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Perturbation series for transition moments of anharmonic oscillators

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Abstract. The off-diagonal hypervirial theorems and a matrix product rule are applied to the perturbed one-dimensional harmonic oscillator in a new method of obtaining perturbation series for the off-diagonal elements $\langle m|x|n\rangle$. The present work gives the Rayleigh-Schrödinger series for $\langle 0|x|1\rangle$ to eighth order for a quartic perturbation.

1. Introduction

The quantum mechanical hypervirial theorems were introduced by Hirschfelder (1960) in a generalisation of the classical hypervirial theorems arising from the Poisson bracket representation of the classical equations of motion. The time average of the Poisson bracket vanishes for a bound system. This corresponds to the vanishing of the expectation value of the commutator in quantum mechanics. For a quantum mechanical system described by a Hamiltonian operator H , with energy eigenvectors $|n\rangle$, a time-independent operator $W = q^\alpha p^\beta$ yields diagonal hypervirial theorems when used in the relation

$$\langle n|[H, W]|n\rangle = 0. \quad (1)$$

Each α, β combination in W yields a dynamical relationship obeyed by the system.

In a perturbation problem H is of the form $H_0 + \lambda V$, where λ is the perturbation parameter. With suitable choices of W , a recurrence relation may be produced from (1) to obtain perturbation series for expectation values of various powers of the position coordinate. Using these results, the Hellmann-Feynman theorem can then be employed to give an energy perturbation series. This procedure has been carried out by Swenson and Danforth (1972) for the perturbed one-dimensional harmonic oscillator, and by Killingbeck (1978) for the hydrogen atom with radial perturbation λr . The method possesses the advantage over wave mechanical methods that the calculation of perturbed wavefunctions and the consequent integration over the space region considered is not required. Expectation values are treated as variables and are calculated directly as power series in λ .

The off-diagonal hypervirial theorems are derived by placing the commutator $[H, W]$ between the energy eigenvectors $|m\rangle$ and $|n\rangle$ to give

$$\langle m|[H, W]|n\rangle = (E_m - E_n)\langle m|W|n\rangle. \quad (2)$$

In a non-perturbative application, Banerjee (1977) has used (2) to obtain a linear recurrence relation between the transition moments of anharmonic oscillators, valid

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for any polynomial potential. For even parity potentials the recurrence relation requires the provision of a certain minimum number of the lowest power moments in order to calculate the higher ones.

The present work presents a new method of producing perturbation series for the off-diagonal matrix elements $\langle m|x|n \rangle$ of the perturbed one-dimensional harmonic oscillator. A recurrence relation is derived from (2) relating the perturbation coefficients of transition moments between two arbitrary perturbed eigenstates. For the perturbed oscillator potential energy $V = \mu x^2 + \lambda x^{2\nu}$ the recurrence relation can be analysed with an appropriate algebra to determine the positions of vanishing elements in the matrix perturbation coefficients (MPCs) of $x^{2h+1}(\lambda)$. The remaining matrix elements are left undetermined by the algebra and their positions in the MPCs obey a definite structural law. A product rule is then constructed relating a diagonal element of a MPC of $x^2(\lambda)$ to a sum involving off-diagonal elements of MPCs of $x(\lambda)$. The positions of the undetermined elements participating in this product rule are then given by the structural law, which sets finite limits to the sums over states. The product rule subsequently serves as the basis for the calculation of off-diagonal perturbation series.

The production of diagonal perturbation series (which are needed to start off the off-diagonal calculations) presents an immediate problem. The range of the coupling constant λ for which the series sum to γ th order satisfactorily converges is confined to low values, $\lambda \ll 1$. This led Killingbeck (1981) to devise a renormalisation method which, by regrouping the terms in the Hamiltonian operator, alters the rate of divergence of the perturbation coefficients and extends the useful range of λ . The application of this method to the off-diagonal problem by the present author has converted off-diagonal series which are strongly divergent at relatively small λ into renormalised series which give satisfactorily convergent results to a γ th-order approximation.

To illustrate the off-diagonal calculation presented in this work, the procedure has been described to fourth order for a quartic perturbation, and the Rayleigh-Schrödinger series are given for $\langle 0|x|1 \rangle$, $\langle 1|x|2 \rangle$ and $\langle 0|x|3 \rangle$ from an eighth-order calculation.

It is emphasised that the essence of the calculation lies in the property that it simultaneously produces many $\langle m|x|n \rangle$ series. In the calculation for $\langle 0|x|1 \rangle$ to eighth order a total of 365 perturbation coefficients are produced. As the calculation order is raised all the $\langle m|x|n \rangle$ are gradually produced.

2. Hypervirial recurrence relation

Consider the Hamiltonian operator

$$H = -\alpha D^2 + V(x). \quad (3)$$

If we place this Hamiltonian into (2), first with $W = x^k$ then with $W = x^{k-1}D$, the operator D can be eliminated from the two equations obtained. Substitution of the operator D^2 from (3) into the result yields

$$\begin{aligned} \alpha^2 k(k-1)(k-2)(k-3)\langle m|x^{k-4}|n \rangle + 2\alpha k(k-1)(E_m + E_n)\langle m|x^{k-2}|n \rangle \\ - 4\alpha k(k-1)\langle m|x^{k-2}V|n \rangle - 2\alpha k\langle m|x^{k-1}DV|n \rangle \\ + (E_m - E_n)^2\langle m|x^k|n \rangle = 0. \end{aligned} \quad (4)$$

For the perturbed harmonic oscillator with potential energy

$$V(x) = \mu x^2 + \lambda x^{2\nu} \quad (5)$$

we postulate that the matrices x^k (with elements $\langle m|x^k|n\rangle$) and the eigenenergies E_m can be expressed as perturbation series in λ , thus

$$x^k(\lambda) = \sum_{i=0}^{\infty} Q_i^k \lambda^i \tag{6}$$

$$E_m(\lambda) = \sum_{i=0}^{\infty} E_i \lambda^i. \tag{7}$$

The matrix coefficients Q_i^k and the E_i clearly have state-dependent values. For the sake of brevity it will be useful to define E_{mn}^+ and E_{mn}^- as

$$E_{mn}^+ = (E_m + E_n) \quad E_{mn}^- = (E_m - E_n).$$

It then follows from (7) that there will be series expansions of the form

$$E_{mn}^+(\lambda) = \sum_{i=0}^{\infty} E_i^+ \lambda^i \tag{8}$$

$$E_{mn}^-(\lambda) = \sum_{i=0}^{\infty} E_i^- \lambda^i \tag{9}$$

where the coefficients E_i^+ and E_i^- have a dependence on m and n .

Substituting (5), (6), (8) and (9) into (4) and equating coefficients of like powers of λ produces the relation

$$\begin{aligned} \alpha^2 k(k-1)(k-2)(k-3)Q_\gamma^{k-4} + 2\alpha k(k-1) \sum_{i+j=\gamma} E_i^+ Q_j^{k-2} - 4\alpha\mu k^2 Q_\gamma^k \\ + \sum_{r+s+u=\gamma} E_r^- E_s^- Q_u^k - 4\alpha k(k+\nu-1)Q_{\gamma-1}^{k+2(\nu-1)} = 0. \end{aligned} \tag{10}$$

By separating out all Q of order γ to the left side of (10) we arrive at the result

$$\begin{aligned} \alpha^2 k(k-1)(k-2)(k-3)Q_\gamma^{k-4} + 2\alpha k(k-1)E_0^+ Q_\gamma^{k-2} + 4\alpha\mu[(m-n)^2 - k^2]Q_\gamma^k \\ = 4\alpha k(k+\nu-1)Q_{\gamma-1}^{k+2(\nu-1)} - 2\alpha k(k-1) \sum_{i+j=\gamma-1} E_{i+1}^+ Q_j^{k-2} \\ - \sum_{u=0}^{\gamma-1} \sum_{r+s=\gamma-u} E_r^- E_s^- Q_u^k \end{aligned} \tag{11}$$

having noted that the unperturbed energies E_m are given by $E_m = (\alpha\mu)^{1/2}(2m+1)$.

Equation (11) is the hypervirial recurrence relation for the Q matrices associated with the anharmonic oscillator potential energy (5).

To produce the recurrence relation for renormalised series we regroup the terms in (5) in the form

$$V(x) = Mx^2 + \lambda(x^{2\nu} - Rx^2) \tag{5a}$$

so that $M = \mu + R\lambda$. The fixed constants of the problem considered are μ and λ so that R is varied to obtain the best series convergence. The effect this procedure has on the recurrence relation (11) is to change μ into M and to add the term $4\alpha k^2 RQ_{\gamma-1}^k$ to the right-hand side.

Our first task is to examine what information can be obtained from the recurrence relation (11).

3. Consequences of the recurrence relation

Consider the power series (6) of the odd power matrices

$$x^{2h+1}(\lambda) = \sum_{\gamma=0}^{\infty} Q_{\gamma}^{2h+1} \lambda^{\gamma}, \quad h = 0, 1, \dots \tag{12}$$

It is possible to show (Clarke 1984a) by analysing the recurrence relation (11) with an appropriate algebra, that matrix elements in Q_{γ}^{2h+1} vanish for states m, n which do not satisfy

$$|m - n| = 2s + 1, \quad s = 0, 1, \dots, h + \gamma(\nu - 1) \tag{13}$$

where $h, \gamma \geq 0; \nu \geq 1$; and 2ν is the power of the perturbing potential energy. Those matrix elements with state numbers conforming to (13) are left undetermined by the algebra. If we assume that these undetermined elements are non-vanishing then the result (13) provides some justification within our perturbative approach for the truncation hypothesis used in matrix methods, e.g. Li *et al* (1975). This hypothesis assumes that the transition moments of $x(\lambda)$ fall off rapidly as $|m - n|$ increases. We see from (13) at $\nu = 2$ that a new family of elements comes into play at each order γ and the greater the difference between their state numbers $|m - n|$ then the greater is the order at which they first appear. We can see that for small λ the $x(\lambda)$ elements will presumably decrease rapidly as $|m - n|$ increases.

Only certain families of elements may be directly evaluated from the recurrence relation (11). These are given (Clarke 1984a) by the reduced recurrence relation

$$Q_{\gamma}^{2h+1} = \mu^{-1}[(2s + 1)^2 - (2h + 1)^2]^{-1} \\ \times \left((2h + 1) \sum_{t=1}^{\nu} (2h + t) A_t Q_{\gamma-1}^{2(h+t)-1} - \alpha h(h - 1)(4h^2 - 1) Q_{\gamma}^{2h-3} \right. \\ \left. - h(2h + 1) E_0^+ Q_{\gamma}^{2h-1} \right) \tag{14}$$

valid for $0 \leq s \leq h - 1; \gamma = 0$, and for $h + (\gamma - 1)(\nu - 1) + 1 \leq s \leq h + \gamma(\nu - 1); \gamma > 0$. Provision of initial zeroth-order moments $\langle m | Q_0^{2j+1} | n \rangle$ permits the γ th-order moment $\langle m | Q_{\gamma}^{2h+1} | n \rangle$ to be determined. The results (13) and (14) are valid when the potential energy is expressed as

$$V(x) = \mu x^2 + \lambda \sum_{t=1}^{\nu} A_t x^{2t}. \tag{5b}$$

This fact is important for conducting a renormalised series calculation.

Finally, a third relation arises if we place $k = 1$ ($h = 0$) in the recurrence relation (11). This produces the i th-order equation

$$\langle m | Q_i^1 | m + 2s' + 1 \rangle = A \langle m | Q_{i-1}^{2\nu-1} | m + 2s' + 1 \rangle \\ + B \sum_{u=0}^{i-1} \sum_{r+s=i-u} E_r^- E_s^- \langle m | Q_u^1 | m + 2s' + 1 \rangle \tag{15}$$

having taken the $\langle m | m + 2s' + 1 \rangle$ element. (Of course, additional terms arise in (15) when the potential (5b) is used.) The constants are

$$A = \nu / \mu [(2s' + 1)^2 - 1], \quad B = -1/4\alpha\mu [(2s' + 1)^2 - 1].$$

Providing $s' \neq 0$ then A and B are defined and (15) can be used. Recourse to the structural result (13) for the Q_i^1 ($h = 0$) therefore gives the range of validity for s' in (15) as

$$s' = 1, 2, \dots, i(\nu - 1), \quad i > 0.$$

All that remains is to set up a product rule calculation to which (13), (14) and (15) will supply information.

4. Product rule calculation of perturbation series for $\langle m|x|n \rangle$

The product rule employed to find the elements of the Q_γ^1 —the γ th-order MPCS of $x(\lambda)$ —is based on knowledge of the perturbation series for the diagonal elements of $x^2(\lambda)$. The matrices are related by the matrix product equation

$$x^2(\lambda) = x(\lambda)x(\lambda). \tag{16}$$

We can make use of (6) to express $x(\lambda)$ and $x^2(\lambda)$ as perturbation series of the form

$$x(\lambda) = \sum_{i=0}^{\infty} Q_i^1 \lambda^i \tag{17}$$

$$x^2(\lambda) = \sum_{\gamma=0}^{\infty} Q_\gamma^2 \lambda^\gamma. \tag{18}$$

Placing (17) and (18) in (16) and equating coefficients of like powers of λ gives

$$Q_\gamma^2 = \sum_{i+j=\gamma} Q_i^1 Q_j^1. \tag{19}$$

Equation (19) relates matrix perturbation coefficients of $x(\lambda)$ and $x^2(\lambda)$. Each matrix product $Q_i^1 Q_j^1$ can be expressed as a sum over products of matrix elements. We are therefore interested only in the positions of the undetermined elements in the i th-order matrix Q_i^1 in order to exclude the determined vanishing elements from the calculation. These positions are given by the choice $h = 0$ in the general structural equation (13) which then shows that only elements having states satisfying the condition

$$|m - n| = 2s_i + 1, \quad s_i = 0, 1, \dots, i(\nu - 1)$$

are undetermined in Q_i^1 . Consequently, taking the $\langle m|m \rangle$ element in (19) produces a sum over states (characterised by a sum over the integers $s_i = s_j$) for the term

$$\sum_{\oplus=+,-} \langle m|Q_i^1|m \oplus (2s_i + 1) \rangle \langle m \oplus (2s_j + 1)|Q_j^1|m \rangle.$$

Since one factor in each product must vanish when we transcend the range of s_i or s_j then the sum over states must have an upper limit equal to the lower value of $i(\nu - 1)$ and $j(\nu - 1)$ —the upper limits of s_i and s_j . The $\langle m|m \rangle$ element of (19) therefore becomes

$$\langle m|Q_\gamma^2|m \rangle = \sum_{i+j=\gamma} \sum_{s=0}^P \sum_{\oplus=+,-} \langle m|Q_i^1|m \oplus (2s + 1) \rangle \langle m \oplus (2s + 1)|Q_j^1|m \rangle \tag{20}$$

where $P = [i(\nu - 1), j(\nu - 1)]$ min.

The substitution $j = \gamma - i$ finally gives

$$\langle m|Q_\gamma^2|m\rangle = \sum_{i=0}^{\gamma} \sum_{s=0}^{P'} \sum_{\oplus=+,-} \langle m|Q_i^1|m \oplus (2s+1)\rangle \langle m \oplus (2s+1)|Q_{\gamma-i}^1|m\rangle \tag{21}$$

so that $P' = [i(\nu - 1), (\gamma - i)(\nu - 1)]$ min.

We note from the limit P' that at $i = \gamma$ —the highest order—we have $P' = 0$ giving only one value of s in (21), $s = 0$. This means that only two γ th-order elements occur, namely, $\langle m|Q_\gamma^1|m+1\rangle$ and $\langle m|Q_\gamma^1|m-1\rangle$. The symmetric nature of the Q matrices means that if the former is determinable at $m = n$ then the latter is already evaluated at $m = n + 1$. We therefore focus on the element $\langle m|Q_\gamma^1|m+1\rangle$. Since it is the highest term in the indices γ, m , we make it the subject of the calculation (i.e. we set out to determine it in terms of the other elements in (21)). Each γ, m combination therefore characterises one calculation using (21) to find $\langle m|Q_\gamma^1|m+1\rangle$.

The diagonal elements $\langle m|Q_\gamma^2|m\rangle$ may be found from the diagonal hypervirial theorems used by Swenson and Danforth (1972). This leaves the question: is it possible to systematically determine all the elements $\langle m|Q_i^1|m+2s+1\rangle$ in (21) for every order γ and state m ? To illustrate that this is possible we concentrate on the quartic perturbation problem—with $\nu = 2$ in P' —and make out a list of all the matrix elements generated by the sums in (21), for ascending orders γ with arbitrary state m . This list is given in table 1 to fourth order ($\gamma = 4$). The members of the list at each order γ are determined by the permissible values of s in the coefficients Q_i^1 . We see from table 1 that the elements at order γ consist of the elements at order $(\gamma - 1)$ accompanied by additional elements. The previously calculated $(\gamma - 1)$ th-order elements are used in the γ th-order calculations and are shown within the dotted region in table 1. The

Table 1. Matrix elements $\langle m|Q_i^1|m \pm (2s+1)\rangle$ generated at each order of the product-rule calculation for the Hamiltonian $H = -\alpha D^2 + \mu x^2 + \lambda x^4$.

Order of perturbation coefficient Q_γ^2 in $x^2(\lambda)$ γ	Order of perturbation coefficient Q_i^1 in $x(\lambda)$ i	$\langle m Q_i^1 m \pm (2s+1)\rangle$ elements generated s
0	0	0
1	0	0
	1	0
2	0	0
	1	0 ①
	2	0
3	0	0
	1	0 1
	2	0 1
	3	0
4	0	0
	1	0 1
	2	0 1 ②
	3	0 1
	4	0

problem therefore reduces to finding the additional elements at each order (undotted region).

The additional elements consist of the highest-order elements— $\langle m|Q_\gamma^1|m+1\rangle$ and $\langle m|Q_\gamma^1|m-1\rangle$ —and calculable elements which we shall discuss shortly. We recall that if the subject of the calculation $\langle m|Q_\gamma^1|m+1\rangle$ is determinable then $\langle m|Q_\gamma^1|m-1\rangle$ is known at the next highest m . For each order γ a calculation is made for $\langle m|Q_\gamma^1|m+1\rangle$ at each m in ascending order from $m=0$. The element $\langle m|Q_\gamma^1|m-1\rangle$ may then be taken from calculations at previous m and providing the above-mentioned calculable elements and $\langle m|Q_\gamma^2|m\rangle$ are given we can find $\langle m|Q_\gamma^1|m+1\rangle$. If these calculations are carried out at each γ in ascending order from $\gamma=0$, with appropriate ranges of m , the lower-order calculations support the higher-order ones. We can then find $\langle m|Q_\gamma^1|m+1\rangle$ for any γ , $m \geq 0$.

The question that remains is: how are the calculable elements found? To answer this we make use of equations (14) and (15) of § 3.

Equation (14) at $h=0$ will give the elements $\langle m|Q_i^1|m+2s+1\rangle$ for any order $i > 0$ and state $m \geq 0$ providing s satisfies the condition,

$$(i-1)(\nu-1)+1 \leq s \leq i(\nu-1).$$

For a quartic perturbation ($\nu=2$) we have $s=i$, the order of the element. These elements are shown with a full circle in table 1.

Equation (15) provides the remaining elements for the calculation. For a quartic perturbation ($\nu=2$) s' must satisfy the condition

$$s' = 1, 2, \dots, i.$$

We note that at order i , both (14) and (15) are valid for $s=s'=i$; however, the calculation in terms of zeroth order elements with (14) is easier. The r th-order energy differences E_r^- can be found from the diagonal hypervirial theorems and the u th-order elements $\langle m|Q_u^1|m+2s'+1\rangle$, having order $u < i$, can be taken from previous order calculations. This leaves the $(i-1)$ th-order element $\langle m|Q_{i-1}^{2(\nu-1)+1}|m+2s'+1\rangle$ which is found by constructing a product rule. For example, for a quartic perturbation ($\nu=2$) we require a product rule for $\langle m|Q_{i-1}^3|m+2s'+1\rangle$. This involves the matrix product $Q_a^1 Q_b^1 Q_c^1$ where Q_{i-1}^3 arises from summing over the combinations of orders a, b, c satisfying

$$a+b+c=i-1.$$

Each $Q_a^1 Q_b^1 Q_c^1$ must then involve a sum over states n, n' for the term $\langle m|Q_a^1|n\rangle\langle n|Q_b^1|n'\rangle\langle n'|Q_c^1|m+2s'+1\rangle$. The ranges of these sums are taken from the structural result (13) at $h=0$; $\nu=2$; $\gamma=a, b, c$. Since each element generated in these sums has order less than i , their values may be drawn from previous order calculations.

The elements calculated with (15) at $\nu=2$ are shown with a square in table 1. The calculation of the $\langle m|Q_i^1|m-(2s+1)\rangle$ for (21) is superfluous since the symmetric nature of the Q matrices and the calculation with ascending values of m in (21) guarantees that the $\langle m|Q_i^1|m+2s+1\rangle$ are sufficient.

As an aside, it is interesting to note that the $\langle m|n\rangle$ element of the commutator equation

$$[H, [H, x]] = 2\alpha \, dV/dx$$

also leads to (15) when the $\langle m|x^{2h+1}|n\rangle$ and the energies E_m are expressed as perturbation series.

5. Results

For a general $\lambda x^{2\nu}$ perturbation a BASIC computer program has been produced which calculates renormalised perturbation series for any $\langle m|x|n \rangle$ to arbitrary order.

With the selection $\alpha = \mu = 1$ in (3) and (5) and for a quartic perturbation ($\nu = 2$), the energy perturbation coefficients required by the fourth-order $\langle 0|x|1 \rangle$ moment calculation are given by Drummond (1981) and are shown in table 2. The energy coefficients can also be calculated with the microcomputer program of Killingbeck (1983). This program has been used to calculate the required $\langle m|Q_\gamma^2|m \rangle$ coefficients presented in table 3. We recall that each γ, m combination corresponds to one $\langle m|Q_\gamma^2|m \rangle$ coefficient and characterises one calculation for $\langle m|Q_\gamma|m+1 \rangle$ with (21).

The Rayleigh-Schrödinger series for $\langle 0|x|1 \rangle$ to eighth order is shown in table 4 together with the series for $\langle 1|x|2 \rangle$ and $\langle 0|x|3 \rangle$ to seventh order; the latter series emerge as some of the by-products of the $\langle 0|x|1 \rangle$ calculation.

If we choose $k = 1$ in (6) and take the $\langle 0|1 \rangle$ element we have, to eighth order

$$\langle 0|x|1 \rangle = \sum_{i=0}^8 \langle 0|Q_i^1|1 \rangle \lambda^i \tag{22}$$

Selecting the value $\lambda = 0.02$ and using the coefficients $\langle 0|Q_\gamma^1|1 \rangle$ in the first column of table 4 we can make up a table of the sum of the truncated series (22) to order $i = \gamma$. These partial sums are given in table 5.

Table 2. Energy perturbation coefficients for various states m for the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$.

State m	Energy perturbation coefficient E_γ at order γ		
	E_0	E_1	E_2
0	1.0	0.75	-1.3125
1	3.0	3.75	
2	5.0	9.75	
3	7.0	18.75	-203.0625
4	9.0	30.75	

Table 3. Diagonal elements of perturbation coefficient Q_γ^2 of $x^2(\lambda)$ for the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$.

State m	$\langle m Q_\gamma^2 m \rangle$ perturbation coefficient of $x^2(\lambda)$ at order γ				
	$\langle m Q_0^2 m \rangle$	$\langle m Q_1^2 m \rangle$	$\langle m Q_2^2 m \rangle$	$\langle m Q_3^2 m \rangle$	$\langle m Q_4^2 m \rangle$
0	0.5	-0.75	3.281 25	-20.8125	165.886 25
1	1.5	-3.75	25.781 25	-244.6875	
2	2.5	-9.75	96.093 75		
3	3.5	-18.75	246.093 75		
4	4.5	-30.75	507.656 25		
5	5.5	-45.75	912.656 25		
6	6.5	-63.75			
7	7.5	-84.75			

Table 4. Off-diagonal elements of perturbation coefficient Q_γ^1 of $x(\lambda)$ for the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$.

Order γ	$\langle m Q_\gamma^1 n\rangle$ coefficient of $x(\lambda)$ at order γ		
	$\langle 0 Q_\gamma^1 1\rangle$	$\langle 1 Q_\gamma^1 2\rangle$	$\langle 0 Q_\gamma^1 3\rangle$
0	0.707 106 7812	1.0	0
1	-0.530 330 0859	-1.5	0.216 506 3509
2	2.088 174 713	10.054 6875	-2.110 936 922
3	-12.504 189 06	-94.570 3125	23.749 731 83
4	94.404 711 14	1 065.576 508	-300.360 698 4
5	-836.645 493 7	-13 566.953 29	4 204.975 928
6	8 396.630 153	189 561.747 7	-64 095.223 22
7	-93 535.925 02	-2857 992.657	1051 351.205
8	1143 303.25	—	—

Table 5. Sum of series $\langle 0|x|1\rangle$ to eighth order for $\lambda = 0.02$ in the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$.

Order of truncation of series, γ	Value of sum $\langle 0 x 1\rangle$ to order γ
0	0.707 106 7812
1	0.696 500 1795
2	0.697 335 4494
3	0.697 235 4158
4	0.697 250 5206
5	0.697 247 8433
6	0.697 248 3807
7	0.697 248 2610
8	0.697 248 2903
GP extrapolation	0.697 248 2845

Replacing the seventh-order term in (22) by a geometrical progression term

$$\frac{-\lambda^7 \langle 0|Q_7^1|1\rangle}{(1 - \lambda \langle 0|Q_8^1|1\rangle / \langle 0|Q_7^1|1\rangle)}$$

extrapolates the series (22) to infinite order. This result is also given in table 5.

An upper bound variational principle has been used (Clarke 1984b) to obtain the result for $\langle 0|x|1\rangle$ for the Hamiltonian

$$H = -D^2 + x^2 + 0.02x^4.$$

This result is

$$\langle 0|x|1\rangle = 0.697 248 2852$$

agreeing with the GP result of table 5 to nine decimal places.

Two interesting points stand out from the results of tables 4 and 5.

(a) The series produced are alternating series and thus show the typical feature of the diagonal perturbation series arising from perturbed oscillator problems.

(b) Successive values of the sums for $\langle 0|x|1 \rangle$ in table 5 provide an upper limit and a lower limit of the 'true' result. This is also a typical feature of diagonal perturbation series for perturbed oscillator problems.

The usefulness of the renormalised series method can be best illustrated by selecting a strong coupling, $\lambda = 1$, for the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$. Table 6 shows the sum of the untreated Rayleigh-Schrödinger series ($R = 0$) for $\langle 0|x|1 \rangle$ alongside the sum of the renormalised series (with $R = 3.3$). Compared with the variational result for this problem (Clarke 1984b) which gives

$$\langle 0|x|1 \rangle = 0.552\ 565\ 9594$$

the renormalised sum gives agreement to five decimal places. In contrast, the sum of the untreated series is strongly diverging and yields no useful result.

The algorithm presented in this work has the disadvantage that the number of operations required to calculate the products $\langle m|Q_{i-1}^{2\nu-1}|m+2s+1 \rangle$ in (15) rapidly escalate with the order i and the perturbation potential power 2ν due to a calculation of sums over products of $x(\lambda)$ elements. This has a noticeable effect on the running time of the program. It is conceivable that the introduction of off-diagonal even power moments into this calculation could considerably reduce the number of operations.

Table 6. Sum of series $\langle 0|x|1 \rangle$ to eighth order for $\lambda = 1$ in the Hamiltonian $H = -D^2 + x^2 + \lambda x^4$ with $R = 0$ and $R = 3.3$.

Order of truncation of series, γ	$R = 0$	$R = 3.3$
0	0.707 106 7812	0.491 041 1501
1	0.176 776 6953	0.543 950 0213
2	2.264 951 409	0.551 907 1063
3	-10.239 237 65	0.552 625 1583
4	84.165 473 5	0.552 599 6847
5	-752.480 020 2	0.552 570 0737
6	7 644.150 133	0.522 568 4942
7	-85 891.774 88	0.552 565 3873
8	1057 411.475	0.552 566 9939
GP extrapolation		0.552 566 4463

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