Convergence Behavior of Variational Perturbation Expansions

Wolfhard Janke\textsuperscript{1} and Hagen Kleinert\textsuperscript{2}

\textsuperscript{1} Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany
\textsuperscript{2} Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

Abstract

Variational weak-coupling perturbation theory yields converging approximations, uniformly in the coupling strength. This allows us to calculate directly the coefficients of strong-coupling expansions. For the anharmonic oscillator we explain the physical origin of the empirically observed convergence behavior which is exponentially fast with superimposed oscillations.

1 Introduction

An important problem of perturbation theory is the calculation of physically meaningful numbers from expansions which are usually divergent asymptotic series with coefficients growing $\propto k!$ in high orders $k$. For small expansion parameters $g$ a direct evaluation of the series truncated at a finite order $k \approx 1/g$ can yield a reasonably good approximation, but for larger couplings such series become completely useless and require some kind of resummation. Well-known examples are field theoretical $\epsilon$-expansions for the computation of critical exponents of phase transitions, but also the standard Stark and Zeeman effects in atomic physics lead to divergent perturbation expansions.

The paradigm for studying this problem is the quantum mechanical anharmonic oscillator with a potential $V(x) = \frac{1}{2}\omega^2 x^2 + \frac{1}{4}gx^4$ ($\omega^2, g > 0$). The Rayleigh-Schrödinger perturbation theory yields for the ground-state energy a power-series expansion

$$E^{(0)}(g) = \omega \sum_{k=0}^{\infty} E_k^{(0)} \left( \frac{g/4}{\omega^2} \right)^k,$$

where the $E_k^{(0)}$ are rational numbers $1/2, 3/4, -21/8, 333/16, -30885/128, \ldots$, which can easily be obtained to very high orders from the recursion relations of
Bender and Wu [1]. Their large-order behavior is analytically known to exhibit the typical factorial growth,

\[ E_k^{(0)} = -(1/\pi)(6/\pi)^{1/2}(-3)^k k^{-1/2} k!(1 + \mathcal{O}(1/k)). \]  

Standard resummation methods are Padé or Borel techniques whose accuracy, however, decreases rapidly in the strong-coupling limit. In this note we summarize recent work on a new approach based on variational perturbation theory [2, 3]. Our results demonstrate that by this means the divergent series expansion (1) can be converted into a sequence of exponentially fast converging approximations, uniformly in the coupling strength \( g \) [4–7]. This allows us to take all expressions directly to the strong-coupling limit, yielding a simple scheme for calculating the coefficients \( \alpha_i \) of the convergent strong-coupling series expansion,

\[ E^{(0)}(g) = (g/4)^{1/3} \left[ \alpha_0 + \alpha_1(4\omega^3/g)^{2/3} + \alpha_2(4\omega^3/g)^{4/3} + \ldots \right]. \]

## 2 Variational Perturbation Theory

The origin of variational perturbation theory can be traced back to a variational principle for the evaluation of quantum partition functions in the path-integral formulation [3, 8]. While in many applications the accuracy was found to be excellent over a wide range of temperatures, slight deviations from exact or simulation results at very low temperatures motivated a systematic study of higher-order corrections [2, 3].

In the zero-temperature limit the calculations simplify and lead to a resummation scheme for the energy eigenvalues which can be summarized as follows. First, the harmonic term of the potential is split into a new harmonic term with a trial frequency \( \Omega \) and a remainder, \( \omega^2 x^2 = \Omega^2 x^2 + (\omega^2 - \Omega^2) x^2 \), and the potential is rewritten as \( V(x) = \frac{1}{2}\Omega^2 x^2 + \frac{1}{4}g(-2\sigma x^2/\Omega + x^4) \), where \( \sigma = \Omega(\Omega^2 - \omega^2)/g \). One then performs a perturbation expansion in powers of \( \hat{g} \equiv g/\Omega^3 \) at a fixed \( \sigma \),

\[ \hat{E}_{N}^{(0)}(\hat{g}, \sigma) = \sum_{k=0}^{N} \varepsilon_k^{(0)}(\sigma) (\hat{g}/4)^k, \]  

where \( \hat{E}_N^{(0)} \equiv E_N^{(0)}/\Omega \) is the dimensionless reduced energy. The new expansion coefficients \( \varepsilon_k^{(0)} \) are easily found by inserting \( \omega = \sqrt{\Omega^2 - g\sigma/\Omega} = \Omega\sqrt{1 - g\sigma} \) in (1) and reexpanding in powers of \( \hat{g} \),

\[ \varepsilon_k^{(0)}(\sigma) = \sum_{j=0}^{k} E_j^{(0)} \binom{(1 - 3j)/2}{k-j} (-4\sigma)^{k-j}. \]  

The truncated power series \( \hat{W}_N(\hat{g}, \Omega) \equiv \Omega \hat{E}_N^{(0)}(\hat{g}, \sigma) \) is certainly independent of \( \Omega \) in the limit \( N \to \infty \). At any finite order, however, it does depend on \( \Omega \), the approximation having its fastest speed of convergence where it depends least on \( \Omega \), i.e., at points where \( \partial \hat{W}_N/\partial \Omega = 0 \). If we denote the order-dependent optimal value of \( \Omega \) by \( \Omega_N \), the quantity \( \hat{W}_N(\hat{g}, \Omega_N) \) is the new approximation to \( E^{(0)}(g) \).
At first sight the extremization condition $\partial W_N/\partial \Omega = 0$ seems to require the determination of the roots of a polynomial in $\Omega$ of degree $3N$, separately for each value of $g$. In Ref. [4] we observed, however, that this task can be greatly simplified. While $W_N$ does depend on both $g$ and $\Omega$ separately, we could prove that the derivative can be written as $\partial W_N/\partial \Omega = (\hat{g}/4)^{N} P_N(\sigma)$, where $P_N(\sigma) = -2d\varepsilon_{N+1}^{(0)}(\sigma)/d\sigma$ is a polynomial of degree $N$ in $\sigma$. The optimal values of $\sigma$ were found to be well fitted by

$$\sigma_N = cN \left(1 + 6.85/N^{2/3}\right),$$

with $c = 0.186047272\ldots$ determined analytically (cp. Sec. 3). This observation simplifies the calculations considerably and shows that the optimal solutions $\Omega_N$ depend only trivially on $g$ through $\sigma_N = \Omega_N(\Omega_N^2 - \omega^2)/g$. Since the explicit knowledge of $\Omega_N$ is only needed in the final step when going back from $\hat{E}_N^{(0)}$ to $E_N^{(0)}$, this suggests that the variational resummation scheme can be taken directly to the strong-coupling limit.

To this end we introduce the reduced frequency $\hat{\omega} = \omega/\Omega$, write the approximation as $W_N = (g/\hat{g})^{1/3} w_N(\hat{g}, \hat{\omega}^2)$, and expand the function $w_N(\hat{g}, \hat{\omega}^2)$ in powers of $\hat{\omega}^2 = (\omega^3/g)^{2/3} \hat{g}^{2/3}$. This gives [5]

$$W_N = (g/4)^{1/3} \left[ \alpha_0 + \alpha_1 \left( 4\omega^3/g \right)^{2/3} + \alpha_2 \left( 4\omega^3/g \right)^{4/3} + \ldots \right],$$

with the coefficients,

$$\alpha_n = (\hat{g}/4)^{(2n-1)/3} \sum_{k=0}^{N} (-1)^{k+n} \sum_{j=0}^{k-n} E_j^{(0)} \left( \begin{array}{c} (1 - 3j)/2 \\ k - j \end{array} \right) \left( k - j \right) \left( n \right) (-\hat{g}/4)^j.$$  

(7)

If this is evaluated at $\hat{g} = 1/\sigma_N$ with $\sigma_N$ given in (5), we obtain the exponentially fast approach to the exact limit as shown in Fig. 1 for $\alpha_0$. The exponential falloff is modulated by oscillations. Our result, $\alpha_0 = 0.66798625915577710827096$, agrees to all 23 digits with the most accurate 62-digit value in the literature. The computation of the higher-order coefficients $\alpha_n$ for $n > 0$ proceeds similarly and the results up to $n = 22$ are given in Table 1 of Ref. [5].

3 Convergence Behavior

To explain the convergence behavior [6, 7] we recall that the ground-state energy $E^{(0)}(g)$ satisfies a subtracted dispersion relation which leads to an integral representation of the original perturbation coefficients,

$$E_k^{(0)} = \frac{4^k}{2\pi i} \int_0^{-\infty} \frac{dg}{g^{k+1}} \text{disc} E^{(0)}(g),$$

(8)

where $\text{disc} E^{(0)}(g) = 2i \text{Im} E^{(0)}(g - i\eta)$ denotes the discontinuity across the left-hand cut in the complex $g$-plane. For large $k$, only its $g \rightarrow 0^-$ behavior is relevant and a semiclassical calculation yields $\text{disc} E^{(0)}(g) \approx -2i\omega(6/\pi)^{1/2}(-4\omega^3/3g)^{1/2} \exp(4\omega^3/3g)$, which in turn implies the large-order behavior (2) of $E_k^{(0)}$. 

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Figure 1: L.h.s.: Exponentially fast convergence of the $N$th approximants for $\alpha_0$ to the exact value. The dots show $\Delta_N = |(\alpha_0)_N - \alpha_0|$. R.h.s.: Cuts in the complex $\hat{g}$-plane. The cuts inside the shaded circle happen to be absent due to the convergence of the strong-coupling expansion for $g > g_s$.

The reexpanded series (3) is obtained from (1) by the replacement of $\omega \rightarrow \Omega \sqrt{1 - \sigma \hat{g}}$. In terms of the coupling constant, the above replacement amounts to $\hat{g} \equiv g/\Omega^3 \rightarrow \hat{g}/(1 - \sigma \hat{g})^{3/2}$. Using this mapping it is straightforward to show [6] that $\hat{E}^{(0)} \equiv E^{(0)}/\Omega$ satisfies a dispersion relation in the complex $\hat{g}$-plane. If $C$ denotes the cuts in this plane and $\text{disc}_C \hat{E}^{(0)}(\hat{g})$ is the discontinuity across these cuts, the dispersion integral for the expansion coefficients $\varepsilon_k^{(0)}$ reads

$$
\varepsilon_k^{(0)} = \frac{4^k}{2\pi i} \int_C \frac{d\hat{g}}{\hat{g}^{k+1}} \text{disc}_C \hat{E}^{(0)}(\hat{g}).
$$

In the complex $\hat{g}$-plane, the cuts $C$ run along the contours $C_1, C_1, C_2, C_2$, and $C_3$, as shown on the r.h.s. of Fig. 1. The first four cuts are the images of the left-hand cut in the complex $g$-plane, and the curve $C_3$ is due to the square root of $1 - \sigma \hat{g}$ in the mapping from $\bar{g}$ to $\hat{g}$.

Let us now discuss the contributions of the various cuts to the $k$th term $S_k$. For the cut $C_1$ and the empirically observed optimal solutions $\sigma_N = cN(1 + b/N^{2/3})$, a saddle-point approximation shows [6] that this term gives a convergent contribution, $S_N(C_1) \propto e^{-b \log(-\gamma) + (\gamma)^{-2/3}} N^{1/3}$, only if one chooses $c = 0.186047272 \ldots$ and $\gamma = -0.242964029 \ldots$. Inserting the fitted value of $b = 6.85$ this yields an exponent of $-b \log(-\gamma) = 9.7$, in rough agreement with the convergence seen in Fig. 1. If this was the only contribution the convergence behavior could be changed at will by varying the parameter $b$. For $b < 6.85$, a slower convergence was indeed observed. The convergence cannot be improved, however, by choosing $b > 6.85$, since the optimal convergence is limited by the contributions of the other cuts.

The cut $C_1$ is still harmless; it contributes a last term $S_N(C_1)$ of the negligible order $e^{-N \log N}$. The cuts $C_{2,2,3}$, however, deserve a careful consideration. If they would really start at $\hat{g} = 1/\sigma$, the leading behavior would be $\varepsilon_k^{(0)}(C_{2,2,3}) \propto \sigma^k$, and therefore $S_N(C_{2,2,3}) \propto (\sigma \hat{g})^N$, which would be in contradiction to the empirically
observed convergence in the strong-coupling limit. The important point is that the
cuts in Fig. 1 do not really reach the point $\sigma \hat{g} = 1$. There exists a small circle of
radius $\Delta \hat{g} > 0$ in which $\hat{E}^{(0)}(\hat{g})$ has no singularities at all, a consequence of the fact
that the strong-coupling expansion (6) converges for $g > g_*$. The complex conjugate
pair of singularities gives a contribution,
$$S_N(C_{2,2,3}) \approx e^{-N^{1/3}a \cos \theta} \cos(N^{1/3}a \sin \theta),$$
with $a = 1/(|\bar{g}_s|c)^{2/3}$. By analyzing the convergence behavior of the strong-coupling
series we find $|\bar{g}_s| \approx 0.160$ and $\theta \approx -0.467$, which implies for the envelope an asymptotic falloff of $e^{-9.23N^{1/3}}$, and furthermore also explains the oscillations in the data [6].

4 Conclusions

To summarize, we have shown how variational perturbation theory can be used to
convert the divergent weak-coupling perturbation series of the anharmonic oscillator
into a sequence of converging approximations for the strong-coupling expansion. By
making use of dispersion relations and identifying the relevant singularities we are
able to explain the exponentially fast convergence with superimposed oscillations in
the strong-coupling limit.

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