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LETTER TO THE EDITOR

Some extensions of the renormalised series approach

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Abstract. The non-Stieltjes renormalised series given by the hypervirial approach are empirically found to be summable by Padé methods (using the plateau criterion). The resulting energy estimates are exact, as shown by using an alternative power series method also based on the renormalisation approach.

In a recent work Killingbeck (1981) has used the hypervirial method to obtain renormalised perturbation series for the perturbed oscillator and for the s states of the perturbed hydrogen atom Hamiltonian

$$H = -\tfrac{1}{2}\nabla^2 - Zr^{-1} + \lambda r. \tag{1}$$

The renormalisation approach involves partitioning the potential energy so that the unperturbed part involves a modified nuclear charge, and uses the potential

$$V(r) = -\mu r^{-1} + \lambda(r - Kr^{-1}) \tag{2}$$

with $\mu = Z - K\lambda$. The unperturbed eigenvalue then takes the form $E_0 = -\mu^2/2n^2$ and it is the only information needed to start off a hypervirial calculation which gives the perturbation series for the energy and $\langle r^n \rangle$ values (Swenson and Danforth 1972, Killingbeck 1978). Since the exact energy is K independent it seems reasonable, when given only a finite number of terms of the perturbation series, to choose K so that $\partial E_N/\partial K$ is zero, when E_N is the sum to N terms of the energy series (for a given λ). This criterion produces ground state energies better than those obtained from Padé approximants to the usual ($K = 0$) perturbation series. The $K = 0$ series is an alternating one of Stieltjes type, but for $K \neq 0$ the coefficients stick together in blocks of the same sign. Table 1 shows some ground state (1s) energy coefficients for three K values at $\lambda = 1$.

Since the $K \neq 0$ series are not of Stieltjes type, Killingbeck (1981) did not try a Padé approximant analysis, but noted that use of the plateau criterion $\partial E_N/\partial K = 0$ gives an energy estimate which, although fairly good, fluctuates as N increases. In this work we extend his work in three respects. First, we show that use of the plateau criterion gives energy results which tend smoothly to a stable (and exact) energy value as N increases, if E_N is the $[N/2, N/2]$ Padé approximant to $N+1$ terms (including E_0) of the renormalised series. Second, we show that the procedure works equally well for states with $l = 1$ and 2; to treat such states involves adding the usual term $\frac{1}{2}l(l+1)r^{-2}$ to the radial potential and making the appropriate modification of the double-precision hypervirial program used by Austin (1980). Third, we show how

Table 1. Some perturbation coefficients for the 1s state ($\lambda = 1$).

N	$K = 0$	$K = -1.25$†	$K = -3$
0	−5E−1	−2.351 25E0	−8E0
1	1.5E0	3.479 166 666 7E0	1.237 5E0
2	−1.5E0	−4.694 072 931 E−1	−4.224 609 375 E0
3	6.75E0	9.882 188 239 1E−2	1.937 713 623 E−1
4	−4.968 875E1	8.647 494 806 8E−3	1.273 596 882 8E−1
5	4.803 75E2	−7.716 533 692 5E−3	7.535 443 268 7E−2
6	−5.583 E3	−1.818 642 524 7E−3	3.730 355 459 3E−2
7	7.455 733 593 7E4	1.373 422 367 8E−3	1.220 406 346 5E−2
8	−1.114 319 335 E6	4.611 297 080 4E−4	−1.815 910 688 3E−3
9	1.832 917 144 E7	−3.283 226 957 4E−4	−7.370 944 510 6E−3

† $K = -1.25$ is the plateau midpoint for $\lambda = 1$ (see text).

the renormalisation idea can be used to give a power series approach to the Hamiltonian (1) which gives very good eigenvalues for both Dirichlet and Neumann boundary conditions imposed at any r value. Using a large r value enables us to check the results from the hypervirial method.

When λ and $N+1$, the (odd) number of terms used are fixed, it is found that the corresponding diagonal approximant $[N/2, N/2]$ has a plateau region extending over a wide range of K values. If stationarity to a given number of decimal places is demanded then the plateau width increases with N. Table 2 shows some results for the 1s state at $\lambda = 0.2$. The plateau extends between $K_0 \pm \Delta K/2$. Table 3 shows some

Table 2. Plateau midpoint and width for the [N/2, N/2] approximants. (1s state, $\lambda = 0.2$).

N	K_0	ΔK	E†
8	−1.8	0.4	−0.235 648
10	−1.7	0.6	−0.235 6474
12	−2.1	1.2	−0.235 647 41
14	−2.5	2.0	−0.235 647 405
16	−2.75	2.7	−0.235 647 405
18	−2.8	3.6	−0.235 647 405
20	−3.1	5.0	−0.235 647 405

† These digits stable along the plateau.

Table 3. Comparison of energy estimates from different methods. (only digits after the colon shown in last two columns).

State and λ	N	$E(K = 0)$†	E(plateau)	E(exact)‡
1s, 0.2	14	−0.2356 : 5	47 405	47 405
1s, 1.0	22	0.5779 :	21 352	21 352
2s, 0.15	20	0.466 :	659	659 084
3s, 0.02	22	0.137 : 1	0844	084 408
2p, 0.15	18	0.3 : 6	582 967	58 296 694
3d, 0.02	18	0.0926 :	06 733	06 733

† Stable digits from diagonal approximant sequence for $K = 0$ series.
‡ Using the power series method described in the text.

typical results obtained using the approach described above and compares them with the Padé approximant results for the $K = 0$ series and with the results of a power series calculation. This latter calculation involves applying the renormalisation idea in a different form, writing the eigenfunction ψ of the Hamiltonian (1) as a product $\exp(-\beta r)Y_l F(r)$, where Y_l is a solid harmonic of degree l. The first two factors represent a hydrogenic function for some renormalised nuclear charge. If λ is zero in (1) then the choice $\beta = (l+1)^{-1}$ gives $E = -\frac{1}{2}\beta^2$, an unperturbed hydrogenic energy, with $F(r) = 1$. For non-zero λ, however, $F(r)$ will be an infinite series for any choice of β, although varying β will help to speed up convergence. Taking $F(r)$ in the form

$$F(r) = \sum A_n r^n = \sum T_n \tag{3}$$

leads after some tedious algebra, to the recursion relation

$$T_{N+1}(N+1)(N+2l+2) = [(2l+2+2N)\beta - 2]rT_N - (2E+\beta^2)r^2 T_{N-1} + 2\lambda r^3 T_{N-2}. \tag{4}$$

To use (4), T_0 is set equal to 1 and r is made large ($r \sim 15$) if the boundary condition $\psi(\infty) = 0$ is to be simulated. For a given β and two trial energies, E_1 and E_2, the T_N and the sum $F(r)$ are evaluated, starting with $T_0 = 1$ and $T_{-1} = T_{-2} = T_{-3} = 0$. If β is chosen reasonably the series quickly converge and lead to two values $F(r, E_1)$ and $F(r, E_2)$, from which an interpolated energy E can be found which would have given $F(r, E) = 0$. After a few repetitions the eigenvalue corresponding to the boundary condition $\psi(r) = 0$ is determined very accurately. Killingbeck (1982) discusses in detail how to perform the calculation on a microcomputer and how to use it for Neumann as well as Dirichlet boundary conditions.

The results seem to show that the use of Padé approximants gives accurate energies from the renormalised series, even though the series are not of Stieltjes type. The calculations reported here are for positive λ, so that well defined bound states exist. For small negative λ there will be quasi-bound (resonance) states; the real part of the energy of such a state can be estimated using the stabilisation method (Hazi and Taylor 1970) or by using a phase shift analysis (Killingbeck 1980). Since increasing the number of terms in the renormalised series is presumably analogous to increasing the number of basis functions in the stabilisation approach, it may be possible to study resonant states for negative λ by looking for a minimum in $|\partial E/\partial N|$ as both N and K are varied; this point is still under investigation.

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