International Journal of Theoretical Physics, Vol. 39, No. 10, 2000

Large-Order Strong Coupling Perturbation Coefficients for Anharmonic Oscillators

J. Zamastil,[1,2] L. Skála,[1,2,3] and J. Čížek[1,2]

Received January 27, 2000

A large-order formula for the perturbation coefficients of the strong-coupling perturbation expansion for anharmonic oscillators with Hamiltonian $H = p^2 + x^2 + \beta x^{2m}$ is derived and parameters in this formula are determined for the ground and first excited states of the quartic, sextic, octic, and decadic oscillators (m = 2, 3, 4, 5).

1. INTRODUCTION

In this paper, we investigate the Schrödinger equation

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

for the anharmonic oscillators, where

$$H = -d^2/dx^2 + x^2 + \beta x^{2m}, \qquad \beta \geq 0, \quad m \geq 2 \tag{2}$$

The energy $E(\beta)$ can be expressed as the strong-coupling expansion (see, e.g., ref. 1)

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

The series (3) converges if β is sufficiently large, i.e., if $\beta > \beta_{\min}$, where $\beta_{\min} > 0$. The large-order behavior of the K_n coefficients was investigated in ref. 2, where the large-order formula for the K_n coefficients

[1] Faculty of Mathematics and Physics, Charles University, 12116 Prague, 2, Czech Republic.
[2] Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.
[3] To whom correspondence should be addressed at Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic; e-mail: skala@quantum.karlov.mff.cuni.cz

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

where $\varphi = \arg z_K$, was derived. Here, A and δ are constants, z_K denotes the complex square root branch point of the energy $\epsilon(z)$ with the smallest distance to the origin [1, 3–5],

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

$z = \beta^{-2/(m+1)}$, and $K = 0, 1, \ldots$ is the index of the excitation. The minimal value of β for which the series (3) converges can be computed from the equation [6, 7]

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

The values of z_K for the ground and first excited states of the quartic, sextic, octic, and decadic oscillators ($m = 2, 3, 4, 5$) can be found in refs. 6 and 7. Since the derivation of Eq. (4) in ref. 2 is very brief and there are typos in the expressions for the constants A and δ found in there, we give independent derivation of this equation here. Further, we compute the numerical values of the constants A and δ for the ground and first excited states of the quartic, sextic, octic, and decadic oscillators and perform numerical tests of Eq. (4).

2. LARGE-ORDER FORMULA

In agreement with refs. 1, 3–5, and 8, the energy $\epsilon(z)$ has the following analytic structure. Because of the symmetry $\epsilon(z) = [\epsilon(z^*)]^*$, where the asterisk denotes complex conjugation, we restrict our discussion to the upper half-plane $\arg z \in (0, \pi)$. The energy $\epsilon(z)$ is analytic in the region $\arg z < 2\pi/3$. For $\arg z > 2\pi/3$ and $|z| \geq |z_0|$, the energy $\epsilon(z)$ has square-root branch points. At these points, two neighboring states of the same parity have the same (degenerate) complex energy $\epsilon(z)$. For example, at the branch point $z_0 = z_2$ with the smallest distance to the origin the ground and second excited states have the same complex energy $\epsilon(z_0) = \epsilon(z_2)$. Going to larger values of $|z|$, another branch point $z_1 = z_3$ where the first and third excited states have the same degenerate energy exists. Continuing, we find two branch points where the energies of the second and fourth excited states are degenerate, three branch points where the energies of the fourth and sixth excited states are degenerate, etc. An analogous picture is obtained for the odd-parity states. For $K > 3$, the absolute value of the branch point z_K, which has the smallest distance to the origin of all the branch points corresponding to the degenerate energies of the $(K-2)$th and Kth states, determines the radius of convergence of the series (3) for the Kth state. The absolute value of z_K increases with increasing K. We note that the absolute values of the branch points belonging to the degenerate energies of the $(K-2)$th and Kth states are similar, so that these points lie approximately on a part of the circle with the center in the origin.

To derive Eq. (4) we consider the ground and second excited states. Discussion for the first and third excited states is analogous. It follows from the analytic structure of the energy $\epsilon(z)$ that to calculate K_n we can use the Cauchy formula with the integration path C shown in Fig. 1:

$$K_n = \frac{1}{2\pi i}\oint_C dz\, \frac{\epsilon(z)}{z^{n+1}} \tag{7}$$

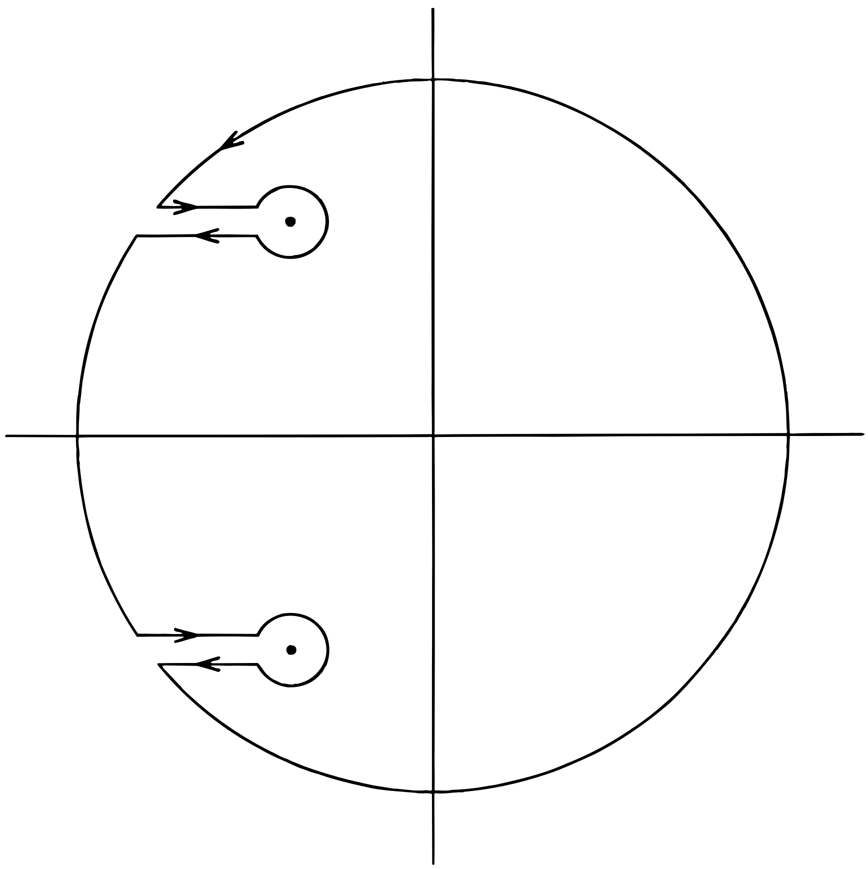

Fig. 1. The integration path C in the complex z-plane. The dots denote z_0 and z_0^*.

Using the square-root character of the branch points, we can write for z close to z_0

$$\epsilon(z) = \epsilon(z_0) + c(z - z_0)^{1/2} + \cdots \tag{8}$$

where c is a complex constant. Neglecting the integrals along the circle-like parts of the contour C and assuming large n, we can extend the lower bound of the integration to $z_0 - \infty$ and get

$$K_n = \frac{1}{2\pi i} \int_{z_0-\infty}^{z_0} dz \, \frac{\Delta\epsilon(z)}{z^{n+1}} + \text{c.c.} \tag{9}$$

where $\Delta\epsilon(z) = 2i(z_0 - z)^{1/2}c$ for the ground state and $\Delta\epsilon(z) = -2i(z_0 - z)^{1/2}c$ for the second excited state. Further, introducing the variable $t = (z_0 - z)/|z_0|$, where $z_0 = |z_0|e^{i\arg z_0}$, we get

$$K_n = \frac{\pm c|z_0|^{3/2}}{\pi z_0^{n+1}} \int_0^{\infty} dt \, \frac{t^{1/2}}{(1 - t\, e^{-i\arg z_0})^{n+1}} + \text{c.c.} \tag{10}$$

Here, the plus sign is valid for the ground state and the minus sign for the second excited state. The last integral can be written in the form

$$I = \int_0^{\infty} dt \, t^{1/2} \, e^{-(n+1)\ln(1+t\exp i\theta)} \tag{11}$$

where

$$\theta = \pi - \arg z_0 \tag{12}$$

For large n, the dominant contribution to this integral is given by $t \to 0$. Therefore, we can replace $\ln(1 + t \exp i\theta)$ by $t \exp i\theta$, which leads to

$$I = \frac{\sqrt{\pi}}{2} \, e^{-i3\theta/2} \, \frac{1}{n^{3/2}} \tag{13}$$

Inserting this result into Eq. (10), we get after some manipulation the final result

$$K_n = \pm \sqrt{\frac{1}{\pi}} \, |c| \cdot |z_0|^{1/2} \, \frac{1}{|z_0|^n n^{3/2}} \times \cos\left[n \arg z_0 + \frac{3\pi - \arg z_0}{2} - \arg c \right] \tag{14}$$

Comparing this equation with Eq. (4), we see that

$$A = \pm \sqrt{\frac{1}{\pi}}\, |c| \cdot |z_0|^{1/2} \tag{15}$$

and

$$\delta = (3\pi - \arg z_0)/2 - \arg c \tag{16}$$

Our Eq. (14) differs from the formula given in ref. 2 in the values of A and δ. We note also that the form of Eq. (14) agrees with the form of Eq. (19) in ref. 6,

$$K_n = \frac{1}{|z_0|^{n-1} n^{3/2}} \left[e_1 \cos(n\varphi) + f_1 \sin(n\varphi)\right] \tag{17}$$

where the large-order behavior of the coefficients K_n was investigated by another method. Comparing the first two terms of Eq. (7) in ref. 6

$$\epsilon(z) = \epsilon(z_0) + c_1[(z - z_0)(z - z_0^*)]^{1/2} + \cdots \tag{18}$$

with Eq. (8), we get for z in the neighborhood of z_0

$$c = c_1(z_0 - z_0^*)^{1/2} \tag{19}$$

3. NUMERICAL RESULTS

The numerical values of the coefficients K_n, the branch points z_K, and the constants c_1 and $\beta_{\min}$ for the ground and first excited states of the quartic, sextic, octic, and decadic oscillators can be found in refs. 6 and 7. Using the values of z_K and c_1 given in these papers, we calculated the constants A and δ from Eqs. (15), (16), and (19) (see Tables I and II). It follows from Eq. (20) of ref. 6,

Table I. Constants A and δ and Value of the Branch Point z_0 in Eq. (4) Describing the Large-Order Behavior of Coefficients K_n for the Ground State ($K = 0$) of the Quartic, Sextic, Octic, and Decadic Oscillators ($m = 2, 3, 4, 5$)[a]

m	A	δ	z_0
2	2.17	5.73	$-4.193 + 2.169i$
3	2.94	5.82	$-6.438 + 5.011i$
4	3.41	5.87	$-8.099 + 7.545i$
5	3.67	5.89	$-9.445 + 9.702i$

[a] The values of z_0 were taken from ref. 6.

Table II. Constants A and δ and Value of the Branch Point z_1 in Eq. (4) Describing the Large-Order Behavior of Coefficients K_n for the First Excited State ($K = 1$) of the Quartic, Sexic, Octic, and Decadic Oscillators ($m = 2, 3, 4, 5$)[a]

m	A	δ	z_1
2	3.22	5.83	$-4.987 + 4.023i$
3	4.48	5.97	$-7.029 + 10.02i$
4	5.04	6.04	$-7.863 + 15.46i$
5	5.86	6.08	$-8.255 + 20.05i$

[a] The values of z_1 were taken from ref. 7.

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

that the accuracy of Eq. (4) is $O(1/n)$.

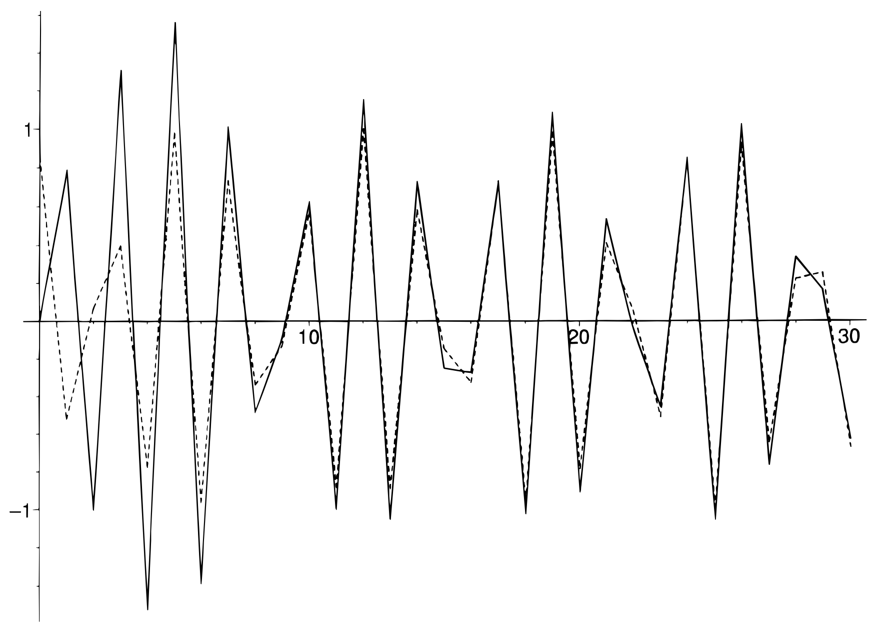

Fig. 2. Comparison of the large-order formula (14) with the numerical values of the K_n coefficients for the ground state of the quartic oscillator. The dashed line shows $\cos[n \arg z_0 + (3\pi - \arg z_0)/2 - \arg c]$ from Eq. (14) and the full line shows $K_n/[\sqrt{(1/\pi)}|c| \cdot |z_0|^{1/2}(1/|z_0|^n n^{3/2})]$, where K_n are the numerical values of the coefficients, $n = 0, \ldots, 30$.

Comparison of the numerical values of the K_n coefficients with Eq. (14) for the ground state of the quartic oscillator is done in Figs. 2 and 3. It is seen that Eq. (14) is qualitatively applicable already for n about 10. For larger n, Eq. (14) describes the behavior of the numerical coefficients K_n very well. The results for other oscillators ($m = 3, \ldots, 5$) and the first excited state ($K = 1$) are similar.

We tried to apply Eq. (4) also to the higher excited states. However, for $K > 3$ and n less than 100 the formula (4) cannot be used. The problem is apparently in the fact that the number of the branch points increases with increasing K and the absolute values of these points are very close [see the discussion above Eq. (7)]. To suppress the contribution of the other branch points it would be necessary to consider n much larger than 100 or to generalize Eq. (4) to a larger number of the branch points.

4. CONCLUSIONS

Concluding, we derived the expressions (15) and (16) for A and δ, calculated the values of these constants for the ground and first excited states

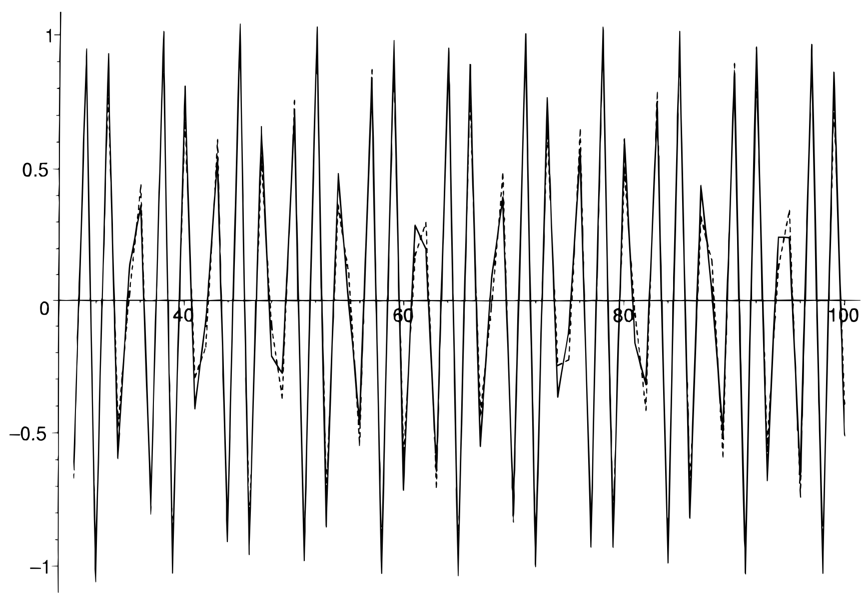

Fig. 3. Comparison of the large-order formula (14) with the numerical values of the K_n coefficients for the ground state of the quartic oscillator. The dashed line shows $\cos[n \arg z_0 + (3\pi - \arg z_0)/2 - \arg c]$ from Eq. (14) and the full line shows $K_n/[\sqrt{(1/\pi)}|c| \cdot |z_0|^{1/2}(1/|z_0|^n n^{3/2})]$, where K_n are the numerical values of the coefficients, $n = 30, \ldots, 100$.

of the quartic, sextic, octic, and decadic oscillators, and showed that the large-order formula (14) describes well the behavior of the numerical coefficients K_n starting from low values of n. Equation (14) cannot be used for the excited states with $K > 3$ and n about 100. For these cases, further generalization of this equation is necessary.

ACKNOWLEDGMENTS

This work was supported in part by the NSERC of Canada and the GACR (grant No. 202/00/1026), GAUK (grant No. 166/2000), UK (grant No. 190-01/206053), and FRVS (grant No. 1923) of the Czech Republic.

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