Asymptotic series in quantum mechanics: anharmonic oscillator

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Abstract: This thesis deals with the study of the asymptotic series that one obtains for the ground state energy of the anharmonic oscillator, that is, an harmonic oscillator with a quartic perturbation term in its Hamiltonian. First we study a simplified field theory model as an introductory example, and then we use the path integral formulation and semiclassical methods to obtain analytically the behaviour of the series at large order.

I. INTRODUCTION

Quantum field theory is one of the most accurate physical theories constructed so far, but only a few problems can be solved exactly. To obtain meaningful results, we usually consider an exactly solvable problem H_0 and then add a perturbation so it describes our model. That is, we consider a small dimensionless parameter λ such that

$$H = H_0 + \lambda H_1$$

and we compute the results as a power series in λ. However, many of the series that we encounter are not convergent. A typical method used in quantum mechanics is the Rayleigh-Schrödinger perturbation theory (it can be found in many quantum mechanics books, [1] for example). If we consider the one-dimensional harmonic oscillator perturbed by a quartic term, which is called anharmonic oscillator (first studied by Bender and Wu [2]), the method shows that the series for the ground state energy is

$$E_0 = \hbar\omega \left(\frac{1}{2} + \frac{3}{4}\lambda - \frac{21}{8}\lambda^2 + \frac{333}{16}\lambda^3 + ... \right).$$

As we can see, the coefficients grow at an alarming rate. However, as Dyson argued in [3] this divergence is expected, because for λ negative the system is unstable and so the radius of convergence of the series must be zero. These divergent series that appear usually behave similarly, and we call them asymptotic series.

An asymptotic series is a divergent series which truncated after a finite number of terms gives an approximation of a function. Formalisation of this concept is what is known as Gevrey asymptotics. We say that a power series is α-Gevrey, with $\alpha \in (0, 1]$ if $CK^n n!^\alpha$ is an upper bound for the modulus of the coefficients, where C, K are constant to be determined, and we say that a formal power series $\hat{f}$ is the α-Gevrey asymptotic expansion of f if

$$\left| z^{-n} \left(f(z) - \sum_{k=0}^{n-1} f_k z^k \right) \right| \leq CK^n n!^\alpha.$$

For the formal definitions and some results see [4].

So, the point is that even if we obtain non convergent series, we are able to describe their behaviour and understand them as an expansion of some analytic function, giving them a physical meaning. Borel summation method can be used to obtain uniqueness theorems for these functions, and to sum the asymptotic series in order to obtain the exact solution.

In the calculations for the anharmonic oscillator we will use the path integral formulation of quantum mechanics. The idea of this formulation is that in quantum mechanics we have to take into account all possible paths that connect our initial and final states. Also, we will use the partition function $Z(\beta)$ to describe our system. It can be seen (see, for instance, [5]) that

$$Z(\beta) = \mathrm{Tr}e^{-\beta H} = \int [\mathrm{d}q(t)] e^{-\frac{S(q)}{\hbar}}, \quad (1)$$

where $S(q)$ is the Euclidean action, and the notation $[\mathrm{d}q(t)]$ indicates that this is a path integral, that is, that we are taking into account all possible paths.

If H is bounded from below, we can obtain the ground state energy by taking the large β limit; as the temperature (β^{-1}) becomes lower, the term corresponding to the ground state becomes more important in the series because there is no energy for excited states. Therefore,

$$E_0 = \lim_{\beta \to \infty} \left(-\frac{1}{\beta} \ln \mathrm{Tr}e^{-\beta H} \right). \quad (2)$$

We will also use the partition function for the harmonic oscillator, which is

$$Z_0(\beta) = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{1 - e^{-\beta\hbar\omega}}. \quad (3)$$

II. 0-DIMENSIONAL EXAMPLE

In quantum field theory we deal with fields that depend on spatial and temporal coordinates, $\Phi(\vec{x}, t)$. In this sense, we can understand quantum mechanics as a 0+1 QFT, because the states are fields which depend only on time, $\Phi(t)$. Going one step further, we can consider a theory where the fields are constants of the space

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time. In this section we consider a model described by an integral where Φ does not depend on any coordinate,

$$Z(\lambda) = \int_{-\infty}^{\infty} \mathrm{d}\Phi \frac{1}{\sqrt{2\pi}} e^{-\left(\frac{1}{2}\Phi^2 + \frac{\lambda}{4!}\Phi^4\right)}. \qquad (4)$$

A. Analyticity

First of all we prove that this function is analytic on the cut plane, that is, on the complex λ plane minus the negative real axis. On the real line, it is clear that the integral converges for $\lambda \geq 0$ and diverges for $\lambda < 0$. Now, let $\lambda \in \mathbb{C}$. Since the imaginary is bounded, analyticity is also clear for $\mathrm{Re}(\lambda) \geq 0$; we are in the same case as when $\lambda \in \mathbb{R}^+ \cup \{0\}$. Therefore, our only concern is $\mathrm{Re}(\lambda) < 0$.

For $\mathrm{Re}(\lambda) < 0$ the integral diverges, and so we have to perform an analytic continuation, as proposed by [5]. We need the integral to remain finite, and thus we need $\mathrm{Re}(\lambda\Phi^4)$ to remain positive. Hence we rotate the contour of integration as we change the argument of λ in a way that $\arg(\Phi) = -\frac{1}{4}\arg(\lambda)$. Depending on the direction in which we rotate on the λ-plane, we obtain two different contours of integration. In both cases, the integral is dominated by the saddle point at the origin, because the contribution of the other saddle points is of order $e^{3/2\lambda} \ll 1$, for $\lambda \to 0^-$.

In the next chapter we will need to calculate the discontinuity of the integral on the cut to obtain the imaginary part of the energy. As a guide, let us see what is obtained here. If we calculate it, we see that the contribution of the origin cancels, and the integral is dominated by the other saddle points aforementioned. Therefore,

$$\mathrm{Im}Z(\lambda) \sim e^{\frac{3}{2\lambda}}.$$

B. Perturbative expansion

Now we will write $Z(\lambda)$ as a power series. Here we will be able to obtain it exactly, and see its behaviour. This will be an illustrative example of this kind of series, as for the anharmonic we will not be able to obtain an exact analytic expression. So, if we set

$$e^{-\frac{\Phi^4}{4!}\lambda} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\Phi^4\lambda}{4!}\right)^2,$$

substitute it in the integral, apply the dominated convergence theorem, integrate and simplify, we obtain

$$Z(\lambda) = \sum_{n=0}^{\infty} (-1)^n \frac{(4n-1)!!}{n!(4!)^n} \lambda^n =: \sum_{n=0}^{\infty} c_n (-\lambda)^n. \qquad (5)$$

If we compute its radius of convergence, we see that it is indeed 0, as expected from the previous section.

We present in figure 1 the behaviour of the series up to order 5 and 10, and we compare it with the exact result

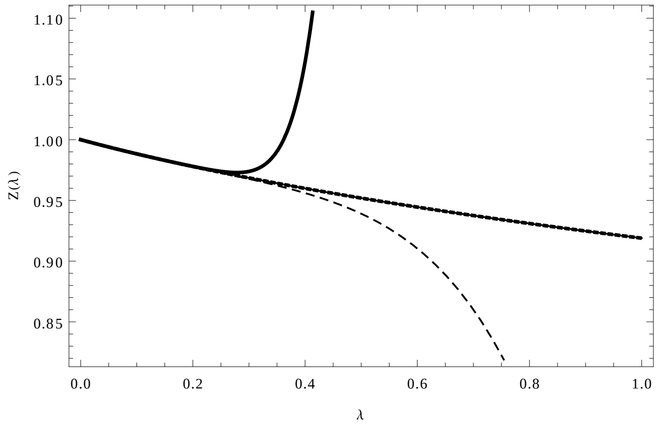

FIG. 1: Values of $Z(\lambda)$ given by power series (5) up to order $n = 5$ (dashed line), $n = 10$ (thick line), computing the Borel sum of (5) (thick dashed line) and computing exactly the integral (4), which coincides with the Borel sum.

(the integral, computed with Mathematica). We see that considering more terms does not assure a better estimate of the original function, as expected for an asymptotic series. As we said in the introduction though, we can use the Borel summation method to obtain a better result.

If we have a factorially divergent series, we can consider its Borel transform (divide each term by $n!$), compute the sum, which now converges, and then undo the transformation, that is, apply the Laplace transform (for the formal definitions see [4]). This way we can sum the series and obtain an analytic function as a result. If we do it in this case, we obtain the thick dashed line of figure 1. As we can see, the correspondence with the original function is perfect. In fact, it is straightforward to see that in this case the Borel sum of the power series is equal to the original function $Z(\lambda)$.

Power series (5) is the asymptotic expansion of our integral (4), and it can be seen that the series coefficients behave like

$$c_n \leq \frac{3}{16}\left(\frac{2}{3}\right)^n n!,$$

i.e. that the series is 1-Gevrey.

C. Semiclassical method

To obtain (5) we had to compute an integral, which we were able to solve exactly. However, as we said before this is not always the case. So, we are going to compute the integral using steepest descent. The integral that we want to approximate is

$$\int_{-\infty}^{\infty} \mathrm{d}\Phi \frac{1}{\sqrt{2\pi}} e^{-\frac{\Phi^2}{2} + \ln \Phi^{4n}}. \qquad (6)$$

The steepest descent method gives an approximation for this kind of integrals, even in the complex plane. It is presented in [4]. However, here we just need the following: let $f(x)$ be a function with a minimum at x_0. Then,

$$\int_{-\infty}^{+\infty} \mathrm{d}x \; e^{-f(x)} \approx e^{-f(x_0)} \sqrt{\frac{2\pi}{f''(x_0)}}.$$

Applying this formula to (6) we obtain

$$\int_{-\infty}^{\infty} \mathrm{d}\Phi \frac{1}{\sqrt{2\pi}} e^{-\frac{\Phi^2}{2} + \ln \Phi^{4n}} \approx \frac{1}{\sqrt{2}} e^{-2n} (4n)^{2n}.$$

The exact result for this integral is $(4n-1)!!$. Using Stirling's approximation for $n!$ we see that both results are the same, up to a term $\ln \sqrt{2}$ which is negligible because the approximation is for n large.

III. ANHARMONIC OSCILLATOR

Our objective now is to obtain the perturbative series for the ground-state energy of the anharmonic oscillator. We will understand the anharmonic oscillator as a field theory in a one-dimensional space time, described by the Hamiltonian

$$H = \frac{1}{2}\dot{\varphi}^2 + \frac{1}{2} m^2 \varphi^2 + \lambda \varphi^4.$$

We want to obtain the coefficients A_n in

$$E_0(\lambda) = \frac{1}{2} m + \sum_{n=1}^{\infty} m A_n \left(\frac{\lambda}{m^3}\right)^n. \qquad (7)$$

First, to obtain an easy formula to be calculated with Mathematica, we consider the coordinate representation of this Hamiltonian,

$$\begin{cases} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{4}x^2 + \frac{1}{4}\lambda x^4\right)\Phi(x) = E(\lambda)\Phi(x), \\ \lim_{x\to\pm\infty} \Phi(x) = 0. \end{cases} \qquad (8)$$

If we set

$$\Phi(x) = \sum_{n=0}^{\infty} \lambda^n e^{-\frac{x^2}{4}} B_n(x)$$

with $B_{-1} = 0, B_0 = 1$, and substitute it in (8), we obtain the following equation:

$$\sum_{n=0}^{\infty} \lambda^n \left(x B'_n(x) - B''_n(x) + \frac{1}{4} x^4 B_{n-1}(x) \right) = \\ = \left(\sum_{n=1}^{\infty} A_n \lambda^n \right) \left(\sum_{m=0}^{\infty} \lambda^m B_m(x) \right). \qquad (9)$$

We have written a small script with Mathematica which obtains the coefficients from this equation (see [4] for the code). We notice that they grow very fast, and just like in the 0-dimensional case, it can be seen that (7) is a 1-Gevrey power series, but with different constants.

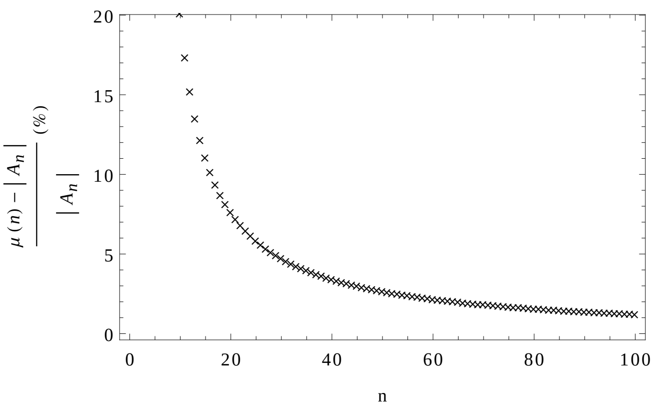

FIG. 2: Difference between Rayleigh-Schrödinger coefficients and the asymptotic behaviour.

Using the Borel summation method with these coefficients, Simon et al. prove in [6] that the Borel sum converges to the exact eigenvalue.

Bender and Wu guessed correctly the asymptotic behaviour of the series in their original paper [2]; it is

$$A_n \sim (-1)^{n+1} \left(\frac{6}{\pi^3}\right)^{\frac{1}{2}} \Gamma\left(n + \tfrac{1}{2}\right) 3^n =: \mu(n). \qquad (10)$$

We present in figure 2 the relative difference between the coefficients A_n computed with Mathematica (up to $n = 100$) and the asymptotic behaviour of the series. As expected, the difference goes to 0 for large values of n.

Our goal now is to obtain this behaviour analytically. This can be done rigorously using perturbation theory, as Simon and Dicke showed in [7]. However, the mathematics involved are beyond our reach. What we will do instead is obtain this result using semiclassical methods.

A. Semiclassical methods

Let $E(\lambda)$ be an analytic function on the cut plane. By Cauchy's theorem, we write

$$E(\lambda) = \frac{1}{2\pi i} \oint_C \mathrm{d}\lambda' \frac{E(\lambda')}{\lambda' - \lambda},$$

where C is a circle in the λ' cut plane. As Bender and Wu show in [8], changing the contour of integration we can write

$$E(\lambda) = \frac{1}{\pi} \int_{-\infty}^{0} \mathrm{d}\lambda' \frac{\mathrm{Im} E(\lambda')}{\lambda' - \lambda}.$$

If we now expand $E(\lambda)$ in a power series of λ, it is straightforward to see that

$$A_n = \frac{1}{\pi} \int_{-\infty}^{0} \mathrm{d}\lambda' \frac{\mathrm{Im} E(\lambda')}{(\lambda')^{n+1}}. \qquad (11)$$

Hence we need to calculate Im$E(\lambda)$. To do so, we are going to use instanton solutions.

Without loss of generality, we will set the mass $m = 1$. So, we will work with the Hamiltonian

$$H = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 + \frac{1}{2}q^2 + \lambda q^4.$$

As we said, we will use the path integral representation of the partition function, (1). In our case the Euclidean action is

$$S(q) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left(\frac{1}{2}\dot{q}(t)^2 + \frac{1}{2}q(t)^2 + \lambda q(t)^4\right),$$

and we need to compute (2). The path integral is now also analytic on the cut plane, and so to obtain the imaginary part we will compute the discontinuity on the cut.

Analogous to the previous section, we rotate the contour of integration in the $q(t)$ space, $q(t) \to q(t)e^{-i\theta}$, in such a way that $\mathrm{Re}[\lambda q^4(t)]$, $\mathrm{Re}[\dot{q}^2(t)] > 0$, so we take paths regular enough. The saddle points at the origin of the two path integrals corresponding to the continuations cancel when we take the difference, and so we have to find non-trivial saddle points. However, if we go to the Euclidean classical equation,

$$-\ddot{q}(t) + q(t) + 4\lambda q^3(t) = 0 \quad (\lambda < 0) \qquad (12)$$
$$q(-\beta/2) = q(\beta/2)$$

we see that a solution is

$$q^2(t) = -\frac{1}{4\lambda}.$$

The contribution of this saddle point to the integral is of order $e^{\beta/16\lambda}$, and so is negligible in the large β limit (λ is negative). We need solutions with an action that remains finite for $\beta \to +\infty$. These solutions are called instantons.

They will correspond to a periodic motion in real time around the minima of the potential $V(q) = q^2/2 + \lambda q^4$. Integrating equation (12),

$$\frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2 - \lambda q^4 = \varepsilon, \qquad \varepsilon < 0. \qquad (13)$$

The period of the solution will be

$$\beta = 2\int_{q_0}^{q_1} \mathrm{d}q \frac{1}{\sqrt{q^2 + 2\lambda q^4 + 2\varepsilon}}.$$

In the infinite β limit, $\varepsilon, q_0 \to 0$. If we solve then (13) for q we can check that the classical solution becomes

$$q_c(t) = \pm\sqrt{-\frac{1}{2\lambda}}\frac{1}{\cosh(t - t_0)},$$

and the corresponding classical action is

$$S(q_c) = -\frac{1}{3\lambda} + O\left(\frac{e^{-\beta}}{\lambda}\right). \qquad (14)$$

Since the classical action is invariant under time translations, for β finite the classical solution has a free parameter t_0, $0 \le t_0 < \beta$. So, we now have two one-parameter families of saddle points. We have to evaluate their contribution at leading order. To do so, we will use the Gaussian approximation.

We expand the action around the saddle point we just obtained. If we set $q(t) = q_c(t) + r(t)$ and plug it in (1), we can express the integral in terms of an operator M, which is just the second functional derivative of the action;

$$\mathrm{ImTr}e^{-\beta H} = \frac{1}{i}e^{\frac{1}{3\lambda}}\int [\mathrm{d}r(t)] e^{-\frac{1}{2}\int \mathrm{d}t_1 \mathrm{d}t_2 r(t_1)M(t_1,t_2)r(t_2)}$$

with

$$M(t_1, t_2) = \left[-\left(\frac{\mathrm{d}}{\mathrm{d}t_1}\right)^2 + 1 + 12\lambda q_c^2(t_1)\right]\delta(t_1 - t_2).$$

Here we face another setback though. The Gaussian integration leads to a solution which is infinite, because it is proportional to $(\det M)^{-1/2}$ and $\dot{q}_c(t)$ is an eigenvector of M with eigenvalue 0. To solve this, we have to integrate exactly over the time translation parameter t_0, which is then called a collective coordinate.

If we insert the identity

$$1 = \frac{1}{\sqrt{2\pi\xi}}\int \mathrm{d}t_0 \left[\int \mathrm{d}t \dot{q}_c(t)\dot{q}(t + t_0)\right] \cdot$$
$$\cdot e^{-\frac{1}{2\xi}\left[\int \mathrm{d}t \dot{q}_c(t)(q(t+t_0) - q_c(t))\right]^2}$$

to (1), the new action is

$$S(q) + \frac{1}{2\xi}\left[\int \mathrm{d}t \dot{q}_c(t)(q(t + t_0) - q_c(t))\right]^2.$$

Notice that it is no longer invariant under time translation. With this action, instead of the operator M, the determinant generated by Gaussian integration around the saddle point is

$$\det\left(\frac{\partial^2 S}{\partial q_c(t_1)\partial q_c(t_2)} + \frac{1}{\xi}\dot{q}_c(t_1 - t_0)\dot{q}_c(t_2 - t_0)\right).$$

Now, instead of the eigenvalue 0 we have $\|\dot{q}_c\|^2/\xi$, as we wanted. Only the normalisation of the path integral and the determinant remain to be computed.

To normalise the path integral, we compare it to its value at $\lambda = 0$, which is just the partition function $Z_0(\beta)$ of the harmonic oscillator, (3). Let M_0 be the operator M for $\lambda = 0$. As is shown in [5], what can be calculated is $\det(M + \varepsilon)\det(M_0 + \varepsilon)^{-1}$, where ε is an arbitrary constant. So, if we denote by $|1\rangle$ the unitary eigenvector proportional to $\dot{q}_c$ and define $\nu := \|\dot{q}_c\|^2/\xi$, what we have to calculate is

$$\det(M + \nu|1\rangle\langle 1|)M_0^{-1} =$$
$$= \lim_{\varepsilon\to 0}\det(M + \varepsilon + \nu|1\rangle\langle 1|)(M_0 + \varepsilon)^{-1}.$$

If we define

$$\det{}' M M_0^{-1} := \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \det(M+\varepsilon)(M_0+\varepsilon)^{-1},$$

after some algebra it is easy to see that the contribution of the determinant is

$$\det{}' M M_0^{-1} \frac{\|\dot{q}_c\|^2}{\xi}.$$

Noticing that all functions in the determinant depend on $t - t_0$, the integration yields

$$\frac{\beta}{\sqrt{2\pi}} Z_0(\beta) \|\dot{q}_c\| (\det{}' M M_0^{-1})^{-1/2}.$$

Taking into account that we have two families of saddle points, and that we have to divide by $2i$ to obtain the imaginary part, taking the $\beta \to +\infty$ limit we obtain, recalling that (3) $\to e^{-\beta/2}$ when $\beta \to +\infty$,

$$\mathrm{Im}\mathrm{Tr} e^{-\beta H} \sim \frac{1}{i} \frac{\beta}{\sqrt{2\pi}} e^{-\beta/2} \|\dot{q}_c\| (\det{}' M M_0^{-1})^{-1/2} e^{1/3\lambda} \tag{15}$$

It is not straightforward to compute the determinant, as [5] shows. It can be seen that

$$\det{}' M M_0^{-1} = -\frac{1}{12}.$$

Putting everything together, along with the value of $\|\dot{q}_c\|$, which can be easily computed with Mathematica, we obtain

$$\mathrm{Im}\mathrm{Tr} e^{-\beta H} \sim -\frac{2\beta}{\sqrt{2\pi}} \frac{e^{-\beta/2}}{\sqrt{-\lambda}} e^{1/3\lambda} (1 + O(\lambda)). \tag{16}$$

Now, for $\lambda \to 0^-$,

$$\mathrm{Im}\mathrm{Tr} e^{-\beta H} \sim -\beta e^{-\beta/2} \mathrm{Im} E_0(\lambda).$$

Therefore,

$$\mathrm{Im} E_0(\lambda) = \frac{2}{\sqrt{2\pi}} \frac{e^{\frac{1}{3\lambda}}}{\sqrt{-\lambda}} (1 + O(\lambda)). \tag{17}$$

If we insert (17) into (11), and compute the integral, we reproduce the asymptotic behaviour of the series (10), as expected:

$$A_n = \frac{1}{\pi} \int_{-\infty}^{0} \mathrm{d}\lambda' \frac{\mathrm{Im} E(\lambda')}{(\lambda')^{n+1}} =$$
$$= (-1)^{n+1} \left(\frac{6}{\pi^3}\right)^{\frac{1}{2}} \Gamma\left(n + \tfrac{1}{2}\right) 3^n. \tag{18}$$

IV. CONCLUSIONS

- Some series that naturally appear in quantum mechanics and quantum field theory are not convergent. However they are asymptotic series, and so they grow in a controlled way which we can describe and obtain analytically.
- Borel summation method can often be used to obtain the exact solution from the asymptotic series.
- Classical solutions are related to very large order in perturbation theory. If we can obtain the imaginary part of the energy using semiclassical methods, Cauchy's theorem allows us to obtain the coefficients.
- Path integral formulation of quantum mechanics allows us to use semiclassical methods which can be easily generalised to field theory, such as the instanton solutions.

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