



ELSEVIER

19 October 1995

PHYSICS LETTERS B

Physics Letters B 360 (1995) 65–70

Variational resummation of divergent series with known large-order behavior

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Received 19 July 1995; revised manuscript received 26 August 1995

Editor: P.V. Landshoff

Abstract

Recently-developed variational perturbation expansions converge exponentially fast for positive coupling constants. They do not, however, possess the proper left-hand cut in the complex coupling constant plane, implying a wrong large-order behavior of their Taylor expansion coefficients. We correct this deficiency and present a method for resumming divergent series in which the leading large-order behavior is incorporated. For a given set of expansion coefficients, knowledge of the large-order behavior considerably improves the quality of the approximation.

PACS: 03.20.+i; 04.20.Fy; 02.40.+m

1. There exist various resummation procedures which turn divergent perturbation expansions for quantum mechanical energy eigenvalues into convergent approximation schemes [1]. These procedures involve some variational rescaling parameter to be optimized at each order of the expansion. The order-dependent rescaling reduces the factorial growth of the expansion coefficients to an algebraic growth sufficient for convergence. The convergence was initially observed empirically, and proved rigorously for finite coupling strengths and temperatures [2].

Independently of this development, Feynman and the author [3] proposed a variational approximation to path integrals at any temperature on the basis of a quasiharmonic local trial path integral. This approximation contains an arbitrary frequency *function* to be optimized at the end, leading to very accurate results

for partition functions, magnetization curves, and particle distributions [4]. In the past years, this approximation was systematically extended to a fast convergent *variational perturbation theory* for path integrals [5,4]. In this theory, the convergence of the approximants to the partition function is at any T better than at $T = 0$, where only the ground state energy is involved. At this point the convergence properties of the two approaches turned out to coincide.

Recently, the variational perturbation theory of path integrals was also extended to amplitudes with an unstable potential [7–9]. One distinguishes *sliding* and a *tunneling regimes*. The first is accessible by the above rescaling manipulations of the perturbation expansions, the second requires an additional calculation of classical tunneling solutions. Also here the result is improved beyond the semiclassical limit by a subsequent optimization of a trial frequency. Related to this is an approximation developed for quantum parti-

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tion functions of potentials with level splitting due to tunneling [10] (non-Borel summable systems).

In the quantum mechanical systems where variational perturbation expansions were carried to high orders, the approximations turned out to converge *uniformly* in the coupling strength [4]. This has made it possible to take the formalism directly to the limit of infinite coupling strength and find a simple direct approximation scheme for the expansion coefficients of strong-coupling series [11,12]. It was found that even in this limit, the approximations converge exponentially fast, with interesting superimposed oscillations, a result unforeseen by the theoretical work in Refs. [2]. This oscillatory behavior was explained only recently [13]; the convergence was proved rigorously in [14].

Making use of the pleasant properties of the reexpansions in the strong-coupling limit, a convergent approximation scheme was set up for functions with a known limited number of weak- and strong-coupling expansion coefficients [15]. This scheme should prove useful in studying phase transitions in models of statistical mechanics, for which one often knows many terms of their high- and low-temperature expansions (see, for example, the textbook [16] and the references therein).

The purpose of this note is to address another important resummation problem which arises in the field theory of critical phenomena. For a ϕ^4 field theory near zero mass, one possesses divergent series for critical exponents, with maximally 5 or 6 expansion coefficients in $4 - \epsilon$ [17] or three dimensions [18], respectively. To extract from these accurate results, additional information is needed. This is provided by the large-order behavior of the expansions which is available from semiclassical tunneling theory [4,19]. There exist well-developed and sophisticated methods for combining power series with large-order information via Borel-Padé-Leroy and analytic mapping techniques [20,21,19]. In this note we present an alternative method which combines the exponentially-fast convergence of variational perturbation theory with the information on the large-order behavior, thus laying the grounds for a further efficient resummation of perturbative expressions in the quantum field theory of critical phenomena.

The method is completely general and holds for any physical system whose quantities, for instance energy eigenvalues E , possess divergent power series expan-

sions of the type $E(g) = \omega^p \sum E_n \times (g/\omega^q)^n$, with coefficients behaving for large orders like

$$E_k = \gamma s k^\beta (-a)^k \Gamma(sk + \beta + 1) \times \left[1 + \frac{c_1}{sk + \beta} + \frac{c_2}{(sk + \beta)(sk + \beta - 1)} + \dots \right], \quad (1)$$

where s is some parameter. A behavior of the type (1) arises from a cut in the complex coupling constant plane, across which $E(g)$ has a discontinuity

$$\text{disc } E(-|g|) \equiv E(-|g| - i\eta) - E(-|g| + i\eta) = 2i \text{Im } E(-|g| - i\eta) \quad (2)$$

$$= 2\pi i \gamma \omega^p (a|g'|)^{-(\beta+1)/s} e^{-1/(a|g'|)^s} \times [1 + c_1(a|g'|)^{1/s} + c_2(a|g'|)^{2/s} + \dots]. \quad (3)$$

Here a frequency scale ω is introduced so that $g' = g/\omega^q$ becomes a dimensionless coupling constant.

A typical example is the ground state energy $E(g)$ of the anharmonic oscillator which has $p = 1$, $q = 3$, $s = 1$ and a large-order behavior

$$E_k = -\frac{\omega}{\pi} \sqrt{\frac{6}{\pi}} (-3/\omega^3)^k \Gamma(k + 1/2) \times [1 - 95/72k + \dots], \quad (4)$$

corresponding to a discontinuity [22]

$$2i \text{Im } E(-|g| - i\eta) = -2i\omega \sqrt{\frac{6}{\pi}} \sqrt{\frac{\omega^3}{3|g|}} e^{-\omega^3/3|g|} \times [1 - (95/72)(3|g|/\omega^3) + \dots]. \quad (5)$$

We shall explain the method for this particular example and illustrate how the information on the large-order behavior accelerates the convergence of variational perturbation expansions.

2. Following the procedure explained in [4], we take the weak coupling expansion of order N ,

$$E_N = \omega^p \sum_{n=0}^N E_n \left(\frac{g}{\omega^q} \right)^n, \quad (6)$$

replace ω by the identical expression involving an arbitrary trial frequency Ω ,

$$\omega \rightarrow \sqrt{\Omega^2 + \omega^2 - \Omega^2}, \quad (7)$$

and reexpand E_N^w in powers of g treating $\omega^2 - \Omega^2$ as a quantity of order g . The reexpanded series is truncating after the order $n > N$. The resulting expansion has the form

$$W_N(g, \Omega) = \Omega^p \sum_{n=1}^N a_n f_n(\Omega) \left(\frac{g}{\Omega^q}\right)^n, \quad (8)$$

with

$$f_n(\Omega) = \sum_{j=0}^{N-n} \binom{(p-qn)/2}{j} (-)^j \left(1 - \frac{\omega^2}{\Omega^2}\right)^j. \quad (9)$$

Forming the first and second derivatives of $W_N(g, \Omega)$ with respect to Ω , we find the positions of the extrema. The one with the smallest curvature is denoted by Ω_N . If there are no extrema, the smoothest turning point defines the optimal trial frequency Ω_N . The resulting $W_N(g) \equiv W_N(g, \Omega_N)$ constitutes the desired approximation to the energy.

3. The perturbation expansion of the anharmonic oscillator looks like (6) with $E_n = 1/2, 3/4, -21/8, 333/16, -30885/128, 916731/256 \dots$. The lowest-order approximation to the energy reads

$$W_1(g, \Omega) = \left(\frac{\Omega}{2} + \frac{1}{2\Omega}\right) E_0 + E_1 \frac{g}{\Omega^2}. \quad (10)$$

Extremizing this yields

$$\Omega_1 = \begin{cases} \frac{2}{\sqrt{3}} \omega \cosh \left[\frac{1}{3} \operatorname{arccosh}(g/g_1) \right] & \text{for } g > g_1, \\ \frac{2}{\sqrt{3}} \omega \cos \left[\frac{1}{3} \arccos(g/g_1) \right] & \text{for } g < g_1, \end{cases} \quad (11)$$

with $g_1 \equiv 2\omega^3 E_0 / 3\sqrt{3} E_1$. The result is shown in Fig. 1, where the approximation is seen to have a maximal error of 2% for large couplings.

For sufficiently negative couplings $g < 0$, the imaginary part of the energy is reproduced with the same type of error, as shown in Fig. 2. This is the *sliding regime* discussed in Ref. [7]. In the *tunneling regime* $g \lesssim 0$, however, the approximation $W_1(g)$ has an important qualitative deficiency: In contradiction to the semiclassical expression (5), it does not have any imaginary part in the interval $g \in (-g_1, 0)$ where $g_1 \approx 0.2566$.

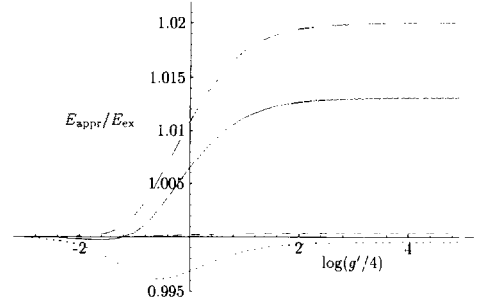


Fig. 1. Plot of the ratio of the resummed ground-state energy of the anharmonic oscillator $\bar{W}'_1(g)$ (solid curve) with respect to the exact energy $E_{ex}(g)$ as a function of the dimensionless coupling constant $g' = g/\omega^3$ for the anharmonic oscillator. The dashed curve shows the old approximation $W_1(g)$. The short-dashed curve indicates the approximation $W_3(g)$. The dotted curve indicates the approximation derived in Ref. [15] making use of the known strong-coupling behavior (which is not done here).

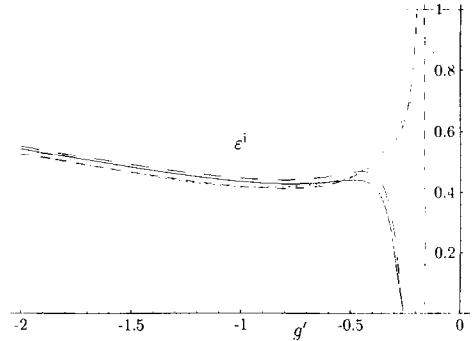


Fig. 2. The reduced approximate imaginary part $\operatorname{Im} \bar{W}'_1(g)$ (solid curve) of the ground-state energy in comparison with the exact one (dotted). The curve vanishes for $g \in (-0.26459, 0)$, where it is replaced by the semiclassical imaginary part. The dashed curve shows the approximation $\operatorname{Im} W_1(g)$. The short-dashed curve indicates the approximation $\operatorname{Im} W_3(g)$.

By going on to the approximation $W_3(g)$, the energy at positive g is found correctly to within 0.05% (see Figs. 1 and 3). The same is true for the imaginary part at sufficiently negative g (see Figs. 2, 4, and 5). Again, however, the imaginary part at $g \lesssim 0$ is being missed, although the interval is now smaller: $g \in (-g_3, 0)$ with $g_3 \approx 0.16$

4. Let us now extend the variational perturbation expansion by the information on the imaginary part (5) derived from tunneling theory for $g \lesssim 0$. First we consider the approximation $W_1(g)$ where the missing

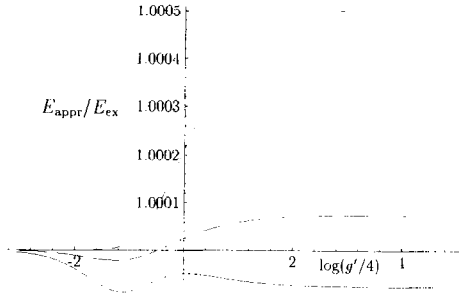


Fig. 3. The ratio of the approximation $\bar{W}'_3(g)$ to the ground-state energy of the anharmonic oscillator with respect to the exact ground-state energy $E_{\text{ex}}(g)$ of the anharmonic oscillator (solid curve). The short-dashed curve shows the old approximation $W_3(g)$, the long-dashed curve the approximation obtained for $g_3 = 0.16$ rather than the proper value $g_3 = 0.166$.

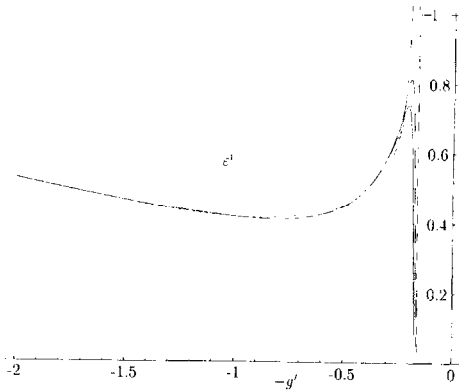


Fig. 4. The imaginary part of the approximation $\bar{W}'_3(g)$ (solid curve) to the ground-state energy of the anharmonic oscillator. It vanishes for $g \in (-0.166, 0)$, where it is replaced by the semiclassical imaginary part. The dotted curve is the exact imaginary part. The dashed curve is obtained for $g_3 = 0.16$. The short-dashed curve shows the old approximation $W_3(g)$.

interval is $(-g_1, 0)$ with $g_1 = 4/9\sqrt{3} \approx 0.2566$. The dispersion relation for $E(g)$ reads (with one subtraction to ensure convergence and setting $\omega = 1$)

$$E(g) = \frac{\omega}{2} + 2\omega g \int_0^\infty \frac{d\lambda}{2\pi} \frac{1}{\lambda(\lambda + g)} \times \sqrt{\frac{6}{\pi}} \sqrt{\frac{\omega^3}{3\lambda}} e^{-\omega^3/3\lambda} \varepsilon^i(\lambda), \quad (12)$$

where $\varepsilon^i(g)$ is a reduced imaginary part starting out like $1 - (95/72)(3|g|) + \dots$. Its full behavior is shown

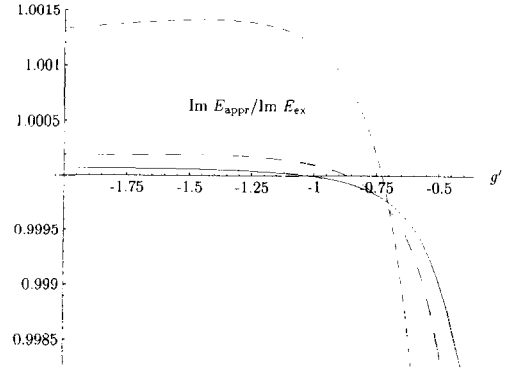


Fig. 5. Plot of the ratio of the approximate imaginary part $\text{Im } W'_3(g)$ of the ground-state energy of the anharmonic oscillator with respect to the exact $\text{Im } E_{\text{ex}}(g)$ as a function of $g' = g/\omega^3$ (solid curve). The dashed curve shows the old approximation $W_3(g)$, the short-dashed curve is obtained for $g_3 = 0.16$ rather than the proper value $g_3 = 0.166$.

in Fig. 2 (taken from [4]). By expanding $1/(\lambda + g)$ in a power series in g , we obtain the expansion coefficients as the moment integrals of the imaginary part as a function of $1/g$:

$$E_k = (-1)^{k-1} 2\omega \int_0^\infty \frac{dg}{2\pi} \frac{1}{g^{k+1}} \times \sqrt{\frac{6}{\pi}} \sqrt{\frac{\omega^3}{3g}} e^{-\omega^3/3g} \varepsilon^i(g). \quad (13)$$

We now assume only the knowledge of the leading semiclassical imaginary part (5), which corresponds to $\varepsilon^i(g) \equiv 1$. This is used to approximate the imaginary part in the entire regime where $W_1(g)$ is real for negative g , i.e., in the interval $g \in (-g_1, 0)$. There it contributes to the expansion coefficients

$$\Delta_{g_1}^{1.0} E_k = (-1)^{k-1} 2\omega \int_0^{g_1} \frac{dg}{2\pi} \frac{1}{g^{k+1}} \times \sqrt{\frac{6}{\pi}} \sqrt{\frac{\omega^3}{3g}} e^{-\omega^3/3g}. \quad (14)$$

These numbers are subtracted from the full expansion coefficients E_k forming E'_k . For the new coefficients E'_k , the imaginary part of $W_1(g)$ starts out at another value of $g_1 \equiv 2\omega^3 E'_0/3\sqrt{3} E'_1$, for which we calculate from (14) new coeffi-

Table 1

Comparison between the exact perturbation coefficients, the semiclassical ones, and those from our variational approximation $\bar{W}'_1(g)$ and $\bar{W}'_3(g)$ by forming the moment integrals over the imaginary parts. An alternating sign $(-1)^{k-1}$ has been omitted and ω is set equal to 1

k	E_k	E_k^{sc}	$E_{k,1}^{disp}$	$E_{k,3}^{disp}$
1	0.75	1.16954520	0.75	0.75
2	2.625	5.26295341	2.505524433	2.625
3	20.8125	39.4722	19.6119	20.8308
4	241.289063	414.457581	236.904087	241.882
5	3580.98047	5595.17734	3763.97503	3605.37152
6	63982.8135	92320.4261	71620.4682	65010.3990
7	1329733.73	1800248.43	1551691.33	1371000.52
8	31448214.7	40505587.0	33031401.4	33031401.4
9	833541603	1032892468	992802856	892574746
10	24478940700	29437435332	28909365063	26655844721

coefficients E'_k , and so on. The iteration converges at $g_1 \approx 0.166$. For the associated coefficients $E'_k \approx 0.50117, 0.72905, -2.24059, 13.54295, -98.64571, \dots$, we now evaluate the variational perturbation expansion $W'_1(g)$. To this we add the energy associated with the coefficients (14), which is determined by the dispersion integral

$$\Delta_{g_1}^{1,0} E(g) = -2\omega \int_0^{g_1} \frac{d\lambda}{2\pi} \frac{1}{\lambda + g} \times \sqrt{\frac{6}{\pi}} \sqrt{\frac{\omega^3}{3\lambda}} e^{-\omega^3/3\lambda} e^{i(\lambda)}. \quad (15)$$

No subtraction is necessary. For positive g , the new approximation $\bar{W}'_1(g) \equiv W'_1(g) + \Delta_{g_1}^{1,0} E(g)$ is shown in Fig. 1. It is seen to be better roughly by about 30% than the previous approximation $W_1(g)$.

The important qualitative advantage of the approximation $\bar{W}'_1(g)$ is displayed in Fig. 2. Now the imaginary part starts out at $g = 0$, as it should, remains constant until $g = -g_1$, and is approximated by $\text{Im } W'_1(g)$ for $g < -g_1$. Inserting the entire imaginary part into the dispersion relation (13), we find the expansion coefficients shown in the third column of Table 1. They have the leading growth behavior of Eq. (4) and agree reasonably well with the exact expansion coefficients in the first column. They approach the exact coefficients from above, since the constant imaginary parts at $g \lesssim 0$ ignores the falloff in the true $e^i(g)$.

We now proceed to extend the approximation $W_3(g)$, which for $g > 0$ and sufficiently negative g was accurate to within 0.02%, but which failed to produce any imaginary part for $g \in (-g_3, 0)$ with $g_3 \approx -0.16$. For this g_3 we calculate $\Delta_{g_3}^{1,0} E_k$ from the dispersion relation (14), and form the subtracted expansion coefficients $E'_k = E_k - \Delta_{g_3}^{1,0} E_k$. For these, $W'_3(g)$ renders a new value of g_3 , etc., until the method converges at $g_3 \approx 0.166$. The resulting subtracted expansion coefficients are $E'_k \approx 0.5000477, 0.74871, -2.58993, 19.84402, -214.12062, \dots$. To the associated $W'_3(g)$ we add the contribution $\Delta_{g_3}^{1,0} E(g)$ from the dispersion integral (15), and obtain the final result $\bar{W}'_3(g)$. In Fig. 3 we see that for $g > 0$ the new approximation is better than the previous one $W_3(g)$ by roughly a factor 5. To judge the convergence of the iteration in g_3 , we also plot $W'_3(g)$ for the initial value $g_3 \approx 0.16$.

The important qualitative advantage of the new approximation is shown in Figs. 4 and 5. There is now an imaginary part for all negative g which ensures the correct leading large-order behavior of the new approximation (4). The cut in the interval $g \in (-0.166, 0)$ is approximated by leading term in the semiclassical expression (5).

Inserting the entire imaginary part into the dispersion relation (13), we find the expansion coefficients shown in the fourth column of Table 1. They have again the leading growth behavior of Eq. (4), and agree better with the true expansion coefficients than those obtained from the approximation $\bar{W}'_1(g)$.

In the special case of the anharmonic oscillator, the convergence could of course be accelerated by using our knowledge of the correction factor for the imaginary part in the brackets of Eq. (5). In fact, if only the slope is known, a variational treatment allows us to calculate very well the entire initial tunneling portion of the imaginary part [7] (see also [8]). In field theories, however, the slope is usually hard to find. Since we want to develop methods applicable to field theories we shall not make use of the slope information.

Remarkably, one may deduce phenomenologically an initial section of the imaginary part from an eyeball fit to the sliding branch in Fig. 4. This could obviously be quite accurate and used to improve the approximation procedure in the absence of slope information.

5. Since the new resummation method incorporates into the variational perturbation expansion the initial tunneling section of the left-hand cut, it correctly accounts for the leading large-order behavior of the expansion coefficients. This should prove useful in calculations of critical exponents in quantum field theory, where the tip of the cut is accessible by tunneling theory. It will be interesting to see whether the new resummation method will help improving upon the results of traditional resummation theory [20,21,19].

Certainly, any available knowledge of the strong-coupling behavior can be used to obtain better approximations with the help of the procedure developed in Ref. [15].

The present method can also be used to improve upon our earlier results [10] on the non-Borel summable double-well potential. The connections with the present problem is a consequence of the scaling relation

$$E(g, \omega) = \omega E(g/\omega^3, 1) \quad (16)$$

first noted by Symanzik, which links the double well with the anharmonic oscillator at imaginary coupling constant.

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