, the 'particle in a box' approach, with each energy eigenvalue being a function of $X$. $X$ was varied to locate the $X$ and $E$ for which $|\partial E/\partial X|$ is a minimum. The $E$ values can be calculated either by finite difference or power series methods (Killingbeck 1983). Since the box approach gives results which agree with those of other techniques for calculating the real part of resonant state energies, our

**Table 3.** Quasi-bound state energies for the perturbed oscillator ground state with small negative $\lambda$. The three methods used (see text) give results which agree to the digit shown.

| $\|\lambda\|$ | $E$ |
|---|---|
| 0.01 | 0.992 363 22 |
| 0.02 | 0.984 427 67 |
| 0.03 | 0.976 146 2 |
| 0.04 | 0.967 45 |
| 0.05 | 0.958 2 |

results indicate the value of the two inner product formalisms (numerical and perturbation-theoretic) for resonant state calculations. The detailed comparison of the three methods was only carried out for the even parity ground state, but the numerical method of § 3 easily gives results for higher resonant states as well.

## 6. A special perturbation problem

The most common problem arising in perturbation theory is that of taming a divergent series to get a finite (and correct) result; both Padé approximants (Simon 1970) and renormalised series (Killingbeck 1981a) can be used to handle the problem. In some cases, however, the energy perturbation series may converge and yet not give the correct energy, even for a well defined bound state. The methods of §§ 3 and 4 are suitable to explore such a case. The Schrödinger equation with the Hamiltonian

$$-D^2+x^2+\lambda(8x^4-12x^2)+16\lambda^2x^6 \tag{20}$$

has the exact eigenfunction

$$=\exp(-\tfrac{1}{2}x^2-\lambda x^4) \tag{21}$$

with energy 1, as may be verified directly. The Hamiltonian (20) clearly has bound states for real $\lambda$ of either sign, whereas the function (21) is not square integrable if $\lambda$ is negative. For $\lambda<0$ the numerical inner product method of § 3 can be used to compute the ground state energy, which takes the form $1+\Delta$, with $\Delta$ small. Table 4 shows some results. Alternatively, the approach of § 4 permits the calculation of the energy perturbation series in $\lambda$, since the formalism allows the perturbation to involve different powers of $\lambda$ as well as $x$. We would intuitively suspect that the energy series

**Table 4.** $\Delta$ values for the Hamiltonian of equation (20) for small negative $\lambda$. (Twenty-digit computer precision used, with $N_0=1000$.)

| $\|\lambda\|$ | $\Delta$ (numerical) | $\Delta(\lambda)$, equation (22) |
|---|---|---|
| 0.0030 | $7E-19$ | $7.14E-19$ |
| 0.0035 | $2.749E-16$ | $2.747E-16$ |
| 0.0040 | $2.384E-14$ | $2.386E-14$ |
| 0.0045 | $7.666E-13$ | $7.685E-13$ |
| 0.0050 | $1.231E-11$ | $1.236E-11$ |
| 0.010 | $3.246E-6$ | $3.317E-6$ |

would have $E_0 = 1$ and all higher $E_n$ zero, so that it would give the correct $E$ for $\lambda > 0$ and a wrong $E$ for $\lambda < 0$. For a finite computer to give zero for all the $E_n$ (with $n > 0$) is not possible, since the coefficients $S_M$ in equation (15) increase with both $K$ and $M$ and the rounding error will eventually spoil the exact cancellations needed to yield $E_n$ values which are identically zero. Problems with computer overflow were avoided by using the definition $S_N^K = 8^N T_N^K$ and rewriting the equations in terms of the $T_N^K$. Problems with rounding error could not be removed, however, and so an empirical approach was tried. The computation of the $E_n$ was carried out using three levels of increasing precision. The number of zero $E_n$ coefficients obtained increased with the precision, $E_{10}$ being the highest coefficient obtained as exactly zero (with 20 digit precision). These results suggest that the $E_n$ are (as expected) zero beyond $E_0$. In this case the quantity $\Delta = E - 1$ (which is zero for $\lambda > 0$) presumably is some non-analytic function of $\lambda$. The values of $\Delta$ as obtained from the numerical calculation give a graph of $\ln \Delta$ versus $|\lambda|^{-1}$ which is very closely linear for small $|\lambda|$ and we estimate the leading term in $\Delta$ to be of the form

$$\Delta(\lambda) = A \exp(-B|\lambda|^{-1}) \tag{22}$$

for $\lambda \to 0_-$, with $A = 0.890$ and $B = 0.1250$. As table 4 shows, this function fits the numerical $\Delta$ values quite well over several orders of magnitude.

The preceding results seem to imply that the energy values $E(\lambda)$ for $\lambda < 0$ are not obtainable by perturbation theory. However, we managed to make the perturbation formalism of § 4 yield $\Delta$ values with an error of less than one percent by the simple device of linearising the theory in $\lambda$. The perturbing terms in (20) were written in the form

$$\lambda[8x^4 - 12x^4 + 16\mu x^6] = \lambda V(\mu) \tag{23}$$

with $\mu$ set numerically equal to $\lambda$ during the computation of the energy coefficients. Each $\lambda$ value thus produces its own series of $E_n$ coefficients and this flexibility is apparently sufficient to let the series (summed to its smallest term) give a reasonable fit to the non-analytic function $\Delta(\lambda)$. The ratios $E_{n+1}/E_n$ were observed to approach a roughly constant value just before the smallest $E_n$ term, and a geometric continuation of the series improved the $\Delta$ estimate still further, making it correct to 1 part in $10^3$ for $|\lambda|$ values greater than 0.015.

## 7. Perturbed Coulomb potentials

The methods of §§ 3 and 4 can be modified fairly easily to deal with the radial Hamiltonian

$$-\tfrac{1}{2}D^2 + \tfrac{1}{2}l(l+1)r^{-2} - Zr^{-1} + V_M r^M. \tag{24}$$

The comparison function (for states of angular momentum $l$) is taken to be

$$\phi = r^{l+1} \exp(-\beta r) \tag{25}$$

and the $S_N$ are defined as

$$S_N = \langle \phi | r^N | \psi \rangle \tag{26}$$

where $\psi$ is the unknown eigenfunction of the Hamiltonian (24). The recurrence relation for the $S_N$ is then

$$(E+\tfrac{1}{2}\beta^2)S_N=[\beta(M+l+1)-Z]S_{N-1}-\tfrac{1}{2}N(2l+1+N)S_{N-2}+V_MS_{N+M} \tag{27}$$

and it can be converted to 'downhill' form to give numerical calculations analogous to those of § 3 or to 'uphill' form to give a perturbation calculation analogous to that of § 4. The perturbation formalism refers to the ground state of each $l$ value. Since the Coulomb potential has its energy levels densely packed just below $E=0$, it requires great care to pick out the excited states numerically if $V_M$ is zero. However, use of a non-zero $V_M r^M$ term in (24) usually gives a sufficient splitting of the energy levels to make their separate location easy. We have checked that the perturbation formalism based on (27) gives the correct energy series for the perturbations $\lambda r$ and $\lambda r^2$ acting on the 1s ground state; the coefficients were given previously by Killingbeck and Galicia (1980). We have also checked that the numerical formalism based on (27) gives the correct energies for a perturbation $\lambda r^2$, as required for calculations on the quadratic Zeeman effect (Killingbeck 1981b). For the perturbation $\lambda r$ with small negative $\lambda$, the numerical formalism gives quasi-bound state energies which agree with those found by other techniques, just as for the oscillator problem of § 5. The numerical formalism also leads to interlaced zeros and singularities in the function $(E_c-E)$ for excited states of each $l$. Thus the various characteristics of the inner product method which were discovered for even and odd parity states in the oscillator problem also apply for each angular momentum family of states in the perturbed Coulomb potential problem.

## 8. Some double precision tests

Most of the results reported in this work were obtained using a Sinclair Spectrum microcomputer, for which simple programs were written to apply the methods of §§ 3 and 4 (Killingbeck 1984b). However, in order to test the method of § 3 more severely we carried out double precision calculations for various energy levels of the perturbed oscillator Hamiltonian $H(\mu,\lambda)$ given by equation (8). The expectation values $\langle x^2\rangle$ and $\langle x^4\rangle$ were also calculated for each state by using the energy differencing approach (Killingbeck 1979). An internal check on the results was provided by noting that the independently calculated values of $E$, $\langle x^2\rangle$ and $\langle x^4\rangle$ correctly satisfied the virial theorem $E=2\mu\langle x^2\rangle+3\lambda\langle x^4\rangle$. A value of $N_0=1000$ was more than adequate to give energies good to 20 significant digits. Only one energy value, the ground state energy for $H(0,1)$, appears to have been calculated to this kind of accuracy previously (Richardson and Blankenbecler 1979). We obtained a result which agrees with theirs to 20 digits,

$$E=1.060\,362\,090\,484\,182\,8996.$$

We note that the energy quoted by Crandall (1983) and attributed to Penk is incorrect in having a seventeenth (and last) digit of 0 instead of 9. These double precision results seem to establish clearly that the use of the initial condition $R_N=0$ for $N>N_0$ gives numerical energy values of any desired accuracy, even though the asymptotic behaviour of the $R_N$ as determined by analysis (Blankenbecler *et al* 1980) is quite different. This appears to be a case in which the 'downhill' use of the recurrence relation picks out a dominant solution which is independent of the initial values provided that $N_0$ is large enough. The studies of Hautot and Ploumhans (1979) may be relevant in explaining this effect which our numerical investigations have demonstrated.

## 9. Conclusion

The present work has shown clearly the accuracy and simplicity of the inner product method, in both its numerical and perturbation theoretic forms. However, it has also produced a few new mathematical problems which we wish to point out to interested readers. First, although the energy shift formula of § 2 is based on a nodeless reference function, it leads to excited state energies in § 3. Why this is so is not clear, but it may be related to the way in which the gap between the zeros and the singularities increases with $b$. Varying $b$ will vary the overlap of $\phi$ with excited state functions $\psi_n$. We suspect that there is some more inclusive theory, based on the resolvent $(H-E)^{-1}$ and on the inner products $\langle\phi|\psi_n\rangle$, which will explain both the presence of the singularities and the way in which excited state energies appear in the calculation. The second problem arising out of this work is that of why using zero initial $R_N$ values works so well, even though the exact $R_N$ should increase with $N$. The theory of dominant and subdominant solutions of recurrence relations is presumably relevant to the resolution of this problem. It also remains to be investigated how far the $\Delta(\lambda)$ values can be improved by performing a full Padé approximant analysis of the perturbation series obtained by the linearisation procedure of § 6.

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