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Variational perturbation theory for summing divergent tunnelling amplitudes

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Abstract

We present a method for evaluating divergent series with factorially growing coefficients of *equal* sign. The method is based on an analytic continuation of variational perturbation theory from the regime of alternating signs. We demonstrate its power first by applying it to the exactly known partition function of the anharmonic oscillator in zero space–time dimensions (the simple integral). Then we consider the quantum-mechanical case of one space–time dimension and derive the imaginary part of the ground-state energy of the anharmonic oscillator for *all* negative values of the coupling constant g, including the non-analytic tunnelling regime at small $-g$. As a highlight of the theory we extract, from the divergent perturbation expansion, the action of the critical bubble and the contribution of the higher loop fluctuations around the bubble.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Most of the presently known resummation schemes [1, 2] rely on Borel summability. Typical perturbation series of quantum field theory possess factorially growing expansion coefficients with alternating or equal signs. If the signs are alternating and if the underlying functions are free of special difficulties like renormalons [3], there exist well-developed resummation techniques. For equal signs, these techniques fail. This happens for all tunnelling phenomena, where physical amplitudes have cuts whose imaginary parts have such divergent expansions. In this paper we show that these can be summed up by an analytic continuation of variational perturbation theory from the regime of opposite coupling constants where the signs of the expansions coefficients alternate.

In the path integral approach, tunnelling processes are dominated by non-perturbative contributions coming from nontrivial classical solutions called *critical bubbles* [4, 5] or *bounces* [6], and fluctuations around these. Our method will enable us to derive such nonperturbative contributions from perturbation expansions. It will work reliably only if amplitudes are not strongly influenced by extra singularities in the complex Borel plane such as those caused by renormalons.

Variational perturbation theory has a long history [7–10]. It is based on the introduction of a dummy variational parameter Ω on which the full perturbation expansion does not depend, while the truncated expansion does. An optimal Ω is selected by the principle of minimal sensitivity [11], requiring the quantity of interest to be stationary as a function of the variational parameter. The optimal Ω is usually taken from a zero of the derivative with respect to Ω. If the first derivative has no zero, a zero of the second derivative is chosen. For Borel-summable series, these zeros are always real, in contrast with statements in the literature [12–15], which have proposed the use of complex zeros. Complex zeros produce, in general, wrong results for Borel-summable series, as was recently shown in [16].

In this paper we show that there does exist a wide range of applications of complex zeros if one wants to resum divergent series whose coefficients have equal signs, which have so far remained intractable. These arise typically in tunnelling problems, and we shall see that variational perturbation theory provides us with an efficient method for evaluating these series, rendering their real and imaginary parts with any desirable accuracy, if only enough perturbation coefficients are available. An important problem which had to be solved is the specification of the proper choice of the optimal zero from the many possible candidates existing in higher orders. The series to be summed are associated with functions which have an essential singularity at the origin in the complex g-plane, which is the starting point of a left-hand cut. Near the tip of the cut, the imaginary part of the function approaches zero rapidly like $\exp(-\alpha/|g|)$ for $g \to 0-$. If the variational approximation is plotted against g with an enlargement factor $\exp(\alpha/|g|)$, oscillations become visible near $g = 0$. The choice of the optimal complex zeros of the derivative with respect to the variational parameter is fixed by the requirement of obtaining, in each order, the least oscillating imaginary part when approaching the tip of the cut. We may call this selection rule the *principle of minimal sensitivity and oscillations*.

In section 2, we will explain and test the new principle on the exactly known partition function $Z(g)$ of the anharmonic oscillator in zero space–time dimensions. In section 3, we apply the method to the critical-bubble regime of small $-g$ of the anharmonic oscillator and find the action of the critical bubble and the corrections caused by the fluctuations around it. In section 4 we present yet another method of calculating the properties of the critical-bubble regime. This method is restricted to quantum mechanical systems. Its results for the anharmonic oscillator give more evidence for the correctness of the general method of sections 2 and 3.

2. Test of resummation

The partition function $Z(g)$ of the anharmonic oscillator in zero space–time dimensions is

$$Z(g) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-x^2/2 - gx^4/4)\, \mathrm{d}x = \frac{\exp(1/8g)}{\sqrt{4\pi g}} K_{1/4}(1/8g), \qquad (2.1)$$

where $K_\nu(z)$ is the modified Bessel function. For small g, the function $Z(g)$ has a divergent Taylor series expansion, to be called *weak-coupling expansion*,

$$Z_{\mathrm{weak}}^{(L)}(g) = \sum_{l=0}^{L} a_l g^l \quad \text{with} \quad a_l = (-1)^l \frac{\Gamma(2l + 1/2)}{l!\sqrt{\pi}}. \qquad (2.2)$$

For $g < 0$, the expansion coefficients have equal signs which make resummation difficult. For large $|g|$ there exists a convergent *strong-coupling expansion*

$$Z_{\text{strong}}^{(L)}(g) = g^{-1/4} \sum_{l=0}^{L} b_l g^{-l/2} \quad \text{with} \quad b_l = (-1)^l \frac{\Gamma(l/2 + 1/4)}{2l!\sqrt{\pi}}. \tag{2.3}$$

As is obvious from the integral representation (2.1), $Z(g)$ obeys the second-order differential equation

$$16g^2 Z''(g) + 4(1 + 8g)Z'(g) + 3Z(g) = 0, \tag{2.4}$$

which has two independent solutions. One of them is $Z(g)$, which is finite for $g > 0$ with $Z(0) = a_0$. The weak-coupling coefficients a_l in (2.2) can be obtained by inserting the Taylor series into (2.4) and comparing coefficients. The result is the recursion relation

$$a_{l+1} = -\frac{16l(l + 1) + 3}{4(l + 1)} a_l. \tag{2.5}$$

A similar recursion relation can be derived for the strong-coupling coefficients b_l in equation (2.3). We observe that the two independent solutions $Z(g)$ of (2.4) behave like $Z(g) \propto g^\alpha$ for $g \to \infty$ with the powers $\alpha = -1/4$ and $-3/4$. The function (2.1) has $\alpha = -1/4$. It is convenient to remove the leading power from $Z(g)$ and define a function $\zeta(x)$ such that $Z(g) = g^{-1/4}\,\zeta(g^{-1/2})$. The Taylor coefficients of $\zeta(x)$ are the strong-coupling coefficients b_l in equation (2.3). The function $\zeta(x)$ satisfies the differential equation and initial conditions

$$4\zeta''(x) - 2x\zeta'(x) - \zeta(x) = 0 \quad \text{with} \quad \zeta(0) = b_0 \quad \text{and} \quad \zeta'(0) = b_1. \tag{2.6}$$

The Taylor coefficients b_l of $\zeta(x)$ satisfy the recursion relation

$$b_{l+2} = \frac{2l + 1}{4(l + 1)(l + 2)} b_l. \tag{2.7}$$

Analytic continuation of $Z(g)$ around $g = \infty$ to the left-hand cut gives:

$$Z(-g) = (-g)^{-1/4} \zeta((-g)^{-1/2}) \tag{2.8}$$

$$= (-g)^{-1/4} \sum_{l=0}^{\infty} b_l (-g)^{-l/2} \exp\left[-\frac{\mathrm{i}\pi}{4}(2l + 1)\right] \quad \text{for } g > 0, \tag{2.9}$$

so that we find an imaginary part

$$\operatorname{Im} Z(-g) = -(4g)^{-1/4} \sum_{l=0}^{\infty} b_l (-g)^{-l/2} \sin\left[-\frac{\mathrm{i}\pi}{4}(2l + 1)\right] \tag{2.10}$$

$$= -(4g)^{-1/4} \sum_{l=0}^{\infty} \beta_l (-g)^{-l/2}, \tag{2.11}$$

where

$$\beta_0 = b_0, \quad \beta_1 = b_1, \qquad \beta_{l+2} = -\frac{2l + 1}{4(l + 1)(l + 2)} \beta_l. \tag{2.12}$$

It is easy to show that

$$\sum_{l=0}^{\infty} \beta_l x^l = \zeta(x) \exp(-x^2/4), \tag{2.13}$$

so that

$$\mathrm{Im}\, Z(-g) = -\frac{1}{\sqrt{2}} g^{-1/4} \exp(-1/4g) \sum_{l=0}^{\infty} b_l g^{-l/2}. \tag{2.14}$$

From this we may re-obtain the weak-coupling coefficients a_l by means of the dispersion relation

$$Z(g) = -\frac{1}{\pi} \int_0^\infty \frac{\mathrm{Im}\, Z(-z)}{z+g}\, \mathrm{d}z \tag{2.15}$$

$$= \frac{1}{\pi\sqrt{2}} \sum_{j=0}^{\infty} b_j \int_0^\infty \frac{\exp(-1/4z) z^{-j/2-1/4}}{z+g}\, \mathrm{d}z. \tag{2.16}$$

Indeed, replacing $1/(z+g)$ by $\int_0^\infty \exp(-x(z+g))\, \mathrm{d}x$, and expanding $\exp(-xg)$ into a power series, all integrals can be evaluated to yield

$$Z(g) = \frac{1}{\pi} \sum_{j=0}^{\infty} 2^j b_j \sum_{l=0}^{\infty} (-g)^l \Gamma(l + j/2 + 1/4). \tag{2.17}$$

Thus, we find for the weak-coupling coefficients a_l an expansion in terms of the strong-coupling coefficients

$$a_l = \frac{(-1)^l}{\pi} \sum_{j=0}^{\infty} 2^j b_j \Gamma(l + j/2 + 1/4). \tag{2.18}$$

Inserting b_j from equation (2.3), this becomes

$$a_l = \frac{(-1)^l}{2\pi^{3/2}} \sum_{j=0}^{\infty} \frac{2^j(-1)^j}{j!} \Gamma(j/2 + 1/4)\Gamma(l + j/2 + 1/4) = (-1)^l \frac{\Gamma(2l + 1/2)}{l!\sqrt{\pi}}, \tag{2.19}$$

coinciding with (2.2).

Variational perturbation theory is a well-established method for obtaining convergent strong-coupling expansions from divergent weak-coupling expansions in quantum-mechanical systems such as the anharmonic oscillator [5, 17] as well as in quantum field theory [2, 18]. We have seen in equation (2.8) that the strong-coupling expansion can easily be continued analytically to negative g. This continuation can, however, be used for an evaluation only if $|g|$ is sufficiently large, where the strong-coupling expansion converges. In the tunnelling regime near the tip of the left-hand cut, the expansion diverges. In this paper we shall see that an evaluation of the weak-coupling expansion according to the rules of variational perturbation theory but with an accompanying analytic continuation into the complex plane gives extremely good results on the entire left-hand cut with a fast convergence even near the tip at $g = 0$.

The Lth variational approximation to $Z(g)$ is given by (see [2, 18])

$$Z_{\mathrm{var}}^{(L)}(g, \Omega) = \Omega^p \sum_{j=0}^{L} \left(\frac{g}{\Omega^q}\right)^j \epsilon_j(\sigma), \tag{2.20}$$

with

$$\sigma \equiv \Omega^{q-2}(\Omega^2 - 1)/g, \tag{2.21}$$

where $q = 2/\omega = 4$, $p = -1$ and

$$\epsilon_j(\sigma) = \sum_{l=0}^{j} a_l \binom{(p - lq)/2}{j - l} (-\sigma)^{j-l}. \tag{2.22}$$

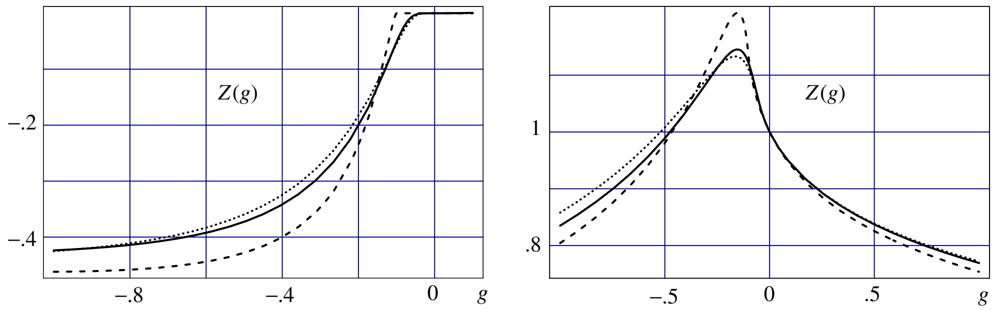

Figure 1. Result of the first- and second-order calculation for the region $g < 0$ where coefficients have equal signs and the function has a cut with non-vanishing imaginary part: imaginary (left) and real parts (right) of $Z_{\text{var}}^{(1)}(g)$ (– – –) and $Z_{\text{var}}^{(2)}(g)$ (——) are plotted against g and compared with the exact values of the partition function (· · · · · ·). The root of (2.21) giving the optimal variational parameter Ω has been chosen to reproduce the weak-coupling result near $g = 0$.

To apply the principle of minimal sensitivity, the zeros of the derivative of $Z_{\text{var}}^{(L)}(g, \Omega)$ with respect to Ω are needed. They are given by the zeros of the polynomials in σ:

$$P^{(L)}(\sigma) = \sum_{l=0}^{L} a_l(p - lq + 2l - 2L) \binom{(p - lq)/2}{L - l} (-\sigma)^{L-l} = 0, \tag{2.23}$$

since it can be shown[1] that the derivative depends only on σ:

$$\frac{\mathrm{d}Z_{\text{var}}^{(L)}(g, \Omega)}{\mathrm{d}\Omega} = \Omega^{p-1} \left(\frac{g}{\Omega^q}\right)^L P^{(L)}(\sigma). \tag{2.24}$$

Consider in more detail the lowest nontrivial order with $L = 1$. From equation (2.23) we obtain

$$\sigma = \tfrac{5}{2} \quad \text{corresponding to} \quad \Omega = \tfrac{1}{2}(1 \pm \sqrt{1 + 10g}). \tag{2.25}$$

To ensure that our method reproduces the weak-coupling result for small g, we have to take the positive sign in front of the square root. In figure 1 we have plotted $Z_{\text{var}}^{(1)}(g)$ (dashed curve) and $Z_{\text{var}}^{(2)}(g)$ (solid curve) and compared these with the exact result (dotted curve) in the tunnelling regime. The agreement is quite good even at these low orders[2]. Next we study the behaviour of $Z_{\text{var}}^{(L)}(g)$ to higher orders L. For selected coupling values along the left-hand cut, $g = -0.01, -0.1, -1, -10$, we will see the error as a function of the order. We will find from this model system the rule for selecting systematically the best zero of $P^{(L)}(\sigma)$ solving equation (2.23), which leads to the optimal value of the variational parameter Ω. For this purpose we plot the variational results of all zeros. This is shown in figure 2, where the logarithm of the deviations from the exact value is plotted against the order L. The outcome of different zeros cluster strongly near the best value. Therefore, choosing any zero out of the middle of the cluster is reasonable, in particular, because it does not depend on the knowledge of the exact solution, so that this rule may be taken over to realistic cases.

We wish to emphasize that for large negative coupling constants, say $g > 0$, variational perturbation theory has the usual fast convergence in this model. In fact, for $g = 10$, probing deeply into the strong-coupling domain, we find rapid convergence like $\Delta(L) \simeq 0.02 \exp(-0.73L)$ for $L \to \infty$, where $\Delta(L) = \log |Z_{\text{var}}^{(L)} - Z_{\text{exact}}|$ is the logarithmic error as a

[1] This was proved in [19] for $p/q = 1$ (see also [5], appendix 5A), but can easily be generalized to hold for arbitrary p and q.
[2] The low-order results were first obtained by Kleinert [20] and extended by Karrlein and Kleinert [21].

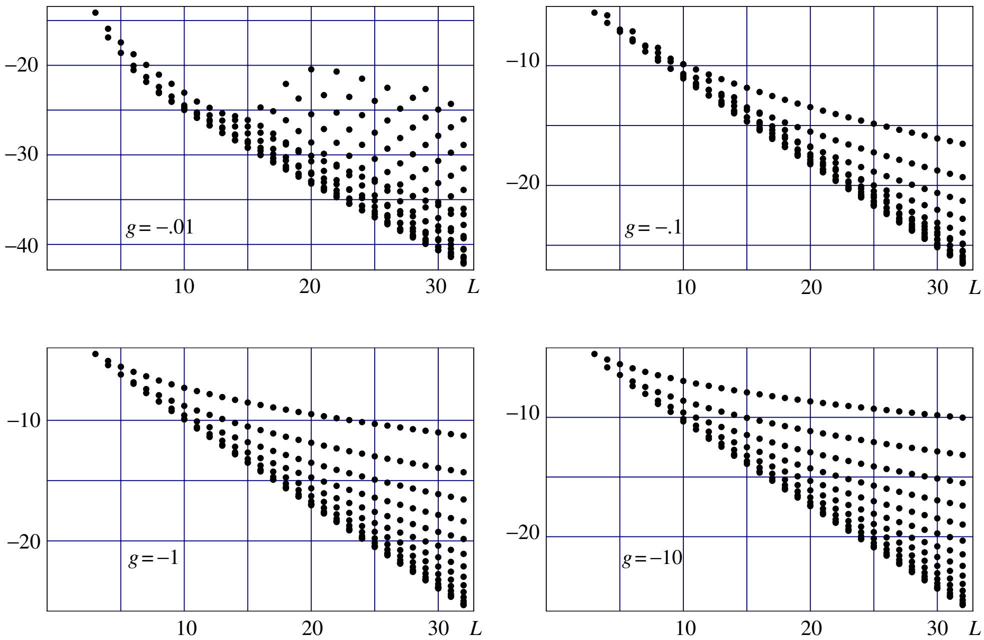

Figure 2. Logarithm of deviation of the variational results from exact values $\log|Z^{(L)}_{\rm var} - Z_{\rm exact}|$ plotted against the order L for different values of $g < 0$ along the left-hand cut. All complex optimal Ωs have been used.

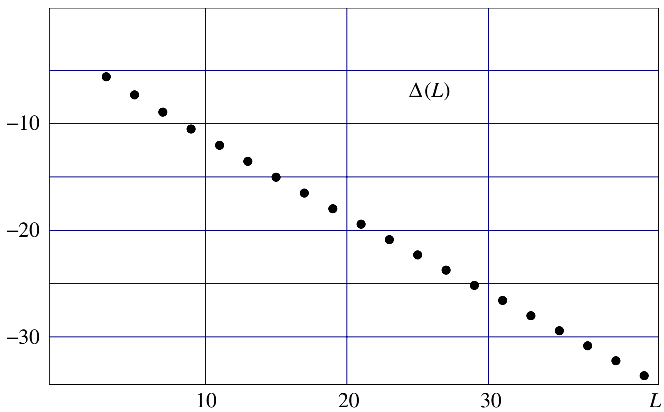

Figure 3. Logarithm of deviation of variational results from exactly known value $\Delta(L) = \log|Z^{(L)}_{\rm var} - Z_{\rm exact}|$, plotted against the order L for $g = 10$ in the regime of equal signs of the expansion coefficients. The real positive optimal Ω have been used. There is only one real zero of the first derivative in every odd order L and none for even orders. There is excellent convergence $\Delta(L) \simeq 0.02 \exp(-0.73L)$ for $L \to \infty$.

function of the order L. This is shown in figure 3. Furthermore, the strong-coupling coefficients b_l of equation (2.3) are reproduced quite satisfactorily. Having solved $P^{(L)}(\sigma) = 0$ for σ, we obtain $\Omega^{(L)}(g)$ by solving equation (2.21). Inserting this and (2.22) into (2.20), we bring $g^{1/4}\, Z^{(L)}_{\rm var}(g)$ into a form suitable for expansion in powers of $g^{-1/2}$. The expansion coefficients

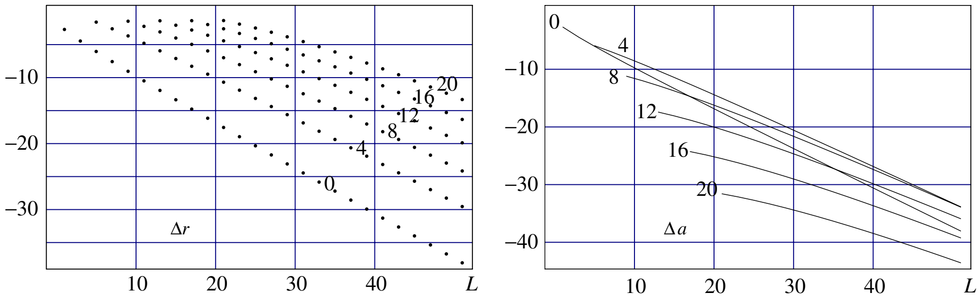

Figure 4. Relative logarithmic error $\Delta_r = \log|1 - b_l^{(L)}/b_l^{(\mathrm{exact})}|$ on the left, and the absolute logarithmic error $\Delta_a = \log|b_l^{(L)} - b_l^{(\mathrm{exact})}|$ on the right, plotted for some strong-coupling coefficients b_l with $l = 0, 4, 8, 12, 16, 20$ against the order L.

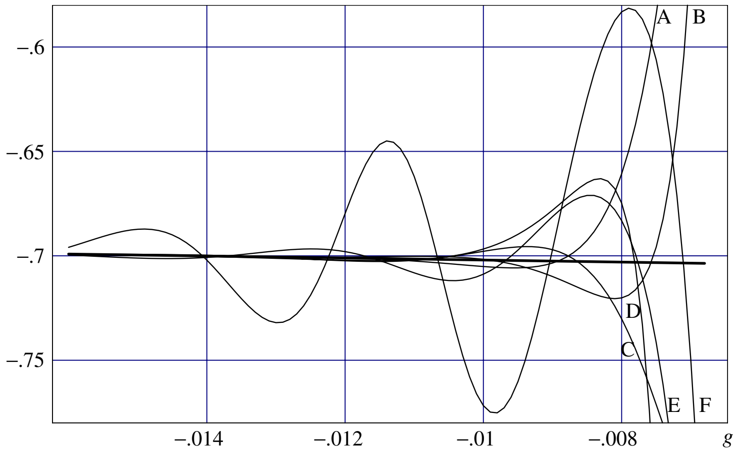

Figure 5. Normalized imaginary part $\mathrm{Im}[Z_{\mathrm{var}}^{(16)}(g)\exp(-1/4g)]$ as a function of g based on six different complex zeros (thin curves). The fat curve represents the exact value, which is $Z_{\mathrm{exact}}(g) \simeq -0.7071 + 0.524g - 1.78g^2$. Oscillations of varying strength can be observed near $g = 0$. Curves A and C carry most smoothly near up to the origin. Evaluation based on either of them yields equally good results. We have selected the zero belonging to curve C as our best choice to this order $L = 16$.

are the strong-coupling coefficients $b_l^{(L)}$ to order L. In figure 4 we have plotted the logarithms of their absolute and relative errors over the order L, and find very good convergence, showing that variational perturbation theory works well for our test-model $Z(g)$.

A better selection of the optimal Ω values comes from the following observation. The imaginary parts of the approximations near the singularity at $g = 0$ show tiny oscillations. The exact imaginary part is known to decrease extremely fast, like $\exp(1/4g)$, for $g \to 0-$, practically without oscillations. We can make the tiny oscillations more visible by taking this exponential factor out of the imaginary part. This is done in figure 5. The oscillations differ strongly for different choices of $\Omega^{(L)}$ from the central region of the cluster. To each order, L we see that one of them is smoothest in the sense that the approximation approaches the singularity most closely before oscillations begin. If this $\Omega^{(L)}$ is chosen as the optimal one, we obtain excellent results for the entire region of negative coupling constant. As an example, we pick the best zero for the order $L = 16$. Figure 5 shows the normalized imaginary part

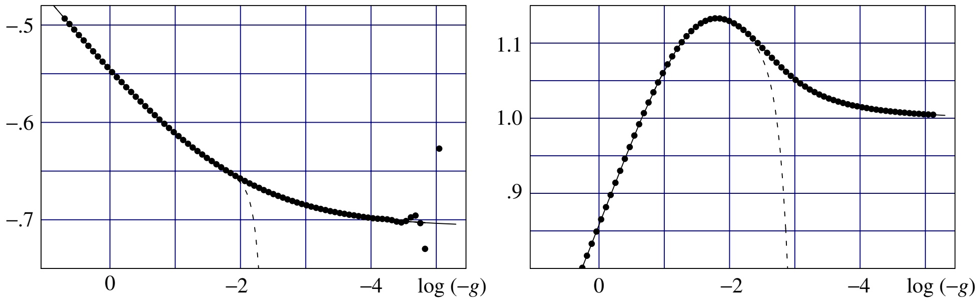

Figure 6. Normalized imaginary part $\mathrm{Im}[Z_{\mathrm{var}}^{(16)}(g)\exp(-1/4g)]$ to the left and the real part $\mathrm{Re}[Z_{\mathrm{var}}^{(16)}(g)]$ to the right, based on the best zero C from figure 5, are plotted against $\log|g|$ as dots. The solid curve represents the exact function. The dashed curve is the order $L = 16$ of the strong-coupling expansion $Z_{\mathrm{strong}}^{(L)}(g)$ of equation (2.3).

calculated to this order, but based on different zeros from the central cluster. Curve C appears optimal. Therefore, we select the underlying zero as our best choice at order $L = 16$ and calculate with it real and imaginary parts for the region $-2 < g < -0.008$, to be compared with the exact values. Both are shown in figure 6, where we have again renormalized the imaginary part by the exponential factor $\exp(-1/4g)$. The agreement with the exact result (solid curve) is excellent as was to be expected because of the fast convergence observed in figure 2. It is indeed much better than the strong-coupling expansion to the same order, shown as a dashed curve. This is the essential improvement of our present theory as compared with previously known methods probing into the tunnelling regime (see footnote 2).

This regime will now be investigated for the quantum-mechanical anharmonic oscillator.

3. Tunnelling regime of quantum-mechanical anharmonic oscillator

The divergent weak-coupling perturbation expansion for the ground-state energy of the anharmonic oscillator in the potential $V(x) = x^2/2 + gx^4$ to order L:

$$E_{0,\mathrm{weak}}^{(L)}(g) = \sum_{l=0}^{L} a_l g^l, \tag{3.1}$$

where $a_l = (1/2,\ 3/4,\ -21/8,\ 333/16,\ -30885/128, \ldots)$ cannot be summed by available methods for $g < 0$. It may be treated in the same way as $Z(g)$ of the previous model, making use as before of equations (2.20)–(2.23), provided we set $p = 1$ and $\omega = 2/3$, so that $q = 3$, accounting for the correct power behaviour $E_0(g) \propto g^{1/3}$ for $g \to \infty$. According to the principle of minimal dependence and oscillations, we pick a best zero for the order $L = 64$ from the cluster of zeros of $P_L(\sigma)$, and use it to calculate the logarithm of the normalized imaginary part:

$$f(g) := \log[\sqrt{-\pi g/2}\,E_{0,\mathrm{var}}^{(64)}(g)] - 1/3g. \tag{3.2}$$

This quantity is plotted in figure 7 against $\log(-g)$ close to the tip of the left-hand cut for $-0.2 < g < -0.006$. Comparing our result with older values from semi-classical calculations (see [22]; the first 10 coefficients of (3.3) are calculated)

$$f(g) = b_1 g - b_2 g^2 + b_3 g^3 - b_4 g^4 + \cdots, \tag{3.3}$$

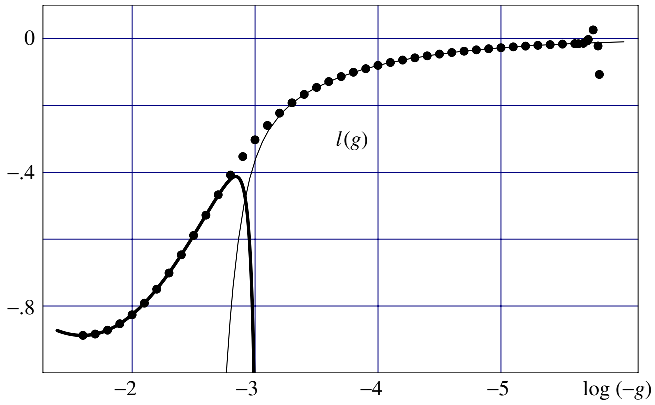

Figure 7. Logarithm of the imaginary part of the ground-state energy of the anharmonic oscillator with the essential singularity factored out for better visualization, $l(g) = \log[\sqrt{-\pi g/2}\, E^{(64)}_{0,\mathrm{var}}(g)] - 1/3g$, plotted against small negative values of the coupling constant $-0.2 < g < -0.006$, where the series is not summable by standard methods. The thin curve represents the divergent expansion around a critical bubble of Zinn-Justin [22]. The fat curve is the 22nd-order approximation of the strong-coupling expansion, analytically continued to negative g in the sliding regime calculated in chapter 17 of the textbook [5].

with

$$b_1 = 3.95833, \qquad b_2 = 19.344, \qquad b_3 = 174.21, \qquad b_4 = 2177, \tag{3.4}$$

shown in figure 7 as a thin curve, we find very good agreement. This expansion contains the information on the fluctuations around the critical bubble. It is divergent and not summable for $g < 0$ by standard methods. In appendix A we have re-derived it in a novel way which allowed us to extend and improve it considerably.

Remarkably, our theory allows us to retrieve the first three terms of this expansion from the perturbation expansion. Since our result provides us with a regular approximation to the essential singularity, the fitting procedure depends somewhat on the interval over which we fit our curve by a power series. A compromise between a sufficiently long interval and the runaway of the divergent critical-bubble expansion is obtained for a lower limit $g > -0.0229 \pm 0.0003$ and an upper limit $g = -0.006$. Fitting a polynomial to the data, we extract the following first three coefficients:

$$b_1 = 3.9586 \pm 0.0003, \qquad b_2 = 19.4 \pm 0.12, \qquad b_3 = 135 \pm 18. \tag{3.5}$$

The agreement of these numbers with those in (3.3) demonstrates that our method is capable of probing deeply into the critical-bubble region of the coupling constant.

Further evidence for the quality of our theory comes from a comparison with the analytically continued strong-coupling result plotted to order $L = 22$ as a fat curve in figure 7. This expansion was derived by a resummation procedure developed in chapter 17 of the textbook [5]. It was based on a two-step process: the derivation of a strong-coupling expansion of the type (2.3) from the divergent weak-coupling expansion, and an analytic continuation of the strong-coupling expansion to negative g. This method was applicable only for large enough coupling strength where the strong-coupling expansion converges, the so-called *sliding regime*. It could not invade into the tunnelling regime at small g governed by critical bubbles, which was treated in [5] by a separate variational procedure. The present work fills the missing gap by extending variational perturbation theory to *all* g arbitrarily close to zero, without the need for a separate treatment of the tunnelling regime.

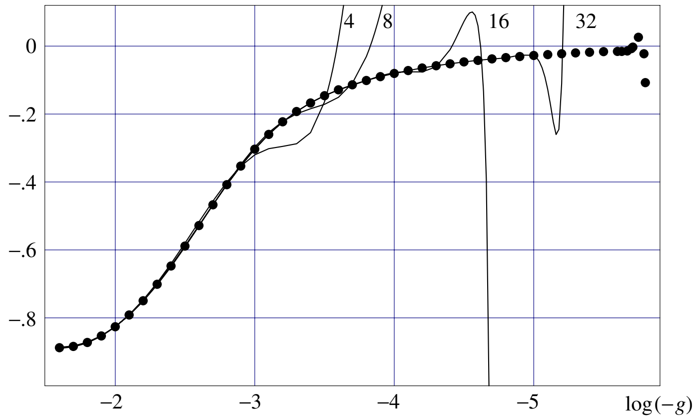

Figure 8. Logarithm of the normalized imaginary part of the ground-state energy $\log(\sqrt{-\pi g/2}\, E^{(L)}_{0,\mathrm{var}}(g)) - 1/3g$, plotted against $\log(-g)$ for orders $L = 4,\ 8,\ 16,\ 32$ (curves). It is compared with the corresponding results for $L = 64$ (points). This is shown for small negative values of the coupling constant $-0.2 < g < -0.006$, i.e. in the critical-bubble region. Fast convergence is easily recognized; lower orders oscillate more heavily. Increasing orders allow closer approach to the singularity at $g = 0-$.

It is interesting to see how the correct limit is approached as the order L increases. This is shown in figure 8, based on the optimal zero in each order. For large negative g, even the small orders give excellent results. Close to the singularity the scaling factor $\exp(-1/3g)$ will always win over the perturbation results. It is surprising, however, how fantastically close to the singularity we can go.

4. Dynamic approach to the critical-bubble regime

Regarding the computational challenges connected with the critical-bubble regime of small $g < 0$, it is worth developing an independent method to calculate imaginary parts in the tunnelling regime. For a quantum-mechanical system with an interaction potential $gV(x)$, such as the harmonic oscillator, we may study the effect of an infinitesimal increase in g upon the system. It induces an infinitesimal unitary transformation of the Hilbert space. The new Hilbert space can be made the starting point for the next infinitesimal increase in g. In this way, we derive an infinite set of first-order ordinary differential equations for the change of the energy levels and matrix elements (see appendix B for details):

$$E_n'(g) = V_{nn}(g), \tag{4.1}$$

$$V_{mn}'(g) = \sum_{k\neq n} \frac{V_{mk}(g)V_{kn}(g)}{E_m(g) - E_k(g)} + \sum_{k\neq m} \frac{V_{mk}(g)V_{kn}(g)}{E_n(g) - E_k(g)}. \tag{4.2}$$

This system of equations holds for any one-dimensional Schrödinger problem. Individual differences come from the initial conditions, which are the energy levels $E_n(0)$ of the unperturbed system and the matrix elements $V_{nm}(0)$ of the interaction $V(x)$ in the unperturbed basis. A truncation is necessary for a numerical integration of the system. The obvious way is to restrict the Hilbert space to the manifold spanned by the lowest N eigenvectors of the unperturbed system. For cases like the anharmonic oscillator, which are even, with even

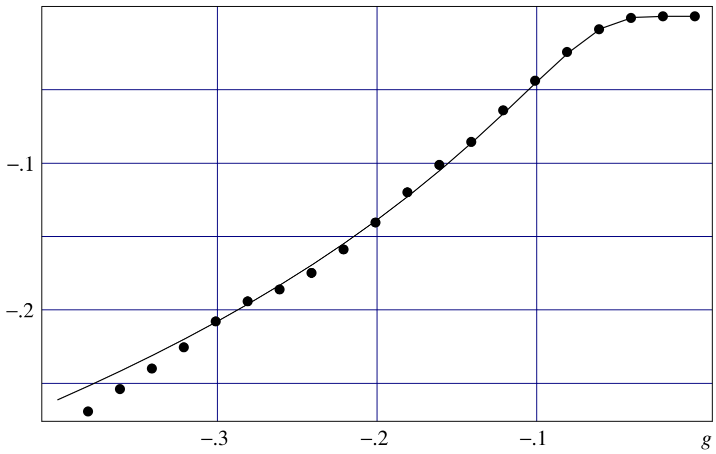

Figure 9. Imaginary part of the ground-state energy of the anharmonic oscillator as solution of the coupled set of differential equations (4.1), truncated at the energy level of $n = 64$ (points), compared with the corresponding quantity from the order $L = 64$ of variational perturbation theory (curve), both shown as functions of the coupling constant g.

perturbation and with only an even state to be investigated, we may span the Hilbert space by even basis vectors only. Our initial conditions are thus for $n = 0,\ 1,\ 2, \ldots, N/2$:

$$E_{2n}(0) = 2n + 1/2, \tag{4.3}$$

$$V_{2n,2m} = 0 \qquad \text{if } m < 0 \text{ or } m > N/2, \tag{4.4}$$

$$V_{2n,2n}(0) = 3(8n^2 + 4n + 1)/4, \tag{4.5}$$

$$V_{2n,2n\pm 2}(0) = (4n + 3)\sqrt{(2n + 1)(2n + 2)}/2, \tag{4.6}$$

$$V_{2n,2n\pm 4}(0) = \sqrt{(2n + 1)(2n + 2)(2n + 3)(2n + 4)}/4. \tag{4.7}$$

For the anharmonic oscillator with a $V(x) = x^4$ potential, all sums in equation (4.1) are finite with at most four terms due to the near-diagonal structure of the perturbation.

To find a solution for some $g < 0$, we first integrate the system from 0 to $|g|$, then around a semi-circle $g = |g| \exp(\mathrm{i}\varphi)$ from $\varphi = 0$ to π. The imaginary part of $E_0(g)$ obtained from a calculation with $N = 64$ is shown in figure 9, where it is compared with the variational result for $L = 64$. The agreement is excellent. It must be noted, however, that the necessary truncation of the system of differential equations introduces an error, which cannot be made arbitrarily small by increasing the truncation limit N. The approximations are asymptotic sharing this property with the original weak-coupling series. Its divergence is, however, reduced considerably, which is the reason why we obtain accurate results for the critical-bubble regime, where the weak-coupling series fails completely to reproduce the imaginary part.

Appendix A

We determine the ground-state energy function $E_0(g)$ for the anharmonic oscillator on the cut, i.e. for $g < 0$ in the bubble region, from the weak-coupling coefficients a_l of equation (3.1).

The behaviour of the a_l for large l can be cast into the form

$$a_l/a_{l-1} = -\sum_{j=-1}^{L} \beta_j l^{-j}. \tag{A.1}$$

The β_j can be determined by a high-precision fit to the data in the large l region of $250 < l < 300$ to be

$$\begin{aligned}\beta_{-1,0,1,\ldots} = \Bigg\{ & 3, -\frac{3}{2}, \frac{95}{24}, \frac{113}{6}, \frac{391691}{3456}, \frac{40783}{48}, \frac{1915121357}{248832}, \frac{10158832895}{124416}, \\ & \frac{70884236139235}{71663616}, \frac{60128283463321}{4478976}, \frac{286443690892}{1423}, \frac{144343264152266}{43743}, \\ & \frac{351954117229}{6}, \frac{2627843837757582}{2339}, \frac{230619387597863}{10}, \\ & \frac{12122186977970425}{24}, \frac{41831507430222441029}{3550}, \ldots \Bigg\},\end{aligned} \tag{A.2}$$

where the rational numbers up to $j = 6$ are found to be exact, whereas the higher ones are approximations.

Equation (A.1) can be read as recurrence relation for the coefficients a_l. Now we construct an ordinary differential equation for $E(g) := E^{(L)}_{0,\mathrm{weak}}(g)$ from this recurrence relation and find

$$\left[\left(g\frac{\mathrm{d}}{\mathrm{d}g} \right)^L + g \sum_{j=0}^{L+1} \beta_{L-j} \left(g\frac{\mathrm{d}}{\mathrm{d}g} + 1 \right)^j \right] E(g) = 0. \tag{A.3}$$

All coefficients being real, real and imaginary parts of $E(g)$ each have to satisfy this equation separately. The point $g = 0$, however, is not a regular point. We are looking for a solution, which is finite when approaching it along the negative real axis. Asymptotically, $E(g)$ has to satisfy $E(g) \simeq \exp(1/g\beta_{-1}) = \exp(1/3g)$. Therefore we solve (A.3) with the ansatz

$$E(g) = g^{\alpha} \exp\left(\frac{1}{3g} - \sum_{k=1} b_k (-g)^k \right), \tag{A.4}$$

to obtain $\alpha = -1/2$ and

$$\begin{aligned} b_{1,2,3,\ldots} = \Bigg\{ & \frac{95}{24}, \frac{619}{32}, \frac{200689}{1152}, \frac{2229541}{1024}, \frac{104587909}{3072}, \frac{7776055955}{12288}, \frac{9339313153349}{688128}, \\ & \frac{172713593813181}{524288}, \frac{1248602386820060039}{139886592}, \frac{1453180839940270416031663 1}{54391637278720}, \\ & \frac{125798367202796417369605679 21}{1435939224158208}, \frac{1090518247175478978847946457467 23}{348951880031797248}, \\ & \frac{45574017678173074497482074500364087}{3780312033677803520} \ldots \Bigg\}. \end{aligned} \tag{A.5}$$

This is in agreement with equation (3.4) and an improvement compared with the WKB results of Zinn-Justin [22]. Again, the first six rational numbers are exact, followed by approximate ones.

Appendix B

Given a one-dimensional quantum system

$$(H_0 + gV)|n, g\rangle = E_n(g)|n, g\rangle \tag{B.1}$$

with Hamiltonian $H = H_0 + gV$, eigenvalues $E_n(g)$ and eigenstates $|n, g\rangle$, we consider an infinitesimal increase dg in the coupling constant g. The eigenvectors will undergo a small change

$$|n, g + \mathrm{d}g\rangle = |n, g\rangle + \mathrm{d}g \sum_{k \neq n} u_{nk}|k, g\rangle \tag{B.2}$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}g}|n, g\rangle = \sum_{k \neq n} u_{nk}|k, g\rangle. \tag{B.3}$$

Given this, we take the derivative of (B.1) with respect to g and multiply by $\langle m, g|$ from the left to obtain

$$\langle m, g|V - E'_n(g)|n, g\rangle = \sum_{k \neq n} u_{nk}\langle m, g|H_0 + gV - E_n(g)|k, g\rangle. \tag{B.4}$$

Setting now $m = n$ and $m \neq n$ in turn, we find

$$E'_n(g) = V_{nn}(g), \tag{B.5}$$

$$V_{mn}(g) = u_{nm}(E_m(g) - E_n(g)), \tag{B.6}$$

where $V_{mn}(g) = \langle m, g|V|n, g\rangle$.

Equation (B.5) governs the behaviour of the eigenvalues as functions of the coupling constant g. To have a complete system of differential equations, we must also determine how the $V_{mn}(g)$ change, when g changes. With the help of equations (B.3) and (B.6), we obtain

$$V'_{mn} = \sum_{k \neq m} u^*_{mk}\langle k, g|V|n, g\rangle + \sum_{k \neq n} u_{nk}\langle m, g|V|k, g\rangle, \tag{B.7}$$

$$V'_{mn} = \sum_{k \neq m} \frac{V_{mk}V_{kn}}{E_m - E_k} + \sum_{k \neq n} \frac{V_{mk}V_{kn}}{E_n - E_k}. \tag{B.8}$$

Equations (B.5) and (B.8) together describe a complete set of differential equations for the energy eigenvalues $E_n(g)$ and the matrix-elements $V_{nm}(g)$. The latter determine via (B.6) the expansion coefficients $u_{mn}(g)$. Initial conditions are given by the eigenvalues $E_n(0)$ and the matrix elements $V_{nm}(0)$ of the unperturbed system.

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