Large-order behavior of the convergent perturbation theory for anharmonic oscillators

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Using the large-order formula for the coefficients of the divergent weak-coupling series for the energy of the anharmonic oscillators, we derive a simple analytic large-order formula for the coefficients of the convergent renormalized strong-coupling series. This formula is valid for all the states of the anharmonic oscillators defined by the Hamiltonians $H=p^2+x^2+\beta x^{2m}$ with $m\geqslant 2$. A further generalization of this formula is also proposed. Numerical tests of the formula are performed for the quartic, sextic, octic, and decadic oscillator with the help of asymptotic analysis. Further it is shown that the renormalized strong-coupling perturbation expansion converges for all the states of these oscillators and for all physically relevant $\beta\in[0,\infty)$.
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I. INTRODUCTION

We investigate the Schrödinger equation $H\psi=E(\beta)\psi$ for the anharmonic oscillators, where

$$H=p^2+x^2+\beta x^{2m}, \quad \beta\geqslant 0, \quad m\geqslant 2. \tag{1}$$

As is well known, $E(\beta)$ can be expressed as a *weak-coupling* perturbation series in powers of β,

$$E(\beta)=\sum_{n=0}^{\infty} b_n\beta^n, \tag{2}$$

which diverges for every $\beta>0$ [1–6]. The large-order behavior of the coefficients b_n follows from [3]

$$b_n=(-1)^{n+1}\frac{(m-1)2^K}{\pi^{3/2}K!2^{2n-1}}\Gamma(n(m-1)+K+1/2)a^{n(m-1)+K+1/2}, \quad K\geqslant 0, \tag{3}$$

$$a=\frac{\Gamma(2m/(m-1))}{\Gamma^2(m/(m-1))}, \tag{4}$$

where K is the index of the excitation.

With the help of the scaling transformation $x\to\beta^{-1/[2(m+1)]}x$, H can be expressed as [2]

$$H=\beta^{1/(m+1)}[p^2+\beta^{-2/(m+1)}x^2+x^{2m}]. \tag{5}$$

Consequently, $E(\beta)$ also possesses the *strong-coupling* expansion

$$E(\beta)=\beta^{1/(m+1)}\sum_{n=0}^{\infty} K_n\beta^{-2n/(m+1)}, \tag{6}$$

which converges if β is sufficiently large [2].

Alternative perturbative approaches based upon renormalization (Wick ordering [7] or scaling [7–11]) have considerable conceptual and technical advantages. In the quartic case, Wick ordering and scaling are closely related and they differ by a numerical factor in the effective coupling constant. In this paper we do scaling according to $x\to\sqrt{\tau}x$, where τ and β are related by the m-dependent equation

$$\beta=(1-\tau^2)/(B_m\tau^{m+1}), \tag{7}$$

with $B_m=m(2m-1)!!/2^{m-1}$ [9]. This transformation maps the physically relevant *unbounded* interval $\beta\in[0,\infty)$ onto the *bounded* interval $\tau\in[1,0)$. With the help of Eq. (7), the Hamiltonian (1) can be expressed in terms of a renormalized Hamiltonian H_R [9,10],

$$H=H_R/\tau, \tag{8}$$

$$H_R(\tau)=p^2+x^2+(1-\tau^2)(x^{2m}/B_m-x^2) \tag{9}$$

$$=p^2+x^{2m}/B_m+\tau^2(x^2-x^{2m}/B_m). \tag{10}$$

The *renormalized* energy

$$E_R(\tau)=\tau E(\beta) \tag{11}$$

can either be expressed as a divergent *renormalized weak-coupling* expansion in $1-\tau^2$ [10],

$$E_R(\tau)=\sum_{n=0}^{\infty} c_n(1-\tau^2)^n, \tag{12}$$

or as a *renormalized strong-coupling* expansion in τ^2 [11],

$$E_R(\tau)=\sum_{n=0}^{\infty} \Gamma_n\tau^{2n}. \tag{13}$$

The weak-coupling expansion (12) diverges almost as strongly as the weak-coupling expansion (2) [7,10]. However, the strong-coupling expansion (13) has some very useful properties [11,12].

For the ground and first excited states of the quartic anharmonic oscillator, we computed numerically 200 coeffi-

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cients Γ_n with high accuracy [12]. From these data, we obtained the following large-order behavior:

$$\Gamma_n = A^{(K)}(2n)^{(K-1)/2} e^{-2\sqrt{2n}} \left(1 + \sum_{\nu=1}^{\infty} \frac{a_\nu^{(K)}}{(2n)^{\nu/2}} \right). \quad (14)$$

The leading coefficient

$$A^{(K)} = -\frac{12^K}{K!} \frac{4\sqrt{6}}{\pi e^2} \quad (15)$$

was determined from the summation rules for Γ_n. In addition, a few coefficients $a_\nu^{(K)}$ were also determined analytically. The leading term of the large-order formula (14) shows that the renormalized strong-coupling expansion (13) converges for all $\tau \in [0,1)$ [12].

Our results for the quartic anharmonic oscillator and further numerical results for the sextic and octic anharmonic oscillators [11] indicate that the renormalized strong-coupling expansion (13) actually converges for arbitrary $m \geqslant 2, K \geqslant 0$, and $\tau \in [0,1)$.

The main purpose of this paper is to investigate *analytically* the large-order behavior of the renormalized strong-coupling coefficients Γ_n of general anharmonic oscillators with Hamiltonian (1). We show in Sec. II that their large-order behavior is described by a simple analytic formula which is a generalization of the leading term in Eq. (14) to arbitrary $m \geqslant 2$. In contrast to [12], where Eq. (14) was conjectured from numerical analysis, we use here an analytic approach. We propose also further generalization of the series (14). In Sec. III we compare the large-order formula with the actual values of the Γ_n coefficients and test the validity of the summation rule for Γ_n. These numerical results and the large-order formula for Γ_n show that the renormalized strong-coupling expansion (13) converges for all $\tau \in [0,1)$, $m \geqslant 2$, and $K \geqslant 0$.

Finally, let us mention that our final goal is the resummation of renormalized series both for the case of oscillators ($\tau \in [0,1]$) and double wells [$\tau \in (-\infty,0)$]. Consideration of the large-order behavior of these coefficients is a step in this program.

II. LARGE-ORDER FORMULA

For the determination of the large-order behavior of Γ_n, we start from Eq. (3) for the coefficients b_n. For large n, it follows from [7,10] that $c_n = b_n/[e^3(B_m)^n]$ for $m=2$, and $c_n = b_n/(B_m)^n$ for $m \geqslant 3$. This leads to the large-order behavior valid for $m \geqslant 3$,

$$c_n = (-1)^{n+1} C \Gamma((m-1)n + K + 1/2)/D^n, \quad (16)$$

$$C = \frac{(m-1)}{\pi^{3/2}} \frac{2^{K+1}}{K!} a^{K+1/2}, \quad (17)$$

$$D = 4 B_m a^{1-m}. \quad (18)$$

For $m=2$, the constant C in Eq. (17) has to be divided by e^3.

For the derivation of the large-order formula for Γ_n we use Eq. (16). First we substitute Eq. (16) into the remainder of the series (12),

$$\Delta E_R(\kappa) = E_R(\kappa) - \sum_{\nu=0}^{n-1} c_\nu \kappa^\nu$$
$$= C \sum_{\nu=n}^{\infty} (-1)^{\nu+1} \left(\frac{\kappa}{D} \right)^\nu \Gamma((m-1)\nu + K + 1/2), \quad (19)$$

where $\kappa = 1 - \tau^2$ and n is large. Then, we use the integral representation of the Γ function, exchange summation and integration, and obtain

$$\Delta E_R(\kappa) = -C \int_0^\infty \sum_{\nu=n}^{\infty} \left[\frac{-\kappa t^{m-1}}{D} \right]^\nu t^{K-1/2} e^{-t} dt. \quad (20)$$

The geometric series in this equation can be summed in the Borel sense

$$\Delta E_R(\kappa) = (-1)^{n+1} C (\kappa/D)^n \int_0^\infty \frac{t^{(m-1)n+K-1/2} e^{-t} dt}{1 + \kappa t^{m-1}/D}. \quad (21)$$

To find the large-order formula for Γ_n, we compute the coefficients of the Taylor expansion of E_R with respect to $\mu = \tau^2 = 1 - \kappa$,

$$\Gamma_n = \frac{1}{n!} \left. \frac{d^n E_R(\mu)}{d\mu^n} \right|_{\mu=0}. \quad (22)$$

If we combine Eqs. (19) and (22), we see that the sum $\Sigma_{\nu=0}^{n-1} c_\nu (1-\mu)^\nu$ does not contribute to Γ_n. Consequently, the large-order formula for Γ_n can be obtained by differentiating the remainder of the sum ΔE_R only. Thus, if we replace in Eq. (22) E_R by ΔE_R, and interchange in Eq. (21) integration and differentiation with respect to $\mu = 1 - \kappa$, we get

$$\Gamma_n = -\frac{C}{D^n} \int_0^\infty \frac{t^{(m-1)n+K-1/2} e^{-t} dt}{(1 + t^{m-1}/D)^{n+1}}. \quad (23)$$

We derive an analytic large-order formula for Γ_n by constructing an asymptotic approximation according to the Laplace method [13]. We have applied this method for different values of m and K and found

$$\Gamma_n = -C D^{(K+1/2)/(m-1)} I_n, \quad (24)$$

where

$$I_n = J_{m,K} \frac{e^{-[m/(m-1)][D(m-1)n]^{1/m}}}{n^{(m-K-1)/m}}, \quad (25)$$

$$J_{2,K} = \frac{e\sqrt{\pi}}{D^{K/2}}, \quad (26)$$

$$J_{m,K} = \frac{\sqrt{2\pi} D^{(m/2-K-1)/[m(m-1)]}}{(m-1)^{(m-K-1)/m} m^{1/2}}, \quad m \geqslant 3. \quad (27)$$

TABLE I. Comparison of the numerical values of the coefficients Γ_n with their values Γ_n^{LO} given by the large-order formula (28) for the ground state ($K=0$) of the quartic, sextic, octic, and decadic oscillators ($m=2,3,4,5$). For the asymptotic analysis of these data, see Table III. Numbers in square brackets are powers of 10.

	Quartic oscillator		Sextic oscillator		Octic oscillator		Decadic oscillator	
n	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}
10	−0.88203[−5]	−0.12314[−4]	−0.63983−[4]	−0.18200[−3]	−0.10130[−3]	−0.21369[−3]	−0.10402[−3]	−0.19836[−3]
25	−0.35367[−7]	−0.43060[−7]	−0.28977[−5]	−0.61652[−5]	−0.99835[−5]	−0.16084[−4]	−0.14801[−4]	−0.21856[−4]
50	−0.76355[−10]	−0.86997[−10]	−0.13891[−6]	−0.25088[−6]	−0.11772[−5]	−0.16529[−5]	−0.25970[−5]	−0.33955[−5]
75	−0.71513[−12]	−0.79322[−12]	−0.16773[−7]	−0.28016[−7]	−0.28464[−6]	−0.37581[−6]	−0.84276[−6]	−0.10457[−5]
100	−0.14217[−13]	−0.15531[−13]	−0.31476[−8]	−0.50082[−8]	−0.95738[−7]	−0.12185[−6]	−0.36076[−6]	−0.43422[−6]
125	−0.45589[−15]	−0.49297[−15]	−0.77117[−9]	−0.11855[−8]	−0.39115[−7]	−0.48549[−7]	−0.18138[−6]	−0.21388[−6]

By substituting the expressions for C, D, and I_n into Eq. (24), we get after some manipulation a remarkably simple large-order formula

$$\Gamma_n = -\frac{2^{K+3/2}a^{K+1/2}b}{\pi K!\sqrt{m}}(bn)^{[(K+1)/m-1]}e^{-\{[m/(m-1)](bn)^{1/m}\}}, \tag{28}$$

$$b=(m-1)D=4(m-1)B_m a^{1-m}, \quad m\geqslant 3. \tag{29}$$

For $m=2$, the right-hand side of Eq. (28) has to be divided by e^2, which yields the leading term of Eq. (14).

Analogously to Eq. (14), we assume that the general large-order behavior of Γ_n can be described by the series

$$\Gamma_n = -\frac{2^{K+3/2}a^{K+1/2}b}{\pi K!\sqrt{m}}(bn)^{[(K+1)/m-1]}e^{-\{[m/(m-1)](bn)^{1/m}\}} \times\left(1+\sum_{\nu=1}^{\infty}\frac{a_\nu^{(K,m)}}{(bn)^{\nu/m}}\right), \quad m\geqslant 3 \tag{30}$$

where $a_\nu^{(K,m)}$ are expansion coefficients. For $m=2$, the right-hand side of Eq. (30) has to be divided by e^2. Four expansion coefficients $a_\nu^{(K,m)}$ are known for the ground state of the quartic oscillator ($K=0, m=2, \nu=1,\ldots,4$), when they equal the coefficients $a_\nu^{(0)}$ given in [12]. The calculation of the $a_\nu^{(K,m)}$ coefficients for the sextic and higher-order oscillators is more involved and leads to transcendental expressions. We plan to publish results for these oscillators in the future [14]. The series (30) is expected to be only asymptotic.

We note at the end of our calculations that the integrals in Eqs. (21) and (23) for $m=2$ can be expressed in terms of the Kummer function $U(a,b,z)$ [15],

$$\Delta E_R(\kappa)=(-1)^{n+1}C(D/\kappa)^{K+1/2}\Gamma(n+k+1/2) \times U(n+K+1/2, n+K+1/2, D/\kappa), \tag{31}$$

$$\Gamma_n=-CD^{K+1/2}\Gamma(n+K+1/2)U(n+K+1/2, K+1/2, D). \tag{32}$$

III. NUMERICAL RESULTS

For the quartic oscillator ($m=2$), the large-order formula (28) was tested in [12]. It was shown that this formula gives numerical values of the Γ_n coefficients close to the exact ones starting from n about 100. Qualitatively, it can be used from n about 10.

Because of the $(bn)^{1/m}$ dependence in Eqs. (28) and (30), slower convergence of the large-order formulas to the actual values of Γ_n can be expected with increasing m. To clarify this question we performed numerical calculation of the Γ_n coefficients for the ground and first excited state ($K=0,1$) of the sextic, octic, and decadic oscillators ($m=3,4,5$). These results are compared with the results for the quartic oscillator in Tables I–III.

The coefficients Γ_n for $n=0,\ldots,125$ were calculated by the method described in [16]. Numerical values of a few selected Γ_n coefficients are compared with the large-order formula (28) for $m=2,3,4,5$ and $K=0,1$ in Tables I and II. The agreement of the numerical values of Γ_n with the large-order formula (28) goes down with increasing m and K. We see, however, that even for the first excited state of the dec-

TABLE II. Comparison of the numerical values of the coefficients Γ_n with their values Γ_n^{LO} given by the large-order formula (28) for the first excited state ($K=1$) of the quartic, sextic, octic, and decadic oscillators ($m=2,3,4,5$). For the asymptotic analysis of these data, see Table III. Numbers in square brackets are powers of 10.

	Quartic oscillator		Sextic oscillator		Octic oscillator		Decadic oscillator	
n	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}	Γ_n	Γ_n^{LO}
10	−0.25353[−3]	−0.66088[−3]	−0.12410[−2]	−0.47993[−2]	−0.16890[−2]	−0.44625[−2]	−0.16329[−2]	−0.37599[−2]
25	−0.19383[−5]	−0.36537[−5]	−0.80553[−4]	−0.22064[−3]	−0.21047[−3]	−0.42235[−3]	−0.27466[−3]	−0.49760[−3]
50	−0.69940[−8]	−0.10439[−7]	−0.52767[−5]	−0.11312[−4]	−0.30768[−4]	−0.51616[−4]	−0.56558[−4]	−0.88795[−4]
75	−0.86211[−10]	−0.11658[−9]	−0.76277[−6]	−0.14460[−5]	−0.84682[−5]	−0.12987[−4]	−0.20266[−4]	−0.29658[−4]
100	−0.20541[−11]	−0.26357[−11]	−0.16180[−6]	−0.28451[−6]	−0.31195[−5]	−0.45252[−5]	−0.93129[−5]	−0.13044[−4]
125	−0.75313[−13]	−0.93534[−13]	−0.43444[−7]	−0.72553[−7]	−0.13661[−5]	−0.19063[−5]	−0.49460[−5]	−0.67184[−5]

TABLE III. Asymptotic analysis of the ratio $\Gamma_n/\Gamma_n^{\mathrm{LO}}$ for the ground and first excited state ($K=0,1$) of the quartic, sextic, octic, and decadic oscillators ($m=2,3,4,5$). The leading term a_0 of the asymptotic expansion (33) corresponding to $n\to\infty$ was obtained by means of the diagonal Padé approximants based on the values $\Gamma_n/\Gamma_n^{\mathrm{LO}}$ for $n=115,\ldots,125$.

m	Ground state a_0	First excited state a_0
2	1.000037	1.003079
3	1.000747	1.021083
4	1.008496	0.984731
5	0.993720	0.978293

adic oscillator ($m=5$ and $K=1$) these values agree relatively well. We note that the absolute values of the Γ_n coefficients obtained from the large-order formula (28) are larger than the actual values of Γ_n. We have studied also the ratio appearing in Eq. (30),

$$\Gamma_n/\Gamma_n^{\mathrm{LO}}=a_0+\frac{a_1^{(K,m)}}{(bn)^{1/m}}+\frac{a_2^{(K,m)}}{(bn)^{2/m}}+\cdots, \qquad (33)$$

where Γ_n are numerical values of the expansion coefficients and Γ_n^{LO} are given by the large-order formula (28). For very large n, this ratio should converge to $a_0=1$. Using the Thiele extrapolation built in MAPLE, we extrapolated $\Gamma_n/\Gamma_n^{\mathrm{LO}}$ to $n\to\infty$ and obtained values of a_0 shown in Table III. These values are very close to one and confirm correctness of Eq. (28).

Similarly to [12], we have tested also the validity of the summation rule

$$\Sigma_0=\sum_{n=0}^{\infty}\Gamma_n=2K+1. \qquad (34)$$

First we calculated the partial sum $\Sigma_0^N=\Sigma_{n=0}^N\Gamma_n$ for $N=125$ from the numerical values of Γ_n. The remaining part of the sum $\Sigma_0^{\mathrm{LO}}=\Sigma_{n=N+1}^{\infty}\Gamma_n$ was calculated numerically with the use of Eq. (28). The infinite limit in this sum was replaced by 5000. Results are shown in Table IV. Since we use only the leading term of Eq. (30) here, the summation rules are obeyed with lower accuracy than in the case of the ground state of the quartic oscillator for which four analytic coefficients $a_\nu^{0,2}$, $\nu=1,\ldots,4$ were used [12]. It is seen that the summation rule is obeyed with very good accuracy for $m=2$ and $K=0$. With increasing m and K, the accuracy goes down. We see, however, that the summation rule is obeyed with reasonable accuracy even for the first excited state of the decadic oscillator ($m=5$ and $K=1$). In any case, the inclusion of the large-order formula (28) improves the accuracy of the rule. We note that $\Sigma_0^N+\Sigma_0^{\mathrm{LO}}-\Sigma_0$ is always negative. It confirms again that the absolute value of Γ_n given by the large-order formula (28) is larger than the absolute value of the actual coefficients Γ_n.

TABLE IV. Summation rules Σ_0^N and $\Sigma_0^N+\Sigma_0^{\mathrm{LO}}$ in comparison with the exact value of the summation rule $\Sigma_0=2K+1$ for the coefficients Γ_n of the strong-coupling expansion for the ground and first excited state ($K=0,1$) of the quartic, sextic, octic, and decadic oscillators ($m=2,3,4,5$). $N=125$. Numbers in square brackets are powers of 10.

	Ground state		First excited state	
m	$\Sigma_0^N-\Sigma_0$	$\Sigma_0^N+\Sigma_0^{\mathrm{LO}}-\Sigma_0$	$\Sigma_0^N-\Sigma_0$	$\Sigma_0^N+\Sigma_0^{\mathrm{LO}}-\Sigma_0$
2	0.339[−14]	−0.265[−15]	0.582[−12]	−0.134[−12]
3	0.160[−7]	−0.805[−8]	0.965[−6]	−0.592[−6]
4	0.142[−5]	−0.298[−6]	0.543[−4]	−0.183[−4]
5	0.951[−5]	−0.139[−5]	0.286[−3]	−0.849[−4]

IV. CONCLUSIONS

The results of this paper may be summarized as follows: Starting from known large-order behavior of the divergent weak-coupling expansion coefficients b_n, we derived the general large-order formula (28) for the strong-coupling expansion coefficients Γ_n. In contrast to [12], where the form of this formula was for $m=2$ conjectured from numerical analysis, Eq. (28) was derived analytically. The large-order formula (28) is very simple and holds for all anharmonicities x^{2m} with $m\geqslant 2$, and for all states $K\geqslant 0$. We suggested also the more general series (30) which is expected to be only asymptotic. The numerical tests of Eq. (28) were performed for the quartic, sextic, octic, and decadic oscillator. Our results show that the absolute values of the Γ_n coefficients obtained from Eq. (28) are upper bounds to the absolute values of actual Γ_n (see also [12]). This result and the large-order formula (28) show that the renormalized strong-coupling expansion (13) converges for all $\tau\in[0,1)$, for all anharmonicities x^{2m} with $m\geqslant 2$, and for all states $K\geqslant 0$. Therefore the energy $E(\beta)$ can for all physically relevant $\beta\in[0,\infty)$ be computed via the *convergent* renormalized strong-coupling expansion (13).

It is remarkable that starting from the large-order behavior (16) of the divergent series (12) it is possible to derive the large-order behavior (28) of the convergent series (13). This can be understood as follows. The weak-coupling expansion $E_R(\kappa)=\Sigma_n c_n\kappa^n$ is expanded at the singular point $\kappa=0$ and, therefore, diverges for any $\kappa\in(0,1)$. From the physical point of view, this point is singular since the Hamiltonian $H_R=p^2+x^2+\kappa(x^4/3-x^2)$ does not have bound states for any $\kappa<0$ and the energy $E_R(\kappa)$ is not analytic at the point $\kappa=0$. In the strong-coupling case when $E_R(\kappa)=\Sigma_n\Gamma_n(1-\kappa)^n$, the Hamiltonian $H_R=p^2+x^4/3+(1-\kappa)(x^2-x^4/3)$ becomes for $1-\kappa<0$ the Hamiltonian of the double-well problem which has bound states and the energy $E_R(\kappa)$ can be, at the point $\kappa=1$, analytic. From this point of view, our derivation of Eq. (28) from Eq. (16) is nothing but transformation from the singular point $\kappa=0$ to the physically more reasonable point $\kappa=1$. We plan to publish a more detailed discussion in the future.

The large-order formula (28) has been derived from the formula for the coefficients b_n which is of semiclassical (JWKB) character. Therefore our formula (28) has the same semiclassical character. In addition, in Eq. (30) we consider the higher-order corrections [17].

The results of this paper can be applied also to more general oscillators such as, for example, to one-dimensional oscillators which have in addition to the x^2 and x^{2m} terms other even powers in the potential [7] as well as for isotropic multidimensional problems considered in [18].

Our results show that the renormalized strong-coupling expansion (13) is both from the physical and mathematical point of view the most advantageous perturbative approach to the anharmonic oscillators. Since the perturbation theory of anharmonic oscillators is important not only as model systems in quantum mechanics and quantum field theory but also in many applications [19], we believe that our results are of some interest.

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