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Renormalised perturbation series

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Abstract. Renormalised perturbation series are obtained directly (by the hypervirial method) for the perturbed oscillator and hydrogen atom, and indirectly (by series transformation) for the helium atom.

In the study of the perturbed Hamiltonian $H = T + U + \lambda V$, where T is the kinetic energy operator and U and V are local potential operators, the most commonly treated perturbation series is that for the energy

$$E = \sum E_n \lambda^n. \quad (1)$$

The perturbed expectation value of any other operator A can be similarly written

$$\langle A \rangle = \sum A_n \lambda^n \quad (2)$$

but in general higher order perturbed wavefunctions are needed to calculate A_n than to calculate E_n for given n . Killingbeck (1977) discussed ways in which the calculation of A_1 and A_2 can be simplified using interchange theorems. The first point which we wish to make in this note is that for *particular* A it is possible to make more headway; we can illustrate this for the example of the Hamiltonian

$$H = -D^2 + mx^2 + \lambda x^4 \quad (3)$$

studied (with $m = 1$) by Reid (1967) and Simon (1970) and many other workers. For the case $m = 1$ the Hellmann–Feynman theorem shows that $\langle x^4 \rangle = \partial E / \partial \lambda$, so the series for $\langle x^4 \rangle$ is obtained by formally differentiating the energy series. The virial theorem states that $E = 2\langle x^2 \rangle + 3\lambda \langle x^4 \rangle$, so that the series for $\langle x^2 \rangle$ follows from those for E and $\langle x^4 \rangle$. The energy equation $E = \langle H \rangle$ then allows the $\langle T \rangle$ series to be found from the three series already known. Thus the energy series directly yields the series for $\langle T \rangle$, $\langle x^2 \rangle$ and $\langle x^4 \rangle$, and the series for $\langle x^6 \rangle$ etc. then follow by using hypervirial relations. This observation would have considerably simplified the calculations of Reid (1967), who computed the series for $\langle T \rangle$ and $\langle x^2 \rangle$ by a method which required the off-diagonal matrix elements of these operators between the unperturbed states.

Recently Grubb (1980) tried to attack the problem of calculating the coefficients A_n by using commutator algebra, and encountered most of the difficulties pointed out by Killingbeck (1977). Grubb (1980) did not complete the calculation of A_1 for her perturbed hydrogen atom example, and apparently overlooked the fact that her quadrature expressions for the first-order perturbed wavefunction are only valid for ground states, as discussed, for example, by Killingbeck (1977) and Aharonov and Au (1979). The second point which we make here is that for perturbed hydrogen atom and

perturbed oscillator problems the A_n for many operators *can* be obtained using a formalism which is based on commutators and which does not need the explicit calculation of perturbed wavefunctions. The method which achieves this is the hypervirial method (Swenson and Danforth 1972, Killingbeck 1978, Caswell 1979, Austin 1980), which is the ultimate refinement of the argument used in the previous paragraph.

The third and main point of this note is to report some remarkable results which have been obtained using the hypervirial method. We can most clearly describe them by using the Hamiltonian (4), and rewriting it as

$$H = -D^2 + \mu x^2 + \lambda[x^4 - Kx^2] \quad (4)$$

with $\mu = m + \lambda K$. If the values of K and μ (for particular λ) are fixed *numerically*, then the hypervirial method permits direct evaluation of the coefficients in the expansions

$$E = \sum E_n(\lambda, K)\lambda^n \quad (5)$$

and

$$\langle x^p \rangle = \sum A_n^p(\lambda, K)\lambda^n. \quad (6)$$

All previous applications of the hypervirial method have found the series for $K = 0$, although Caswell (1979) found the series for non-zero K by performing a transformation on the $K = 0$ series. He dealt only with the energy series for the Hamiltonian (4). In fact the series (5) and (6) can be calculated *directly* from the hypervirial equations for the Hamiltonian (4) and also for a perturbed hydrogen atom Hamiltonian such as (for s states)

$$\begin{aligned} H &= -\frac{1}{2}D^2 - Zr^{-1} + \lambda r \\ &= -\frac{1}{2}D^2 - \mu r^{-1} + \lambda[r - Kr^{-1}] \end{aligned} \quad (7)$$

with $\mu = Z - \lambda K$. (States of higher l can be handled by including a centrifugal potential term.) The details of the hypervirial method have been discussed in the cited works, so we give only a brief sketch in this note. The bound state functions of the Hamiltonian

$$H = -\alpha D^2 + V \quad (8)$$

give expectation values which obey the hypervirial relation

$$0 = \frac{1}{2}\alpha \langle f''' \rangle + 2\langle f'(E - V) \rangle - \langle fV' \rangle \quad (9)$$

where f is any smooth function and E is the energy. Making the choice $f = x^{N+1}$ in (9), taking V from equation (4) or (7), and expanding all quantities as series in λ , we obtain an infinite hierarchy of equations for the coefficients E_n and A_n^p . These equations can be solved sequentially and rapidly on a mini-computer, provided that E_0 is known. E_0 equals $(m + \lambda K)^{1/2}$ for the groundstate of Hamiltonian (4) and $-\frac{1}{2}(Z - \lambda K)^2$ for the groundstate of Hamiltonian (7).

The *exact* results for the Hamiltonians (4) and (7) are independent of K , so we take as a plausible criterion the following one: if $S_N(K)$ is the sum (up to the λ^N term) of the series for any quantity, then K is chosen so that $\partial S_N / \partial K = 0$. It turns out that S_N for alternate N has an extremum in K (so that the criterion works) while for the intervening N the quantity $|\partial S_N / \partial K|$ shows a clear (but non-zero) minimum. The results for a few sets of parameters are shown in tables 1 and 2. (The exact results were obtained by an accurate numerical integration). We note for comparison that the [20, 20] Padé approximant for the $m = 1$ oscillator energy at $\lambda = 1$ is 1.3923375 (as derived from the

Table 1. Perturbed oscillator energy and K values.

N	(m, λ)	(1, 1)	(1, 10)	(-1, 1)
6		1.392 342 02 (4.10)	2.449 101 59 (2.01)	0.657 467 43 (4.11)
8		1.392 350 91 (3.80)	2.449 166 74 (1.87)	0.657 607 83 (4.47)
10		1.392 351 56 (4.20)	2.449 173 07 (2.06)	0.657 645 50 (4.87)
12		1.392 351 64 (4.55)	2.449 174 01 (2.25)	0.657 653 54 (5.25)
Exact		1.392 351 64	2.449 174 07	0.657 653 0

Table 2. Perturbed oscillator $\langle x^2 \rangle$ and K values.

N	(m, λ)	(1, 1)	(1, 10)	(-1, 1)
6		0.305 832 22 (4.44)	0.161 486 49 (2.17)	0.451 044 5 (4.24)
8		0.305 814 74 (3.94)	0.161 457 47 (1.94)	0.450 803 9 (4.60)
10		0.305 813 78 (4.31)	0.161 455 28 (2.12)	0.450 736 6 (4.99)
12		0.305 813 65 (4.75)	0.161 454 93 (2.31)	0.450 721 8 (5.40)
Exact		0.305 813 9	0.161 459 9	0.450 726 1

$K = 0$ energy series); the renormalised series is obviously much better even without the use of any summation procedure. The oscillator results for $m = -1$ are particularly interesting, since an attempt to find the $K = 0$ series would start from an unperturbed Hamiltonian with no bound states, for which E_0 could not be specified. The renormalised series, however, is based on a K value which renders $m + \lambda K$ positive, and gives good results. However, we could not make the method work for the hydrogenic problem with negative Z , which is puzzling, since, for example, a direct numerical integration at $Z = -1$, $\lambda = 0.1$ gives a well-defined bound state with energy 0.762246. The low-order results shown in tables 1 and 2 look very promising, but in principle we expect that even the renormalised series are ultimately divergent; a double precision computation to high order will be needed to investigate this point. Another puzzling feature for the H atom case is the superiority of the $N = 6$ and $N = 10$ results to the others. It remains to be seen whether some other criterion for choosing K will remove this irregularity.

For the two-electron atom groundstate problem, with Hamiltonian

$$\begin{aligned}
 H &= -\frac{1}{2}[\nabla_1^2 + \nabla_2^2] - Z(r_1^{-1} + r_2^{-1}) + \lambda r_{12}^{-1} \\
 &= T - (Z - \lambda K)(r_1^{-1} + r_2^{-1}) + \lambda[r_{12}^{-1} - K(r_1^{-1} + r_2^{-1})]
 \end{aligned}
 \tag{10}$$

the energy perturbation series can be written in the equivalent forms

$$Z^2 \sum E_n \lambda^n Z^{-n} = (Z - K\lambda)^2 \sum \varepsilon_n \lambda^n (Z - K\lambda)^{-n}.
 \tag{11}$$

The E_n were found by Midtdal (1965) using variational methods; so far it has not been possible to find the E_n by the hypervirial method. Comparing coefficients in equation (11) we quickly find that the sum up to the λ^2 term is K -independent. Further we find that

$$\varepsilon_3 = E_3; \quad \varepsilon_4 = E_4 - KE_3
 \tag{12}$$

$$\varepsilon_5 = E_5 - 2KE_4 + K^2E_3
 \tag{13}$$

with the general rule that the coefficients in ε_{N+3} are those for the binomial expansion of $(1-x)^N$. Table 3 shows that the renormalised energy series is superior to the $K=0$ series for this problem also. Of course, the series (11) is convergent here, whereas those arising from the two preceding problems were not.

Table 3. Perturbed H atom energy and K values.

N	(Z, λ)	(1, 0.2)	(1, 0.4)
6		-0.235 647 52 (-1.95)	-0.008 352 86 (-1.48)
8		-0.235 644 35 (-2.83)	-0.008 320 16 (-2.07)
10		-0.235 647 43 (-2.27)	-0.008 359 44 (-2.05)
12		-0.235 647 81 (-3.67)	-0.008 352 55 (-2.04)
Exact		-0.235 647 41	-0.008 353 65

Table 4. Perturbed H atom $\langle r \rangle$ and K values.

N	(Z, λ)	(1, 0.2)	(1, 0.4)
6		1.204 594 9 (-2.12)	1.080 909 5 (-2.10)
8		1.204 564 5 (-2.83)	1.079 733 6 (-2.07)
10		1.204 596 5 (-2.41)	1.079 993 3 (-2.06)
12		1.204 540 5 (-4.67)	1.079 933 2 (-2.05)
Exact		1.204 595	1.079 945

Table 5. Energy sums for the Helium atom ($Z=2, \lambda=1$).

N	5	7	9
K	0.26	0.34	0.40
E	-2.903 704 9	-2.903 723 7	-2.903 724 3
$E(K=0)$	-2.903 668 6	-2.903 718 6	-2.903 723 6
	('Exact' energy is -2.903 724 4)		

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