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LETTER TO THE EDITOR

Large-order behaviour of the strong coupling perturbation expansion for anharmonic oscillators

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Abstract. A new formula describing the large-order behaviour of the strong coupling perturbation coefficients for the anharmonic oscillators with the Hamiltonian $H = -\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \beta x^{2m}$ is suggested. A new method for the accurate calculation of the square root branch points of the energy from the numerical values of the coefficients is also suggested. The branch points and the related minimal values of the coupling constant β for which the expansion converges are calculated for the ground state of the quartic, sextic, octic and decadic oscillators.

In this letter, we investigate the Schrödinger equation

$$H\psi = E(\beta)\psi \tag{1}$$

for the anharmonic oscillators, where

$$H = p^2 + x^2 + \beta x^{2m} \qquad \beta \geqslant 0, \quad m \geqslant 2 \tag{2}$$

and $p = -i\mathrm{d}/\mathrm{d}x$. As is well known, the energy $E(\beta)$ can be expressed as a strong coupling perturbation series in powers of $\beta^{-2/(m+1)}$ (see e.g. [1–3])

$$E(\beta) = \beta^{1/(m+1)} \sum_{n=0}^{\infty} K_n \beta^{-2n/(m+1)}. \tag{3}$$

The numerical values of the K_n coefficients were investigated, for example, in [4–11]. To the best of our knowledge, the large-order behaviour of the K_n coefficients was investigated only in [5], where the large-order formula for the K_n coefficients

$$K_n = A\frac{\cos(n\varphi + \delta)}{|z_0|^n n^{3/2}} \tag{4}$$

where $\varphi = \arg z_0$ was derived. Here, A and δ are constants, z_0 denotes the square root branch point of the energy $\epsilon(z)$ with the smallest distance to the origin [1, 2, 12, 13]

$$\epsilon(z) = \beta^{-1/(m+1)} E(\beta) = \sum_{n=0}^{\infty} K_n z^n \tag{5}$$

and $z = \beta^{-2/(m+1)}$. The value of $z_0 = -4.193\,684 + 2.169\,740\,i$ for the ground state of the quartic oscillator and a few other states of this oscillator is known from [14]. The importance of the branch point z_0 follows from the fact that it determines the minimal value of β for which the series (3) converges. It follows from equations (3), (4) that

$$\beta_{\min} = \frac{1}{|z_0|^{(m+1)/2}}. \tag{6}$$

The values of the constants A and δ are not known.

The aim of this letter is (i) to generalize equation (4), (ii) to suggest a new general method of calculating z_0 and (iii) to calculate z_0 and $\beta_{\min}$ for the ground state of the quartic, sextic, octic and decadic oscillators.

First we generalize equation (4). The energy $\epsilon(z)$ can be in the neighbourhood of the points z_0 and z_0^* described by the series [1, 12, 15]

$$\begin{aligned}\epsilon(z) &= c_1[(z-z_0)(z-z_0^*)]^{1/2} + c_2[(z-z_0)(z-z_0^*)]^{3/2} + \cdots \\ &\quad + d_0 + d_1(z-z_0)(z-z_0^*) + d_2[(z-z_0)(z-z_0^*)]^2 + \cdots \\ &= c_1|z_0|(t^2 - 2t\cos\varphi + 1)^{1/2} + c_2|z_0|^3(t^2 - 2t\cos\varphi + 1)^{3/2} + \cdots \\ &\quad + d_0 + d_1|z_0|^2(t^2 - 2t\cos\varphi + 1) + d_2|z_0|^4(t^2 - 2t\cos\varphi + 1)^2 + \cdots \end{aligned} \tag{7}$$

where c_i and d_i are constants and $t = z/z_0$. The terms with the d_i coefficients do not contribute to the large-order behaviour of the K_n coefficients. Now we observe that the function $(t^2 - 2t\cos\varphi + 1)^{-\alpha}$ is the generating function of the Gegenbauer polynomials $C_n^{(\alpha)}(\cos\varphi)$ [16]:

$$(t^2 - 2t\cos\varphi + 1)^{-\alpha} = \sum_{n=0}^{\infty} t^n C_n^{(\alpha)}(\cos\varphi) \tag{8}$$

where $\alpha = -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$. Therefore, a general large-order formula for the K_n coefficients following from equations (5), (7) and (8) equals

$$K_n = \frac{1}{|z_0|^{n-1}}[c_1 C_n^{(-1/2)}(\cos\varphi) + c_2|z_0|^2 C_n^{(-3/2)}(\cos\varphi) + \cdots]. \tag{9}$$

To find the relation of this formula to equation (4) we proceed as follows. The Gegenbauer polynomials can be expressed as [16]

$$C_n^{(\alpha)}(\cos\varphi) = \sum_{i=0}^{n} a_i^{(\alpha)} \cos((n-2i)\varphi) \tag{10}$$

where

$$a_i^{(\alpha)} = a_{n-i}^{(\alpha)} = \frac{\Gamma(\alpha+i)\Gamma(\alpha+n-i)}{i!(n-i)![\Gamma(\alpha)]^2}. \tag{11}$$

It follows from equation (10) that equation (9) can also be written in the form

$$\begin{aligned}K_n = \frac{1}{|z_0|^{n-1}}\Bigg[&\cos(n\varphi)\sum_{i=0}^{n}(c_1 a_i^{(-1/2)} + c_2|z_0|^2 a_i^{(-3/2)} + \cdots)\cos(2i\varphi) \\ &+ \sin(n\varphi)\sum_{i=0}^{n}(c_1 a_i^{(-1/2)} + c_2|z_0|^2 a_i^{(-3/2)} + \cdots)\sin(2i\varphi)\Bigg]. \end{aligned} \tag{12}$$

The large-order behaviour of the coefficients $a_i^{(\alpha)}$ equals

$$a_0^{(-1/2)} = -\frac{1}{2\sqrt{\pi}n^{3/2}}[1 + 3/(8n) + 25/(128n^2) + \cdots] \tag{13}$$

$$a_1^{(-1/2)} = \frac{1}{4\sqrt{\pi}n^{3/2}}[1 + 15/(8n) + 385/(128n^2) + \cdots] \tag{14}$$

$$a_2^{(-1/2)} = \frac{1}{16\sqrt{\pi}n^{3/2}}[1 + 27/(8n) + 1225/(128n^2) + \cdots] \tag{15}$$

$$\cdots$$

$$a_0^{(-3/2)} = \frac{3}{4\sqrt{\pi}n^{5/2}}[1 + 15/(8n) + 385/(128n^2)\cdots] \tag{16}$$

$$a_1^{(-3/2)} = -\frac{9}{8\sqrt{\pi}n^{5/2}}[1 + 35/(8n) + 1785/(128n^2)\cdots] \tag{17}$$

$$a_2^{(-3/2)} = -\frac{9}{32\sqrt{\pi}n^{5/2}}[1 + 55/(8n) + 4305/(128n^2)\cdots] \tag{18}$$

$$\cdots$$

First we restrict ourselves to the $\alpha = -\frac{1}{2}$ term in equation (12). If we take the leading $1/n^{3/2}$ term in equations (13)–(15) we get from equation (12)

$$K_n = \frac{1}{|z_0|^{n-1}n^{3/2}}[e_1\cos(n\varphi) + f_1\sin(n\varphi)] \tag{19}$$

where e_1 and f_1 are constants. Introducing further $\cos\delta = e_1/\sqrt{e_1^2 + f_1^2}$ and $\sin\delta = -f_1/\sqrt{e_1^2 + f_1^2}$ we see that this equation can be re-written in the form of equation (4). Thus, equation (4) corresponds to the leading $1/n^{3/2}$ term of equations (9) and (12). Corrections to equation (19) can be found analogously. It is obvious that the large-order formula (12) can also be written in the form

$$K_n = \frac{1}{|z_0|^{n-1}n^{3/2}}[(e_1 + e_2/n + e_3/n^2 + \cdots)\cos(n\varphi) + (f_1 + f_2/n + f_3/n^2 + \cdots)\sin(n\varphi)] \tag{20}$$

where e_i and f_i are constants.

We now suggest a general method of calculating the value of the branch point z_0 from the numerical values of the K_n coefficients. To calculate $|z_0|$ and φ we can use equation (9) and the recurrence relation for the Gegenbauer polynomials [16]

$$(n + 2\alpha - 1)C_{n-1}^{(\alpha)} - 2(n + \alpha)\cos(\varphi)C_n^{(\alpha)} + (n + 1)C_{n+1}^{(\alpha)} = 0. \tag{21}$$

Taking only the first $\alpha = -\frac{1}{2}$ term in equation (9) we get from equation (21) the equation used in [6]

$$(n - 2)K_{n-1} - (2n - 1)\mathrm{Re}\,(z_0)K_n + (n + 1)|z_0|^2K_{n+1} = 0. \tag{22}$$

If we take $n = n_0$ and $n = n_0 + 1$, where n_0 is a large integer, we obtain two equations for two unknowns from which $\mathrm{Re}\,(z_0)$ and $|z_0|^2$ can be calculated. It is seen from equations (12)–(18) that equation (22) correctly respects only the terms depending on $1/n^{3/2}$.

Considering the $\alpha = -\frac{1}{2}$ and $\alpha = -\frac{3}{2}$ terms in equation (9) we analogously get

$$(n - 2)x_{n-1} - (2n - 1)\mathrm{Re}\,(z_0)x_n + (n + 1)|z_0|^2x_{n+1} = 0 \qquad n = n_0, \ldots, n_0 + 3 \tag{23}$$

$$(n - 4)y_{n-1} - (2n - 3)\mathrm{Re}\,(z_0)y_n + (n + 1)|z_0|^2y_{n+1} = 0 \qquad n = n_0, \ldots, n_0 + 3 \tag{24}$$

$$K_n = x_n + y_n \qquad n = n_0 - 1, \ldots, n_0 + 4 \tag{25}$$

where

$$x_n = \frac{c_1}{|z_0|^{n-1}}C_n^{(-1/2)}(\cos\varphi) \tag{26}$$

$$y_n = \frac{c_2}{|z_0|^{n-3}}C_n^{(-3/2)}(\cos\varphi). \tag{27}$$

Equations (23)–(25) are a system of 14 nonlinear equations for 14 unknowns x_n, y_n, $\mathrm{Re}(z_0)$ and $|z_0|^2$ which can be solved numerically. If x_n, y_n, $\mathrm{Re}(z_0)$ and $|z_0|^2$ are known we can return to equations (26), (27) for $n = n_0$ and calculate the coefficients c_1 and c_2. Equations (23)–(25) correctly respect all the terms depending on $1/n^{3/2}$ and $1/n^{5/2}$.

Table 1. The square root branch point z_0, $\beta_{\min}$ and the constants c_i for the ground state of the quartic, sextic, octic and decadic oscillators ($m = 2, 3, 4, 5$) for different number of terms in equation (9) ($j = 1, \ldots, 4$). For these oscillators, we used the values $n_0 = 104$, $n_0 = 90$, $n_0 = 92$ and $n_0 = 90$. Because of their larger dependence on n_0, the values of the c_i coefficients are less reliable than the values of z_0 and $\beta_{\min}$.

m	j	z_0	$\beta_{\min}$	c_1	c_2	c_3	c_4
2	1	−4.193 853 43 + 2.169 896 90 *i*	0.097 457 940 8	−0.858 4970			
2	2	−4.193 685 91 + 2.169 736 66 *i*	0.097 464 827 2	−0.850 6593	0.254 839e-1		
2	3	−4.193 684 15 + 2.169 739 64 *i*	0.097 464 833 1	−0.850 6123	0.259 139e-1	−0.252 91e-3	
2	4	−4.193 684 13 + 2.169 739 77 *i*	0.097 464 831 4	−0.850 6134	0.259 109e-1	−0.255 56e-3	−0.1776e-5
3	1	−6.438 219 23 + 5.011 037 59 *i*	0.015 023 775 5	−0.582 1553			
3	2	−6.438 074 09 + 5.010 772 56 *i*	0.015 024 796 9	−0.578 2958	0.375 112e-2		
3	3	−6.438 070 60 + 5.010 772 42 *i*	0.015 024 807 4	−0.578 2492	0.384 978e-2	−0.841 19e-5	
3	4	−6.438 070 38 + 5.010 772 54 *i*	0.015 024 807 8	−0.578 2477	0.385 552e-2	−0.947 53e-5	−0.4804e-7
4	1	−8.099 162 89 + 7.545 791 80 *i*	0.002 452 861 2	−0.470 8212			
4	2	−8.099 057 67 + 7.545 508 45 *i*	0.002 453 010 85	−0.468 4753	0.927 710e-3		
4	3	−8.099 054 62 + 7.545 506 72 *i*	0.002 453 012 74	−0.468 4380	0.958 470e-3	−0.218 32e-5	
4	4	−8.099 054 41 + 7.545 506 75 *i*	0.002 453 012 82	−0.468 4364	0.960 602e-3	−0.249 84e-5	−0.5096e-8
5	1	−9.445 967 30 + 9.702 660 53 *i*	0.000 402 730 909	−0.403 2380			
5	2	−9.445 874 63 + 9.702 337 30 *i*	0.000 402 757 342	−0.401 7092	0.236 347e-3		
5	3	−9.445 871 57 + 9.702 334 52 *i*	0.000 402 757 710	−0.401 6768	0.246 656e-3	−0.711 07e-5	
5	4	−9.445 871 33 + 9.702 334 51 *i*	0.000 402 757 726	−0.401 6748	0.247 643e-3	−0.850 38e-5	−0.1785e-8

It is obvious that equations (23)–(25) can be generalized to an arbitrary number of terms in equation (9). Taking $j > 1$ terms in equation (9) with the coefficients $c_1, \ldots, c_j$ we have to solve $2(j^2 + j + 1)$ equations for the same number of unknowns. In general, these equations can be reduced to two nonlinear equations for $\mathrm{Re}(z_0)$ and $|z_0|^2$. The coefficients c_i, $i = 1, \ldots, j$ can be calculated analogously to the case $j = 2$.

In numerical calculations, we used the K_n coefficients for the ground state of the quartic, sextic, octic and decadic oscillators computed by the method described in [17, 18] and found the values of the branch point z_0, $\beta_{\min}$ and the constants c_i (see table 1). It is seen that the values of z_0, $\beta_{\min}$ and c_i coefficients stabilize with increasing j. We also note that the values of the coefficients c_i, $i > 1$ go down with increasing i so that we can restrict ourselves to a few terms in equation (9). The value of the branch point $z_0 = -4.193\,6841 + 2.169\,7397\,i$ for the quartic oscillator following from table 1 is more exact than the value $z_0 = -4.193\,684 + 2.169\,740\,i$ found in [14]. A more detailed discussion will be published elsewhere.

Summarizing, we suggested the general large-order formula (9) for the K_n coefficients, showed that equation (4) is equivalent to the leading term (19) of equation (9) and derived equation (20) describing the large-order corrections to equation (19). Further, we suggested a new more general method of calculating the branch point z_0 and the expansion coefficients c_i from the numerical values of the K_n coefficients. The values of the branch point z_0, $\beta_{\min}$, and the constants c_i were computed for the ground state of the quartic, sextic, octic and decadic oscillators.

Our discussion is based on the existence of the expansion (7). It is obvious that our method can be applied not only to the anharmonic oscillators but also to more general problems with the same character of the branch points. Extension to a more general fraction-like character of the branch points also seems to be possible. For this reason, we believe that the results of this letter contribute to better understanding of the large-order perturbation expansions in general.

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References

[1] Simon B 1970 *Ann. Phys., NY* **58** 76
[2] Simon B 1972 *Cargese Lectures in Physics 1970* **5** ed D Bessis (New York: Gordon and Breach) p 383
[3] Löwdin P O and Öhrn Y (ed) 1981 *Proc. of the Sanibel Workshop on Perturbation Theory at Large Order(Sanibel, Florida)*
Simon B and Bender C M 1982 *Int. J. Quantum Chem.* **21** 1
[4] Weniger E J 1996 *Ann. Phys., NY* **246** 133
[5] Ushveridze A G 1989 *Bulg. J. Phys.* **16** 137 (in Russian)
[6] Fernández F M and Guardiola R 1997 *J. Phys. A: Math. Gen.* **30** 7187
[7] Weniger E J 1996 *Phys. Rev. Lett.* **77** 2859
[8] Turbiner A V and Ushveridze A G 1998 *J. Math. Phys.* **29** 2053
[9] Guardiola R, Solís M A and Ros J 1992 *Nuovo Cimento* B **107** 713
[10] Fernández F M and Guardiola R 1993 *J. Phys. A: Math. Gen.* **26** 7169
[11] Janke W and Kleinert H 1995 *Phys. Rev. Lett.* **75** 2787
[12] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
[13] Loeffel J J and Martin A 1972 *Cargese Lectures in Physics 1970* vol 5 ed D Bessis (New York: Gordon and Breach) p 415
[14] Shanley P E 1986 *Phys. Lett.* **117** 161
[15] Fernández F M, Arteca G A and Castro E A 1987 *J. Math. Phys.* **28** 323
[16] Abramowitz M and Stegun I E (ed) 1972 *Handbook of Mathematical Functions* (New York: Dover)
[17] Skála L and Čížek J 1996 *J. Phys. A: Math. Gen.* **29** L129
[18] Skála L and Čížek J 1996 *J. Phys. A: Math. Gen.* **29** 6467