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Further applications of the renormalised series technique

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Abstract. The renormalised series technique is applied to two quantum mechanical problems, the octically perturbed oscillator and the hydrogen Stark effect. Modification of the method is required for the latter problem; the results yield the Stark shifted energies and an estimate of the widths of the states studied.

1. Introduction

The renormalised series approach (Killingbeck 1981, Austin and Killingbeck 1982) has been found to be a useful technique for dealing with divergent perturbation series, particularly when combined with the use of Padé approximants (Austin and Killingbeck 1982).

In this paper the renormalised series technique is applied to two further quantum mechanical problems: the harmonic oscillator with an octic perturbation and the hydrogen Stark effect. The octically perturbed oscillator problem is of interest since the unrenormalised series violates one of the conditions for Padé summation, although it is of Stieltjes type (Graffi *et al* 1971, Graffi and Grecchi 1978). The Stark problem is an example involving a system which has no bound states; direct summation of the perturbation series yields the real part of the resonance energy $E_{\mathrm{RES}} = E - \frac{1}{2}\mathrm{i}\Gamma$. The series also contains information about the width Γ (Silverstone *et al* 1979, Drummond 1981, Reinhardt 1982), but not in a directly accessible form. In § 3, it is shown that a modification of the renormalised series method allows an estimate of Γ to be obtained, as well as good values of E.

2. The octically perturbed oscillator

2.1. *The unrenormalised and renormalised series for the octically perturbed oscillator*

The Hamiltonian

$$H = -D^2 + x^2 + \lambda x^{2n} \qquad (\lambda > 0) \tag{2.1}$$

is often used as a test case in perturbation theory. The energy perturbation series for this type of system has been shown (Simon 1970, Loeffel and Martin 1970) to take the form $E_0 + \lambda S$, where S is a series of Stieltjes, i.e. the terms of the energy series

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have the form:

$$C_n = (-)^n \int_0^\infty x^n \, d\rho(x), \qquad n \geq 1, \tag{2.2}$$

where $\rho(x)$ is non-decreasing. The applicability of Padé summation to series of Stieltjes is closely related to the existence of a unique solution $\rho(x)$ to (2.2). From the study of the continued fraction representation of Stieltjes series, it has been proved (Wall 1929, 1948) that the moment problem does not have a unique solution if the sum of the continued fraction coefficients converges. Under these conditions the $[N+j/N]$ sequences of Padé approximants converge to different Stieltjes functions

$$F_j(t) = \int_0^\infty \frac{d\rho_j(x)}{1+xt}.$$

The F_j are bounded by the limits of the $[N/N]$ and $[N-1/N]$ sequences (Bender and Orszag 1978).

For oscillator perturbation series, the continued fraction analysis has not been performed. It is known, however, that a sufficient (but not necessary) condition for a unique solution of the moment problem and convergence of the Padé sequences to a common limit is that

$$\sum_n |E_n|^{-1/(2n+1)}$$

should diverge. This condition is obeyed for x^{2n} perturbations $m = 2$, 3 but not for $m > 3$; the indeterminancy of the moment problem for $m > 3$ has been rigorously proved by Graffi and Grecchi (1978).

In numerical work, it is of interest to investigate the differences between the $[N+1/N]$ and $[N/N]$ sequence limits. Although these sequences do not converge to a common limit, they may still be used to give bounds on the energy. (The energy series has the form $\alpha + \lambda S$ where S is a series of Stieltjes, so $[N+1/N]$ and $[N/N]$ replace $[N/N]$ and $[N-1/N]$ in the previous discussion on bounds.) It is also of interest to compare results for the unrenormalised and renormalised series. (For the latter the series is not necessarily of Stieltjes form, so no convergence theorems are available.)

The unrenormalised energy series for the ground state of the octically perturbed oscillator was calculated using the hypervirial method (Swenson and Danforth 1972, Killingbeck 1978a, b), as described in previous work (Austin 1980). The number of terms obtainable is limited by the strong (asymptotically $(3n)!$) divergence of the series coefficients. The series is strongly divergent, but the Padé approximants do converge for reasonably small λ values; results are presented in table 1. For small λ, the $[N+1/N]$ and $[N/N]$ sequences converge to a common limit, within the accuracy of the calculation. For larger λ the $[N+1/N]$ and $[N/N]$ provide upper and lower bounds as expected; these bounds move further apart and thus become less useful as λ increases. To illustrate the gap between the limits reached by the $[N/N]$ and $[N+1/N]$ approximants the ratio $[N/N]/[N+1/N]$ was studied as a function of N for various λ values. For small λ the ratio converges to a value close to unity; for larger λ values the limit is considerably different from unity and decreases with increasing λ. Similar results are found for the $n = 1$ and $n = 2$ states of the perturbed oscillator. Table 2 shows typical results for two λ values. For $\lambda = 0.001$ the ratio is close to unity and the Padé approximants are clearly providing reasonable upper and

Table 1. Comparison of results for the octically perturbed oscillator. $[N/N]$ and $[N+1/N]$ are the unrenormalised series results; $[M/M]_{\text{PLATEAU}}$ and $[M+1/M]_{\text{PLATEAU}}$ are results for the renormalised series. The $[7/6]_{\text{DP}}$ were obtained by the method of Dmitrieva and Plindov (1980a, b); E_{EXACT} values are those of Banerjee (1978), truncated to ten decimal places.

λ	N	$[N/N]$	$[N+1/N]$	M	$[M/M]_{\text{PLATEAU}}$	$[M+1/M]_{\text{PLATEAU}}$	$[7/6]_{\text{DP}}$	E_{EXACT}
10^{-5}	2	1.000 065 5203		—	—	—	—	1.000 065 5203
10^{-4}	12	1.000 646 3699		—	—	—	—	1.000 646 3699
10^{-3}	16	1.005 85	1.005 86	16	1.005 8573	1.005 858	1.005 864	1.005 857 5141
10^{-2}	16	1.0387	1.41	12	1.039	1.0407	1.041 268	1.039 496 7787
10^{-1}	10	1.07	1.42	12	1.17	1.19	1.187 902	1.168 970 8957
10^{0}	10	1.08	5.0	10	1.7	1.6	1.550 991	1.491 019 8957
10^{1}	—	—	—	—	—	—	2.238 098	2.114 544 6219
10^{2}	—	—	—	—	—	—	3.405 332	3.188 654 3465
10^{3}	—	—	—	—	—	—	5.307 470	4.949 487 4400
10^{4}	—	—	—	—	—	—	8.354 811	7.778 272 2143
4×10^{4}	—	—	—	—	—	—	11.003055	10.238 868 2355

Table 2. Values of the $[N+1/N]$ and $[N/N]$ approximants and their ratio for the octically perturbed oscillator.

λ	N	$[N/N]$	$[N+1/N]$	Ratio
0.001	1	1.005 6536	1.005 9574	0.999 6980
	2	1.005 8020	1.005 8962	0.999 9063
	3	1.005 8308	1.005 8790	0.999 9520
	4	1.005 8410	1.005 8718	0.999 9693
	5	1.005 8458	1.005 8680	0.999 9779
0.1	1	1.038 4334	1.516 2366	0.684 8755
	2	1.051 4476	1.467 6822	0.716 4000
	3	1.058 2672	1.442 2288	0.733 7720
	4	1.062 5760	1.426 2364	0.745 0209
	5	1.065 5596	1.415 1064	0.752 9896

lower bounds. For $\lambda = 0.1$, the ratio has converged to 0.75 and is clearly converging at a more rapid rate than the $[N+1/N]$ sequence and at a comparable rate to the $[N/N]$ sequence. The known smooth convergence of the $[N+1/N]$ and $[N/N]$ to their respective limits should guarantee that the ratio, having converged to 0.75, will not diverge again. This technique of studying the convergence of the ratio of two quantities has been successfully applied in other types of quantum mechanical calculations (Killingbeck 1983).

The limiting factor in the study of this problem is the rapid growth of the terms of the energy series, which limits both the number of terms available and their precision. The present calculation was carried out using double precision; a higher precision and higher-order calculation would yield more information the gap between the sequence limits. It should be noted that, whilst Padé summation alone is of only limited utility, a combination of Padé and Borel summation techniques has been successfully applied to the octic oscillator perturbation series, giving good numerical results (Graffi and Grecchi 1978).

The application of the Padé approximant technique to the ordinary perturbation series for the octically perturbed oscillator is thus limited. The renormalised Hamiltonian

$$H = -D^2 + (1 + K\lambda)x^2 + \lambda(x^8 - Kx^2) \tag{2.3}$$

was also studied. The perturbation series remains strongly divergent, even for small λ, so analysis of the partial series sums as in (Killingbeck 1981) was not possible. The Padé approximants, however, show a plateau as a function of K as found previously for the radial Stark problem (Austin and Killingbeck 1982). The results of these calculations are shown in table 1. The $[N/N]$ results are considerably better than the $K = 0$ results; the $[N+1/N]$ are more variable. As well as the improved energies obtained by using the renormalised $[N/N]$, a feature of great interest is that the $[N/N]$ and $[N+1/N]$ plateau values are similar for larger λ. There are no formal convergence theorems for the renormalised series, so it is not clear that there should be a gap between the $[N+1/N]$ and $[N/N]$ limits; clearly if such a gap exists, it is numerically smaller than for the unrenormalised series. This agreement indicates that correct eigenvalues are in fact being obtained from this 'difficult' series. The method fails, however, for $\lambda \geqslant 2$, no plateau being found.

2.2. Alternative series method for the octically perturbed oscillator

Dmitrieva and Plindov (1979, 1980a, b) have introduced a transformed perturbation series for oscillator problems which resembles the renormalised series. Their work, however, involves both a coordinate scaling of the Hamiltonian and a transformation of the perturbation parameter. The transformed parameter allows the correct asymptotic behaviour of $E(\lambda)$ as $\lambda \to \infty$ to be obtained, whilst retaining the usual ψ_0 as the unperturbed wavefunction. This method would thus be expected to be most effective at large λ.

For the octically perturbed oscillator, the transformations are:

$$\lambda = \lambda'/(1 - A\lambda')^{5/2}$$

$$H' = -D^2 + x^2 + \lambda'(x^8 - Ax^2) \qquad E' = (1 - A\lambda')^{1/2}E \tag{2.4}$$

where $A = 4\langle x^8\rangle_0/\langle x^2\rangle_0$; this choice allows ψ_0 to satisfy the virial theorem.

H' gives rise to a divergent series, of which the first fourteen terms were obtained. Results obtained from the [7/6] approximants are shown in table 1; the [6/6] results are less good. This calculation extends the very low-order results of Dmitrieva and Plindov (1979) and shows that remarkably good eigenvalues can be obtained over a wide λ range. The calculation is, however, less accurate than for the quartically perturbed oscillator (Dmitrieva and Plindov 1980b); a calculation on the intermediate sextically perturbed oscillator would be of interest in this context.

Comparison of the entries in table 1 shows that the renormalised series approach gives the best results for small λ. The method described in this section, as expected, is poor for small λ, but improves relative to the other methods as λ increases; for large λ it is the only successful technique involving summation of a perturbation series.

3. The Stark effect

The renormalised series approach works well for the radial Stark problem (Killingbeck 1981, Austin and Killingbeck 1982); it is of interest to extend this work to the more realistic Stark effect problem. The renormalised Hamiltonian is

$$H=-\tfrac{1}{2}\nabla^2-(1+K\lambda)/r+\lambda(z+K\lambda/r). \tag{3.1}$$

The Schrödinger equation for this problem can be separated in parabolic coordinates; the calculation of the perturbation series is as described by Austin (1980), with the inclusion of extra terms due to the $K\lambda/r$ part of the perturbation. Unfortunately, it is found for this problem that neither the partial series sums nor the Padé approximants show any sign of plateau behaviour. A similar effect is also found for the radial Stark problem with $\lambda<0$. This indicates that the breakdown of the method is related to the non-existence of bound states in both problems. It has been suggested (Austin and Killingbeck 1982) that as the effect of increasing the order of perturbation theory is analogous to increasing the number of basis functions in a variational calculation, results analogous to those of the stabilisation method (Hazi and Taylor 1970) should be obtainable. This would involve searching for a stable $E^{\mathrm{PADE}}(N,K)$ as a function of both N and K. This search was performed, but difficulties were found because the values of the Padé approximants fluctuate as N and K are varied and any stability found is no better than the unrenormalised series results. It has been pointed out by Reinhardt (1982) that there are mathematical grounds for expecting fluctuations as a function of N for $K=0$, since the Padé approximants to the perturbation series have real-axis poles. Reinhardt notes that the range of such fluctuations is expected to be comparable to the width Γ of the state concerned. Assuming similar arguments apply to the renormalised series, in the present calculation the stabilisation phenomenon would be masked by these fluctuations. It therefore seems reasonable to proceed by combining the stabilisation idea with a version of the least squares technique (Killingbeck 1978b). The optimum value of E is found by searching for the value of K for which the terms of the sum

$$S_N=\sum_N E^{\mathrm{PADE}}(K,N)$$

show least fluctuation about their mean (as measured by the RMS deviation Δ), the sum being taken over the higher-order Padé approximants.

Table 3 presents results obtained for the ground and $n=2$ states of hydrogen. The averaging was performed by summing the $[N/N]$ from $N=0$ to $N=16$; the energies thus obtained are relatively insensitive to changes in the range of N values; the Δ values are more variable, but remain of the same order of magnitude. The optimum energies are seen to be in good agreement with calculations of other workers (Benassi and Grecchi 1980, Hehenberger *et al* 1974, Cerjan *et al* 1978, Damburg and Kolosov 1976) and the range of validity of the perturbation approach has been extended to larger λ values than for the unrenormalised series (Austin 1980), for example for the ground state from $\lambda=0.05$ to $\lambda=0.12$. In addition, as predicted, the value of Δ provides a reasonable estimate of Γ.

The results obtained for the hydrogen ground state were compared with the results of a conventional least squares calculation using the trial function $e^{-r}+\alpha z\, e^{-\beta r}$. Calculations of this type give values of E and the RMS deviation Δ is thought (Killingbeck 1978b) to provide an estimate of the width Γ, provided the trial function is appropriately chosen. The E values obtained from the renormalised series calculation are found to be more accurate than those obtained by the least squares technique. The Δ values of the least squares calculation considerably overestimate Γ (presumably due to the

Table 3. Results of renormalised series calculations for the Stark effect for four values of the parabolic quantum numbers. Δ is the minimum value found for the RMS deviation of $\Sigma_{N=6}^{16}[N/N]$; E is the corresponding mean. The E_{ex} and Γ values were obtained from the following: [a] Benassi and Grecchi (1980), [b] Hehenberger *et al* (1974), [c] Cerjan *et* (1978), [d] Damburg and Kolosov (1976).

Parabolic quantum numbers	λ	E	Δ	E_{ex}	Γ
n_1 n_2 m					
0 0 0	0.04	−0.503 772	2.8×10^{-6}	−0.503 772[a]	4.0×10^{-6}[a]
= 1s	0.05	−0.506 076	8.6×10^{-5}	−0.506 1054[a]	7.8×10^{-5}[a]
	0.06	−0.509 205	4.2×10^{-4}	−0.509 2035[a]	5.2×10^{-4}[a]
	0.07	−0.513 250	2.1×10^{-3}	−0.513 0768[a]	1.85×10^{-3}[a]
	0.08	−0.517 121	2.8×10^{-3}	−0.517 5606[a]	4.54×10^{-3}[a]
	0.09	−0.522 215	6.3×10^{-3}	−0.522 4128[a]	8.78×10^{-3}[a]
	0.10	−0.526 333	1.1×10^{-2}	−0.527 4182[a]	1.45×10^{-2}[a]
	0.11	−0.536 196	2.5×10^{-2}	−0.532 45[b]	2.16×10^{-2}[b]
	0.12	−0.542 484	4.6×10^{-2}	−0.537 4[b]	2.99×10^{-2}[b]
1 0 0	0.004	−0.114 305 30	9.2×10^{-8}	−0.114 3053[c]	1.4×10^{-7}[c]
= $(2s-2p_z)$	0.005	−0.112 063	4.5×10^{-6}	−0.120 62†[d]	5.72×10^{-6}[d]
	0.008	−0.106 606	6.1×10^{-4}	−0.106 6684[c]	8.5×10^{-4}[c]
	0.010	−0.104 138	3.2×10^{-3}	−0.103 89[d]	3.28×10^{-3}[d]
	0.015	−0.096 880	5.4×10^{-3}	−0.096 945[d]	1.51×10^{-2}[d]
	0.020	−0.088 274	9.9×10^{-3}	−0.088 941[d]	3.10×10^{-2}[d]
0 1 0	0.004	−0.138 5518	6.6×10^{-6}	−0.138 5488[c]	4.4×10^{-6}[c]
= $(2s+2p_z)$	0.005	−0.142 608	1.1×10^{-5}	−0.142 62[d]	1.06×10^{-4}[d]
	0.008	−0.155 666	8.6×10^{-3}	−0.156 3768[c]	4.2×10^{-3}[c]
	0.010	−0.166 526	1.4×10^{-2}	−0.166 09[d]	1.09×10^{-2}[d]
	0.015	−0.185 851	2.3×10^{-2}	−0.187 62[d]	3.38×10^{-2}[d]
0 0 ±1	0.004	−0.126 315 36	2.2×10^{-6}	−0.126 3169[c]	8.1×10^{-7}[c]
= $2p_x$, $2p_y$	0.005	−0.127 153	2.2×10^{-5}	−0.127 15[d]	2.62×10^{-5}[d]
	0.008	−0.131 22	4.5×10^{-3}	−0.131 1886[c]	2.0×10^{-3}[c]
	0.010	−0.134 793	5.9×10^{-3}	−0.134 53[d]	6.28×10^{-3}[d]

† This value believed to be in error (Cerjan 1982). Holt (1983) has obtained the value −0.1121 using the perturbation theory results of Alliluev and Malkin (1974).

simple form of the trial function); the renormalised series in contrast provides good estimates of Γ, even though the calculation involves the use of only one parameter. It is clearly of interest to investigate other model problems involving resonance states to see if this is generally true; if so the renormalised series method could be used to confirm or check the results of least squares calculations.

The renormalised series calculation is also of interest in providing a method of obtaining an approximate value of Γ from the perturbation series in a simple manner. Previous Γ calculations have used indirect methods, involving the large order behaviour of perturbation series coefficients (Silverstone *et al* 1979) or complex-λ techniques (Reinhardt 1982). These methods give more accurate results, but the direct method described here is certainly of interest; in particular order of magnitude estimates of Γ could be very useful in pinpoint the regions of the complex E plane to be searched in non-perturbative calculations.

4. Conclusion

In this paper the application of the renormalised series technique to two problems of interest in quantum mechanics has been studied. The radius of convergence of the Padé approximants to the perturbation series for the octically perturbed oscillator is improved by this method; the large-λ technique (Dmitrieva and Plindov 1979, 1980a, b) is also found to be useful. The Stark effect problem is successfully treated by a modified renormalised series method; this has the advantage of yielding an estimate of the width Γ as well as the energy; in addition the radius of convergence of the Padé approximants is increased.

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