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Quantum mechanics as classical mechanics plus quantum corrections: the cubic anharmonic oscillator

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Abstract. The Rayleigh-Schrödinger perturbation series for the cubic anharmonic oscillator can be formally rearranged as the classical Birkhoff series plus quantum corrections proportional to successive powers of $\hbar^2$. Each of the individual quantum corrections is a convergent power series expansion (with the same radius of convergence as the classical series) of the corresponding term in the Jeffreys-Wentzel-Kramers-Brillouin series.

1. Introduction

The relation between the Birkhoff normal form for a classical Hamiltonian and the Rayleigh-Schrödinger perturbation series for the corresponding quantum operator has been the subject of several recent investigations. Ali (1985) and Eckhardt (1986) pointed out that replacing the Poisson brackets in the Lie transformation formulation of classical perturbation theory by quantum commutators changes the classical algorithm to calculate the Birkhoff normal form into a quantum algorithm to generate the Rayleigh-Schrödinger perturbation series. Transforming to the Bargmann representation, Graffi and Paul (1987) have shown that (for multidimensional non-resonant perturbed harmonic oscillators) the algorithm of classical perturbation theory can be used to solve the quantum mechanical perturbation theory, with terms in powers of $\hbar$ 'correcting' the classical potential. Wood and Ali (1987) reviewed the problem of direct quantisation of the classical Birkhoff series using as a model a general cubic and quartic anharmonic oscillator, and showed that no quantisation rule can recover the quantum series starting *only* from the classical series, pointing out the differences in term-by-term quantisation in the pure cubic and quartic cases. More recently Alvarez *et al* (1988) provided a complete description of the transition between classical mechanics and quantum mechanics for the x^4 perturbed harmonic oscillator. It turns out that the quantum perturbation series rearranges directly into the classical Birkhoff expansion plus quantum corrections proportional to successively higher powers of $\hbar^2$ converging (subseries by subseries) to the terms of the Jeffreys-Wentzel-Kramers-Brillouin (JWKB) semiclassical expansion. The aim of the present paper is to prove similar results for the x^3 perturbed harmonic oscillator, in which the $x \to -x$ symmetry is absent and the role of $\hbar$ in the scaling quite different. In the quartic anharmonic oscillator $V = x^2/2 + gx^4$, for coupling constant $g \geq 0$ all the classical motions are bounded while for $g < 0$ there exists a separatrix. For fixed energy $E > 0$ the classical action J is defined as an analytic function in the complex g plane cut along the negative real axis from $g = -(16E)^{-1}$ to ∞. The situation in the cubic anharmonic oscillator

$V = x^2/2 + gx^3$ is completely different. For any value of $g \neq 0$, there exist both bounded and unbounded classical motions and therefore a separatrix (in quantum mechanics bound states no longer exist, only resonances). For fixed energy $E > 0$ the classical action J is defined as an analytic function in the complex g plane cut along both the positive and negative real axes from $g = \pm(54E)^{-1}$ to ∞. Despite these differences, it will be shown that the full Rayleigh-Schrödinger perturbation series can be recovered from the semiclassical JWKB expansion and, through this construction, that the semiclassical series determines the exact resonant eigenvalues of the cubic oscillator. The analogous fact for the eigenvalues of even-perturbed oscillators was first noticed by Graffi and Grecchi (1985). The structure of the quantum mechanical perturbation series is exposed in a complementary way to that in terms of Feynman diagrams suggested by Wood and Ali (1987).

The practical relevance of this analysis is emphasised by the work of Fried and Ezra (1988), in which they propose an algorithm to generate the classical series plus a finite number of quantum corrections in multidimensional systems.

2. Analysis of the quantum mechanical perturbation series

Consider the Schrödinger equation for the cubic anharmonic oscillator

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tfrac{1}{2}m\omega^2x^2 - m^{3/2}\omega^{5/2}gx^3\right)\psi = \varepsilon\psi \tag{1}$$

for which the scaling transformation $x \to (\hbar/m\omega)^{1/2}x$, $E = \varepsilon/\omega$, renders the equivalent form

$$\hbar\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tfrac{1}{2}x^2 - g\hbar^{1/2}x^3\right)\Psi = E\Psi. \tag{2}$$

The intuitive conjecture is that under the cubic perturbation the bound states of the harmonic oscillator will become resonances: the particle, initially in the potential well, will escape to $x = \infty$ by tunnelling. Mathematically the problem is complicated because the potential goes so strongly to $-\infty$. Nevertheless, it has been proved (Caliceti *et al* 1980, Caliceti and Maioli 1983) that there is a natural concept of resonances and that the Rayleigh-Schrödinger perturbation series is Borel summable to these resonance eigenvalues.

Equation (2) is invariant under the simultaneous substitutions $x \to -x$, $g \to -g$. Consequently, all odd-order coefficients of the perturbation series are null:

$$E(g) \sim \hbar \sum_{N=0}^{\infty} E^{(N)}(g^2\hbar)^N \tag{3}$$

and the series is divergent, since the non-vanishing coefficients behave asymptotically (Alvarez 1988):

$$E^{(N)} \sim -\frac{(60)^{N+n+1/2}}{n!(2\pi)^{3/2}8^N}\Gamma(N+n+\tfrac{1}{2}) \qquad \text{as } N \to \infty \tag{4}$$

where n is the usual harmonic oscillator quantum number. Moreover, using a Fourier representation (Silverstone 1978) it can be proved that $E^{(N)}$ is a polynomial in $(n + \frac{1}{2})$

of degree $N+1$ and parity $(-1)^{N+1}$:

$$E^{(N)} = \sum_{k=0}^{[(N+1)/2]} (n+\tfrac{1}{2})^{N+1-2k} E_k^{(N)} \tag{5}$$

where $[r]$ stands for the interger part of r. Table 1 gives the values of these polynomial coefficients up to $N=10$.

By virtue of equation (5) and denoting by $J=(n+1/2)\hbar$ the 'classical action' (see the discussion in § 3), the Rayleigh-Schrödinger series (3) can be formally rearranged as follows:

$$\begin{aligned} E(g) \sim\ & (n+\tfrac{1}{2})\hbar \\ & + g^2\{E_0^{(1)}[(n+\tfrac{1}{2})\hbar]^2 + \hbar^2 E_1^{(1)}\} \\ & + g^4\{E_0^{(2)}[(n+\tfrac{1}{2})\hbar]^3 + \hbar^2 E_1^{(2)}[(n+\tfrac{1}{2})\hbar]\} \\ & + g^6\{E_0^{(3)}[(n+\tfrac{1}{2})\hbar]^4 + \hbar^2 E_1^{(3)}[(n+\tfrac{1}{2})\hbar]^2 + \hbar^4 E_2^{(3)}\} \\ & + \ldots \\ = {} & E_0(J, g^2) + \hbar^2 E_1(J, g^2) + \hbar^4 E_2(J, g^2) + \ldots \end{aligned} \tag{6}$$

with the E_k defined by

$$E_0(J, g^2) = J + J \sum_{N=1}^{\infty} E_0^{(N)} (g^2 J)^N \tag{7}$$

$$E_k(J, g^2) = J^{-2k+1} \sum_{N=2k-1}^{\infty} E_k^{(N)} (g^2 J)^N \qquad \text{if } k>0. \tag{8}$$

Table 1. Rayleigh-Schrödinger perturbation theory energy coefficients for the x^3 perturbed harmonic oscillator as polynomials in $n+\frac{1}{2}$: coefficients $E_k^{(N)}$ of (5) in the text multiplied by -4^N.

N	k	$-4^N E_k^{(N)}$	N	k	$-4^N E_k^{(N)}$
1	0	60	7	0	201 158 359 894 103 040
1	1	7	7	1	1 034 954 374 948 623 360
			7	2	1 354 179 181 521 479 040
2	0	11 280	7	3	454 335 713 959 279 680
2	1	4 620	7	4	17 170 481 745 607 092
3	0	3 704 160	8	0	113 999 847 953 961 784 320
3	1	3 344 880	8	1	777 192 185 748 823 004 160
3	2	202 958	8	2	1 491 257 719 745 410 409 856
			8	3	895 492 413 985 388 281 920
4	0	1 533 962 304	8	4	114 892 678 503 242 999 604
4	1	2 473 621 920			
4	2	517 773 396	9	0	66 769 249 690 003 994 664 960
			9	1	584 129 752 829 918 521 712 640
5	0	723 154 199 040	9	2	1 554 154 955 972 830 234 383 360
5	1	1 844 044 392 960	9	3	1 482 588 050 328 357 994 728 960
5	2	849 337 282 080	9	4	416 470 110 232 500 563 672 160
5	3	38 008 581 072	9	5	14 171 193 177 483 475 548 800
6	0	370 492 639 165 440	10	0	40 141 485 640 273 528 509 972 480
6	1	1380 009 990 078 720	10	1	439 288 308 727 505 086 103 654 400
6	2	1137 723 951 981 120	10	2	1 554 436 081 034 982 981 520 312 320
6	3	173 935 618 884 720	10	3	21 775 880 736 476 692 174 992 611 440
			10	4	1 094 056 746 964 689 583 045 696 320
			10	5	125 793 460 743 631 174 290 997 200

Thus, the Rayleigh-Schrödinger series decomposes formally as a power series in $\hbar^2$. The purpose of the following section is to show that E_0 is the convergent classical Birkhoff series, to determine its radius of convergence, and to show that the E_k with $k>0$ are also convergent series, with the same radius of convergence, for the corresponding terms of the JWKB expansion.

3. The Jeffreys–Wentzel–Kramers–Brillouin series

By means of the $\hbar$-independent scaling $x \to (m\omega)^{-1/2}x$, $E=\varepsilon/\omega$, the Schrödinger equation (1) turns into the equivalent form

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\tfrac{1}{2}x^2-gx^3\right)\Phi=E\Phi. \tag{9}$$

The JWKB expansion for the wavefunction is

$$\Phi=\exp\left(\frac{\mathrm{i}}{\hbar}\int S\,\mathrm{d}x\right) \tag{10}$$

$$S=\sum_{N=0}^{\infty}\hbar^N S^{(N)}(x) \tag{11}$$

and the JWKB function $S(x)$ satisfies the Riccati equation

$$\tfrac{1}{2}S^2-\frac{\mathrm{i}}{2}\hbar\frac{\mathrm{d}S}{\mathrm{d}x}+\tfrac{1}{2}x^2-gx^3-E=0 \tag{12}$$

which allows recursive evaluation of the $S^{(N)}$. In particular, one obtains

$$S^{(0)}=\sqrt{2E-x^2+2gx^3} \tag{13}$$

$$S^{(1)}=\frac{\mathrm{i}}{2}\frac{\mathrm{d}}{\mathrm{d}x}(\ln S^{(0)}) \tag{14}$$

$$S^{(2)}=\tfrac{1}{2}[S^{(0)}]^{-1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}[S^{(0)}]^{-1/2}. \tag{15}$$

The quantisation condition is given by Dunham's formula (Dunham 1932):

$$\frac{1}{2\pi}\oint S\,\mathrm{d}x=n\hbar \tag{16}$$

where the path of integration in the complex plane encloses the two turning points x_- and x_+ in the well $[x_\pm \sim \pm(2E)^{1/2}+\mathrm{O}(g)]$. For later reference, x_1 will denote the third turning point $[x_1 \sim (2g)^{-1}+\mathrm{O}(g)]$. From the computational point of view the main difference between the cubic and the quartic oscillators (Alvarez *et al* 1988) is that in the quartic case parity reduces the determination of the turning points to the solution of a simple quadratic equation. Although it is possible to find closed form expressions for the three turning points in the cubic oscillator (roots of a cubic polynomial), it is more convenient for our present purpose to work directly with the convergent expansions for x_-, x_+, and x_1 given in the appendix.

To lowest order in $\hbar$, equation (12) is equivalent to the classical Hamilton-Jacobi equation. The classical action is

$$J = \frac{1}{2\pi}\oint S^{(0)}\,\mathrm{d}x = \frac{1}{4}\sqrt{\frac{g}{2}}(x_+ - x_-)^2(x_1 - x_-)^{1/2}F(-\tfrac{1}{2},\tfrac{3}{2};3;\alpha) \tag{17}$$

where F stands for Gauss's hypergeometric function and $\alpha = (x_+ - x_-)/(x_1 - x_-)$. Equation (17) can be readily expanded in a convergent series whose first terms are

$$J = E + \tfrac{15}{4}g^2E^2 + \tfrac{1155}{16}g^4E^3 + \ldots \tag{18}$$

and inversion of this series gives the classical Birkhoff expansion:

$$E = J - \tfrac{15}{4}g^2J^2 - \tfrac{705}{16}g^4J^3 - \ldots. \tag{19}$$

Its radius of convergence can be determined by the same argument used by Turchetti (1984) in the quartic case: the value of J at the energy $E = 1/54g^2$ corresponding to the separatrix is given by

$$\frac{1}{2\pi}\oint\sqrt{2E - x^2 + 2gx^3} = \frac{1}{15\pi g^2}. \tag{20}$$

Consequently, the series converges for $|g^2J| < 1/15\pi$, and according to equation (16), to this order quantisation amounts to the substitution $J = n\hbar$.

Since $S^{(1)}$ is essentially the logarithmic derivative of $S^{(0)}$, the next term from equation (16) is simply

$$\frac{\hbar}{2\pi}\oint S^{(1)}\,\mathrm{d}x = -\frac{\hbar}{2} \tag{21}$$

which induces the substitution $J = (n + \frac{1}{2})\hbar$ in the classical Birkhoff expansion (equation (19)) giving rise to the leading contribution $E_0(J, g^2)$ (equations (6) and (7)) in the analysis of the Rayleigh-Schrödinger perturbation series.

The general method to evaluate higher-order terms is as follows. First, evaluate the corresponding $S^{(N)}$. For odd $N \geq 3$, the integral $\oint S^{(N)}\,\mathrm{d}x$ vanishes. For even N, repeated integration by parts can be used to reduce the integral to an equivalent expression which can be calculated by shrinking the path to the interval (x_-, x_+) in the real axis (Krieger *et al* 1967). For example, for $N = 2$

$$\begin{aligned}\frac{1}{2\pi}\oint S^{(2)}\,\mathrm{d}x &= -\frac{1}{64\pi\sqrt{2}}\oint\frac{(V')^2}{(E-V)^{5/2}}\,\mathrm{d}x \\ &= -\frac{1}{48\pi\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}E}\oint\frac{V''}{(E-V)^{1/2}}\,\mathrm{d}x \\ &= -\frac{1}{24\sqrt{2g}}\frac{\mathrm{d}}{\mathrm{d}E}\left(\frac{1-6gx_-}{(x_1-x_-)^{1/2}}F(\tfrac{1}{2},\tfrac{1}{2};1;\alpha) - \frac{3g(x_+-x_-)}{(x_1-x_-)^{1/2}}F(\tfrac{1}{2},\tfrac{3}{2};2;\alpha)\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}E}I_1(E).\end{aligned} \tag{22}$$

Then, expand the energy in equation (16) as a power series in $\hbar$ and collect terms of the same order. Since only even powers of $\hbar$ are non-zero on the left-hand side of equation (16) (except the first which gets absorbed in the definition of J), only even powers of $\hbar$ occur in the expansion of E (in agreement with equation (6)). The result is that the E_k with $k>0$ are given *explicitly* in terms of hypergeometric functions, x_+, x_-, x_1 and their derivatives evaluated at E_0. Only E_0 itself is given as the solution of an implicit equation. For example,

$$E_1(J, g^2) = -\frac{\mathrm{d}}{\mathrm{d}J} I_1(E_0(J, g^2))$$
$$= -g^2\left(\frac{7}{4^2}+\frac{4620}{4^4}g^2J+\ldots\right) \tag{23}$$

whose first terms can be identified with the corresponding coefficients in table 1. Moreover, from the closed form expression for each E_k that gives rise to the power series in g it is easy to see that all the substitution of power series are carried inside their radii of convergence, the final radius of convergence being determined by E_0.

4. Numerical behaviour

Graffi and Grecchi (1985) have already observed that for even-perturbed harmonic oscillators the JWKB expansion determines the exact eigenvalues. A similar conclusion with respect to the resonances of the cubic anharmonic oscillator can be drawn from the preceding analysis. By power series expansion and rearrangement of the terms of the JWKB series, the Rayleigh-Schrödinger perturbation series can be recovered, and from the latter the exact resonances can be calculated via Borel summation.

As far as partial sums are concerned, the analysis of the Rayleigh-Schrödinger series as the classical series plus quantum corrections provides insight into the asymptotic nature of the full quantum series. Figure 1 shows the partial sums of the first four quantum corrections $E_1, \ldots, E_4$ for the ground state $n=0$ and coupling constant $g=0.15$ (inside the radius of convergence of the individual series). The kth quantum correction starts at $2k-1$ (see equation (8)) and since all the terms have the same sign, the partial sums converge monotonically towards the JWKB value. Note that this converged value decreases in magnitude from E_1 to E_2 (which in this case would be the 'optimal' term to keep in the asymptotic expansion) and then increases

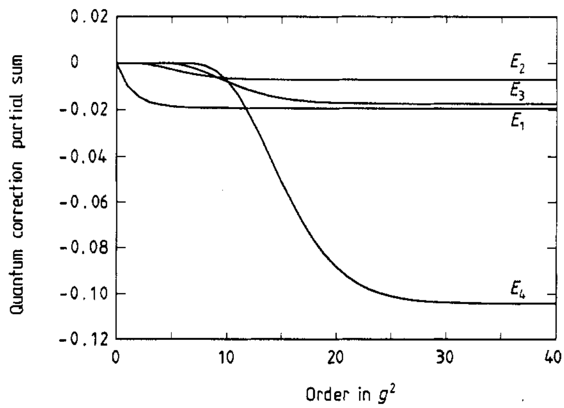

Figure 1. Partial sums of the perturbation series for the quantum corrections E_k, $k=1,\ldots,4$, as a function of perturbation theory order, for the ground state $n=0$ and coupling constant $g=0.15$ (inside the radius of convergence).

in magnitude from E_2 on, leading to the overall divergence. Besides, the convergence of the individual series is of course non-uniform in k. This behaviour is also manifest in the partial sums of the JWKB series shown in figure 2 for $n=0$ and $g=0.01$ (E_0 is not displayed to allow for an appropriate scale).

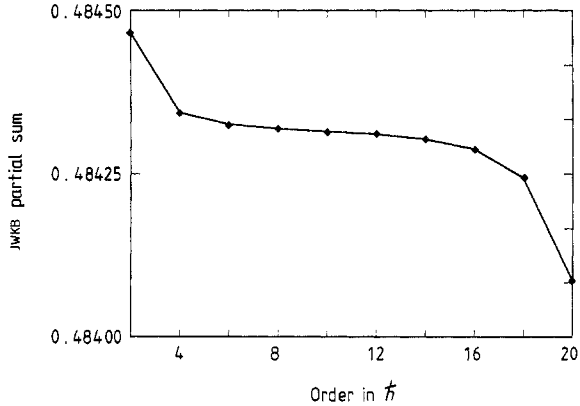

Figure 2. Partial sums of the JWKB series as a function of the order in $\hbar$, for the ground state $n=0$ and coupling constant $g=0.01$. The value of E_0 (not displayed to allow for an appropriate scale) is 0.490 009 0975....

5. Summary

To examine in full detail the relation between the classical Birkhoff expansion and the quantum Rayleigh-Schrödinger perturbation theory for the cubic anharmonic oscillator, the quantum series has been rearranged as the classical series plus quantum corrections proportional to successive powers of $\hbar^2$. Each of the individual quantum corrections turns out to be a convergent power series expansion (with the same radius of convergence as the classical series) of the corresponding term in the Jeffreys-Wentzel-Kramers-Brillouin series. As a by-product of this analysis, it has been shown that the JWKB series determines completely the resonances of the cubic anharmonic oscillator.

From the numerical point of view, inside the classical radius of convergence the partial sums of the classical series plus a finite number k of quantum corrections tend (as the order of perturbation tends to infinity) to the corresponding JWKB partial sum $E_0+\hbar^2E_1+\ldots+\hbar^{2k}E_k$. The JWKB series itself seems to be asymptotic and, for any fixed values of g and J, it will ultimately diverge if enough number of quantum corrections are added.

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Appendix

The purpose of this appendix is to provide convergent series representations for the three real roots of

$$E - \tfrac{1}{2}x^2 + gx^3 = 0 \tag{A1}$$

when $g \geqslant 0$ and $0 \leqslant E < 1/54g^2$. With the notation $z = 2gx$, $\varepsilon = 8g^2E$ $(0 \leqslant \varepsilon < \frac{4}{27})$, consider the roots $z_\pm$, z_1 of $z^3 - z^2 + \varepsilon = 0$ as an algebraic function of ε in a neighbourhood of $\varepsilon = 0$. The root which comes from $z = 1$ can be readily expanded in Taylor series, with radius of convergence $|\varepsilon| < \frac{4}{27}$,

$$z_1 = \sum_{n=0}^{\infty} c_n \varepsilon^n \tag{A2}$$

where

$$c_0 = 1 \qquad c_1 = -1 \qquad c_{n+1} = -\sum_{k=1}^{n} \sum_{i=0}^{k} c_i c_{k-i} c_{n-k+1}. \tag{A3}$$

The first terms of the series are

$$z_1 = 1 - \varepsilon - 2\varepsilon^2 - 7\varepsilon^3 - 30\varepsilon^4 - 143\varepsilon^5 - 728\varepsilon^6 - \ldots. \tag{A4}$$

The roots $z_\pm$ which come from $z = 0$ are the two branches of a Puiseux series (Taylor series in $z^{1/2}$),

$$z_\pm = \sum_{n=1}^{\infty} c_n \varepsilon^{n/2} \tag{A5}$$

with radius of convergence $|\varepsilon^{1/2}| < (\frac{4}{27})^{1/2}$, and

$$c_1 = 1 \qquad c_2 = \tfrac{1}{2}$$
$$c_{n+1} = \frac{1}{2}\left[c_n + \sum_{k=2}^{n}\left(c_{k-1} - c_k + \sum_{i=1}^{k-1} c_i c_{k-i}\right) c_{n+2-k}\right]. \tag{A6}$$

The first terms of this series are

$$z_\pm = \varepsilon^{1/2} + \tfrac{1}{2}\varepsilon + \tfrac{5}{8}\varepsilon^{3/2} + \varepsilon^2 + \tfrac{231}{128}\varepsilon^{5/2} + \tfrac{7}{2}\varepsilon^3 + \ldots. \tag{A7}$$

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