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On an alternative perturbation method in quantum mechanics

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Abstract
We investigate the convergence properties of a perturbation method proposed some time ago and reveal some of its most interesting features. Anharmonic oscillators in the strong-coupling limit prove to be appropriate illustrative examples and a suitable benchmark.

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1. Introduction

Some time ago Bessis and Bessis (BB from now on) [1] proposed a new perturbation approach in quantum mechanics based on the application of a factorization method to a Riccati equation derived from the Schrödinger one. They obtained reasonable results for some of the energies of the quartic anharmonic oscillator by means of perturbation series of order fourth and sixth, without resorting to a resummation method. In spite of this success, BB's method has passed unnoticed as far as we know.

The purpose of this paper is to investigate BB's perturbation method in more detail. In section 2, we write it in a quite general way and derive other approaches as particular cases. In section 3, we carry out perturbation calculations of sufficiently large order and try to find out numerical evidence of convergence. One-dimensional anharmonic oscillators prove to be a suitable benchmark for present numerical tests. For simplicity, we restrict to ground states and choose straightforward logarithmic perturbation theory instead of the factorization method proposed by BB [1]. Finally, in section 4 we discuss the results and draw some conclusions.

2. The method

In the standard Rayleigh–Schrödinger perturbation theory we try to solve the eigenvalue equation

$$\hat{H}\Psi = E\Psi, \qquad \hat{H} = \hat{H}_0 + \lambda \hat{H}' \tag{1}$$

by expanding the energy E and eigenfunction Ψ in a Taylor series about $\lambda = 0$. This method is practical provided that we can solve the eigenvalue equation for $\lambda = 0$.

In some cases it is more convenient to construct a parameter-dependent Hamiltonian operator $\hat{H}(\beta)$ that one can expand in a Taylor series about $\beta = 0$

$$\hat{H}(\beta) = \sum_{j=0} \hat{H}_j \beta^j \tag{2}$$

in such a way that we can solve the eigenvalue equation for $\hat{H}(0) = \hat{H}_0$. In this case we expand the eigenfunctions $\Psi(\beta)$ and eigenvalues $E(\beta)$ in Taylor series:

$$\Psi(\beta) = \sum_{j=0}^{\infty} \Psi_j \beta^j, \qquad E(\beta) = \sum_{j=0}^{\infty} E_j \beta^j. \tag{3}$$

There are many practical examples of application of this alternative approach [2]. In particular, BB [1] suggested the following form of $\hat{H}(\beta)$:

$$\hat{H}(\beta) = \hat{H} + (\beta - 1)\hat{W}(\beta), \qquad \hat{W}(\beta) = \sum_{j=0} \hat{W}_j \beta^j, \tag{4}$$

where $\hat{H}(1) = \hat{H}$. Comparing equations (2) and (4) we conclude that

$$\hat{H}_0 = \hat{H} - \hat{W}_0, \qquad \hat{H}_j = \hat{W}_{j-1} - \hat{W}_j, \quad j > 0. \tag{5}$$

In principle there is enormous flexibility in the choice of the operator coefficients $\hat{W}_j$ as we show below by derivation of two known particular cases.

If we restrict expansion (4) to just one term $\hat{W}(\beta) = \hat{W}(0) = \hat{W}_0$ then $\hat{H}(\beta) = \hat{H} - \hat{W}_0 + \beta\hat{W}_0$. Choosing $\hat{W}_0 = \hat{H} - \hat{H}_0(\alpha) = \hat{H}'(\alpha)$, where $\hat{H}_0(\alpha)$ is a parameter-dependent Hamiltonian operator with known eigenvalues and eigenfunctions, we obtain the method proposed by Killingbeck [3] some time ago. The main strategy behind this approach is to choose an appropriate value of the adjustable parameter α leading to a renormalized perturbation series with the best convergence properties [2, 3].

If we consider two terms of the form $\hat{W}_0 = \hat{H} - \hat{H}_0(\alpha)$ and $\hat{W}_1 = \lambda\hat{H}'$, then we derive the Hamiltonian operator $\hat{H}(\beta) = \hat{H}_0(\alpha) + \beta[\hat{H}_0 - \hat{H}_0(\alpha)] + \beta^2\lambda\hat{H}'$ that Killingbeck *et al* [4] have found to be even more convenient for the treatment of some perturbation problems. Those approaches are practical if we can solve the eigenvalue equation for $\beta = 0$ and all relevant values of α.

We should mention that it was not the aim of BB to obtain renormalized series with an adjustable parameter but to choose the operator coefficients $\hat{W}_j$ in such a way that they could solve the perturbation equations

$$(\hat{H}_0 - E_0)\Psi_j = \sum_{i=1}^{j} (E_i - \hat{W}_i + \hat{W}_{i-1})\Psi_{j-i} \tag{6}$$

in exact algebraic form [1].

For simplicity in this paper, we concentrate on a one-dimensional eigenvalue equation of the form

$$\Psi''(x) = [U(x) - E]\Psi(x), \qquad U(x) = V(x) + \frac{l(l+1)}{x^2}. \tag{7}$$

If $\Psi(0) = \Psi(\infty) = 0$ and $l = 0, 1, 2, \ldots$ is the angular-momentum quantum number, this equation applies to central-field models. If $\Psi(-\infty) = \Psi(\infty) = 0$ and $l = -1$, we have a one-dimensional model. In particular, when $V(x) = V(-x)$ then $l = -1$, and $l = 0$, select the spaces of even and odd solutions, respectively. In any case the regular solution to the eigenvalue equation (7) behaves asymptotically as x^{l+1} at the origin.

In order to calculate perturbation corrections of sufficiently large order by means of BB's method we define

$$f(x) = \frac{s}{x} - \frac{\Psi'(x)}{\Psi(x)}, \qquad s = l + 1 \tag{8}$$

that satisfies the Riccati equation

$$f' + \frac{2s}{x} f - f^2 + V - E = 0. \tag{9}$$

The corresponding equation for the Hamiltonian $\hat{H}(\beta)$ in equation (4) reads

$$f' + \frac{2s}{x} f - f^2 + V - E + (\beta - 1)W = 0, \tag{10}$$

if we restrict to the case that $\hat{W}(\beta) = W(\beta, x)$ depends only on β and the coordinate. The coefficients of the expansion

$$f = \sum_{j=0}^{\infty} f_j \beta^j \tag{11}$$

satisfy the perturbation equations

$$f_j' + \frac{2s}{x} f_j - \sum_{k=0}^{j} f_k f_{j-k} + V\delta_{j0} - E_j + W_{j-1} - W_j = 0. \tag{12}$$

3. Results

Simple one-dimensional anharmonic oscillators $V(x) = x^2 + \lambda x^{2K}$, $K = 2, 3, \ldots$, are a suitable demanding benchmark for testing new perturbation approaches. We easily increase the degree of difficulty by increasing the values of the coupling parameter λ and anharmonicity exponent K. BB applied their method to the first four energy levels of the model with $K = 2$ and several values of λ, restricting their calculation to perturbation theory of order four and six [1]. Here we consider the strong-coupling limit ($\lambda \to \infty$) of the oscillators mentioned above:

$$V(x) = x^{2K}. \tag{13}$$

Note that if the perturbation series gives acceptable results for this case, then it will certainly be suitable for all $0 < \lambda < \infty$. Moreover, the perturbation corrections for these models are simpler enabling us to proceed to higher orders with less computational requirement.

In order to make present discussion clearer we first illustrate the main ideas of the method with the pure quartic oscillator $K = 2$. We try polynomial solutions of the form

$$f_j(x) = \sum_{m=0}^{j+1} c_{j,2m+1} x^{2m+1}, \qquad j = 0, 1, \ldots \tag{14}$$

in the perturbation equations (12) for the ground state ($s = 0$). Substitution of $f_0(x)$ into the perturbation equation of order zero leads to

$$-c_{0,3}^2 x^6 + (1 - 2c_{0,1}c_{0,3})x^4 + \left(3c_{0,3} - c_{0,1}^2\right)x^2 + c_{0,1} - E_0 - W_0 = 0. \tag{15}$$

In order to have a solution with $c_{0,3} \neq 0$ we choose $W_0 = -c_{0,3}^2 x^6$; then $c_{0,3} = 1/(2c_{0,1})$, and $3c_{0,3} - c_{0,1}^2 = 0$ becomes a cubic equation with two complex and one real root. If we select the later we finally have

$$f_0 = \frac{12^{1/3}}{2} x + 12^{-1/3} x^3, \qquad W_0 = -12^{-2/3} x^6, \qquad E_0 = \frac{12^{1/3}}{2} \approx 1.1447. \tag{16}$$

Table 1. Padé approximants $[N, N]$ for the ground states of the quartic ($K = 2$) sextic ($K = 3(b)$) and octic ($K = 4$) oscillators.

N	$K = 2$	$K = 3(b)$	$K = 4$
1	1.060 996 335 262 11	1.130 792 741 075 56	1.210 520 271
2	1.060 358 707 944 51	1.145 013 857 041 72	1.203 379 654
3	1.060 362 220 792 74	1.144 794 069 904 71	1.225 903 753
4	1.060 362 043 227 21	1.144 807 763 229 51	1.225 811 686
5	1.060 362 100 291 30	1.144 802 298 405 45	1.225 826 780
6	1.060 362 090 588 62	1.144 802 434 896 11	1.225 839 331
7	1.060 362 090 607 31	1.144 802 453 936 88	
8	1.060 362 090 488 82	1.144 802 453 343 62	
9	1.060 362 090 482 95		
10	1.060 362 090 482 46		
11	1.060 362 090 483 01		
12	1.060 362 090 484 23		
13	1.060 362 090 484 20		
14	1.060 362 090 484 17		
15	1.060 362 090 484 17		
16	1.060 362 090 484 08		
17	1.060 362 090 484 18		
18	1.060 362 090 484 18		
19	1.060 362 090 484 18		
20	1.060 362 090 484 17		
21	1.060 362 090 484 18		
22	1.060 362 090 484 18		
23	1.060 362 090 484 18		
Exact	1.060 362 090 484 183	1.144 802 453 80	1.225 820 11

We expect the resulting unperturbed wavefunction

$$\Psi_0 \propto \exp\left(-\frac{12^{1/3}}{4}x^2 - \frac{x^4}{4\times 12^{1/3}}\right) \tag{17}$$

to be an improvement on the harmonic-oscillator one in the standard Rayleigh–Schrödinger perturbation theory [2–4]. The zeroth-order energy (16) is reasonably close to the exact value shown in table 1 which was obtained with the Riccati–Padé method [5].

At first order we have

$$-\frac{12^{2/3}}{6}c_{1,5}x^8 - 12^{1/3}\left(c_{1,5} + \frac{12^{1/3}c_{1,3}}{6} + \frac{1}{12}\right)x^6 + \left(5c_{1,5} - 12^{1/3}c_{1,3} - \frac{12^{2/3}c_{1,1}}{6}\right)x^4$$
$$+(3c_{1,3} - 12^{1/3}c_{1,1})x^2 + c_{1,1} - E_1 - W_1 = 0. \tag{18}$$

We easily solve this equation if $W_1 = -12^{2/3}c_{1,5}x^8/6$; the result is

$$f_1 = -\frac{5}{112}12^{1/3}\left(x + \frac{12^{1/3}}{3}\right) - \frac{3x^5}{56}, \qquad W_1 = \frac{12^{2/3}x^8}{112},$$
$$E_1 = -\frac{5}{112}12^{1/3} \approx -0.1022. \tag{19}$$

The energy corrected through first order is somewhat closer to the exact value: $E_0 + E_1 \approx 1.0425$.

The systematic calculation of perturbation corrections of larger order offers no difficulty if we resort to a computer algebra system. Since we are unable to prove rigorously whether the

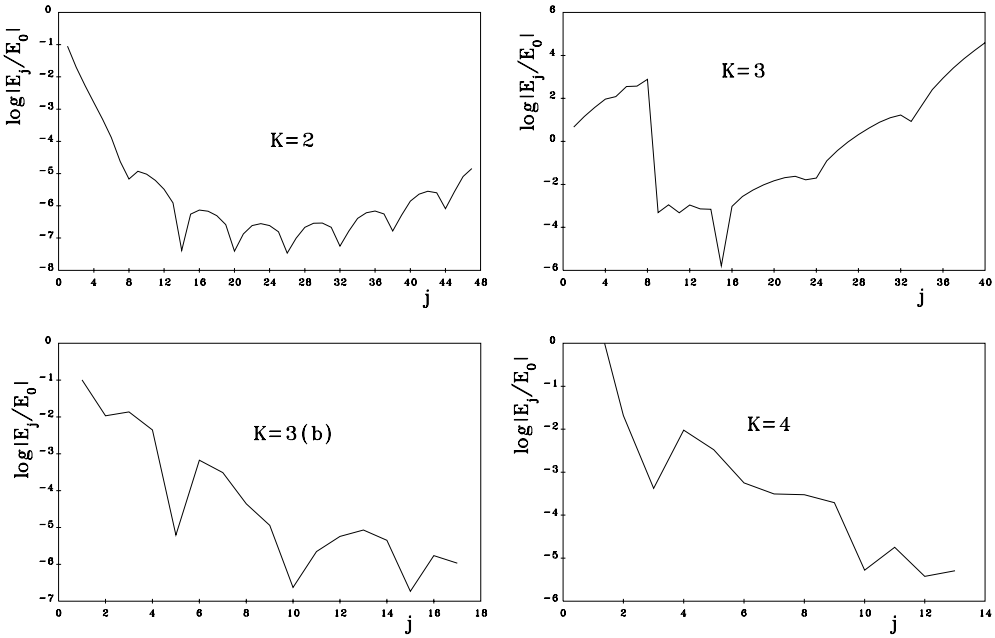

Figure 1. $\log|E_j/E_0|$ versus j for the ground states of the quartic ($K = 2$), sextic ($K = 3$ and $K = 3$ (b)) and octic ($K = 4$) oscillators.

perturbation series converges for $\beta = 1$, we resort to numerical investigation. Figure 1 shows that $\log|E_j/E_0|$ first decreases rapidly as j increases, but then it increases slowly suggesting that the series does not converge. If we assume that the error on the energy estimated by the partial sum

$$E^{[M]} = \sum_{j=0}^{M} E_j \tag{20}$$

is proportional to the first neglected term $|E - E^{[M]}| \approx |E_{M+1}|$, then it is reasonable to truncate the perturbation series at the smallest value of $|E_{M+1}|$ [6]. In this case we find that $E_{26} = -0.389\,768\,6104 \times 10^{-7}$ is the energy coefficient with the smallest absolute value so that our best estimate is $E^{[25]} = 1.060\,362\,15$ (compare with the exact value in table 1).

We proceed exactly in the same way for the pure sextic oscillator $K = 3$. Figure 1 shows values of $\log|E_j/E_0|$ that clearly suggest poorer convergence properties than in the preceding example. The energy coefficient with the smallest absolute value is $E_{15} = 0.275\,911\,8288 \times 10^{-5}$, and our best estimate $E^{[14]} = 1.144\,70$ is reasonably close to the exact eigenvalue in table 1. It is not surprising that perturbation theory yields poorer results for $K = 3$ than for $K = 2$ [2] because the former potential is more singular at infinity than the latter.

For the pure octic anharmonic oscillator $K = 4$ we look for polynomial solutions of the form

$$f_j(x) = \sum_{m=0}^{j+3} c_{j,2m+1} x^{2m+1}, \qquad j = 0, 1, \ldots. \tag{21}$$

In this case we have calculated less perturbation coefficients because they require more computer memory and time. Surprisingly, the values of $\log|E_j/E_0|$ in figure 1 suggest that

the perturbation series for $K = 4$ exhibits better convergence properties than the one for $K = 3$ just discussed. The energy coefficient with the smallest absolute value (among those we managed to calculate) is $E_{12} = -0.520\ 549\ 3999 \times 10^{-5}$ so that our best estimate is $E^{[11]} = 1.225\ 822$ which is quite close to the exact one in table 1.

The surprising fact that the convergence properties of the perturbation series are clearly poorer for $K = 3$ than for $K = 4$ suggests that there should be better solutions for the former case. If we try

$$f_j(x) = \sum_{m=0}^{j+2} c_{j,2m+1} x^{2m+1}, \qquad j = 0, 1, \ldots \tag{22}$$

then the values of $\log|E_j/E_0|$ are smaller than those obtained earlier (compare $K = 3(b)$ with $K = 3$ in figure 1). The coefficient with the smallest absolute value is $E_{15} = -0.234\ 406\ 6313 \times 10^{-6}$ and our best estimate results to be $E^{[14]} = 1.144\ 8015$.

It is well known that Padé approximants give considerably better results than power series [6]. We have tried diagonal Padé approximants $[N, N]$ on the perturbation series for the cases $K = 2$, $K = 3(b)$ and $K = 4$, and show results in table 1. Note that the Padé approximants sum the $K = 2$ series to a great accuracy but they are less efficient for $K = 3(b)$ and $K = 4$. This is exactly what is known to happen with the standard perturbation series for anharmonic oscillators [7]. However, Padé approximants appear to improve the accuracy of present perturbation results in all the cases discussed above.

4. Conclusions

Present numerical investigation on the perturbation method proposed by Bessis and Bessis [1] suggests that although the series may be divergent they are much more accurate than those derived from the standard Rayleigh–Schrödinger perturbation theory. One obtains reasonable eigenvalues for difficult anharmonic problems of the form $V(x) = x^{2K}$, and results deteriorate much less dramatically than those from the standard Rayleigh–Schrödinger perturbation series as the anharmonicity exponent K increases. In order to facilitate the calculation of perturbation corrections of sufficiently large order we restricted our analysis to polynomial solutions that are suitable for the ground state. The treatment of rational solutions for excited states (such as those considered by BB [1]) is straightforward but increasingly more demanding.

Following BB [1] we have implemented perturbation theory by transformation of the linear Schrödinger equation into a nonlinear Riccati one. In this way, the appropriate form of each potential coefficient W_j reveals itself more clearly as shown in section 3 for the quartic model. However, in principle one can resort to any convenient algorithm because the perturbation method is sufficiently general as shown in section 2.

A remarkable advantage of the method of BB [1], which may not be so clear in their paper, is its extraordinary flexibility as shown by the two solutions obtained above for the case $K = 3$. Moreover, the method of BB, unlike two other renormalization approaches derived above as particular cases [3, 4], does not require and adjustable parameter to give acceptable results.

One may rise doubts about the practical usefulness of perturbation theory to treat problems of actual interest in quantum mechanics. When one is able to obtain the perturbation coefficients in terms of the quantum numbers, then it takes as little effort to calculate the ground-state energy as well as highly excited ones [2]. On the other hand, the computation time increases with the quantum number when one resorts to a numerical method. In some other cases, perturbation theory provides analytical functions of the perturbation parameter

that yield, for example, the energies of an atom or molecule for any chosen value of an external field [2]. Since perturbation theory is likely to be one of the first approaches commonly tried on problems in quantum mechanics, statistical mechanics and other fields of theoretical physics, there has been great interest in the convergence properties of the perturbation series [2].

The implementation of present perturbation theory by means of logarithmic perturbation theory is not as practical as other strategies for the calculation of highly excited energy levels [2]. We have chosen it because it greatly facilitates the systematic calculation of perturbation coefficients of sufficiently large order for the ground state that are necessary for testing the convergence properties of the method. In principle, the generalization of the method outlined in section 2 is expected to facilitate the application of any alternative implementation of perturbation theory [2]. We believe that further investigation on the method of BB [1] will produce more unexpected surprises.

References

[1] Bessis N and Bessis G 1997 *J. Math. Phys.* **38** 5483
[2] Fernández F M 2001 *Introduction to Perturbation Theory in Quantum Mechanics* (Boca Raton: CRC Press)
[3] Killingbeck J 1981 *J. Phys. A: Math. Gen.* **14** 1005
[4] Killingbeck J P, Grosjean A and Jolicard G 2001 *J. Phys. A: Math. Gen.* **34** 8309
[5] Fernández F M, Ma Q and Tipping R H 1989 *Phys. Rev.* A **39** 1605
[6] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
[7] Graffi S and Grecchi V 1978 *J. Math. Phys.* **19** 1002