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Rayleigh–Schrödinger perturbation theory with a strong perturbation: anharmonic oscillators

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Abstract. The bound state solutions of Schrödinger's equation for the anharmonic oscillator potentials $V = x^2 + \lambda x^{2k}$ $(k = 2, 3, \ldots)$ have been investigated, using elementary techniques of low-order variational perturbation theory. For the quartic oscillator $(k = 2)$ a scaled harmonic potential provides a remarkably accurate model for all λ. Although this model is slightly less satisfactory for higher-order anharmonicities $(k \geq 3)$, our perturbation procedures remain effective, and can be applied successfully provided that higher-order terms are calculated.

1. Introduction

In the last few years, there has been renewed interest in the application of Rayleigh-Schrödinger (RS) perturbation theory (PT), particularly for cases in which the standard RSPT energy series is known to be divergent or asymptotic. Considerable analytical and computational effort has led to a rich variety of summation techniques which extract useful information from the calculated RSPT coefficients. The recent review of Cizek and Vrscay (1982) contains a fairly comprehensive bibliography of many of these developments.

Some of the problems which normally lead to a singular RSPT energy expansion can be treated effectively by other (non-perturbative) means. However, it is often also possible to obtain accurate solutions from a variant of RSPT which appears to avoid the formal difficulties of the standard theory. The procedure has been described previously (Cohen and Kais 1984). It is based on rewriting the system Hamiltonian

$$H(\lambda) = H_0 + \lambda H_1 \tag{1}$$

in which H_0 and H_1 are λ-independent operators, in an equivalent form with λ-dependent operators,

$$H(\lambda) = H(\lambda; \mu = 1), \qquad H(\lambda, \mu) = \bar{H}_0(\lambda) + \mu \bar{H}_1(\lambda). \tag{2}$$

The essential difference between (1) and (2) stems from the observation that whereas the physical perturbation parameter λ may assume very large values, the formal parameter μ is limited to the range $0 \leq \mu \leq 1$. The improved convergence of the RSPT energy expansion based on (2) depends on the possibility of choosing $\bar{H}_1(\lambda)$ small by comparison with $\bar{H}_0(\lambda)$, for each λ of interest.

Clearly, the success of this procedure, which yields a renormalised energy series (Killingbeck 1977), depends critically on the choice of $\bar{H}_0(\lambda)$. This must be a soluble

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model Hamiltonian and should reflect (as far as possible) the λ dependence of the given (physical) Hamiltonian $H(\lambda)$. In our earlier treatment of the problem of a hydrogen atom in the presence of a strong magnetic field (Cohen and Kais 1984) and of the Stark effect of a rigid rotor (Cohen *et al* 1984), $\bar{H}_0(\lambda)$ could be chosen to reproduce the essential features of $H(\lambda)$ at both limits, $\lambda \to 0$ and $\lambda \to \infty$. This is not possible in the present case.

Here, we treat general anharmonic oscillators, with

$$H(\lambda) = -\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \lambda x^{2k}, \tag{3}$$

and have adopted a scaled harmonic oscillator model,

$$\bar{H}_0(\lambda) = -\mathrm{d}^2/\mathrm{d}x^2 + \alpha^2 x^2, \tag{4}$$

where $\alpha = \alpha(\lambda)$ remains to be selected. As we show in the following, this choice is most appropriate for the quartic anharmonic oscillator ($k = 2$) but becomes progressively less satisfactory for higher k. Since this $\bar{H}_0(\lambda)$ approaches $H(\lambda)$ only as $\lambda \to 0$ (but not as $\lambda \to \infty$, no matter how α is chosen), we might expect to encounter convergence difficulties for large λ. We shall see, however, that α may be chosen so that individual terms of the RSPT series which arise from $\bar{H}_0(\lambda)$ remain finite no matter how large λ becomes. Furthermore, energy calculations based on $\bar{H}_0(\lambda)$, and taken to first order only, yield results which are qualitatively correct for all λ for $k = 2, 3, 4$. These calculations require nothing more than the well known harmonic oscillator eigenfunctions.

For the quartic anharmonic oscillator ($k = 2$), highly accurate energies are obtained by calculating in addition second- and third-order energy corrections. This enables us to calculate variational upper bounds for the lowest states of even and odd parity and leads to results more accurate for the ground state than those obtained by Schönhammer and Cederbaum (1975) using a similar procedure. To achieve similar accuracy for higher k (≥ 3), it will probably be necessary to calculate increasingly higher-order energy corrections. This will present no great difficulty in practice, since the RSPT wavefunction corrections may be obtained analytically to any desired order (cf Bender and Wu 1969) or, alternatively, the hypervirial theorem method (Swenson and Danforth 1972, Killingbeck 1981) may be employed to obtain energy corrections directly.

2. Energy expansions

It is convenient to make a change of scale $x \to x/\alpha^{1/2}$, $E \to \alpha E$ so that, effectively,

$$\bar{H}_0(\lambda) = \alpha(-\mathrm{d}^2/\mathrm{d}x^2 + x^2), \qquad \bar{H}_1(\lambda) = \alpha(px^2 + qx^{2k}), \tag{5}$$

where

$$p = (1/\alpha^2 - 1), \qquad q = \lambda/\alpha^{k+1}. \tag{6}$$

Now it is clear that E has a formal RSPT expansion, which arises naturally if we apply two perturbations px^2 and qx^{2k} to $\bar{H}_0(\lambda)$:

$$E = \alpha \sum_i \sum_j E_{ij} p^i q^j. \tag{7}$$

By combining the two perturbing terms into a single perturbation $\bar{H}_1(\lambda)$, we are simply rewriting the double sum (7) in the equivalent form

$$E = \alpha \sum_t \varepsilon_t, \qquad \varepsilon_t = \sum_{i+j=t} \sum E_{ij} p^i q^j. \tag{8}$$

However, we may equally absorb the px^2 perturbation into $\bar{H}_0(\lambda)$, make a further change of scale $x \to x/(1+p)^{1/4}$, $E \to (1+p)^{1/2}E$ and obtain directly an expansion in terms of a single parameter r:

$$E = \alpha(1+p)^{1/2} \sum_t E_t r^t, \qquad r = q/(1+p)^{1/2(k+1)}. \tag{9}$$

Expanding $(1+p)^{1/2}$ and r^t in power series now allows us to obtain the coefficients E_{ij} of (8) from the traditional RSPT coefficients E_t since it is clear from (6) and (9) that

$$\alpha(1+p)^{1/2} = 1, \qquad r = \lambda, \tag{10}$$

so that the total E is independent of α, as it must be.

However, each individual ε_t in the expansion (8) is a function of α and in order for ε_t to remain finite as $\lambda \to \infty$, it is sufficient to choose $\alpha \sim \lambda^{1/(k+1)}$. By contrast, each term in the standard expansion $\Sigma_t E_t \lambda^t$ becomes infinite with λ.

3. Zero-order calculations

All the states of $H(\lambda)$ are of definite parity, and for the lowest even- and odd-parity states, those values of $\alpha(\lambda)$ which minimise the variational energy calculated with a zero-order eigenfunction $\psi_0(\alpha)$ of $\bar{H}_0(\lambda)$,

$$\varepsilon(\alpha) = \langle \psi_0(\alpha) | H(\lambda) | \psi_0(\alpha) \rangle / \langle \psi_0(\alpha) | \psi_0(\alpha) \rangle, \tag{11}$$

yield rigorous upper bounds to the energy for any given λ. Thus, we minimise $\varepsilon(\alpha)$ which is here given explicitly by

$$\varepsilon_n^{(2k)}(\lambda) = \alpha[(2n+1) + \tfrac{1}{2}(2n+1)p + A_n^{(2k)} q] \tag{12}$$

and $A_n^{(2k)} = \langle x^{2k} \rangle_n$ has been evaluated quite generally as

$$A_n^{(2k)} = \frac{n!(2k)!}{2^n \Gamma(\frac{1}{2})} \sum_{m=i}^{n} \frac{2^m \Gamma(\frac{1}{2}+k+m-n)}{(2k+2m-2n)![(n-m)!]^2 m!} \qquad i = \max(0, n-k). \tag{13}$$

The variation yields

$$\varepsilon_n^{(2k)}(\lambda) = \tfrac{1}{2}(2n+1)[(k+1)\alpha + (k-1)/\alpha]/k \tag{14}$$

where α satisfies

$$\alpha^{k-1}(\alpha^2 - 1) = 2kA_n^{(2k)} \lambda/(2n+1) \tag{15}$$

so that for λ sufficiently large

$$\frac{\varepsilon_n^{(2k)}}{\lambda^{1/(k+1)}} = (k+1)\left[\left(\frac{2n+1}{2k}\right)^k A_n^{(2k)}\right]^{1/(k+1)}. \tag{16}$$

In table 1, we present variational energies of the lowest four states ($n = 0, 1, 2, 3$) of the quartic anharmonic oscillator ($k = 2$) calculated from (14), (15) and (16) as compared with the converged Hill determinant values of Biswas *et al* (1973). Our results for the lowest even- and odd-parity states ($n = 0, 1$) are seen to be upper bounds

Table 1. Energy levels of the quartic anharmonic oscillator.

	$n=0$		$n=1$		$n=2$		$n=3$	
λ	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
0.1	1.066 20	1.065 29	3.310 31	3.306 87	5.748 00	5.747 96	8.346 15	8.352 68
0.2	1.120 61	1.118 29	3.546 77	3.539 01	6.276 49	6.277 25	9.243 87	9.257 77
0.5	1.248 03	1.241 85	4.069 92	4.051 93	7.393 08	7.396 90	11.085 1	11.115 2
1	1.403 32	1.392 35	4.678 23	4.648 81	8.647 04	8.655 05	13.109 5	13.156 8
2	1.625 00	1.607 54	5.519 87	5.475 78	10.344 7	10.358 6	15.815 9	15.884 8
5	2.047 04	2.018 34	7.082 28	7.013 48	13.443 8	13.467 7	20.708 8	20.814 0
10	2.488 62	2.449 17	8.691 31	8.599 00	16.602 3	16.635 9	25.666 8	25.806 3
20	3.062 50	3.009 94	10.764 2	10.643 2	20.648 8	20.694 1	31.998 6	32.180 3
50	4.078 52	4.003 99	14.411 2	14.241 7	27.739 2	27.804 0	43.068 5	43.321 6
100	5.095 16	4.999 41	18.046 8	17.830 2	34.790 4	34.874 0	54.062 9	54.385 3
Asymptotic $E/\lambda^{1/3}$	1.08†	1.07	3.85†	3.84	7.44†	7.51	11.6†	11.7

(1) Present results, equations (14) and (15).
(2) Biswas *et al* (1973).
† From equation (16).

as required, but this is not the case for the excited states ($n=2, 3$). Nevertheless, this choice of α clearly yields accurate energies for all calculated λ, extending also to the asymptotic region, $\lambda \to \infty$.

Note that we obtain full agreement with the calculations of Feranchuk and Komarov (1982) for the $n=0, 1$ states but not for the $n=2$ state. Their procedure, though expressed formally in terms of creation and annihilation operators, is evidently very similar to ours and it appears that their numerical results for the $n=2$ state are in error.

Table 2 contains a similar comparison for the even-parity ground states of the sextic ($k=3$) and octic ($k=4$) anharmonic oscillators, from which it is clear that this

Table 2. Ground state energies of the sextic and octic oscillators.

	$k=3$		$k=4$	
λ	(1)	(2)	(1)	(2)
0.1	1.119 93	1.109 09	1.211 27	1.168
0.2	1.192 81	1.173 89	1.300 53	1.240
0.5	1.334 89	1.300 99	1.454 52	1.367
1	1.484 05	1.435 62	1.601 90	1.490
2	1.675 59	1.609 93	1.779 38	1.640
5	2.005 31	1.912 45	2.066 52	1.889
10	2.322 92	2.205 72	2.329 02	2.118
20	2.710 02	2.564 64	2.636 17	2.387
50	3.348 81	3.159 02	3.121 01	2.80
100	3.946 99	3.716 97	3.556 52	3.18
Asymptotic $E_n^{(2k)}/\lambda^{1/(k+1)}$	1.22†	1.17	1.38†	1.27

(1) Present results, equations (14) and (15).
(2) Biswas *et al* (1973).
† From equation (16).

approximation deteriorates in accuracy with increasing k for any given λ. This is due to the fact that eigenfunctions of $H(\lambda)$ behave asymptotically as $\exp(-\lambda^{1/2}|x|^k/k)$ (cf Killingbeck 1985, Schwartz 1985) which differs increasingly from the harmonic oscillator eigenfunctions with increasing k. Nevertheless, the qualitative features of the eigenvalues $\varepsilon_n^{(2k)}(\lambda)$ are adequately reproduced and even the asymptotic limit $\varepsilon_n^{(2k)}/\lambda^{1/(k+1)}$ obtained from (16) remains fairly satisfactory.

4. First-order calculations

A major advantage of our choice of $\bar{H}_0(\lambda)$ is that it leads to RSPT equations which are analytically soluble. If $\psi_0(\alpha)$ provides a good approximation to an exact eigenfunction $\psi(\lambda)$, it is to be expected that the first-order approximation $\psi_0+\psi_1(p, q)$ will yield very accurate results, which may be improved variationally (for ground states retaining the upper bound property) by using $\psi_0+\eta\psi_1(p, q)$.

Since it is always possible to choose $\psi_1(p, q)$ orthogonal to ψ_0, a simple measure of the importance of $\psi_1(p, q)$ is provided by the integral $S_{11}=\langle\psi_1|\psi_1\rangle$, which should be as small as possible by comparison with $\langle\psi_0|\psi_0\rangle=1$. Thus, for any state, it seems sensible to minimise $S_{11}(\alpha)$; this provides an alternative choice of α, but requires that $\psi_1(p, q)$ be calculated explicitly. (This presents no difficulty here; in other cases a variational approximation to $\psi_1(p, q)$ should suffice.) The possibility of minimising S_{11} in order to improve an RSPT expansion has been considered previously by Silverman (1981).

Since first-order solutions contain steadily increasing numbers of terms as k increases, we treat here the quartic anharmonic oscillator only. The zero- and first-order solutions for an arbitrary state (labelled n) are then

$$\psi_0(n)=|n\rangle=N_n\exp(-x^2/2)H_n(x) \tag{17}$$

and

$$\psi_1(n)=a_{n-4}|n-4\rangle+a_{n-2}|n-2\rangle+a_{n+2}|n+2\rangle+a_{n+4}|n+4\rangle, \tag{18}$$

where $H_n(x)$ is the usual Hermite polynomial, N_n the appropriate normalisation factor and the coefficients appearing in $\psi_1(n)$ are explicitly

$$\begin{aligned} a_{n-4}&=2b(n)b(n-2)q, \qquad a_{n-2}=b(n)[p+(2n-1)q], \\ a_{n+2}&=-b(n+2)[p+(2n+3)q], \qquad a_{n+4}=-2b(n+4)b(n+2)q, \end{aligned} \tag{19}$$

where

$$b(n)=\tfrac{1}{8}[n(n-1)]^{1/2}. \tag{20}$$

It is now a straightforward calculation to obtain

$$\begin{aligned} \varepsilon_0&=(2n+1), \\ \varepsilon_1&=\tfrac{1}{2}(2n+1)p+\tfrac{3}{4}(2n^2+2n+1)q, \\ \varepsilon_2&=Ap^2+Bpq+Cq^2, \\ \varepsilon_3&=Dp^3+Fp^2q+Gpq^2+Jq^3, \end{aligned} \tag{21}$$

and

$$S_{11}=Kp^2+Lpq+Mq^2.$$

The coefficients are gathered for convenience in table 3, and the interrelations implied by equations (8) and (9) provide a valuable check.

Table 3. Coefficients appearing in equations (21).

$A=-\frac{1}{8}(2n+1)$	$G=\frac{5}{32}(34n^3+51n^2+59n+21)$
$B=-\frac{3}{4}(2n^2+2n+1)$	$J=\frac{3}{64}(125n^4+250n^3+472n^2+347n+111)$
$C=-\frac{1}{16}(34n^3+51n^2+59n+21)$	$K=\frac{1}{32}(n^2+n+1)$
$D=\frac{1}{16}(2n+1)$	$L=\frac{1}{16}(2n+1)(n^2+n+3)$
$F=\frac{3}{4}(2n^2+2n+1)$	$M=\frac{1}{512}(65n^4+130n^3+487n^2+422n+156)$

We are now able to calculate truncated perturbation sums,

$$E=\alpha\sum_{i=0}^{N}\varepsilon_i, \qquad N=1,2,3, \tag{22}$$

and two variational upper bounds (for ground states),

$$E(\psi_0+\psi_1)=\alpha[\varepsilon_0+\varepsilon_1+(\varepsilon_2+\varepsilon_3)/(1+S_{11})] \tag{23}$$

and

$$E(\psi_0+\eta\psi_1)=\alpha[\varepsilon_0+\varepsilon_1+\eta\varepsilon_2], \tag{24}$$

where (Dalgarno and Stewart 1961)

$$S_{11}\eta^2+(1-\varepsilon_3/\varepsilon_2)\eta-1=0. \tag{25}$$

Note that when S_{11} is sufficiently small, (24) yields the [2/1] Padé approximation to E (the so-called geometric approximation)

$$E_{\text{geom}}=\alpha[\varepsilon_0+\varepsilon_1+\varepsilon_2/(1-\varepsilon_3/\varepsilon_2)]. \tag{26}$$

Up to this point, α remains at our disposal. We have performed two different sets of calculations, with α minimising the first-order energy sum $\alpha(\varepsilon_0+\varepsilon_1)$, and with α minimising S_{11}.

The results for each of the lowest even- and odd-parity states are very similar for both choices of α, but the convergence of the low-order partial sums is slightly more rapid when S_{11} is minimised, and we present these values in tables 4 and 5. It will be

Table 4. Ground state energies of the quartic anharmonic oscillator.

	Perturbation partial sums			Variational estimates			Accurate
λ	(1)	(2)	(3)	(4)	(5)	(6)	(7)
0.1	1.0662	1.0652	1.0653	1.0653	1.0653	1.0653	1.0653
0.2	1.1206	1.1179	1.1185	1.1185	1.1184	1.1184	1.1183
0.5	1.2481	1.2406	1.2429	1.2429	1.2424	1.2424	1.2419
1	1.4036	1.3899	1.3949	1.3949	1.3936	1.3936	1.3924
2	1.6254	1.6034	1.6125	1.6125	1.6098	1.6098	1.6075
5	2.0479	2.0114	2.0277	2.0278	2.0227	2.0227	2.0183
10	2.4899	2.4395	2.4629	2.4630	2.4555	2.4555	2.4492
20	3.0643	2.9970	3.0291	3.0291	3.0187	3.0187	3.0099
50	4.0811	3.9855	4.0320	4.0321	4.0169	4.0168	4.0040
100	5.0985	4.9757	5.0359	5.0360	5.0162	5.0161	4.9994

(1) Equation (22), $N=1$.
(2) Equation (22), $N=2$.
(3) Equation (22), $N=3$.
(4) Equation (23).
(5) Equation (24).
(6) Equation (26).
(7) Hill determinant, Biswas *et al* (1973).

Table 5. First excited state energies of the quartic anharmonic oscillator.

	Perturbation partial sums			Variational estimates			Accurate
λ	(1)	(2)	(3)	(4)	(5)	(6)	(7)
0.1	3.3103	3.3065	3.3070	3.3070	3.3070	3.3070	3.3069
0.2	3.5468	3.5378	3.5396	3.5396	3.5393	3.5393	3.5390
0.5	4.0701	4.0484	4.0544	4.0544	4.0531	4.0531	4.0519
1	4.6787	4.6425	4.6540	4.6540	4.6513	4.6512	4.6488
2	5.5206	5.4658	5.4848	5.4849	5.4800	5.4799	5.4758
5	7.0836	6.9973	7.0294	7.0296	7.0208	7.0207	7.0135
10	8.6931	8.5768	8.6216	8.6218	8.6093	8.6091	8.5990
20	10.7667	10.6139	10.6738	10.6742	10.6571	10.6569	10.6432
50	14.4147	14.2002	14.2857	14.2862	14.2617	14.2613	14.2417
100	18.0513	17.7770	17.8870	17.8877	17.8560	17.8555	17.8302

(1) Equation (22), $N = 1$.
(2) Equation (22), $N = 2$.
(3) Equation (22), $N = 3$.
(4) Equation (23).
(5) Equation (24).
(6) Equation (26).
(7) Hill determinant, Biswas *et al* (1973).

observed that S_{11} is generally so small that the third-order partial sums (22) and the simple upper bounds (23) are indistinguishable, as are the improved upper bounds (24) and the results of the geometric approximation (26). The second-order partial sums (22) are generally too low, but these are not upper bounds even for the ground states.

In table 6, we present similar results for the second excited state ($n = 2$), this being the lowest state for which (23) and (24) are not guaranteed bounds. It turns out that in this case, only (23) yields upper bounds *in practice*, but our procedure yields excellent approximate energies even when these are (slightly) too low. The modified operator method calculations of Feranchuk and Komarov (1984) yield results of similar accuracy to ours for both types of states and it is clear that the procedures have much in common. Other states ($n \geq 3$) and other anharmonicities ($k \geq 3$) may clearly be treated in the

Table 6. Second excited state energies of the quartic anharmonic oscillator.

	Perturbation partial sums			Variational estimates			Accurate
λ	(1)	(2)	(3)	(4)	(5)	(6)	(7)
0.1	5.7502	5.7461	5.7486	5.7486	5.7476	5.7476	5.7480
0.2	6.2804	6.2722	6.2793	6.2793	6.2760	6.2760	6.2772
0.5	7.3998	7.3836	7.4036	7.4036	7.3926	7.3925	7.3969
1	8.6562	8.6320	8.6676	8.6675	8.6465	8.6464	8.6550
2	10.3569	10.3229	10.3789	10.3786	10.3441	10.3441	10.3586
5	13.4608	13.4105	13.5013	13.5008	13.4429	13.4429	13.4677
10	16.6240	16.5583	16.6821	16.6812	16.6012	16.6012	16.6359
20	20.6763	20.5915	20.7556	20.7543	20.6475	20.6474	20.6941
50	27.7767	27.6595	27.8910	27.8891	27.7374	27.7373	27.8040
100	34.8378	34.6889	34.9858	34.9833	34.7882	34.7881	34.8740

(1) Equation (22), $N = 1$.
(2) Equation (22), $N = 2$.
(3) Equation (22), $N = 3$.
(4) Equation (23).
(5) Equation (24).
(6) Equation (26).
(7) Hill determinant, Biswas *et al* (1973).

same way, so that the utility of RSPT is dramatically enhanced for strong perturbations of this type.

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