Construction of the Strong Coupling Expansion for the Ground State Energy of the Quartic, Sextic, and Octic Anharmonic Oscillator via a Renormalized Strong Coupling Expansion

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A recently developed renormalized strong coupling expansion [E. J. Weniger, Ann. Phys. (N.Y.) **246**, 133 (1996)] is employed to compute the coefficients of the standard strong coupling expansion for the ground state energy of the quartic, sextic, and octic anharmonic oscillator. This approach is very simple, both conceptually and technically, and produces more accurate results than previously used techniques which were in most cases applied to the quartic case only. [S0031-9007(96)01319-1]

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Rayleigh-Schrödinger perturbation theory expresses an eigenvalue of a Hamiltonian $\hat{H}(\beta) = \hat{H}_0 + \beta\hat{V}$ as a formal power series in β. Frequently, such a series diverges for every $\beta \neq 0$ and has to be summed [1]. If β is small, this can often be accomplished, for instance, by Padé approximants or by the Borel method. Unfortunately, summation techniques for power series do not work if β is very large, because then the terms diverge individually. Thus, alternative summation methods for the troublesome strong coupling regime are needed.

The anharmonic oscillators, which are defined by the Hamiltonians

$$\hat{H}^{(m)}(\beta) = \hat{p}^2 + \hat{x}^2 + \beta\hat{x}^{2m}, \quad m = 2, 3, 4, \ldots, \tag{1}$$

are well suited to illustrate these problems. The weak coupling perturbation series

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

for the ground state energy eigenvalue $E^{(m)}(\beta)$ of the Hamiltonian (1) diverges quite strongly for every $\beta \neq 0$, since the coefficients $b_n^{(m)}$ grow essentially like $([m-1]n)!$ as $n \to \infty$ [2]. If β is small, this series can be summed by a variety of methods, but if β is large, a straightforward summation of this power series is not possible [3].

With the help of Symanzik scaling, the Hamiltonian (1) can be transformed into an equivalent Hamiltonian $\beta^{1/(m+1)}[\hat{p}^2 + \beta^{-2/(m+1)}\hat{x}^2 + \hat{x}^{2m}]$ [4]. Consequently, $E^{(m)}(\beta)$ possesses also the strong coupling expansion

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

which converges if β is sufficiently large [4].

Hence, the use of this expansion in the strong coupling regime is in principle very desirable. Unfortunately, the computation of the coefficients $K_n^{(m)}$ is very difficult, since the eigenvalues and eigenfunctions of the Hamiltonian $\hat{p}^2 + \hat{x}^{2m}$ are not known in closed form. Consequently, alternative techniques for the computation of the coefficients $K_n^{(m)}$ had to be developed [5–12]. In the quartic case ($m = 2$), the so far best results were obtained by Janke and Kleinert [12]. Very good results were also obtained by Guardiola *et al.* [10] who computed coefficients $K_n^{(m)}$ with $m = 2, 3, 4, 5$.

It is the purpose of this Letter to demonstrate that the coefficients $K_n^{(m)}$ can be computed via some remarkably simple intermediate steps directly from the coefficients $b_n^{(m)}$ of the weak coupling expansion (2). The starting point is a renormalization scheme introduced by Čížek and Vrscay [13] and worked out by Vinette and Čížek [14]. This renormalization scheme replaces $\beta \in [0, \infty)$ by a renormalized coupling constant $\kappa \in [0, 1)$ [14]:

$$\beta = \frac{1}{B_m} \frac{\kappa}{(1-\kappa)^{(m+1)/2}}, \qquad m = 2, 3, 4. \tag{4}$$

Here, $B_m = m(2m-1)!!/2^{m-1}$.

In this scheme, the Hamiltonian (1) is transformed into $(1-\kappa)^{-1/2}\{\hat{p}^2 + \hat{x}^2 + (\kappa/B_m)[\hat{x}^{2m} - B_m\hat{x}^2]\}$. Consequently, $E^{(m)}(\beta)$ can be expressed as follows [3]:

$$E^{(m)}(\beta) = (1-\kappa)^{-1/2} E_R^{(m)}(\kappa). \tag{5}$$

The renormalized ground state energy $E_R^{(m)}(\kappa)$ possesses the following weak coupling perturbation expansion [3]:

$$E_R^{(m)}(\kappa) = \sum_{n=0}^{\infty} c_n^{(m)} \kappa^n. \tag{6}$$

The coefficients $c_n^{(m)}$ can be computed via nonlinear difference equations [3]. However, they can also be computed from the coefficients $b_n^{(m)}$ in Eq. (2). In the weak coupling expansion (2), β is substituted according to Eq. (4), and the product $(1-\kappa)^{1/2}E^{(m)}(\beta)$ is expanded in powers of κ. Comparison with Eq. (6) yields

$$c_n^{(m)} = \sum_{\nu=0}^{n} \frac{([(m+1)\nu - 1]/2)_{n-\nu}}{(n-\nu)!} \frac{b_\nu^{(m)}}{[B_m]^\nu}. \tag{7}$$

Here, $([(m+1)\nu - 1]/2)_{n-\nu}$ is a Pochhammer symbol.

The renormalized perturbation expansion (6) diverges almost as strongly as the weak coupling expansion (2) and has to be summed [3,15,16]. Thus, its main advantage seems to be the bounded domain of κ. However, there are several advantages if $E^{(m)}(\beta)$ is computed via Eq. (5). For example, Eq. (4) implies that

$$\beta^{1/(m+1)} \sim (1 - \kappa)^{-1/2}, \qquad \beta \to \infty. \tag{8}$$

The prefactor $(1 - \kappa)^{-1/2}$ in Eq. (5) guarantees that the terms and partial sums of the renormalized perturbation series $E^{(m)}(\beta) = (1 - \kappa)^{-1/2} \sum_{n=0}^{\infty} c_n^{(m)} \kappa^n$ possess the correct asymptotic behavior as $\beta \to \infty$. This greatly facilitates summation even for small values of β [3,17,18].

Moreover, $E_R^{(m)}(\kappa)$ is finite at $\kappa = 1$ and can be computed by summing the renormalized perturbation series (6). In contrast, $E^{(m)}(\beta)$ diverges according to Eq. (3) like $\beta^{1/(m+1)}$ as $\beta \to \infty$. This has far-reaching consequences. For example, the infinite coupling limit $k_m = \lim_{\beta\to\infty} E^{(m)}(\beta)/\beta^{1/(m+1)}$, which is identical with the ground state eigenvalue of the Hamiltonian $\hat{p}^2 + \hat{x}^{2m}$ and with the leading term $K_0^{(m)}$ of the strong coupling expansion (3), cannot be computed by a straightforward summation of the weak coupling expansion (2). However, k_m can be computed comparatively easily by summing the renormalized perturbation expansion (6) [3,15,16].

It is even possible to compute higher derivatives of $E_R^{(m)}(\kappa)$ at $\kappa = 1$ via the renormalized perturbation expansion (6). Consequently, it makes sense to express $E_R^{(m)}(\kappa)$ by a Taylor expansion around $\kappa = 1$ [18]:

$$E_R^{(m)}(\kappa) = \sum_{n=0}^{\infty} \Gamma_n^{(m)} (1 - \kappa)^n. \tag{9}$$

The coefficients $\Gamma_n^{(m)}$ can be computed by summing the following divergent series [18]:

$$\Gamma_n^{(m)} = \frac{(-1)^n}{n!} \sum_{\nu=0}^{\infty} (\nu + 1)_n c_{n+\nu}^{(m)}. \tag{10}$$

Padé approximants are not powerful enough to sum this series effectively, in particular in the sextic ($m = 3$) and octic ($m = 4$) case. Much better results were obtained with the help of the sequence transformation $\delta_k^{(n)}(\zeta, s_n)$ [Eq. (8.4-4) of Ref. [19]], which is able to sum effectively many strongly divergent quantum mechanical perturbation expansions [3,15–18,20] and divergent asymptotic series for special functions [19–21]. Further details on $\delta_k^{(n)}(\zeta, s_n)$ and related transformations can be found in Refs. [3,16–19], in Sec. 2.7 of the book by Brezinski and Redivo Zaglia [22], or in an article by Roy, Bhattacharya, and Bhowmick [23].

In Ref. [3], the renormalized coefficients $c_n^{(2)}$ with $n \leq 200$, $c_n^{(3)}$ with $n \leq 165$, and $c_n^{(4)}$ with $n \leq 139$ were computed using the exact rational arithmetics of MAPLE. Using these coefficients, the strong coupling coefficients $\Gamma_n^{(2)}$ with $n \leq 20$, $\Gamma_n^{(3)}$ with $n \leq 9$, and $\Gamma_n^{(4)}$ with $n \leq 5$ could be computed by summing the divergent series (10) (Tables 2–4 of Ref. [18]).

It can be proven that $E_R^{(m)}(\kappa)$ is analytic at $\kappa = 1$ (Theorems 1 and 2 of Ref. [18]). Hence, the renormalized strong coupling expansion (9) converges in a neighborhood of $\kappa = 1$. Moreover, there is strong numerical evidence that this series converges also for $\kappa = 0$ and hence for all $\kappa \in [0, 1]$ (Tables 5, 7, and 8 of Ref. [18]). Thus, $E^{(m)}(\beta)$ can for all physically relevant $\beta \in [0, \infty)$ be computed by the convergent perturbation expansion

$$E^{(m)}(\beta) = (1 - \kappa)^{-1/2} \sum_{n=0}^{\infty} \Gamma_n^{(m)} (1 - \kappa)^n. \tag{11}$$

This perturbation expansion makes the computation of $E^{(m)}(\beta)$ almost trivial (Tables 6–8 of Ref. [18]). Its only disadvantage is that for a given β the corresponding renormalized coupling constant κ has to be computed by solving the nonlinear equation (4). Otherwise, it is even more convenient than the strong coupling expansion (3) which only converges if β is sufficiently large. With the help of the strong coupling expansion (11), effective characteristic polynomials and two-point Padé approximants for $E^{(m)}(\beta)$ could also be constructed [24].

From Eq. (4) we immediately obtain

$$\beta^{-2/(m+1)} = [B_m]^{2/(m+1)} (1 - \kappa) \kappa^{-2/(m+1)}. \tag{12}$$

Obviously, $\beta^{-2/(m+1)}$ can be expressed as a convergent power series in $1 - \kappa$, and the expansions (3) and (11) are closely related. The coefficients $K_n^{(m)}$ can be computed from the coefficients $\Gamma_n^{(m)}$ and vice versa. In the strong coupling expansion (3), β is substituted according to Eq. (4), and the product $(1 - \kappa)^{1/2} E^{(m)}(\beta)$ is expanded in powers of $1 - \kappa$. Comparison with Eq. (6) yields

$$\Gamma_n^{(m)} = \sum_{\nu=0}^{n} [B_m]^{(2\nu-1)/(m+1)} \times \frac{\big((2\nu - 1)/(m + 1)\big)_{n-\nu}}{(n - \nu)!} K_\nu^{(m)}. \tag{13}$$

Thus, the coefficients $\Gamma_n^{(m)}$ can be computed from the coefficients $K_n^{(m)}$. However, Eq. (13) can also be interpreted as a system of linear equations for the coefficients $K_n^{(m)}$. It can be solved recursively starting with $K_0^{(m)} = [B_m]^{1/(m+1)} \Gamma_0^{(m)}$, if the coefficients $\Gamma_n^{(m)}$ are known.

In Tables I and II coefficients $K_n^{(m)}$ of the strong coupling expansion (3) for the ground state energy of the quartic, sextic, and octic anharmonic oscillator are listed. They were computed via Eq. (13) from those coefficients $\Gamma_n^{(m)}$, which are listed in Tables 2–4 of Ref. [18]. The resulting system of linear equations was solved using MAPLE.

In the quartic case, very accurate results could be obtained. The coefficients $K_n^{(2)}$ in Table I are clearly more accurate than the coefficients in the second column of Table IV of Guardiola *et al.* [10]. The coefficients α_n in Table I of Janke and Kleinert [12], which satisfy $\alpha_n = K_n^{(2)}/2^{(2+2n)/3}$, differ at most in the last two digits from the more accurate coefficients in Table I. However, it is not easy to decide whether the summation method used in

TABLE I. Coefficients $K_n^{(2)}$ of the strong coupling expansion (3) for the ground state energy $E^{(2)}(\beta)$ of the quartic anharmonic oscillator, using the coefficients $c_n^{(2)}$ with $n \leq 200$ of the weak coupling expansion (2).

n	$K_n^{(2)}$
0	1.060 362 090 484 182 899 647 046 016 692 66
1	0.362 022 648 788 676 845 644 761 000 340 73
2	−0.034 510 262 723 209 116 511 854 989 055 10
3	0.005 195 302 710 909 514 585 377 423 303 57
4	−0.000 830 834 446 308 314 838 119 005 702 75
5	0.000 129 111 907 760 655 436 096 641 966 25
6	−0.000 018 489 463 440 751 674 937 410 100 91
7	0.000 002 263 664 760 568 938 396 637 753 15
8	−0.000 000 188 772 014 893 399 451 497 796 96
9	−0.000 000 006 523 871 072 063 258 083 651 65
10	0.000 000 007 775 509 229 188 590 256 438 81
11	−0.000 000 002 288 721 886 432 770 916 815 36
12	0.00 000 000 489 940 425 053 978 129 570 84
13	−0.000 000 000 084 084 607 518 223 513 605 1
14	0.000 000 000 011 018 331 561 071 908 96
15	−0.000 000 000 000 724 793 992 899 258 1
16	−0.000 000 000 000 152 212 178 068 284 7
17	0.000 000 000 000 078 626 634 169 299
18	−0.000 000 000 000 021 379 266 380
19	0.000 000 000 000 004 434 152 29
20	−0.000 000 000 000 000 728 030 3

TABLE III. Convergence of the partial sums of the strong coupling expansion (3) for the ground state energy $E^{(2)}(\beta)$ of the quartic anharmonic oscillator.

n	$\beta = 1/5$	$\beta = 1$
0	0.620 103 512	1.060 362 090 484 182 900
1	1.239 153 534	1.422 384 739 272 859 745
2	1.066 602 220	1.387 874 476 549 650 629
3	1.142 558 007	1.393 069 779 260 560 143
4	1.107 040 334	1.392 238 944 814 251 829
5	1.123 179 322	1.392 368 056 722 012 484
6	1.116 421 382	1.392 349 567 258 571 732
7	1.118 840 640	1.392 351 830 923 332 301
8	1.118 250 727	1.392 351 642 151 317 408
9	1.118 191 115	1.392 351 635 627 446 336
10	1.118 398 864	1.392 351 643 402 955 565
11	1.118 220 058	1.392 351 641 114 233 679
12	1.118 331 979	1.392 351 641 604 174 104
13	1.118 275 814	1.392 351 641 520 089 496
14	1.118 297 334	1.392 351 641 531 107 828
15	1.118 293 195	1.392 351 641 530 383 034
16	1.118 290 653	1.392 351 641 530 230 821
17	1.118 294 492	1.392 351 641 530 309 448
18	1.118 291 440	1.392 351 641 530 288 069
19	1.118 293 291	1.392 351 641 530 292 503
20	1.118 292 403	1.392 351 641 530 291 775
Exact	1.118 292 654	1.392 351 641 530 291 856

this Letter or the method of Janke and Kleinert [12] gives better results in the quartic case. Here, the coefficients $c_n^{(2)}$ with $n \leq 200$ were used, whereas Janke and Kleinert apparently used the coefficients $b_n^{(2)}$ with $n \leq 251$ [see the text following Eq. (19) of Ref. [12]].

Table III shows that the partial sums of the strong coupling expansion (3) converge for $m = 2$ remarkably rapidly for coupling constants as small as $\beta = 1$.

The infinite series (10) for $\Gamma_n^{(m)}$ diverges much more strongly in the sextic and octic than in the quartic case. Moreover, fewer coefficients $c_n^{(m)}$ were available in sextic and octic than in the quartic case. Thus, the coefficients $K_n^{(3)}$ and $K_n^{(4)}$ in Table II are slightly more accurate than the coefficients in the third and fourth columns of Table IV of Guardiola *et al.* [10], but not nearly as accurate as the coefficients $K_n^{(2)}$ in Table I.

Nevertheless, the coefficients $K_n^{(3)}$ and $K_n^{(4)}$ in Table II are by no means useless. In Tables IV and V it is shown that the partial sums of the strong coupling expansion (3) provide in the sextic and octic case remarkably accurate approximations to the ground state energy.

Thus, the coefficients $K_n^{(m)}$ of the strong coupling expansion (3) can be computed directly from the coefficients $b_n^{(m)}$ of the weak coupling expansion (2). In the first step, the coefficients $c_n^{(m)}$ of the renormalized weak coupling

TABLE II. Coefficients $K_n^{(3)}$ and $K_n^{(4)}$ of the strong coupling expansion (3) for the ground state energies $E^{(3)}(\beta)$ and $E^{(4)}(\beta)$ of the sextic and octic anharmonic oscillator, using the coefficients $c_n^{(3)}$ with $n \leq 165$ and $c_n^{(4)}$ with $n \leq 139$, respectively, of the weak coupling expansion (2).

n	$K_n^{(3)}$	$K_n^{(4)}$
0	1.144 802 453 80	1.225 814 6
1	0.307 920 303 73	0.277 124 5
2	−0.018 541 664 32	−0.012 634 6
3	0.001 559 742 20	0.000 751 0
4	−0.000 123 901 17	−0.000 038 7
5	0.000 007 971 95	0.000 001 3
6	−0.000 000 267 67	
7	−0.000 000 025 12	
8	0.000 000 006 3	
9	−0.000 000 001	

TABLE IV. Convergence of the partial sums of the strong coupling expansion (3) for the ground state energy $E^{(3)}(\beta)$ of the sextic anharmonic oscillator.

n	$\beta = 1/5$	$\beta = 1$	$\beta = 4$
0	0.765 575 542	1.144 802 454	1.618 995 156
1	1.226 023 793	1.452 722 758	1.836 727 691
2	1.164 026 002	1.434 181 093	1.830 172 223
3	1.175 687 795	1.435 740 835	1.830 447 948
4	1.173 616 352	1.435 616 934	1.830 436 998
5	1.173 914 373	1.435 624 906	1.830 437 350
6	1.173 891 998	1.435 624 639	1.830 437 343
7	1.173 887 302	1.435 624 613	1.830 437 343
8	1.173 889 936	1.435 624 620	1.830 437 343
9	1.173 889 001	1.435 624 619	1.830 437 343
Exact	1.173 889 345	1.435 624 619	1.830 437 344

TABLE V. Convergence of the partial sums of the strong coupling expansion (3) for the ground state energy $E^{(4)}(\beta)$ of the octic anharmonic oscillator.

n	$\beta = 1/5$	$\beta = 1$	$\beta = 4$
0	0.888 44	1.225 81	1.617 47
1	1.270 80	1.502 94	1.827 49
2	1.237 62	1.490 30	1.821 99
3	1.241 37	1.491 06	1.822 19
4	1.241 00	1.491 02	1.822 18
5	1.241 03	1.491 02	1.822 18
Exact	1.241 03	1.491 02	1.822 18

expansion (6) are computed via Eq. (7), which is simple. In the second and most demanding step, the coefficients $\Gamma_n^{(m)}$ of the renormalized strong coupling expansion (9) are computed by summing the divergent series (10) [18]. The final step—the computation of the coefficients $K_n^{(m)}$ via Eq. (13)—is again very simple.

Conceptually, the most important aspect of the renormalization scheme of Vinette and Čížek [14] is that the ground state energy $E^{(m)}(\beta)$ of an anharmonic oscillator is partitioned into $(1 - \kappa)^{-1/2}$, which diverges like $\beta^{1/(m+1)}$ as $\beta \rightarrow \infty$, and the renormalized energy $E_R^{(m)}(\kappa)$, which is analytic at $\kappa = 1$ (Theorems 1 and 2 of Ref. [18]). The analyticity of $E_R^{(m)}(\kappa)$ is the basis of all subsequent manipulations. The renormalized strong coupling expansion (9) is nothing but the Taylor expansion of $E_R^{(m)}(\kappa)$ around $\kappa = 1$, and the defining divergent series (10) for the renormalized strong coupling coefficients $\Gamma_n^{(m)}$ can be derived by doing a Taylor expansion of the weak coupling expansion (6) at $\kappa = 1$ [18].

The results of this Letter show once more that the direct approach to solve a problem need not be the most efficient one. Moreover, it should be worth while investigating whether the indirect approach described here, which is based on the transformation of the Hamiltonian (1) into an equivalent Hamiltonian having advantageous properties in the troublesome strong coupling regime, could also be used profitably in the case of other divergent quantum mechanical perturbation expansions.

Finally, it should be mentioned that numerical techniques, which permit a direct calculation of the coefficients $\Gamma_n^{(m)}$ of the renormalized strong coupling expansion (9) even for large indices n, were recently developed by L. Skála and J. Čížek. A manuscript is in preparation.

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