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1998 J. Phys. A: Math. Gen. 31 5697

(http://iopscience.iop.org/0305-4470/31/26/009)

Sextic and octic anharmonic oscillators: connection between strong-coupling and weak-coupling expansions

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Received 12 December 1997, in final form 23 March 1998

Abstract. For the eigenvalues of the Hamiltonians $\frac{1}{2}\hat{p}^2 + \frac{1}{2}x^2 + \frac{1}{2}\beta x^{2m}$ with $m = 3, 4\ldots$, we propose representations reproducing the well known weak-coupling asymptotic perturbation and strong-coupling expansions as limiting cases. Some analytical relations which the strong-coupling coefficients must satisfy are presented.

1. Introduction

The quantum-mechanical systems described by the Hamiltonians with polynomial interactions and especially the so-called anharmonic oscillators

$$\hat{H}^{(m)} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}x^2 + \frac{1}{2}\beta x^{2m} \tag{1}$$

with $m = 2, 3, 4, \ldots$, have received considerable attention from many workers. One of the reasons for such an interest may be explained by the fact that the anharmonic oscillators provide the simplest examples of the quantum-mechanical systems for which the wave equation cannot be solved exactly. Approximation schemes should be used to study the properties of such systems and, due to their relative simplicity, anharmonic oscillators provide convenient models for the development of such schemes. One can mention, for example, that the studies of the anharmonic oscillators have contributed considerably to the understanding of large-order perturbation theory (Le Guillou and Zinn-Justin 1990), to the development of the methods of handling the divergent expansions in quantum mechanics (Simon 1970, 1982, Graffi *et al* 1970, Hirsbrunner and Loeffel 1975, Arteca *et al* 1990), to the development of 'exact quantization schemes' (Voros 1983, 1994, Ecalle 1981, 1994, Delabaere and Pham 1997, Delabaere *et al* 1997) and many other computational methods (Vinette and Čižek 1991, Fernandez 1992, Janke and Kleinert 1995, Weniger 1996a, b, Ivanov 1996). A review of the works on the anharmonic oscillators can be found in the paper by Killingbeck (1977).

The best studied example of the anharmonic oscillators is provided by the quartic anharmonic oscillator ($m = 2$ in the equation (1)). The properties of eigenvalues of the quartic oscillator are known in detail from the works of Simon (1970), and Bender and Wu (1969, 1971, 1973).

In the present paper we deal with the oscillators of higher anharmonicities, sextic ($m = 3$ in the Hamiltonian (1)) and octic ($m = 4$ in the Hamiltonian (1)). We recall some known properties of eigenvalues of the anharmonic oscillators which we shall need later.

0305-4470/98/265697+08$19.50

For the sake of simplicity we consider the ground-state eigenvalues of the Hamiltonians (1), although the results presented in this present paper can be equally applied to the excited states of the corresponding Hamiltonians (the excited levels of $\hat{H}^{(m)}$ will be briefly considered in the final part of the paper).

It is known from the works of Simon (1970) and Bender and Wu (1969, 1971, 1973) that energy eigenvalues of the Hamiltonians (1) considered as functions of the complex variable β allow analytical continuation onto multi-sheeted Riemann surfaces. On their Riemann surfaces these functions possess a very complex structure of singular points. Thus, for example, the result of such analytic continuation in the case of the quartic anharmonic oscillator is an analytic function defined on the three-sheeted Riemann surface on which the point $\beta = 0$ is *not* an isolated singularity (Simon 1970). This analytic function was shown (Bender and Wu 1969, Simon 1970) to have on its Riemann surface an infinite number of branch-point singularities (the so-called Bender–Wu branch points), the point $\beta = 0$ being the point of accumulation of these branch-point singularities. The Bender–Wu singularities were shown to arise at the points where different anharmonic oscillator eigenvalues coincide. It was shown (Bender and Wu 1969) that all anharmonic oscillator eigenvalues are analytic continuations of each other with respect to the complex anharmonicity constant. The distribution of the Bender–Wu branch points has been studied by many authors (Bender and Wu 1969, Simon 1970, Shanley 1986, Delabaere and Pham 1997).

In the present paper we consider the single-valued branches of the analytic functions emerging as a result of an analytic continuation process of the ground-state eigenvalues of the Hamiltonians (1). The single-valued branches of these analytic functions can be singled out if one cuts the complex β-plane along the negative real axis. We shall be interested in the present paper in those single-valued branches which assume 'physical' values on the real positive β-axis, i.e. which coincide there with the ground-state eigenvalues of the Hamiltonians (1). For these functions we shall adopt the notation $E^{(m)}(\beta)$. The functions $E^{(m)}(\beta)$ are known to be analytic single-valued functions of β, regular everywhere in the cut complex β-plane, except at $\beta = 0$ and $\beta = \infty$ (Loeffel and Martin 1970).

Formal application of Rayleigh–Schrödinger perturbation theory to the Hamiltonians (1), with the term $\beta x^{2m}/2$ being considered as a perturbing operator, yields a divergent expansion for the eigenvalues $E^{(m)}(\beta)$ of the Hamiltonians (1)

$$E^{(m)}(\beta) \sim \sum_{n=0}^{\infty} E_n^{(m)} \beta^n \tag{2}$$

which can be shown to be asymptotic. For the quartic case this fact was proved by Simon (1970). The coefficients $E_n^{(m)}$ rapidly grow with n. The asymptotic behaviour of $E_n^{(m)}$ for the ground-state of the quartic, sextic and octic oscillators is known in analytical form after the works of Bender and Wu (1969, 1971, 1973). The corresponding formulae for the sextic and octic oscillators read

$$E_n^{(3)} \sim (-1)^{n-1} \frac{\sqrt{32}}{\pi^2}\, \Gamma(2n+1/2)(16/\pi^2)^n \tag{3}$$

$$E_n^{(4)} \sim (-1)^{n-1} \sqrt{\frac{135\, [\Gamma(2/3)]^3}{2\pi^5}}\, \Gamma(3n+1/2)\, 250^n \left(\frac{3[\Gamma(2/3)]^3}{4\pi^2}\right)^{3n} \tag{4}$$

where $\Gamma(z)$ is Euler gamma function.

In the opposite limit of the large β-values a convergent expansion can be obtained for the eigenvalues of the Hamiltonians (1) (Simon 1970)

$$E^{(m)}(\beta) = \beta^{1/(m+1)} \sum_{n=0}^{\infty} c_n^{(m)} \beta^{-2n/(m+1)}. \tag{5}$$

This expansion (the so-called strong-coupling expansion) can be viewed as an application of Rayleigh–Schrödinger perturbation theory to the Hamiltonians (1), the term $x^2/2$ being considered as a perturbing operator. One can show that, if the term x^2 is considered in the Hamiltonians (1) as a perturbation, the family of Hamiltonians (1) is an analytic family in the sense of Kato (1976) and, therefore, the strong-coupling expansion (5) has a non-zero radius of convergence. For the quartic case this fact was proved by Simon (1970), and for the higher anharmonicities it was proved by Weniger (1994).

Since the eigenvalues and eigenfunctions of the Hamiltonian $\hat{p}^2/2 + \beta x^{2m}/2$ are not known in closed form, the coefficients of the strong-coupling expansion can only be computed numerically. The first ten coefficients of the strong-coupling expansion for the sextic oscillator and the first six coefficients for the octic oscillator are given in the paper by Weniger (1996b).

Despite the fact that the strong-coupling coefficients $c_n^{(m)}$ can only be computed numerically, one can obtain, as we shall see, some analytical information about $c_n^{(m)}$.

The question we shall be dealing with in the present paper, is how to 'combine' both expansions (2) and (5). We shall show that a representation for the eigenvalues $E^{(m)}(\beta)$ of the Hamiltonians (1) can be constructed from which both expansions (2) and (5) can be obtained as two limiting cases. For the quartic oscillator the corresponding procedure has been described in our paper (Ivanov 1998). In the present paper we give a generalization of this procedure. We show that analogous representations can be constructed for ground and excited states of the anharmonic oscillators of higher anharmonicities ($m = 3, 4 \ldots$ in the (1)). Explicit formulae are given for the sextic ($m = 3$) and octic ($m = 4$) oscillators.

2. Theory

Let us consider the functions $G^{(m)}(\beta) = E^{(m)}(\beta)/\beta$ where we use the notation introduced above for the single-valued branches of the corresponding analytic functions. From the discussion of the analytic properties of $E^{(m)}(\beta)$ it follows that $G^{(m)}(\beta)$ are single-valued analytic functions regular everywhere except at $\beta = 0$ and $\beta = \infty$ in the β-complex plane cut along the negative real axis. From equation (5) it follows that $G^{(m)}(\beta)$ tend uniformly to zero when $\mathrm{Re}\,\beta \to +\infty$. It is known (Markushevitch 1968) that these conditions are sufficient to guarantee that for $\mathrm{Re}\,\beta > 0$ the functions $G^{(m)}(\beta)$ can be represented as Laplace transforms of certain functions $f^{(m)}(\beta)$ and, hence for $\mathrm{Re}\,\beta > 0$, $E^{(m)}(\beta)$ can be represented as

$$E^{(m)}(\beta) = \beta \int_0^\infty f^{(m)}(t)\,\mathrm{e}^{-\beta t}\,\mathrm{d}t \tag{6}$$

where the functions $f^{(m)}(t)$ are determined uniquely as inverse Laplace transforms of $E^{(m)}(\beta)/\beta$. A representation similar to (6) has been considered by Delabaere *et al* (1997) for the quartic anharmonic oscillator. With formula (6) holding for $\mathrm{Re}\,\beta > 0$ and the strong-coupling expansion (5) converging for sufficiently large, $|\beta|$, there is a region of the β-complex plane where both equations (6) and (5) are valid. Therefore, one may expect that a connection can be established between the functions $f^{(m)}(t)$ under the integral sign in equation (6) and the coefficients $c_n^{(m)}$ of the strong-coupling expansion (5). This connection can be easily found. Inverting the Laplace transformation (6), one obtains for $f^{(m)}(t)$

$$f^{(m)}(t) = \frac{1}{2\pi\mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \frac{E^{(m)}(\beta)}{\beta}\,\mathrm{e}^{\beta t}\,\mathrm{d}\beta. \tag{7}$$

The integral in equation (7) can be taken along any straight line Re $\beta = c > 0$. In particular, one can choose the contour of integration so that everywhere on the contour the strong-coupling expansion is applicable. Then, substituting under the integral sign in equation (7) the strong-coupling expansion (5) and performing term-by-term integration with the help of the known formula (Abramovitz and Stegun 1964)

$$\frac{1}{\Gamma(z)} = \frac{1}{2\pi \mathrm{i}} \int_C x^{-z}\, \mathrm{e}^x \, \mathrm{d}x \tag{8}$$

where the contour of integration C is a straight line Re $x =$ constant > 0, one obtains the following formula for the functions $f^{(m)}(t)$:

$$f^{(m)}(t) = \sum_{n=0}^{\infty} \frac{c_n^{(m)}}{\Gamma((2n+m)/(m+1))} t^{(2n-1)/(m+1)}. \tag{9}$$

The coefficients $c_n^{(m)}$ in equation (9) are the coefficients of the strong-coupling expansion (5). It is easy to see that, since the strong-coupling expansion (5) has a non-zero radius of convergence, the series (9) converges for any t.

Formula (9) establishes a connection between the functions $f^{(m)}(t)$ under the integral sign in equation (6) and the coefficients $c_n^{(m)}$ of the strong-coupling expansion (5).

Since formula (6) holds for Re $\beta > 0$ and hence holds also in the region where the asymptotic expansion (2) can be used, one may expect another connection to exist between this formula and the asymptotic expansion (2). This connection can be established as follows. We note that the asymptotic expansion (2) can be obtained from the formula (6) if the functions $f^{(m)}(t)$ can be represented as

$$f^{(m)}(t) = E_0 + g^{(m)}(t) \tag{10}$$

where $E_0^{(m)}$ is the zero-order coefficient of the perturbation expansion (2) and the functions $g^{(m)}(t)$ decay sufficiently rapidly when $t \to \infty$ so that all integrals $\int_0^\infty |g^{(m)}(t)| t^n \, \mathrm{d}t$ for $n > 0$ exist.

If assumption (10) is valid then, expanding the exponential function under the integral sign in equation (6) and integrating the series obtained term-by-term, one obtains for $E^{(m)}(\beta)$ the series (2), where for the coefficients $E_n^{(m)}$ with $n > 0$ one has

$$E_n^{(m)} = \frac{(-1)^{n-1}}{(n-1)!} \int_0^\infty g^{(m)}(t)\; t^{n-1}\, \mathrm{d}t. \tag{11}$$

It is easy to see that the series thus obtained is Poincaré asymptotic when $\beta \to 0$ remaining in the half-plane Re $\beta > 0$. To establish this fact, one should only note that according to our assumption (10) all integrals $\int_0^\infty |g^{(m)}(t)| t^n \, \mathrm{d}t$ for $n > 0$ exist. The remainder of the series obtained as a result of the above-described procedure of term-by-term integration is

$$E^{(m)}(\beta) - E_N^{(m)}(\beta) = \beta \int_0^\infty (\mathrm{e}^{-\beta t} - \mathrm{e}_{N-1}^{-\beta t})\; g^{(m)}(t)\, \mathrm{d}t \tag{12}$$

where $E_N^{(m)}(\beta)$ is Nth partial sum of the series and $\mathrm{e}_{N-1}^{-\beta t}$ is the sum of the first $N-1$ terms of the Taylor series for $\mathrm{e}^{-\beta t}$. For $\mathrm{e}^{-\beta t} - \mathrm{e}_{N-1}^{-\beta t}$ one has for Re $\beta > 0$

$$|\mathrm{e}^{-\beta t} - \mathrm{e}_{N-1}^{-\beta t}| = \frac{1}{N!}\; |(\beta t)^N \;{}_1F_1(1, N+1, -\beta t)| \leqslant \frac{|\beta t|^N}{N!} \tag{13}$$

where ${}_1F_1(1, N+1, -\beta t)$ is a confluent hypergeometric function. For Re $\beta > 0$ the inequality on the right-hand side of equation (13) is easily obtained with the help of the well known integral representation for confluent hypergeometric functions (Abramovitz and Stegun 1964). From equations (12) and (13) one obtains $|E^{(m)}(\beta) - E_N^{(m)}(\beta)| = O(|\beta|^{N+1})$

when $\beta \to 0$, Re $\beta > 0$, i.e. the series obtained is Poincaré asymptotic when $\beta \to 0$ remaining in the half-plane Re $\beta > 0$. Since the asymptotic series of a given function is determined uniquely and the asymptotic expansion (2) is known to represent the functions $E^{(m)}(\beta)$ inside some sectors $|\arg \beta| < \theta_m$, the coefficients $E_n^{(m)}$ defined by formula (11) must coincide with the coefficients of the asymptotic expansion (2).

Table 1. The function $f^{(m)}(t)$ and its asymptotic approximations $\tilde{f}^{(m)}(t)$.

	Sextic oscillator		Octic oscillator	
t	$f^{(3)}(t)$	$\tilde{f}^{(3)}(t)$	$f^{(4)}(t)$	$\tilde{f}^{(4)}(t)$
1	0.627 529 97	0.666 006 00	0.670 650 45	0.698 549 52
5	0.537 200 57	0.552 975 75	0.572 942 75	0.592 524 36
10	0.518 338 18	0.525 914 47	0.546 586 72	0.559 820 13
15	0.511 296 51	0.515 693 13	0.534 769 87	0.544 652 44
20	0.507 707 88	0.510 526 72	0.527 812 00	0.535 612 39
25	0.505 586 64	0.507 513 62	0.523 158 72	0.529 537 88
30	0.504 214 33	0.505 595 52	0.519 803 40	0.525 151 81
35	0.503 268 44	0.504 299 06	0.517 259 62	0.521 827 89
40	0.502 582 90	0.503 383 37	0.515 260 52	0.519 219 26
45	0.502 063 36	0.502 714 38		

In the second column of table 1 we present the numerical values of the function $f^{(3)}(t)$ computed for different t-values with the help of series (9) for the ground-state of the sextic oscillator. In the fourth column of this table we present the numerical values of $f^{(4)}(t)$, computed according to (9) for the ground-state of the octic oscillator. In both cases we used the data for the coefficients of the strong-coupling coefficients calculated by Weniger (1996b). In this work the first ten strong-coupling coefficients for the sextic and the first six strong-coupling coefficients for the octic oscillator were computed. With the presence of the gamma function in the denominator in equation (9) ensuring rapid convergence of the series, we were able to calculate the functions $f^{(m)}(t)$ up to rather large values of t even with the relatively small number of terms of series (9) taken into account. We estimate that taking account of the first ten terms of series (9) for the sextic oscillator allows one to compute $f^{(3)}(t)$ with an accuracy to better than 1 part in 10^6 for $t \approx 10$, 1 part in 10^4 for $t \approx 30$ and 1 part in 10^3 for $t \approx 40$. For the octic oscillator we believe that taking account of the first six terms of the series (9) allows one to compute $f^{(4)}(t)$ with an accuracy to better than 1 part in 10^4 for $t \approx 10$, 1 part in 10^3 for $t \approx 30$ and 1 part in 10^2 for $t \approx 40$.

Based on formula (10) one would expect that both for the sextic and octic oscillators the functions $f^{(m)}(t)$ would tend to the limiting value $E_0^{(m)}$ (which is in both cases, of course, equal to one-half the ground-state energy of the harmonic oscillator). The data from the second and fourth columns of table 1 give enough evidence that this is indeed the case.

More detailed information about the functions $f^{(m)}(t)$ can be obtained if we analyse the large-n asymptotic behaviour of the coefficients $E_n^{(m)}$ following from equation (11). When $n \to \infty$ in equation (11) it is the region of large t-values which contributes mostly to the integral. Therefore, if the large-t asymptotic behaviour of the functions $g^{(m)}(t)$ were known, the large-n asymptotic behaviour of the integrals (11) could be found with the use of the standard asymptotic methods. Usually, in the applications of the Borel method or when finding the large-order asymptotic behaviour of the perturbation coefficients from dispersion relations (Simon 1970, Bender and Wu 1971, Herbst and Simon 1978, Silverstone *et al* 1979, Le Guillou and Zinn-Justin 1990) one knows the required asymptotic properties and finds the asymptotic behaviour of the perturbation coefficients by applying the saddle-point method. In our problem the situation is inverse. The asymptotic behaviour of the perturbation coefficients is known, and is given by formula (2). We will try to find the large-t asymptotic behaviour of functions $g^{(m)}(t)$ which would yield the correct large-n asymptotic behaviour of the integrals (11). To reproduce the leading-order asymptotic behaviour of the coefficients of the perturbation expansion (2) given in the sextic and octic cases by formulae (3) and (4), it is sufficient to suppose that the functional form of the leading term of the asymptotic behaviour of $g^{(m)}(t)$ is

$$g^{(m)}(t) \sim At^{\alpha} \exp\left(-bt^{\gamma}\right) \tag{14}$$

where A, α, b, γ are some constants (which are, of course, different for the sextic and octic oscillators). Substituting this expression into equation (11) and performing the integration one obtains for $n \to +\infty$

$$\begin{aligned} E_n^{(m)} &\sim \frac{(-1)^{n-1}}{(n-1)!}\frac{A}{\gamma}\frac{\Gamma((\alpha+n)/\gamma)}{b^{(\alpha+n)/\gamma}} \\ &\sim (-1)^{n-1}\ \frac{A}{\sqrt{\gamma}b^{(\alpha+n)/\gamma}}\mathrm{e}^{n-(n/\gamma)}\left(\frac{n}{\gamma}\right)^{(\alpha+n)/\gamma} n^{-n} \end{aligned} \tag{15}$$

where deriving the second asymptotic equality in equation (15) we used the well known asymptotic formula (Abramovitz and Stegun 1964) for the gamma function.

Comparing the asymptotic behaviour given by equation (15) with the leading large-n asymptotic behaviour of $E_n^{(m)}$ given by equations (3) and (4), one can easily find the parameters in formula (14) for the sextic and octic oscillators. It is important to note that once the ansatz (14) is assumed to describe the large-t asymptotic behaviour of $g^{(m)}(t)$, all the parameters in (14) are determined uniquely. Thus, one obtains the following large-t asymptotic formulae for the functions $f^{(m)}(t)$ from equation (9) in the sextic and octic cases

$$f^{(3)}(t) = \sum_{n=0}^{\infty} \frac{c_n^{(3)}}{\Gamma((2n+3)/4)} t^{(2n-1)/4} \sim \frac{1}{2} + \frac{8}{\sqrt{3\pi^3}} \exp\left\{-\left(\frac{27\pi^2 t}{64}\right)^{1/3}\right\} \tag{16}$$

$$f^{(4)}(t) = \sum_{n=0}^{\infty} \frac{c_n^{(4)}}{\Gamma((2n+4)/5)} t^{(2n-1)/5} \sim \frac{1}{2} + \sqrt{\frac{135\ [\Gamma(2/3)]^3}{4\pi^4}} \exp\left\{-(bt)^{1/4}\right\} \tag{17}$$

where in the last equation

$$b = \frac{128}{3375}\left(\frac{4\pi^2}{3[\Gamma(2/3)]^3}\right)^3.$$

As we have seen, such asymptotic behaviour of the functions $f^{(m)}(t)$ ensures that equation (11) will reproduce the correct large-n asymptotic behaviour of the coefficients of the perturbation expansion for the sextic and octic oscillators.

In the third column of the table 1 we present the numerical values of the right-hand side of equation (16) (designated $\tilde{f}^{(3)}(t)$), the fifth column of this table contains the numerical values of the right-hand side of equation (17) (designated $\tilde{f}^{(4)}(t)$) for different values of t. Comparison of these values with those computed according to formula (9) gives enough evidence to show that formulae (16) and (17) describe correctly the large-t asymptotic behaviour of functions (9) for the sextic and octic anharmonic oscillator.

3. Remarks

The goal of the present paper was to establish the formulae (6), (16) and (17). As we have seen, the strong-coupling and the weak-coupling expansions for the ground-state energies of the anharmonic oscillators considered can be obtained from equation (6) as two limiting cases.

To avoid confusion we would like to emphasize that the present results have been obtained for the single-valued branches of the corresponding analytic functions. The formula (6) holds for the β-values satisfying $|\arg\,\beta| < \pi/2$. What would happen if we allowed β to quit this region and, in particular, whether analogous formulae could be obtained for other branches of the corresponding analytic functions is an interesting question which we believe deserves separate consideration.

We have given analytic relations which the strong-coupling coefficients $c_n^{(m)}$ must satisfy. The fact that such relations can be obtained is itself rather curious in our opinion, taking into account the fact that $c_n^{(m)}$ can only be computed numerically. Equations (16) and (17) provide the 'sum rules', which can serve to check the accuracy of the calculations of the strong-coupling coefficients. An interesting question is whether one can obtain any analytic information about large-order behaviour of the strong-coupling coefficients with the help of equations (16) and (17). If it were possible, one could hope to find an analytical estimation of the radius of convergence of the strong-coupling expansion (5) for the ground-state of the sextic and octic anharmonic oscillators.

Our derivation of formulae (6), (9), (16) and (17) used only the facts that $E^{(m)}(\beta)$ is analytic and regular for $\operatorname{Re}\beta > 0$, and the fact that the strong-coupling expansion (5) holds for $E^{(m)}(\beta)$. These conditions guarantee that $E^{(m)}(\beta)$ can be represented as a Laplace integral (6). It is easy to see that both these conditions are fulfilled for the excited states of the anharmonic oscillators considered and, moreover, for the states of the oscillators of higher anharmonicities ($m = 5, 6\ldots$) in formula (1). The corresponding formulae are quite analogous to equations (6), (9), (16) and (17) and we do not present them here.

Acknowledgment

The financial support from RFBR (project code 95-02-14284) is acknowledged.

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