Mathematical Methods

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1 Examples of perturbation theory in physics problems

This course is about using perturbation theory, broadly defined, to solve complicated mathematical problems, and I would like to explain why I consider this subject useful. The main point is that in theoretical physics meaningful problems that can be solved exactly *do not exist*, at the first approximation. Yet, when we teach physics, we often discuss problems that can be solved exactly (recall hydrogen atom, harmonic oscillator, two-body problem in mechanics etc.) The reason we do that is that we believe that exactly solvable problems often allow us to start a sequence of approximations that brings us closer to the real-world problems for which exact solutions are impossible. We can call this approach a "perturbation theory".

However, at variance with what we refer to as perturbation theory in e.g. course on quantum mechanics, we can understand perturbation theory broader – as a way to construct approximate, but high-quality, solutions to problems of interest in situations when exact solution is impossible. Understanding how to do this in various circumstances is the main theme of this course.

During the course we will deal with mathematical examples without connecting them to physics most of the time. For this reason it is perhaps useful to begin with a few simple physics examples where the need to develop perturbation theory in the above sense arises. This is what we will do in this lecture. At the end of the lecture we will also discuss if perturbation theory is a good idea, in general.

Expansion of integrals

Consider a particle moving in an *arbitrary* potential $U(x)$ in one dimension, see Fig.1. We imagine that this potential has a local maximum at a point $x = 0$. The height of the maximum is U_0. The energy of the particle E is such that $E - U_0 = \Delta \ll U_0$.

There are two turning points to the left and to the right of $x = 0$; we will call them a and b. The particle moves back and forth between a and b; we would like to find out how the period of oscillations depends on Δ.

To find this dependence, we write the standard formula for the period of oscillations

$$T = \sqrt{2m} \int\limits_a^b \frac{\mathrm{d}x}{\sqrt{E - U(x)}}. \tag{1}$$

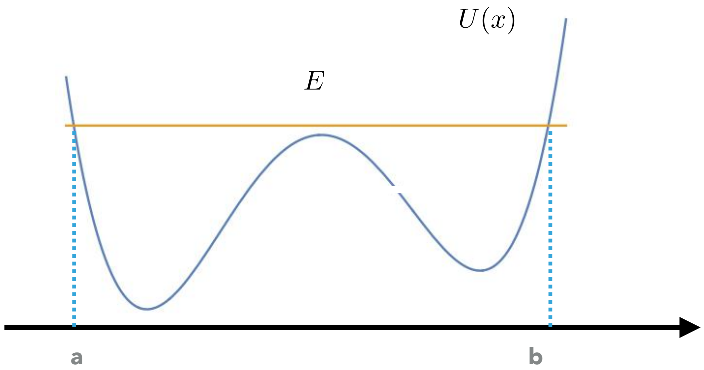

Figure 1: A particle in the potential $U(x)$; the energy of the particle E is slightly larger than the local maximum of the potential energy U_0.

In general, if we want to proceed further, we need to know what $U(x)$ is. However, when Δ is small this is not necessary because the particle spends significant amount of time close to $x = 0$. Since $x = 0$ is the local maximum of the potential, its Taylor expansion at around $x = 0$ reads $U(x) \approx U_0 - |U_0''|x^2/2 + U_0'''x^3/6 + \mathcal{O}(x^4)$. Since the above approximation is only valid at small x, it is convenient to split the integral in Eq.(1) into three integrals that describe two regions away from $x = 0$ and the neighborhood of $x = 0$. Then

$$T = \sqrt{2m}\int_a^{-\epsilon}\frac{\mathrm{d}x}{\sqrt{E-U(x)}} + \sqrt{2m}\int_{-\epsilon}^{\epsilon}\frac{\mathrm{d}x}{\sqrt{E-U(x)}} + \sqrt{2m}\int_{\epsilon}^{b}\frac{\mathrm{d}x}{\sqrt{E-U(x)}}. \tag{2}$$

We can choose ϵ to satisfy the following inequalities

$$\sqrt{\frac{\Delta}{|U_0''|}} \ll \epsilon \ll \frac{|U_0''|}{|U_0'''|}. \tag{3}$$

One of these inequalities allows us to approximate the potential $U(x)$ by a quadratic polynomial in the interval $-\epsilon < x < \epsilon$. The other inequality will be important for connecting the three x-intervals in Eq. (2). Note that the above equation can only be satisfied if

$$\sqrt{\frac{\Delta}{|U_0''|}} \ll \frac{|U_0''|}{|U_0'''|}, \tag{4}$$

and it is important to emphasize that this equation is always satisfied provided that Δ is sufficiently small.

Focusing on the contribution of the region $-\epsilon < x < \epsilon$, we write

$$
\begin{aligned}
&\int\limits_{-\epsilon}^{\epsilon} \frac{\sqrt{2m}\,\mathrm{d}x}{\sqrt{E-U(x)}} \approx \int\limits_{-\epsilon}^{\epsilon} \frac{\sqrt{2m}\,\mathrm{d}x}{\sqrt{\Delta + |U_0''|x^2/2}} = \sqrt{\frac{4m}{|U_0''|}} \int\limits_{-\sqrt{\frac{\epsilon^2|U_0''|}{2\Delta}}}^{\sqrt{\frac{\epsilon^2|U_0''|}{2\Delta}}} \frac{\mathrm{d}\xi}{\sqrt{1+\xi^2}} \\
&\approx \sqrt{\frac{4m}{|U_0''|}} \ln\left[\frac{2\epsilon^2|U_0''|}{\Delta}\right]\left(1+\mathcal{O}\left(\frac{\Delta}{|U_0''|\epsilon^2}\right)\right).
\end{aligned} \tag{5}
$$

The fact that corrections to the above formula really scale as $\Delta/(|U_0''|\epsilon^2)$, i.e. that there is no $\mathcal{O}(\Delta^0)$ term, is not obvious; one has to compute the integral over ξ explicitly and take the limit $\Delta \to 0$.

In principle, the above result can already be used to estimate the period of oscillations since as Δ becomes smaller and smaller the $\ln \Delta$ terms dominates and the above formula gives a better and better approximation to the actual T. However, the logarithm is a slow-growing function so that in practice, it is important to compute T accounting for *both* $\ln \Delta$ and $\mathcal{O}(\Delta^0)$ terms and neglect terms of order Δ and higher.

To this end, we need to use the result in Eq.(5) and add to it contributions of the two outer regions

$$
T \approx \sqrt{\frac{4m}{|U_0''|}} \ln\left[\frac{2\epsilon^2 U''}{\Delta}\right] + \sqrt{2m}\int\limits_a^{-\epsilon} \frac{\mathrm{d}x}{\sqrt{E-U(x)}} + \sqrt{2m}\int\limits_{\epsilon}^{b} \frac{\mathrm{d}x}{\sqrt{E-U(x)}}. \tag{6}
$$

As the next step, we will try to get rid of the parameter ϵ. The key observation is that since we have chosen $|U_0''|\epsilon^2 \gg \Delta$, we can set $E = U_0$ in the remaining integrals in Eq.(6). Then, we find

$$
T \approx \sqrt{\frac{m}{|U_0''|}} \ln\left[\frac{2\epsilon^2|U_0''|}{\Delta}\right] + \sqrt{2m}\int\limits_a^{-\epsilon} \frac{\mathrm{d}x}{\sqrt{U_0-U(x)}} + \sqrt{2m}\int\limits_{\epsilon}^{b} \frac{\mathrm{d}x}{\sqrt{U_0-U(x)}}, \tag{7}
$$

where, in comparison to Eq.(2), we took the limit $E \to U_0$ where appropriate.

In principle, Eq.(7) provides the desired result. However, it does not look satisfactory since Eq.(7) contains the auxiliary parameter ϵ. To get rid of it, we write

$$\int_{\epsilon}^{b} \frac{\mathrm{d}x}{\sqrt{U_0 - U(x)}} = \int_{\epsilon}^{b} \mathrm{d}x \left[\frac{1}{\sqrt{U_0 - U(x)}} - \frac{1}{\sqrt{|U_0''|x^2/2}} \right] + \int_{\epsilon}^{b} \frac{\mathrm{d}x}{\sqrt{\frac{|U_0''|x^2}{2}}}$$
$$= \int_{0}^{b} \mathrm{d}x \left[\frac{1}{\sqrt{U_0 - U(x)}} - \frac{1}{\sqrt{|U_0''|x^2/2}} \right] + \sqrt{\frac{2}{|U_0''|}} \ln \frac{b}{\epsilon} + \mathcal{O}(\epsilon). \tag{8}$$

Repeating the calculation to describe the contribution of the region $a < x < -\epsilon$, we obtain our final result

$$T \approx \sqrt{\frac{4m}{|U_0''|}} \ln \left[\frac{2|ab||U_0''|}{\Delta} \right] + \int_{a}^{b} \mathrm{d}x \left[\frac{1}{\sqrt{U_0 - U(x)}} - \frac{1}{\sqrt{|U_0''|x^2/2}} \right] + \mathcal{O}(\Delta). \tag{9}$$

Note, that the dependence on the auxiliary parameter ϵ is gone.

To summarize, we have found an approximate expression for the period of oscillations of a particle in an *arbitrary* potential under the assumption that the energy of the particle is close to the local maximum of the potential. The leading term in this expansion $\sqrt{\frac{4m}{|U_0''|}} \ln \frac{2|U_0''||ab|}{\Delta}$ depends on the second derivative of the potential at the local maximum and the length of the x interval available to a particle with the energy $E \sim U_0$. The Δ-independent term depends on the *global* properties of the potential; to compute it the exact formula of the potential is needed.

This example shows one of the many ways of how perturbative expansion can appear – we begin with an exact expression, identify a small parameter and simplify the computation setting the small parameter to zero where appropriate. An important trick that we used here to compute an integral that depends on a small parameter is the splitting of the integration region into different intervals chosen in such a way that in each of the intervals we could simplify integrands, albeit for different reasons.

Differential equations

Another class of problems where perturbation theory is often used refers to differential equations that depend on a small parameter. Sometimes the choice of the small parameter is obvious and sometimes it is less so, and sometimes even if the small parameter *is* obvious, it is not clear how a perturbative expansion can be set up.

A good example is the *quasi-classical limit* in quantum mechanics. Consider a Schrödinger equation

$$\left(-\frac{\hbar^2 \mathrm{d}^2}{2m\mathrm{d}x^2} + V(x) - E\right)\Psi = 0. \tag{10}$$

It is well known that $\hbar$ is small.[1] How can the smallness of $\hbar$ be exploited? A systematic approximation that allows us to solve any Schrödinger equation in a closed form assuming of course that $\hbar$ can be considered to be small is known as the WKB approximation. To see that this approximation is non-trivial, we can just take the limit $\hbar \to 0$ in Eq.(10). The result then looks as follows

$$\left(V(x) - E\right)\Psi(x) = 0, \tag{11}$$

which implies $\Psi(x) \sim \delta(V(x) - E)$. This solution, obviously, has nothing to do with the expected behavior of the wave function. We will discuss how to construct a proper perturbation theory for the Schrödinger equation using $\hbar$ as a parameter later in the course; for now let us just say that the reason for this pathological behavior in the limit $\hbar \to 0$ is related to the fact that $\hbar$ multiplies the differential operator in the differential equation. By naively setting $\hbar$ to zero, we completely change the nature of the equation since we turn the differential equation into an algebraic equation.

Next, we will discuss yet another example of a perturbative expansion where the small parameter is not obvious. Consider a pendulum of length l with the mass m attached to its end point; pendulum's pivot moves up and down with an amplitude $a\cos\gamma t$. Suppose that the frequency γ is very large. We would like to describe the pendulum's motion. We choose angle φ to describe the position of the pendulum and construct the Lagrange function[2]

$$L = \frac{ml^2\dot{\varphi}^2}{2} - ma\gamma^2 l\cos(\gamma t)\ \cos(\varphi) + mgl\ \cos(\varphi). \tag{12}$$

The Euler-Lagrange equation of motion then easily follows

$$ml^2\ddot{\varphi} = ma\gamma^2 l\cos(\gamma t)\ \sin(\varphi) - mgl\ \sin(\varphi). \tag{13}$$

We would like to understand how this equation can be solved in the limit when γ is very large. To simplify the discussion we also assume that a/l is small.

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[1] Of course $\hbar$ is a dimensionfull quantity, so in order to say that it is small we need to compare it to something. But we still know that it is small...

[2] To arrive at the Lagrange function shown below, we discard certain total time-derivatives.

To set up a perturbative expansion, we write $\varphi(t) = s(t) + r(t)$ where the two functions $s(t)$ and $r(t)$ describe slow and rapid oscillations. Working in an approximation of small φ, we expand the above equation through terms that are linear in φ and find

$$ml^2\left(\ddot{s} + \ddot{r}\right) = ma\gamma^2 l\cos(\gamma t)\,(s + r) - mgl\,(s + r). \tag{14}$$

We recognize that in this equation there are terms that oscillate fast and there are terms that oscillate slow; of course, these terms should satisfy the equation separately. Since rapid oscillations are driven by the pivot's motion with the amplitude a, we expect $r(t) \sim a/l \ll 1$ whereas $s(t) \sim 1$. Hence, the equation for the leading fast term reads

$$ml^2\ddot{r} = ma\gamma^2 l\cos(\gamma t)\,s(t). \tag{15}$$

To solve this equation, we can neglect the time dependence of the function $s(t)$ since it does not change much on the time scale at which the function $r(t)$ changes. Hence, the solution of Eq. (15) reads

$$r(t) = -\frac{a}{l}\cos(\gamma t)s(t). \tag{16}$$

We now substitute the solution Eq.(16) back into Eq.(14) and average the resulting equation over the period of fast oscillations $2\pi/\gamma$. We then obtain an equation for $s(t)$

$$ml^2\,\ddot{s} = -\frac{ma^2\gamma^2}{2}s - mgls. \tag{17}$$

This equation describes small oscillations of a pendulum with the frequency

$$\omega^2 = \frac{g}{l} + \frac{a^2\gamma^2}{2l^2}. \tag{18}$$

The full solution is then described by the modulated oscillations

$$\varphi(t) = A\left(1 - \frac{a}{l}\cos(\gamma t)\right)\cos(\omega t + \theta_0) \tag{19}$$

We note that since γ is very large, it can compensate smallness of a/l and lead to significant differences between g/l and ω^2.

To summarize, the small parameter in this example is the ratio of frequencies of slow and fast oscillations. As we have seen, developing the perturbation theory in this parameter is not trivial.

Validity of perturbation theory

Having discussed how to set up a calculation of a particular quantity using a perturbation theory, it is interesting to ask if perturbative expansions are helpful. You may think that this is a strange question since we know of plenty of examples in physics were predictions based on perturbation theory are, actually, very important and, apparently, not too wrong.

However, it is instructive to contrast this practical knowledge with the following classic example. We are interested in computing ground state energy of *anharmonic* oscillator described by the Hamiltonian

$$H = \frac{p^2}{2} + \frac{\omega^2 x^2}{2} + \lambda x^4. \tag{20}$$

We would like to solve the Schrödinger equation

$$H\Psi(x) = E_0 \Psi, \tag{21}$$

subject to the boundary condition $\Psi(x) \to 0$ as $|x| \to \infty$ and determine the energy of the ground state E_0 as a function of ω and λ.

It is well-known that we can not solve the Schrödinger equation Eq.(21) exactly but, assuming that λ is sufficiently small, we can use perturbation theory. To this end, we write

$$E_0 = \frac{\omega}{2} + \omega \sum_{k=1}^{\infty} C_k \left(\frac{\lambda}{\omega^3} \right)^k \tag{22}$$

We can compute coefficients C_k using perturbation theory for non-degenerate levels. The coefficient C_1 is given by the following formula

$$\frac{C_1}{\omega^2} = \langle 0 | x^4 | 0 \rangle, \tag{23}$$

whereas the coefficient C_2 reads

$$\frac{C_2}{\omega^5} = \sum_{k \neq 0}^{\infty} \frac{\langle 0 | x^4 | k \rangle \langle k | x^4 | 0 \rangle}{\frac{\omega}{2} - E_k}, \tag{24}$$

where E_k are energy eigenvalues of the Hamiltonian Eq.(20) at $\lambda = 0$.

Both C_1 and C_2 can be computed with some effort using available results for energy eigenvalues and wave functions for the quantum oscillator problem.

However, there is a much more efficient way to compute these coefficients C_k.[3] The result of the computation reads

$$\begin{aligned} &C_1 = \frac{3}{4}, \quad C_2 = -\frac{21}{8}, \quad C_3 = \frac{333}{16}, \quad C_4 = -\frac{30\,885}{128}, \\ &C_5 = \frac{916\,731}{256}, \quad C_6 = -\frac{65\,518\,401}{1\,024}, \quad \dots \quad C_9 = \frac{54\,626\,982\,511\,455}{65\,536}. \end{aligned} \tag{25}$$

We note that these results imply an impressive growth in the expansion coefficients! Indeed, we start with $C_1 = 0.75$ and by the time we get to the ninth term in the expansion, we find $C_9 \sim 10^8$! It can be shown that the explosive growth of perturbative coefficients can be described by the following formula

$$C_k \sim 3^k (-1)^{k+1} \sqrt{\frac{6}{\pi^3}}\, \Gamma\left(k + \frac{1}{2}\right) \left(1 - \frac{95}{72k} + \mathcal{O}(k^{-2})\right). \tag{26}$$

Since $\Gamma(k+1/2) \sim k!$, the perturbative expansion of the ground state energy experiences *factorial growth*. It is then obvious that this series has *vanishing* radius of convergence which implies that no matter how small λ actually is, the series fails to converge to the right answer!

There are several immediate questions that arise:

- why does this happen?
- is the perturbative expansion as we teach it in quantum mechanics (and in quantum field theory etc.) useful after all?
- how can we use this strange series to learn anything about the *true* energy of the ground state of the anharmonic oscillator?

Lets first discuss the answer to the first question – why does it happen.[4] The answer to this question is that the point $\lambda = 0$ is peculiar. Indeed, an existence of the series expansion of the ground state energy in λ in Eq.(21) tacitly implies that the energy of the ground state E is an analytic function of the coupling constant λ meaning that things do not change much between small negative and small positive values of λ. However, it is quite obvious that this can not be the case since the potential at arbitrary small but *negative*

[3] C. Bender and T.T. Wu, 1969.

[4] The first argument that perturbative series in QED can not be convergent was given by F.Dyson in 1952.

λ's is unbounded from below so that the ground state located around $x = 0$ becomes a metastable state. Hence, the perturbative expansion of the ground state in powers of λ should have zero radius of convergence and this is what we see in an explicit computation.

Apart from having the vanishing radius of convergence, the perturbative expansion of the ground state energy has another interesting feature. Indeed, by using perturbative series, we can improve the prediction for the ground state energy up to values of k that are of the order of $\omega^3/(3\lambda)$ but after that series starts to diverge. If λ is small, we can still use quite a large number of terms in the series to get a good estimate of the ground state energy. In fact, the error that we make by truncating series at $k \sim \omega^3/(3\lambda)$ is controlled by $\exp(-\omega^3/(3\lambda))$; so the smaller λ is, the smaller the inevitable error will be. Moreover, it turns out that these divergent perturbative series can be summed up to obtain an estimate of the exact value of the ground state energy even for large values of λ.

To summarize, sometimes the perturbative expansion leads to pathological, divergent series. However, these series can still be used and worked with and, if treated properly, they can give us fairly accurate answers to questions that we try to address to begin with, so not everything is lost.

2 Local analysis of linear differential equations

We begin with discussing approximate solutions of differential equations that can be constructed *locally*; i.e. they provide approximations to solutions of differential equations close to particular points. To make this more precise, consider a homogeneous linear differential equation

$$y^{(n)}(x) + p_{n-1}(x)y^{(n-1)}(x) \cdots + p_1(x)y^{(1)}(x) + p_0(x)y(x) = 0, \tag{27}$$

where we used the notation $y^{(n)}(x) = \mathrm{d}^n y/\mathrm{d}x^n$.

Suppose we pick a point on the x-axis; we will refer to this point x_0. We are interested in understanding how solutions to the differential equation Eq.(27) behave in the immediate vicinity of the point x_0. Not surprisingly, this behavior is controlled by the behavior of the functions $p_n(x)$ at $x = x_0$. In fact, we distinguish three types of points that one refers to as *i*) *regular points* of a differential equation or *ii*) *singular regular* points of a differential equation or *iii*) *irregular singular* points. This nomenclature is explained below.

Regular points. A point $x = x_0$ is a *regular* point of a differential equation Eq.(27) if all coefficient functions $p_k(x)$ in Eq.(27) are analytic in the neighborhood of $x = x_0$. All n solutions of Eq.(27) can be represented as Taylor series at $x = x_0$

$$y(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n. \tag{28}$$

The coefficients a_n of these solutions are determined recursively from the differential equation. The series converge for $|x - x_0|$ smaller than the distance between x_0 and the closest singularity of any of the functions $p_k(x)$ in the complex x-plane.

We will consider a few examples, to illustrate how this works. We begin with the following equation

$$y' - 2xy = 0. \tag{29}$$

The point $x = 0$ is a regular point; therefore, we write

$$y(x) = \sum_{n=0}^{\infty} a_n x^n. \tag{30}$$

Substituting the series into the above equation, we find

$$\sum_{n=0}^{\infty} a_n n x^{n-1} = 2 \sum_{n=0}^{\infty} a_n x^{n+1}. \tag{31}$$

Requiring that coefficients of same powers of x coincide, we find the recurrence relation

$$a_{n+2}(n+2) = 2a_n, \quad a_1 = 0. \tag{32}$$

It follows that $a_3, a_5, .., a_{2k+1} = 0$ and

$$a_{n+2} = \frac{2a_n}{n+2}, \tag{33}$$

for even n. Writing $n = 2k$, we find

$$a_{2k+2} = \frac{a_{2k}}{k+1}, \tag{34}$$

so that

$$a_{2k} = \frac{a_0}{k!}. \tag{35}$$

The function $y(x)$ becomes

$$y(x) = \sum_{k=0}^{\infty} \frac{a_0}{k!} x^{2k} = a_0 e^{x^2}. \tag{36}$$

One can check that this function is indeed the solution of the differential equation Eq.(29). We also observe that the solution is determined up to an unknown constant a_0; this is indeed what should be expected since we have to specify one boundary condition to fully determine a solution of a first-order differential equation.

Regular singular points. A more involved case is that of a *regular singular* point. A point $x = x_0$ is called a regular singular point of the differential equation Eq.(27) if some of the functions $p_k(x)$ are not analytic at $x = x_0$ but *all* functions $(x - x_0)^{n-k} p_k(x)$ are analytic at $x = x_0$. The general theory of differential equations states that in the vicinity of a regular singular point there is *at least one* solution of the differential equation Eq.(27) that has the so-called Frobenius form

$$y(x) = (x - x_0)^{\alpha} \sum_{n=0}^{\infty} a_n (x - x_0)^n. \tag{37}$$

The quantity α is called *indicial exponent*. Of course, one solution is insufficient to fully describe solutions of an n-th order differential equation. We will discuss how other solutions can be obtained after discussing solutions in Frobenius form.

As an example, consider the second-order differential equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \frac{y}{4x^2} = 0. \tag{38}$$

The polynomials $p_{1,0}(x)$ that appear in this equation are $p_1 = 0$ and $p_0 = 1/(4x^2)$. Since $xp_1 = 0$ and $x^2 p_0 = 1/4$ are both analytic functions in the entire complex plane, $x = 0$ is a regular singular point. To find solutions at small x, we make an Ansatz for $y(x)$ in the Frobenius form $y(x) = x^\alpha \sum\limits_{n=0}^{\infty} a_n x^n$, substitute it into the differential equation Eq.(38) and obtain

$$\sum_{n=0}^{\infty} a_n \left((n+\alpha)(n-1+\alpha) + \frac{1}{4} \right) x^{n+\alpha-2} = 0. \tag{39}$$

Suppose $a_0 \neq 0$; this is only possible if

$$\alpha(\alpha - 1) + \frac{1}{4} = \left(\alpha - \frac{1}{2} \right)^2 = 0. \tag{40}$$

It follows that $\alpha = 1/2$. Since for $\alpha = 1/2$,

$$\left((n+\alpha)(n-1+\alpha) + \frac{1}{4} \right) \neq 0, \quad n > 0, \tag{41}$$

we conclude from Eq.(39) that $a_{n>0} = 0$. Hence, $y(x) = a_0 \sqrt{x}$ is a solution in the Frobenius form.

As was stated above, the existence of *only one* solution in the Frobenius form is, in general, guaranteed. However, any second order differential equation must have two independent solutions. We have found one of them and we would like to understand how to find the second one. To this end, we modify the differential equation Eq.(38) as follows

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \frac{1 - 4\epsilon^2}{4x^2} y(x) = 0, \tag{42}$$

where ϵ is a small parameter. The point $x = 0$ remains a regular singular point.

Repeating the above computation, we find an equation for indicial exponent

$$\left(\alpha - \frac{1}{2} \right)^2 = \epsilon^2, \tag{43}$$

so that *two* Frobenius solutions appear

$$\alpha_{\pm} = \frac{1}{2} \pm \epsilon. \tag{44}$$

Therefore,

$$y(x) = y_+(x) + y_-(x) = a_+ x^{1/2+\epsilon} + a_- x^{1/2-\epsilon}. \tag{45}$$

If the limit $\epsilon \to 0$ is taken, the two solutions become degenerate. Hence, two solutions that remain independent also in the $\epsilon \to 0$ limit can be constructed as follows

$$y(x) = a_0 \lim_{\epsilon\to 0} y_+(x) + a_1 \lim_{\epsilon\to 0} \frac{y_+(x) - y_-(x)}{2\epsilon} = a_0\sqrt{x} + a_1\sqrt{x}\ln(x). \tag{46}$$

We note that the second solution $y(x) \sim \sqrt{x}\ln x$ does not have the Frobenius form, cf. Eq. (37).

To discuss this issue from a more general perspective, consider a differential equation with a regular singular point at $x = x_0$

$$y''(x) + \frac{p(x)}{(x-x_0)}\, y'(x) + \frac{q(x)}{(x-x_0)^2} y(x) = 0. \tag{47}$$

The two functions $p(x)$ and $q(x)$ are analytic at $x = x_0$. To construct solutions of the differential equation Eq. (47), we expand these functions in a series around $x = x_0$

$$p(x) = \sum p_n (x-x_0)^n, \quad q(x) = \sum q_n (x-x_0)^n. \tag{48}$$

We will look for the solution in the Frobenius form

$$y(x) = (x-x_0)^{\alpha} \sum_{n=0}^{\infty} a_n (x-x_0)^n. \tag{49}$$

Substituting these expansions in Eq.(47), we find the following recursion relation for the coefficients a_n

$$a_n(n+\alpha)(n-1+\alpha) + \sum_{m=0}^{n} \left(p_m(n-m+\alpha) + q_m\right) a_{n-m} = 0. \tag{50}$$

We take $n = 0$ and find

$$a_0 P(\alpha) = 0, \tag{51}$$

where

$$P(\alpha) = \alpha(\alpha-1) + p_0\alpha + q_0. \tag{52}$$

This function is called *indicial polynomial*. Assuming $a_0 \neq 0$, we find possible values of α by solving the equation

$$P(\alpha) = 0. \tag{53}$$

The solutions read

$$\alpha_\pm = \frac{1 - p_0 \pm \sqrt{(p_0-1)^2 - 4q_0}}{2}. \tag{54}$$

Then,

$$a_1 = -\frac{(p_1\alpha + q_1)a_0}{P(1+\alpha)}, \ldots, \; a_n = -\frac{((p_1(n-1+\alpha)+q_1)\, a_{n-1} + \cdots}{P(n+\alpha)}. \tag{55}$$

It follows from the above discussion that if Eq.(53) admits two solutions $\alpha_\pm$ such that $\alpha_+ - \alpha_-$ is not an integer number, then both independent solutions of the differential equation have Frobenius form.

We will now discuss what happens in two special cases: $\alpha_+ = \alpha_-$ and $\alpha_+ - \alpha_- = N$, where N is integer. We will start with the case $\alpha_+ = \alpha_-$ and explain how to construct the second solution starting from the Frobenius solution. To this end, consider Eq.(47), use the ansatz Eq.(49) there and solve the recurrence relation *ignoring* Eq.(53). We will denote the solution obtained following this procedure $y(x,\alpha)$.

It is easy to check that this function satisfies the following differential equation

$$\hat{L}\; y(\alpha, x) = a_0(x-x_0)^{\alpha-2}P(\alpha), \tag{56}$$

where the differential operator L is defined as

$$\hat{L} = \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{p(x)}{x-x_0}\frac{\mathrm{d}}{\mathrm{d}x} + \frac{q(x)}{(x-x_0)^2}. \tag{57}$$

In case when the two solutions of Eq.(53) are degenerate, the indicial polynomial reads $P(\alpha) = (\alpha-\alpha_1)^2$. Hence, it follows from Eq.(56) that $y(x,\alpha_1)$ is the solution of the original differential equation since the right hand side of Eq.(56) vanishes if we use $\alpha = \alpha_1$ there. This is the solution in the Frobenius form that we have already found.

To construct the second solution, we note that a derivative of Eq.(56) w.r.t. α also has a vanishing right hand side at $\alpha = \alpha_1$ since $\mathrm{d}P(\alpha)/\mathrm{d}\alpha = 0$

for $\alpha = \alpha_1$. Hence, to construct the second solution, we take a derivative of Eq.(56) w.r.t α and, once the derivative is computed, set $\alpha = \alpha_1$. We find

$$\hat{L} \frac{\partial y(x,\alpha)}{\partial \alpha}|_{\alpha=\alpha_1} = 0, \tag{58}$$

which implies that $\partial y(x,\alpha)/\partial\alpha|_{\alpha=\alpha_1}$ is also a solution of the original differential equation.

We can expose the form of the second solution by taking the derivative of $y(x,\alpha) = (x-x_0)^\alpha \sum\limits_{n=0}^{\infty} a_n(\alpha)(x-x_0)^n$ with respect to α. It becomes clear that the second independent solution can be written in the following way

$$y_2(x) = \ln(x-x_0)y_1(x) + (x-x_0)^\alpha \sum_{n=0}^{\infty} b_n(x-x_0)^n, \tag{59}$$

where $y_1(x)$ is the Frobenius solution. To find the coefficients b_n, we make use of the fact that $y_1(x)$ is known, insert Eq.(59) into the differential equation Eq.(47) and obtain recurrence relations for coefficients b_n. We do not show these relations here since it is fairly straightforward to obtain them.

The second special case that we need to consider is $\alpha_1 = \alpha_2 + N$, where N is a positive integer. We assume that we constructed a Frobenius solution for $\alpha = \alpha_1$. Note that if we attempted to construct a Frobenius solution for α_2, we would have run into a problem because for computing a_N we need to divide by $P(\alpha_2 + N) = P(\alpha_1) = 0$. Nevertheless, we can can make use of Eq.(56) by doing the following. Writing

$$\hat{L}(\alpha-\alpha_2)y(x,\alpha) = a_0(x-x_0)^{\alpha-2}(\alpha-\alpha_2)^2(\alpha-\alpha_1) \tag{60}$$

and taking derivative of both sides w.r.t α and evaluating the result at $\alpha = \alpha_2$, we find

$$\hat{L}\frac{\partial}{\partial\alpha}\left[(\alpha-\alpha_2)y(x,\alpha)\right]_{\alpha=\alpha_2} = 0. \tag{61}$$

Hence, the second independent solution is

$$y_2(x) = \lim_{\alpha\to\alpha_2}\frac{\partial}{\partial\alpha}\left[(\alpha-\alpha_2)y(x,\alpha)\right]. \tag{62}$$

We will consider an example to illustrate the construction of the second independent solution. Consider the Bessel equation

$$y''(x) + \frac{1}{x}y'(x) + \frac{x^2-4}{x^2}y(x) = 0. \tag{63}$$

The point $x = 0$ is a regular singular point. Hence, we look for a Frobenius solution

$$y(x) = a_0 x^\alpha \sum_{n=0}^{\infty} r_n x^n. \tag{64}$$

Without loss of generality, we assume that $r_0 = 1$. We then find

$$r_0(\alpha^2 - 4) = 0, \qquad r_{n+2} = -\frac{r_n}{(\alpha + n + 2)^2 - 4}. \tag{65}$$

It follows $r_1, r_3, r_5, .., r_{2n+1} = 0$, $\alpha_1 = 2$ and $\alpha_2 = -2$. Since $\alpha_1 - \alpha_2 = 4$, we need to take $\alpha_1 = 2$ to construct a Frobenius-like solution. It reads

$$y_1(x) = a_0 x^2 \left(1 - \frac{x^2}{12} + \frac{x^4}{384} + \ldots\right). \tag{66}$$

To find the second independent solution, we determine $y(x, \alpha)$. It reads

$$\begin{aligned} y(x, \alpha) = \tilde{a}_0 x^\alpha \Bigg[1 &- \frac{x^2}{\alpha(\alpha + 4)} + \frac{x^4}{\alpha(\alpha + 2)(\alpha + 4)(\alpha + 6)} \\ &- \frac{x^6}{\alpha(\alpha + 2)(\alpha + 4)^2(\alpha + 6)(\alpha + 8)} + \ldots\Bigg]. \end{aligned} \tag{67}$$

We see that the above expression has poles at $\alpha = -2$ so that we can not immediately set α to -2 in that expression.

However, following the above discussion, we multiply $y(x, \alpha)$ with $(\alpha + 2)$ and find

$$\begin{aligned} (\alpha + 2)y(x, \alpha) = \tilde{a}_0 x^\alpha \Bigg[&(\alpha + 2) - (\alpha + 2)\frac{x^2}{\alpha(\alpha + 4)} + \frac{x^4}{\alpha(\alpha + 4)(\alpha + 6)} \\ &- \frac{x^6}{\alpha(\alpha + 4)^2(\alpha + 6)(\alpha + 8)} + \cdots\Bigg]. \end{aligned} \tag{68}$$

This expression is free of singularities at $\alpha = -2$ as expected.

The derivative of Eq. (68) with respect to α at $\alpha = -2$ can be easily computed. We find

$$\begin{aligned} y_2 &= \lim_{\alpha \to -2} \frac{\partial}{\partial \alpha} [(\alpha + 2)y(x, \alpha)] = \tilde{a}_0 \ln x \, x^{-2} \left[\frac{x^4}{(-16)} - \frac{x^6}{(-16)(2)(6)} + \ldots\right] \\ &+ \tilde{a}_0 x^{-2} \left[1 + \frac{x^2}{4} + \frac{x^4}{64} + \cdots\right] \\ &= -\frac{1}{16} \ln x \, y_1(x)|_{a_0 \to \tilde{a}_0} + \tilde{a}_0 x^{-2} \left[1 + \frac{x^2}{4} + \frac{x^4}{64} + \cdots\right]. \end{aligned} \tag{69}$$

This is the second independent solution of the Bessel equation.

Irregular singular points. We will move to the discussion of *irregular singular points* of differential equations. Irregular singular points are all singular points that are not regular. Note that these points can also occur at $x = \infty$; we can access such points by doing a transformation $x \to 1/\xi$ and then studying properties of the differential equation at $\xi = 0$.

To give a simple example of calculations at irregular singular point, consider the following equation

$$y' = \sqrt{x} y. \tag{70}$$

The point $x = 0$ is an irregular singular point since $x\sqrt{x}$ is not analytic at $x = 0$. It is straightforward to solve Eq.(70). We find

$$y(x) = a_0 \exp\left[\frac{2}{3}x^{3/2}\right] = a_0 \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{2}{3}x^{3/2}\right)^n. \tag{71}$$

In this case the solution is represented by absolutely convergent series but these series are not of a Taylor or Frobenius form.

We note, however, that the solution Eq.(71) reads $y(x) = e^{S(x)}$ where $S(x)$ is an algebraic function. We will try to make use of this observation in what follows. For definiteness, consider the following second order equation

$$y'' = x^{-3} y. \tag{72}$$

The point $x = 0$ is an irregular singular point. Motivated by the above observation, we make the ansatz $y(x) = e^{S(x)}$. Then

$$y' = S' y(x), \quad y'' = (S')^2 y(x) + S'' y(x). \tag{73}$$

It follows that

$$(S')^2 + S'' = \frac{1}{x^3}. \tag{74}$$

If we define $W(x) = S'(x)$, we find

$$W^2 + W' - \frac{1}{x^3} = 0, \tag{75}$$

which is the (non-linear) first-order Riccati equation. The Riccati equation is known to be equivalent to a linear second order differential equation so that, from a formal viewpoint, we made no progress.

However, progress can be made if we realise that close to $x = 0$ the two terms on the left hand side of Eq.(74) have very different magnitude.

Indeed, assume that $S(x)$ is a generic algebraic function $S(x) = ax^\beta$. Then $S' = a\beta x^{\beta-1}$ and $S'' = a\beta(\beta-1)x^{\beta-2}$. Then

$$(S')^2 \sim a^2\beta^2 x^{2\beta-2}, \qquad S'' \sim a\beta(\beta-1)x^{\beta-2}. \tag{76}$$

This implies that

$$\lim_{x\to 0} \frac{S''}{(S')^2} \sim \lim_{x\to 0} x^{-\beta} \to 0, \tag{77}$$

where in the last step we assumed that $\beta < 0$. The need to have negative β follows from Eq.(74) where *either* $(S')^2$ or S'' has to match the right hand side of the equation x^{-3}. Hence, there are two options, $\beta = -1/2$ or $\beta = -1$. However, in both case $(S')^2$ dominates over S'' in the $x \to 0$ limit since the required β is negative.

To proceed further, we will introduce the concept of asymptotic equivalence of two functions. Given two functions $f(x)$ and $g(x)$ we will say that $f(x)$ is much smaller than $g(x)$, $f(x) \ll g(x)$, at the point $x = x_0$ if

$$\lim_{x\to x_0} \frac{f(x)}{g(x)} \to 0. \tag{78}$$

We will also say that $f(x)$ is asymptotic to $g(x)$ at $x = x_0$ (the notation is $f(x) \sim g(x)$) if

$$f(x) - g(x) \ll g(x). \tag{79}$$

This implies that

$$\lim_{x\to x_0} \frac{f(x)-g(x)}{g(x)} \to 0, \quad \text{and} \quad \lim_{x\to x_0} \frac{f(x)}{g(x)} \to 1. \tag{80}$$

We note that a function *can not be asymptotic to* 0 (i.e. asymptotic relations probe and compare behaviors of functions around the singular point, not at the singular point).

To analyse Eq.(74) we note that, according to our analysis, $S'' \ll (S')^2$ at $x = 0$. Therefore,

$$S'^2 \sim \frac{1}{x^3}. \tag{81}$$

Taking the square root and solving the differential equation, we find

$$\frac{\mathrm{d}S}{\mathrm{d}x} \sim \pm\frac{1}{x^{3/2}}, \quad \Rightarrow \quad S(x) \sim \pm\frac{2}{\sqrt{x}}. \tag{82}$$

It is tempting to say that

$$y(x) \sim e^{\pm\frac{2}{\sqrt{x}}}, \tag{83}$$

i.e. that $y(x)$ is asymptotic to $e^{\pm\frac{2}{\sqrt{x}}}$. However, this statement is wrong, as we will see in a second.

Let us refine our ansatz by writing

$$S(x) = \pm\frac{2}{\sqrt{x}} + c(x). \tag{84}$$

We assume that at around $x \sim 0$,

$$c(x) \ll \frac{1}{\sqrt{x}}. \tag{85}$$

This implies that

$$c' \ll \frac{1}{x^{3/2}}, \qquad c'' \ll \frac{1}{x^{5/2}}. \tag{86}$$

We re-compute Eq.(74) using the new representation of $S(x)$ in Eq.(84) and find

$$\begin{aligned} &\left(\mp\frac{1}{x^{3/2}} + c'(x)\right)^2 + \left(\pm\frac{3}{2x^{5/2}} + c''\right) = \frac{1}{x^3}, \\ &\mp\frac{2}{x^{3/2}}c'(x) + (c'(x))^2 \pm \frac{3}{2x^{5/2}} + c'' = 0. \end{aligned} \tag{87}$$

We rewrite the last equation as follows

$$c'\left(\mp\frac{2}{x^{3/2}} + c'(x)\right) \pm \frac{3}{2x^{5/2}} + c'' = 0, \tag{88}$$

and use Eq.(86) to discard c' relative to $x^{-3/2}$ in brackets and c'' relative to $x^{-5/2}$. The above equation simplifies to

$$c'(x) \sim \frac{3}{4x}. \tag{89}$$

It's solution reads

$$c(x) \sim \frac{3}{4}\ln(x). \tag{90}$$

Hence, the approximate solution reads

$$y(x) \sim x^{3/4}e^{\pm\frac{2}{\sqrt{x}}}. \tag{91}$$

The reason that we could not have said $y(x)$ is asymptotic to $e^{\pm\frac{2}{\sqrt{x}}}$ at $x \to 0$, is that the prefactor $x^{3/4}$ goes to zero at $x = 0$ and, hence, changes the asymptotic behavior.

To prove that Eq.(91) actually provides a valid asymptotic relation between two functions, we need to check that only terms that do not grow in the limit $x \to 0$ arise if we try to improve the ansatz Eq.(84). We write

$$S(x) = \pm\frac{2}{\sqrt{x}} + \frac{3}{4}\ln(x) + D(x), \tag{92}$$

where $D(x)$ should be small compared to both $\ln(x)$ and $1/\sqrt{x}$. Hence,

$$D(x) \ll \ln(x), \qquad D'(x) \ll \frac{1}{x}, \qquad D''(x) \ll \frac{1}{x^2}. \tag{93}$$

Substituting Eq.(92) into the differential equation Eq.(84), we obtain

$$-\frac{3}{16x^2} + \frac{3}{2x}D' \mp \frac{2}{x^{3/2}}D' + (D')^2 + D'' = 0. \tag{94}$$

We make use of the relations in Eq.(93) and replace Eq.(94) with

$$-\frac{3}{16x^2} \sim \pm\frac{2}{x^{3/2}}D'. \tag{95}$$

The solution is

$$D(x) \sim \ln c_1 \mp \frac{3}{16}\sqrt{x}, \tag{96}$$

where $\ln c_1$ is a constant of integration. It follows that

$$y(x) \sim c_1\, x^{3/4} e^{\pm\frac{2}{\sqrt{x}} - \mp\frac{3}{16}\sqrt{x}}, \tag{97}$$

where all terms neglected in the function $D(x)$ vanish as $x \to 0$. The question of how to construct these series and how they behave is an important one; we will return to this question later.

The method that we have used to work out the asymptotic solution of a differential equation close to an irregular singular point is known as "method of dominant balance". Let us summarize it.

1. We drop all terms in the differential equation that appear to be small and replace an exact equation with an asymptotic relation between functions that appear there;

2. We turn the asymptotic relation into an equation by replacing the asymptotic sign $\sim$ with the equal sign; we integrate the resulting differential equation to find a solution that satisfies the asymptotic relation;

3. We check that the obtained solution is consistent with assumptions in point 1). We then refine approximations made in point 1) to account for smaller contributions to original differential equation and refine the solution.

This method and its minor modifications can be used in very different circumstances, from computing integrals to solving algebraic equations. We will discuss such applications later in this course.

We return to the discussion of the equation Eq. (72) and complete the analysis that we started. Specifically, we would like to improve on the solution to this equation given in Eq.(97). We therefore write

$$y(x) = c_1 x^{3/4} e^{\pm \frac{2}{\sqrt{x}}}\, w(x). \tag{98}$$

From our earlier analysis we know that $\lim\limits_{x\to 0} w(x) = 1$. Using the ansatz Eq.(98) in the differential equation Eq.(72), we find the equation for $w(x)$

$$w''(x) + \left(\frac{3}{2x} \mp \frac{2}{x^{3/2}}\right) w'(x) - \frac{3}{16x^2}\, w(x) = 0. \tag{99}$$

This equation again shows that $x = 0$ is an irregular point but now we are armed with the knowledge that the solution that we would like to find has a particular limit, $w(x) \to 1$ as $x \to 0$.

Therefore, to solve Eq.(99), we write $w(x) = 1 + \epsilon(x)$, assume $\epsilon(x) \ll 1$, consider leading contributions to Eq.(99) and obtain

$$\mp \frac{2}{x^{3/2}} \frac{\mathrm{d}\epsilon}{\mathrm{d}x} \sim \frac{3}{16x^2}, \tag{100}$$

where we have used $\epsilon'' \sim \epsilon'/x \sim \epsilon/x^2 \ll \epsilon'/x^{3/2}$. Hence, we find

$$\epsilon(x) \sim \mp \frac{3}{16}\, \sqrt{x}. \tag{101}$$

Having obtained $\epsilon(x)$, we can check that all the approximations that we have done earlier are valid. We then write

$$w(x) = 1 \mp \frac{3}{16}\sqrt{x} + \epsilon(x) \tag{102}$$

and repeat the calculation. We find the equation

$$2\epsilon' \sim -\frac{15}{256}. \tag{103}$$

It follows that

$$\epsilon(x) \sim -\frac{15}{512}x, \tag{104}$$

and, as the result,

$$w(x) = 1 \mp \frac{3}{16}\sqrt{x} - \frac{15}{512}x + \epsilon(x). \tag{105}$$

We can continue to improve the approximation for the function $w(x)$ but we can also solve the problem in full generality if we realize that $w(x)$ admits an expansion in $\sqrt{x}$. We then write

$$w(x) = \sum_{n=0}^{\infty} a_n x^{n/2}, \tag{106}$$

with $a_0 = 1$, substitute this expression into Eq.(99) and obtain

$$\begin{aligned} \sum_{n=1}^{\infty} a_n \frac{n}{2}\left(\frac{n}{2} - 1\right) x^{n/2-2} + \frac{3}{2}\sum_{n=1}^{\infty} \frac{n}{2} a_n x^{n/2-2} \mp 2 \sum_{n=1}^{\infty} a_n \frac{n}{2} x^{n/2-5/2} \\ - \frac{3}{16}\sum_{n=0}^{\infty} a_n x^{n/2-2} = 0. \end{aligned} \tag{107}$$

The recurrence relation follows

$$a_{n+1} = \pm\frac{4n^2 + 4n - 3}{16(n+1)} a_n = \pm\frac{(2n-1)(2n+3)}{16(n+1)} a_n. \tag{108}$$

The recursion starts with $a_0 = 1$. It is easy to write down the general solution using properties of the so-called Γ-function, defined through

$$z\Gamma(z) = \Gamma(z+1), \quad \Gamma(1) = 1, \quad \Gamma(1/2) = \sqrt{\pi}. \tag{109}$$

We find

$$a_n = -(\pm 1)^n \frac{\Gamma(n-1/2)\Gamma(n+3/2)}{\pi 4^n n!}. \tag{110}$$

The solutions become

$$y(x) \sim -\frac{C_1}{\pi} x^{4/3}\, e^{\pm 2/\sqrt{x}} \sum_{n=0}^{\infty} (\pm 1)^n \frac{\Gamma(n-1/2)\Gamma(n+3/2)}{4^n n!} x^{n/2}. \tag{111}$$

Note that we insist on writing an asymptotic relation between the solution $y(x)$ and the r.h.s. of Eq.(111). This is so because the series that appear on the r.h.s. of Eq.(111) are, actually, divergent and, moreover, their radius of convergence is zero. So eventually we will have to explain what we do with these series or, in other words, we will have to explain the relation between series shown in Eq. (111) and the true solutions of the differential equation Eq. (72).

Finally, we will make a remark concerning the Schrödinger equation. We write it in the following way

$$y'' = Q(x)y. \tag{112}$$

Without loss of generality, we will assume that $x = 0$ is an irregular point of this equation. We then write $y(x) = e^{S(x)}$ and find

$$(S')^2 + S'' = Q(x). \tag{113}$$

Assuming $S'' \ll (S')^2$, we obtain

$$S(x) \sim \pm \int^x \mathrm{d}t \ (Q(t))^{1/2} . \tag{114}$$

We then write

$$S(x) = \pm \int^x \mathrm{d}t \ (Q(t))^{1/2} + c(x), \tag{115}$$

where it is assumed that

$$c(x) \ll \int^x \mathrm{d}t \ (Q(t))^{1/2} . \tag{116}$$

This equation implies

$$c'(x) \ll (Q(x))^{1/2} , \quad c''(x) \ll \frac{Q'}{\sqrt{Q(x)}}. \tag{117}$$

We then substitute the new ansatz Eq.(115) into the differential equation Eq.(112) and obtain

$$\pm 2\sqrt{Q(x)}c' + (c')^2 \pm \frac{Q'}{2\sqrt{Q(x)}} + c'' = 0. \tag{118}$$

Using Eq.(117), we simplify the above equation and find

$$\pm 2\sqrt{Q}c' \sim \mp \frac{1}{2}\frac{Q'}{\sqrt{Q}}, \quad \Rightarrow \quad c' \sim \frac{Q'}{4Q}, \quad c \sim \ln Q^{1/4}. \tag{119}$$

Hence, we obtain the asymptotic form of the solution of the Schrödinger equation in the vicinity of an irregular singular point that we have chosen to be $x = 0$. It reads

$$y(x) \sim (Q(x))^{1/4} e^{\pm \int^{x} \mathrm{d}t \, (Q(t))^{1/2}} . \tag{120}$$

3 Irregular singular points at infinity

In the previous lecture we talked about irregular singular points of linear differential equations. However, we mostly discussed singularities at $x = 0$ which, of course, is equivalent to any other finite point on the x-axis. However, there are many cases when differential equations have irregular singular points at $x = \infty$ and we would like to discuss such cases.

The simplest example is that of a Schrödinger equation. We will consider the Schrödinger equation that describes the harmonic oscillator

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi + \frac{2m}{\hbar^2}\left(E - \frac{m\omega^2 x^2}{2}\right)\Psi = 0. \tag{121}$$

Clearly, any finite point x is a regular point of this differential equation. To analyze what happens at $x = \infty$, we change variables $x = 1/\xi$ and write

$$\frac{\mathrm{d}}{\mathrm{d}x} = -\xi^2\frac{\mathrm{d}}{\mathrm{d}\xi}. \tag{122}$$

This implies

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} = \xi^2\frac{\mathrm{d}}{\mathrm{d}\xi}\,\xi^2\frac{\mathrm{d}}{\mathrm{d}\xi} = \xi^4\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + 2\xi^3\frac{\mathrm{d}}{\mathrm{d}\xi}. \tag{123}$$

We substitute this differential operator into Eq.(121), divide both sides of Eq.(121) by ξ^4 and obtain

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}\xi^2} + \frac{2}{\xi}\frac{\mathrm{d}\Psi}{\mathrm{d}\xi} + \frac{2m}{\hbar^2}\left(\frac{E}{\xi^4} - \frac{m\omega^2}{2\xi^6}\right)\Psi = 0. \tag{124}$$

Clearly, $\xi = 0$ or, equivalently, $x = \infty$ is an irregular singular point.

To analyze the behavior of the wave function at $\xi = 0$, we write $\Psi = e^{S(\xi)}$, substitute this ansatz into Eq.(124) and obtain

$$(S')^2 + S'' + \frac{2}{\xi}S' + \frac{2m}{\hbar^2}\left(\frac{E}{\xi^4} - \frac{m\omega^2}{2\xi^6}\right) = 0. \tag{125}$$

Picking up two terms responsible for the most singular behavior at $\xi \to 0$, we find the simplified equation

$$(S')^2 = \frac{m^2\omega^2}{\hbar^2\xi^6}. \tag{126}$$

It follows

$$S' = \pm\frac{m\omega}{\hbar\xi^3} \quad \to \quad S = \pm\frac{m\omega}{2\hbar\xi^2} = \pm\frac{m\omega x^2}{2\hbar}. \tag{127}$$

If we require that the wave function satisfies the standard boundary condition at infinity, we have to select the solution that decreases in the limit $|x| \to \infty$. To improve the approximation, we write

$$\Psi(x) \sim \exp\left[-\frac{m\omega x^2}{2\hbar} + c(\xi)\right], \tag{128}$$

substitute this ansatz into Eq.(124) and find

$$c'' + c'\left(c' + \frac{2}{\xi} + \frac{2m\omega}{\hbar\xi^3}\right) + \frac{2Em}{\hbar^2\xi^4} - \frac{m\omega}{\hbar\xi^4} = 0. \tag{129}$$

Since $c(\xi)$ should be a small correction to $m\omega/(\hbar\xi^2)$, it follows that

$$c'(\xi) \ll \frac{1}{\xi^3}, \quad c''(\xi) \ll \frac{1}{\xi^4}. \tag{130}$$

Also,

$$c'' \sim \frac{c'}{\xi} \ll \frac{c'}{\xi^3}. \tag{131}$$

Therefore, Eq.(129) simplifies to

$$c'\frac{2m\omega}{\hbar\xi^3} + \frac{2Em}{\hbar^2\xi^4} - \frac{m\omega}{\hbar\xi^4} = 0 \;\Rightarrow\; \xi c' = -\left(\frac{E}{\hbar\omega} - \frac{1}{2}\right), \tag{132}$$

and the solution reads

$$c(\xi) = -\left(\frac{E}{\hbar\omega} - \frac{1}{2}\right)\ln(\xi). \tag{133}$$

Substituting this result back into Eq.(128) and writing the result in terms of $x = 1/\xi$, we find

$$\Psi(x) \sim x^{E/(\hbar\omega)-\frac{1}{2}} e^{-\frac{m\omega x^2}{2\hbar}}. \tag{134}$$

Although this asymptotic behavior may look strange, it all falls into place if we recall that stationary normalizable states are only possible for $E = E_n = \hbar\omega(n + 1/2)$. Hence,

$$\Psi_n(x) \sim x^n e^{-\frac{m\omega x^2}{2\hbar}}, \qquad x \to \infty. \tag{135}$$

An interesting aspect of this analysis is that it allows us to look at the anharmonic oscillator problem from a slightly different perspective. Indeed, let us add an additional term λx^4 to the potential energy in Eq.(121) and study the behavior of the wave function at infinity. We find the leading order equation

$$(S')^2 = \frac{2m\lambda}{\hbar^2}\frac{1}{\xi^8}, \tag{136}$$

so that

$$S = \pm\sqrt{\frac{2m\lambda}{\hbar^2}}\frac{1}{3\xi^3} \tag{137}$$

Computing the sub-leading term we find

$$\Psi_{x\to+\infty} \sim \exp\left[-\sqrt{\frac{2m\lambda}{\hbar^2}}\frac{x^3}{3} - \frac{m^2\omega^2}{2\hbar\sqrt{2\lambda m}}x + \ldots\right] \tag{138}$$

This asymptotic behavior shows that at large x the term λx^4 is not a small perturbation compared to $m\omega^2 x^2$ and that, in fact, the large x asymptotic is controlled by the term λx^4. When we treat λx^4 as a perturbation, we bypass this problem but the theory knows that we do something that is not fully legitimate and tells us about it through perturbative series with vanishing radius of convergence.

In fact, both perturbative series for the ground state energy of an anharmonic oscillator and series that often describe the behavior of the solutions of differential equations close to singular irregular points are so-called *asymptotic series*.

Asymptotic series are defined as follows: a power series $\sum a_n(x-x_0)^n$ is said to be asymptotic to the function $f(x)$ at the point $x = x_0$ if

$$f(x) - \sum^{N} a_n(x-x_0)^n \ll (x-x_0)^N, \tag{139}$$

for every N, as $x \to x_0$. Some variations on this definition exist. For example, if $x_0 = \infty$, the definition of asymptotic series changes. The series $\sum a_n x^{-\alpha n}$, $\alpha > 0$ is asymptotic to the function $f(x)$ at $x = \infty$ if

$$f(x) - \sum_{n}^{N} a_n x^{-n\alpha} \ll x^{-N\alpha}, \tag{140}$$

for every N. The expansion of a function into asymptotic series is unique. However, an asymptotic series does not define a unique function nor does it need to be a convergent series. We will talk more about asymptotic series later in this course. For now, we will continue with other examples of differential equations and irregular singular points at infinity.

We will now compute the asymptotic series of two special functions at $x = \infty$. We begin with the modified Bessel function. It satisfies the differential equation

$$x^2 y'' + xy' - (x^2 + \nu^2)y = 0. \tag{141}$$

The point $x = 0$ is a regular singular point. The point $x = \infty$ is an irregular singular point; one can see this using the $x \to 1/\xi$ transformation as discussed at the beginning of this lecture.

If we accept that the point $x = \infty$ is an irregular singular point, we can try to analyze the differential equation using the x-variable directly, without changing first to the ξ-variable. To this end, we write $y(x) = e^{S(x)}$ and find

$$x^2 \left((S')^2 + S'' \right) + xS' - (x^2 + \nu^2) = 0. \tag{142}$$

We rewrite it as

$$(xS')^2 + xS' + x^2 S'' = (x^2 + \nu^2). \tag{143}$$

Assuming that $(xS')^2 \gg xS' \sim x^2 S''$, we find a simplified version of Eq.(143) and solve it

$$(xS')^2 \sim x^2 \quad \Rightarrow \quad xS' \sim \pm x \quad \Rightarrow \quad S(x) \sim \pm x. \tag{144}$$

We can check that the assumptions that we made above are consistent with the above solution, for large values of x. We now improve the ansatz for the function $S(x)$ and write

$$S(x) = \pm x + C(x). \tag{145}$$

The function $C(x)$ is supposed to be much smaller than x, for large x.

We substitute Eq. (145) into the differential equation Eq. (142) and find

$$x^2 C'' + (xC')^2 + (x \pm 2x^2)C' \pm x - \nu^2 = 0. \tag{146}$$

Using asymptotic relations for the function $C(x)$, e.g. $xC' \ll x$, we rewrite the above equation as

$$2x^2 C' \sim -x \quad \Rightarrow \quad C(x) \sim -\frac{1}{2} \ln x. \tag{147}$$

The above solution for $S(x)$ gives us all the terms that go to infinity as $x \to \infty$; therefore, we write a new Ansatz for the solution

$$y(x) \sim c_1 x^{-1/2} e^{\pm x} w(x), \tag{148}$$

and derive an equation for the function $w(x)$. It reads

$$x^2 w''(x) \pm 2x^2 w'(x) + \left(\frac{1}{4} - \nu^2\right) w(x) = 0. \tag{149}$$

The point $x = \infty$ is an irregular singular point of this differential equation. However, we look for the solution with the property $w(x) \to 1$ for $x \to \infty$. It follows from the differential equation Eq.(149) that the function $w(x)$ can be expanded in powers of $1/x$. We write

$$w(x) = \sum_{n=0}^{\infty} a_n x^{-n}, \tag{150}$$

with $a_0 = 1$. We substitute this ansatz into Eq.(149) and find the recursion relation

$$a_{n+1} = \pm \frac{\left(n(n+1) + \frac{1}{4} - \nu^2\right)}{2(n+1)} a_n. \tag{151}$$

To determine whether or not the series converges, we do the ratio test. We find

$$\lim_{n\to\infty} \frac{a_{n+1} x^{-n-1}}{a_n x^{-n}} \sim \lim_{n\to\infty} \frac{n}{x} \to \infty, \tag{152}$$

for all x. Hence, radius of convergence of our asymptotic series is zero.

Another example is that of an Airy function. We will need the Airy function when discussing the WKB approximation later in the course. The Airy equation reads

$$y'' = xy. \tag{153}$$

Again, $x = \infty$ is an irregular singular point. To construct an asymptotic expansion of the solution, we proceed with the, by now, standard method and write $y(x) = e^{S(x)}$. The equation becomes

$$(S')^2 + S'' = x. \tag{154}$$

Since $(S')^2 \ll S''$, it follows that

$$S \sim \pm \frac{2}{3} x^{3/2}. \tag{155}$$

We then write an "improved" approximation

$$S(x) = \pm \frac{2}{3} x^{3/2} + c(x), \tag{156}$$

and obtain the differential equation for $c(x)$

$$c'' + (c')^2 \pm 2\sqrt{x}c' \pm \frac{1}{2\sqrt{x}} = 0. \tag{157}$$

Since $c \ll x^{3/2}$, $c' \ll \sqrt{x}$, $c'' \ll x^{-1/2}$, we find a simplified equation

$$2\sqrt{x}c' \sim -\frac{1}{2\sqrt{x}} \quad \Rightarrow \quad c \sim -\frac{1}{4}\ln(x). \tag{158}$$

Hence, in order to factor out the leading asymptotic, we make the following ansatz for the solution of the Airy equation

$$y(x) = c_0\, x^{-1/4}\, e^{\pm\frac{2}{3}x^{3/2}}\, w(x), \tag{159}$$

where $w(x) \to 1$ as $x \to \infty$.

There are two solutions to the Airy equation, usually denoted as $Ai(x)$ and $Bi(x)$. The function $Ai(x)$ decreases and the function $Bi(x)$ increases as $x \to \infty$; their asymptotic behaviors correspond to the two asymptotic shown in Eq.(159).

In what follows we will only consider the function $Ai(x)$; it corresponds to $y(x) \sim e^{-2/3x^{3/2}}$ in Eq.(159). We substitute Eq.(159) into the Airy equation Eq.(153) and find

$$x^2 w'' - \left(2x^{5/2} + \frac{1}{2}x\right) w' + \frac{5}{16}w = 0. \tag{160}$$

The function $w(x)$ is given by an expansion in powers of $x^{-3/2}$. Hence, we write

$$w(x) \sim \sum_{n=0}^{\infty} a_n x^{-3/2n}, \tag{161}$$

with $a_0 = 1$. The recursion relation for the coefficients a_n reads

$$a_{n+1} = -\frac{3}{4}\frac{\left(n+\frac{5}{6}\right)\left(n+\frac{1}{6}\right)}{(n+1)}\, a_n. \tag{162}$$

It is straightforward to write the result for the coefficient a_n using properties of the Gamma function. We obtain

$$a_n = (-1)^n \frac{3^n}{4^n}\frac{\Gamma\left(n+\frac{5}{6}\right)\Gamma\left(n+\frac{1}{6}\right)}{2\pi\Gamma(n+1)}, \tag{163}$$

where we used the fact that

$$\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right) = 2\pi. \tag{164}$$

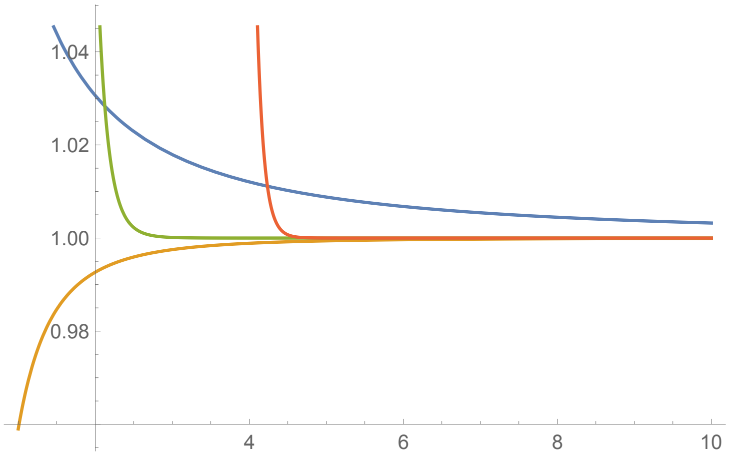

Figure 2: Ratios of asymptotic series to the Airy function. Blue – zero terms are included in the sum, orange – one term, green – ten terms and red – fifty terms.

Hence, we find a representation of the Airy function $Ai(x)$ through asymptotic series

$$Ai(x) \sim c_0 x^{-1/4} e^{-2/3x^{3/2}} \sum_{n=0}^{\infty} \frac{(-1)^n 3^n}{4^n} \frac{\Gamma\left(n+\frac{5}{6}\right)\Gamma\left(n+\frac{1}{6}\right)}{2\pi\Gamma(n+1)} x^{-3/2n}. \tag{165}$$

For the Airy function Ai the normalization coefficient is chosen to be $1/(2\sqrt{\pi})$.

To check the convergence of this series, we do the ratio check

$$\lim_{n\to\infty} \frac{a_{n+1}x^{-3/2(n+1)}}{a_n x^{-3/2n}} \sim \lim_{n\to\infty} \frac{3}{4} n x^{-3/2} \to \infty. \tag{166}$$

Again, similar to the Bessel function, the radius of convergence of these series is zero.

The asymptotic nature of the series is illustrated in Fig. 1 where the ratios of asymptotic approximations to the Airy function obtained by truncating the sum in Eq.(165) at various values of n and the exact Airy function are shown. Naively, we would expect that the more terms we account for in the series in Eq.(165), the better. Whether this statement is true or not depends on the values of x; at lower values of x, e.g. for $x < 5$, including 50 terms in the expansion gives a significantly worse approximation to the correct result than by including just one term. If even more terms are included, series just explodes. Obviously, there is a correlation between values of x that are being studied and the number of terms N that should be kept in the series to achieve best (or even reliable!) results. We will discuss this correlation in the next lecture.

4 Asymptotic series and their properties

In the previous lecture we talked about asymptotic series and explained how they arise when we try to solve differential equations at irregular singular points. The goal of this lecture is to discuss asymptotic series in more detail.

First, as we already know, series $\sum a_n(x-x_0)^n$ are said to be asymptotic to the function $f(x)$ at $x \sim x_0$ if the remainder function $\epsilon_N(x)$ defined as the difference between $f(x)$ and the first $N+1$ terms of the series is much smaller than $(x-x_0)^N$. Mathematically, this condition reads

$$\epsilon_N(x) = f(x) - \sum_{n}^{N} a_n(x-x_0)^n \ll (x-x_0)^N. \tag{167}$$

It is important to understand the difference between convergent and asymptotic series. A series is said to be convergent if the remainder function vanishes

$$\epsilon_N(x) = \sum_{n=N+1}^{\infty} a_n(x-x_0)^n \to 0, \tag{168}$$

in the limit $N \to \infty$, for all $|x-x_0| < R$, where R is independent of N. On the other hand, the series is said to be asymptotic if

$$\epsilon_N(x) \ll (x-x_0)^N, \tag{169}$$

in the limit $x \to x_0$ at fixed N. In another words, we fix N and then find $x-x_0$ for which Eq.(169) holds; if such an x exists, the series is asymptotic.

Let us consider a few examples to make these points clear. First, we discuss the Taylor series of a function $f(x)$ at the point $x = x_0$. We assume that the Taylor expansion has radius of convergence R. Then for all x such that $|x-x_0| < R$,

$$f(x) - \sum_{n=0}^{N} a_n(x-x_0)^n = a_{N+1}(x-x_0)^{N+1} + \cdots \dots \tag{170}$$

Therefore, for all x such that $|x-x_0| < R$,

$$f(x) - \sum_{n=0}^{N} a_n(x-x_0)^n \sim a_{N+1}(x-x_0)^{N+1} \ll (x-x_0)^N, \tag{171}$$

which implies that Taylor series are asymptotic to the original function $f(x)$ within its radius of convergence.

However, asymptotic series *do not need to be convergent*. We will illustrate this point by considering solutions of the following differential equation

$$x^2 y'' + (1+3x)y' + y = 0. \tag{172}$$

It is easy to see that the point $x = 0$ is an irregular singular point of Eq.(172). However, solutions to Eq.(172) admit a power series expansion at $x = 0$. To find this series, we write

$$y(x) = \sum_{n=0}^{\infty} a_n x^n, \tag{173}$$

substitute it into Eq.(172) and obtain the following recurrence relation

$$a_{n+1} = (-1)(n+1)a_n. \tag{174}$$

The solution of this recurrence relation subject to the boundary condition $a_0 = 1$ reads

$$a_n = (-1)^n n!. \tag{175}$$

Hence, the solution to Eq.(172) is given by the following series[5]

$$y(x) = S(x) = \sum_{n=0}^{\infty} (-1)^n n!\, x^n. \tag{176}$$

Because the coefficients a_n grow factorially, series $S(x)$ is not a convergent one; in fact is has vanishing radius of convergence.

We would like to find a function to which $S(x)$ is asymptotic in the sense of Eq.(167). To this end, we use the following representation of the factorial

$$n! = \Gamma(n+1) = \int_0^{\infty} \frac{{\rm d}t}{t}\, t^{n+1}\, e^{-t}. \tag{177}$$

We use this representation in Eq.(176), change the order of summation and integration and find

$$S(x) \to \int_0^{\infty} {\rm d}t\; e^{-t} \sum_{n=0}^{\infty} (-1)^n\, (tx)^n = \int_0^{\infty} \frac{{\rm d}t\; e^{-t}}{1+tx}. \tag{178}$$

Although these manipulations are dubious since the sum is not convergent, we hypothesize that the last integral in Eq.(178) is the solution of the differential equation Eq.(172), i.e.

$$y(x) = \int_0^{\infty} \frac{{\rm d}t\; e^{-t}}{1+tx}. \tag{179}$$

[5] This series is known as the Stieltjes series.

To prove this assertion, we substitute Eq.(179) into Eq.(172), compute derivatives and simplify the result. We require the following derivatives

$$\left(\frac{1}{1+tx}\right)'' = \frac{2t^2}{(1+tx)^3}, \qquad \left(\frac{1}{1+tx}\right)' = -\frac{t}{(1+tx)^2}. \tag{180}$$

Using them in Eq.(172), we find

$$x^2y'' + (1+3x)y' + y = \int_0^\infty \mathrm{d}t\; e^{-t} \left[\frac{2(tx)^2}{(1+tx)^3} - \frac{t(1+3x)}{(1+tx)^2} + \frac{1}{(1+tx)}\right] \tag{181}$$

To simplify the r.h.s. one can do partial fractioning with respect to t to obtain

$$\frac{2(tx)^2}{(1+tx)^3} - \frac{t(1+3x)}{(1+tx)^2} + \frac{1}{(1+tx)} = \frac{2}{(1+tx)^3} + \frac{1-x}{x}\frac{1}{(1+tx)^2} - \frac{1}{x}\frac{1}{1+tx}. \tag{182}$$

It is then convenient to integrate by parts so that all denominators in Eq.(182) become $1/(1+tx)^3$. For example, we can write

$$\begin{aligned} -\frac{1}{x}\frac{1}{1+tx}e^{-t} &= \frac{1}{x}\frac{1}{1+tx}\frac{\mathrm{d}}{\mathrm{d}t}\left[e^{-t}\right] = \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{1+tx}\,e^{-t}\right] - \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{1+tx}\right]\,e^{-t} \\ &= \frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{1+tx}\,e^{-t}\right] + \frac{1}{(1+tx)^2}\,e^{-t}, \end{aligned} \tag{183}$$

integrate the total derivative right away and combine the last term in Eq.(183) with the second term on the right hand side of Eq.(182). Proceeding iteratively, it is easy to show that the integral on the right hand side of Eq.(181) vanishes. This implies that the function $y(x)$ defined in Eq.(179) satisfies the differential equation Eq.(172).

As the next step, we show that the power series in Eq.(176) is asymptotic to the function $y(x)$ defined in Eq.(179). To this end, we will need a formula that describes integration by parts

$$\int_0^\infty \mathrm{d}t\;(1+tx)^{-n}e^{-t} = 1 - nx\int_0^\infty \mathrm{d}t\;(1+tx)^{-n-1}e^{-t}. \tag{184}$$

This result implies that starting from the function $y(x)$ and integrating by part $N+1$ times, we obtain

$$y(x) = 1-x+2!x^2+\cdots+(-1)^N N!\,x^N+(-1)^{N+1}(N+1)!\,x^{N+1}\int_0^\infty \mathrm{d}t\;(1+tx)^{-N-2}e^{-t}. \tag{185}$$

It follows that

$$\epsilon_N(x) = (-1)^{N+1}(N+1)!\, x^{N+1} \int_0^\infty \mathrm{d}t\, (1+tx)^{-N-2} e^{-t}$$
$$< (-1)^{N+1}(N+1)!\, x^{N+1} \int_0^\infty \mathrm{d}t e^{-t} = (-1)^{N+1}(N+1)!\, x^{N+1} \ll x^N, \tag{186}$$

where we used the fact that $(1+tx)^{-N-2} > 1$ and where for the last step x should be chosen appropriately, to beat $N!$. Hence, Eq.(186) proves that the series $S(x)$ is asymptotic to the solution of the differential equation $y(x)$.

There is another application of the above estimate of the remainder ϵ_N. Suppose we would like to obtain a numerical result for the function $y(x)$ from the series $S(x)$. How many terms should we include in the series to obtain the best possible approximation? To find out, we can compute the value of N for which the upper bound of the remainder $\epsilon_N^{\text{upper}}(x)$ is minimal for a given x. We use Eq.(186) and write

$$\left| \frac{\epsilon_{N+1}^{\text{upper}}(x)}{\epsilon_N^{\text{upper}}(x)} \right| = (N+2)x. \tag{187}$$

Hence, for a given x, $\epsilon_N^{\text{upper}}(x)$ decreases as long as $(N+2)x < 1$ and starts increasing after that. Therefore, asymptotic series $S(x)$ should be truncated at

$$N_{\text{opt}} \sim 1/x, \tag{188}$$

to achieve the best approximation to the true value of the function $y(x)$. It follows that the best approximation that series $S(x)$ can ever provide to the exact function $y(x)$ is estimated to be

$$\epsilon_{\text{opt}}^{\text{upper}} \sim \sqrt{2\pi x} e^{-1/x}. \tag{189}$$

To derive this result, we used the Stirling formula for the factorial $n! \sim \sqrt{2\pi n}(n/e)^n$.

Since an upper bound on $\epsilon_N(x)$ in case of Stieltjes series corresponds to the first neglected term in the series, the best possible approximation for such asymptotic series is obtained if one keeps including additional terms into $S(x)$ as long as the new terms are smaller than the previously included one. Once this is not the case anymore, no new terms need to be included because accuracy does not improve and, in fact, deteriorates. Although one can prove this result for Stieltjes series, this also appears to be an accepted procedure to obtain "best" numerical values starting from arbitrary asymptotic series.

Asymptotic series have a number of properties that we will now discuss. The first important point is that *different* functions can have *identical* asymptotic series. Indeed, let us assume that

$$f(x) \sim \sum_n a_n (x-x_0)^n. \tag{190}$$

However, the function $g(x)$

$$g(x) = f(x) + b e^{-1/(x-x_0)^2} \tag{191}$$

can be represented by the same asymptotic series as the function $f(x)$. This is true because

$$e^{-1/(x-x_0)^2} \ll (x-x_0)^n, \tag{192}$$

for any n, as long as $x \to x_0$. Functions that are much smaller than any power (in a sense of asymptotic relations) are called *sub-dominant* function. Hence, a given asymptotic series can be asymptotic to a whole class of functions that differ from each other by sub-dominant functions.

Nevertheless, for each function, there is just one representation in terms of asymptotic series at a given point. This implies that if we have two series that are asymptotic to the same function at the same point, then their coefficients should be the same

$$f(x) \sim \sum a_n (x-x_0)^n \sim \sum b_n (x-x_0)^n, \quad \Rightarrow \quad a_n = b_n. \tag{193}$$

One can perform all arithmetic operations with asymptotic series, working with them as if they were convergent. So, if

$$f(x) \sim \sum_n^{\infty} a_n (x-x_0)^n \quad \text{and} \quad g(x) \sim \sum_n^{\infty} b_n (x-x_0)^n, \tag{194}$$

the following holds

$$\begin{aligned} &\alpha f(x) + \beta g(x) \sim \sum_n^{\infty} (\alpha a_n + \beta b_n)(x-x_0)^n, \\ &f(x) g(x) \sim \sum_n^{\infty} c_n (x-x_0)^n, \end{aligned} \tag{195}$$

where $c_n = \sum\limits_{m=0}^{n} a_m b_{n-m}$.

However, integration and differentiation of asymptotic series is slightly more complex. As far as the integration goes, one can state that asymptotic series $f(x) \sim \sum\limits_{n}^{\infty} a_n (x - x_0)^n$ can be integrated term by term if $f(x)$ itself is integrable near $x = x_0$. In this case,

$$g(x) = \int\limits_{x_0}^{x} \mathrm{d}t \; f(t) \sim \sum_{n=0}^{\infty} \frac{a_n}{n+1} (x - x_0)^{n+1} \tag{196}$$

It is strictly speaking not true that if $f(x) \sim \sum\limits_{n}^{\infty} a_n (x - x_0)^n$, then $\sum\limits_{n}^{\infty} a_n n (x - x_0)^{n-1} \sim f'(x)$. One can construct examples with sub-dominant functions where the derivative of an asymptotic series does not asymptote to the derivative of a function. Nevertheless, if $f'(x)$ exists and it is integrable at $x = x_0$, then $f'(x)$ is asymptotic to the derivative of the asymptotic series of $f(x)$.

One important result that is useful to know and which, to a large extent, justifies what we were doing when we were constructing solutions of differential equations is that if a function $y(x)$ provides a solution of a differential equation $y'' + p(x)y' + q(x) = 0$ and if the functions $p(x)$ $p'(x)$ and $q(x)$ can be expanded in asymptotic series around a singular point $x = x_0$, then the asymptotic expansion of the function y' is obtained by differentiating the asymptotic expansion of $y(x)$.

To illustrate how formal manipulations that we were doing before can be more rigorously justified, we will consider an equation for the modified Bessel function $K_\nu(x)$ that we studied in the previous lecture. The modified Bessel function $K_\nu(x)$ satisfies the differential equation

$$x^2 K_\nu'' + x K_\nu' - (x^2 + \nu^2) K_\nu = 0. \tag{197}$$

We have seen that $x \to \infty$ is an irregular singular point and that approximate solutions at this point have the following asymptotic behavior

$$K_\nu^{\pm}(x) \sim c_1 x^{-1/2} e^{\pm x}. \tag{198}$$

The function $K_\nu(x)$ is defined to behave as $y_-(x)$ at $x \to \infty$ with the coefficient c_1 chosen in a particular way. We write

$$K_\nu = \left(\frac{\pi}{2x}\right)^{1/2} e^{-x} \, w(x), \tag{199}$$

where, according to our analysis in the previous lecture, the function $w(x)$ should have the limit $w(x) \to 1$ as $x \to \infty$. We use ansatz Eq.(199) in Eq.(197) and obtain the following equation for the function $w(x)$

$$w'' - 2w' + \frac{\lambda}{x^2}\, w = 0, \tag{200}$$

where $\lambda = 1/4 - \nu^2$.

Our goal is to find a solution $w(x)$ to Eq.(200) represented by a series in $1/x$. However, we would also like to *prove* that such a series solution is, actually, asymptotic to a true solution of the differential equation Eq.(200).

To achieve this, we derive an *integral equation* for the function $w(x)$. To this end, we re-write Eq.(200) as follows

$$w'' - 2w' = -\frac{\lambda}{x^2} w, \tag{201}$$

and we treat this equation as an *inhomogeneous* differential equation ignoring the fact that its right hand side does depend on the $w(x)$ itself. To "solve" Eq.(201), we write $w' = e^{2x} g$, substitute it into Eq.(201) and obtain

$$e^{2x} g' = -\frac{\lambda}{x^2} w \quad \Rightarrow \quad g' = -\lambda e^{-2x} \frac{w}{x^2} \quad \Rightarrow \quad g(x) = \lambda \int\limits_x^\infty {\rm d}t\; e^{-2t} \frac{w(t)}{t^2}. \tag{202}$$

Hence,

$$w'(x) = \lambda \int\limits_x^\infty {\rm d}t\; e^{2(x-t)} \frac{w(t)}{t^2}. \tag{203}$$

We have chosen the integration boundaries to ensure that the function $w(x)$ has an expansion in $1/x$ at infinity and that the first term can be a constant; this requires that $w'(x)$ vanishes at $x = \infty$. The next step is to integrate Eq.(203). We find

$$w(x) = 1 - \lambda \int\limits_x^\infty {\rm d}\xi \int\limits_\xi^\infty {\rm d}t\; e^{2(\xi - t)} \frac{w(t)}{t^2}. \tag{204}$$

To simplify the right hand side, we change the order of integration and find

$$
\begin{aligned}
w(x) &= 1 - \lambda \int_x^\infty \mathrm{d}t \, \frac{w(t)}{t^2} e^{-2t} \int_x^t \mathrm{d}\xi e^{2\xi} = 1 - \frac{\lambda}{2} \int_x^\infty \mathrm{d}t \, \frac{w(t)}{t^2} e^{-2t} \left(e^{2t} - e^{2x}\right) \\
&= 1 + \frac{\lambda}{2} \int_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{w(t)}{t^2}.
\end{aligned}
\tag{205}
$$

We can use this integral representation to show that the function $w(x)$ is bounded from above. To this end, we write ($x = t_0$)

$$
w(t_0) = 1 + \frac{\lambda}{2} \int_{t_0}^\infty \mathrm{d}t_1 \frac{K(t_0, t_1)}{t_1^2} \, w(t_1), \tag{206}
$$

where $K(t_a, t_b) = e^{2(t_a - t_b)} - 1$. We can solve the above equation iteratively, by repeatedly substituting $w(t_1) \to 1 + \mathcal{O}(\lambda)$ there. We find

$$
w(t_0) = 1 + \sum_{n=1}^\infty \left(\frac{\lambda}{2}\right)^n \int_{t_0}^\infty \mathrm{d}t_1 \, \frac{K(t_0, t_1)}{t_1^2} \int_{t_1}^\infty \mathrm{d}t_2 \, \frac{K(t_1, t_2)}{t_2^2} \cdots \int_{t_{n-1}}^\infty \mathrm{d}t_n \frac{K(t_{n-1}, t_n)}{t_n^2}. \tag{207}
$$

Since $0 < |K(t_a, t_b)| < 1$, it follows, that the n-th term in the above series can be bounded from above

$$
\begin{aligned}
&\left| \int_{t_0}^\infty \mathrm{d}t_1 \, \frac{K(t_0, t_1)}{t_1^2} \int_{t_1}^\infty \mathrm{d}t_2 \, \frac{K(t_1, t_2)}{t_2^2} \cdots \int_{t_{n-1}}^\infty \mathrm{d}t_n \frac{K(t_{n-1}, t_n)}{t_n^2} \right| \\
&< \int_{t_0}^\infty \frac{\mathrm{d}t_1}{t_1^2} \int_{t_1}^\infty \frac{\mathrm{d}t_2}{t_2^2} \cdots \int_{t_{n-1}}^\infty \frac{\mathrm{d}t_n}{t_n^2} = \frac{1}{n!} \frac{1}{t_0^n}.
\end{aligned}
\tag{208}
$$

Using this bound in Eq.

$$
w(x) < e^{\lambda/2/x}. \tag{209}
$$

Given this constraint, we can estimate the integral that appears on the r.h.s. of Eq.(205) since we can claim that, for a given $x > a$, $w(x)$ is bounded by some x-dependent constant B. Then for $x > a$,

$$
\left| \frac{\lambda}{2} \int_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{w(t)}{t^2} \right| < \frac{\lambda B}{2} \int_x^\infty \mathrm{d}t \, \frac{1}{t^2} = \frac{\lambda B}{2x}. \tag{210}
$$

To make use of this result, we write

$$w(x) = 1 + w_1(x), \tag{211}$$

with $w_1(x) < B/x$. This proves that $w(x) \sim 1$, $x \to \infty$.

To do better, we use Eq.(211) to write an integral equation for w_1. It reads

$$\begin{aligned} w_1(x) &= \frac{\lambda}{2} \int\limits_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{w(t)}{t^2} \\ &= \frac{\lambda}{2} \int\limits_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{1}{t^2} + \frac{\lambda}{2} \int\limits_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{w_1(t)}{t^2}. \end{aligned} \tag{212}$$

We can integrate by parts the first term on the right hand side of the previous equation. We find

$$w_1(x) = -\frac{\lambda}{2x} + \frac{\lambda}{4x^2} - \frac{\lambda}{2} \int\limits_x^\infty \frac{e^{2(x-t)}}{t^3} \, \mathrm{d}t + \frac{\lambda}{2} \int\limits_x^\infty \mathrm{d}t \, \left(e^{2(x-t)} - 1\right) \frac{w_1(t)}{t^2}. \tag{213}$$

Since $w_1(t) < B/x$, we find that all remaining integrals are bounded from above by $1/x^2$. Hence,

$$w_1(x) + \frac{\lambda}{2x} < \frac{B_2}{x^2}. \tag{214}$$

Therefore,

$$w(x) \sim 1 - \frac{\lambda}{2x}, \tag{215}$$

at $x = \infty$. One can continue to use the integral equation Eq.(205) for the function $w(x)$ to extract relevant powers of $1/x$ and bound remaining integrals. By doing this we prove that the function $w(x)$ is indeed asymptotic to the series that we have already constructed in Lecture 2.

5 Asymptotic expansion of integrals

There are plenty of examples in physics where the result of the a calculation is expressed as an integral that involves a parameter which can be either large or small. In such cases it is necessary to understand how to compute such integrals by expanding them in small (or large) parameter. We will discuss how such expansions can be constructed. However, before diving into a discussion of how this can be done, we will briefly describe a few mathematical examples where such knowledge may be useful.

Consider the function $\Gamma(z)$. It is defined through the following equations

$$z\Gamma(z) = \Gamma(z+1), \quad \Gamma(1) = 1. \tag{216}$$

$\Gamma(z)$ function has the following integral representation

$$\Gamma(z) = \int\limits_0^\infty \mathrm{d}t \; t^{z-1} e^{-t}. \tag{217}$$

We note that this representation is valid for $z > 0$ but, in fact, it can be used as a starting point for an analytic continuation of $\Gamma(z)$ to an entire complex z-plane.

To prove that Eq.(217) is an integral representation of $\Gamma(z)$, we write

$$z\Gamma(z) = \int\limits_0^\infty \mathrm{d}t \; z t^{z-1} e^{-t} = \int\limits_0^\infty \mathrm{d}t \; \frac{\mathrm{d}}{\mathrm{d}t}\left[t^z\right] \; e^{-t} = \int\limits_0^\infty \mathrm{d}t \; t^z \; e^{-t} = \Gamma(z+1), \tag{218}$$

where in the last step, we integrated by parts and discarded the surface terms.

A typical question that we will address in this lecture is – suppose we are interested in the behavior of $\Gamma(z)$ as very large values of z, $z \to \infty$. Can we systematically derive it from the integral representation in Eq.(217)?

As another example, consider the Airy equation

$$y'' = xy. \tag{219}$$

We have constructed its asymptotic solution at $x \to +\infty$ in the previous lecture by solving the differential equation. However, suppose we do something different and write

$$y(x) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} e^{ipx} f(p) \tag{220}$$

Substituting this ansatz into Eq.(219), using $xe^{ipx} = -i\partial(e^{ipx})/\partial p$ and integrating by parts, we find a first order differential equation for the function $f(p)$

$$p^2 f(p^2) = -i\frac{\partial}{\partial p} f(p). \tag{221}$$

We solve this equation and obtain an integral representation for a possible solution of the Airy equation

$$y(x) = \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} e^{ip(x+p^2/3)}. \tag{222}$$

Again, we may wonder if this integral representation is useful for understanding the behavior of the Airy function at $x \to \infty$.

Finally, similar to the case of the $\Gamma(z)$ function, many special functions possess well-known integral representations. For example, the Bessel function $J_n(x)$ satisfies

$$J_n(x) = \frac{1}{2\pi} \int\limits_0^{2\pi} e^{i(x \sin\theta - n\theta)}\, \mathrm{d}\theta. \tag{223}$$

We may ask if this representation can be used to understand the behavior of $J_n(x)$ as $x \to \infty$ or $n \to \infty$?

1. Taylor and asymptotic expansion of integrals: We will start with a simple intuitive statement. Consider an integral

$$I(x) = \int\limits_a^b \mathrm{d}t\; f(t,x), \tag{224}$$

We would like to understand the behavior of this integral at $x \sim x_0$. If the limit $\lim\limits_{x \to x_0} f(t,x) = f_0(t)$ exists for all $a \leq< t \leq b$, then

$$I(x) \sim \int\limits_a^b \mathrm{d}t\; f_0(t), \tag{225}$$

This result can be generalized as follows. We assume that the function $f(t,x)$ possesses an asymptotic expansion at the point $x = x_0$

$$f(t,x) \sim \sum_n a_n(t)(x - x_0)^{\alpha n}, \tag{226}$$

that is valid for all t from the interval $[a, b]$. Then the asymptotic expansion of the integral $I(x)$ at $x \sim x_0$ is given by the following (natural) formula

$$I(x) \sim \sum (x - x_0)^{\alpha n} \int_a^b \mathrm{d}t \; a_n(t). \tag{227}$$

Let us consider a few examples. We begin with an integral

$$I(x) = \int_0^1 \mathrm{d}t \, \frac{\ln(1 + xt)}{t}. \tag{228}$$

We will study its expansion at $x \sim 0$. The Taylor expansion of the integrand in x converges for all $t \in [0, 1]$.

$$\frac{\ln(1 + xt)}{t} = x \sum_{n=0}^{\infty} \frac{(-1)^n (xt)^n}{n + 1}. \tag{229}$$

Hence,

$$I(x) \sim x - \frac{x^2}{4} + \frac{x^3}{9} - \frac{x^4}{16} + \cdots \tag{230}$$

As the second example, consider an incomplete Gamma-function $\Gamma(\alpha, x)$ defined as

$$\Gamma(\alpha, x) = \int_x^{\infty} \mathrm{d}t \; t^{\alpha - 1} e^{-t}. \tag{231}$$

We are interested in the behavior of this function at small positive x. As we will see, there are three distinct cases that need to be considered: 1) $\alpha > 0$, 2) $\alpha < 0$ but not integer, and 3) $\alpha = 0, -1, -2, -3 \ldots$.

We begin with the first case where $\alpha > 0$. We re-write Eq.(231) in the following way

$$\Gamma(\alpha, x) = \int_0^{\infty} \mathrm{d}t \; t^{\alpha - 1} e^{-t} - \int_0^{x} \mathrm{d}t \; t^{\alpha - 1} e^{-t}. \tag{232}$$

The first integral on the r.h.s. of Eq.(232) evaluates to $\Gamma(\alpha)$. The second integral is such that its integrand can be represented by a convergent series

$$\int_0^x \mathrm{d}t \; t^{\alpha - 1} e^{-t} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^x \mathrm{d}t \; t^{\alpha - 1 + n} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n + \alpha)} x^{\alpha + n} \tag{233}$$

Hence,

$$\Gamma(\alpha, x) \sim \Gamma(\alpha) - \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+\alpha)} x^{\alpha+n}, \tag{234}$$

for $x \to +0$ and $\alpha > 0$.

The second case we want to consider is that of a *non-integer negative* α. We cannot repeat what we just did since the integral over t from 0 to ∞ diverges in this case. To overcome this problem, we define an integer N

$$\alpha = -N - \delta, \tag{235}$$

where $0 < \delta < 1$. To make the integral amenable to an expansion in x, we subtract and add the first $N+1$ terms of the Taylor expansion of the function e^{-t}. We obtain

$$\begin{aligned} \Gamma(\alpha, x) &= \int_x^{\infty} \mathrm{d}t \; t^{-N-\delta-1} e^{-t} \\ &= \int_x^{\infty} \mathrm{d}t \; t^{-N-\delta-1} \left[e^{-t} - \sum_{n=0}^{N} \frac{(-t)^n}{n!} \right] + \int_x^{\infty} \mathrm{d}t \; t^{-N-\delta-1} \sum_{n=0}^{N} \frac{(-t)^n}{n!}. \end{aligned} \tag{236}$$

The first integral on the r.h.s. now converges at $x = 0$ so that we can replace the integral from x to ∞ by a difference of integrals from zero to infinity and from zero to x. We find

$$\begin{aligned} \Gamma(\alpha, x) &= \int_0^{\infty} \mathrm{d}t \; t^{-N-\delta-1} \left[e^{-t} - \sum_{n=0}^{N} \frac{(-t)^n}{n!} \right] \\ &- \int_0^{x} \mathrm{d}t \; t^{-N-\delta-1} \left[e^{-t} - \sum_{n=0}^{N} \frac{(-t)^n}{n!} \right] + \int_x^{\infty} \mathrm{d}t \; t^{-N-\delta-1} \sum_{n=0}^{N} \frac{(-t)^n}{n!}. \end{aligned} \tag{237}$$

The first term on the r.h.s. of the above equation is an x-independent constant that we denote by C_N. The second and the third terms are then computed by representing respective integrands by convergent series. The result, expressed through $\alpha = -N - \delta$ reads

$$\Gamma(\alpha, x) \sim C - \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+\alpha)} x^{\alpha+n}, \tag{238}$$

In fact, one can show that $C = \Gamma(\alpha)$ provided that the Gamma-function is defined for negative α through an analytic continuation. Note that this result appears to be identical to Eq.(234) in spite of a more complicated derivation. In a way, this implies that series Eq.(234) can be analytically continued to the entire complex plane to define $\Gamma(\alpha, x)$, provided that this continuation does not lead to singularities.

Moreover, we can see from Eqs.(234,238) where such singularities are since the series over n can not be evaluated for α being *negative integer or zero*. Since the original integral Eq.(231) does not have singularities for *any* values of α, a singularity in series over n has to be compensated by a singularity of $\Gamma(\alpha)$, see Eqs.(234,238). Hence, according to these equations, $\Gamma(\alpha)$ has simple poles when its argument approaches *negative integers or zero*. These poles read

$$\Gamma(-n+\epsilon) \approx \frac{(-1)^n}{n!\,\epsilon} + \cdots \tag{239}$$

After this remark we return to an incomplete Gamma-function and discuss how to construct its expansion in x for values of α that belong to the third category i.e. negative integers or zero. For simplicity, we will only consider the case $\alpha = 0$. This defines the so-called exponential integral

$$\Gamma(0, x) = E_1(x) = \int\limits_x^\infty \frac{\mathrm{d}t}{t} e^{-t}. \tag{240}$$

The calculation here is more tricky than in the previous examples because the integral does not converge at $x = 0$. Hence, if we replace e^{-t} with its Taylor expansion, we will get an integral that diverges at $t = \infty$; in the previous cases, if was regulated by the non-vanishing $\delta > 0$. To get around this problem, we can *split the integration interval into regions* and do different approximations in each of the regions. We find

$$\begin{aligned} E_1(x) &= \int\limits_1^\infty \frac{\mathrm{d}t}{t} e^{-t} + \int\limits_x^1 \frac{\mathrm{d}t}{t} e^{-t} \\ &= \int\limits_1^\infty \frac{\mathrm{d}t}{t} e^{-t} + \int\limits_x^1 \frac{\mathrm{d}t}{t} (e^{-t} - 1) + \int\limits_x^1 \frac{\mathrm{d}t}{t} \\ &= C - \ln x - \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n! n}, \end{aligned} \tag{241}$$

where C combines contributions of the first integral and the x-independent contributions of the second integral in Eq.(241). One can show that the constant C is related to the Euler constant; it is computed to be

$$C = \lim_{x\to 0}\left(\int_x^\infty \frac{\mathrm{d}t}{t} e^{-t} + \ln(x)\right) = -\gamma_E = \left.\frac{\mathrm{d}\Gamma(1+z)}{\mathrm{d}z}\right|_{z=0}. \tag{242}$$

Numerically, $\gamma_E = 0.5772$.

2. Integration by parts: Integration by parts is a simple method that allows us to compute asymptotic expansions of integrals. We will explain how this method works by considering representative examples.

Consider an integral

$$I(x) = \int_x^\infty \mathrm{d}t\; e^{-t^4}. \tag{243}$$

We would like to understand the behavior of this integral in the limit $x \to \infty$.

What should we expect? If x is very large, not only the argument of the exponential function is very large but it also changes significantly once one moves away from lower integration boundary $t = x$ cutting the integral off. We therefore expect that in the $x \to \infty$ limit, the asymptotic expansion of the integral is defined through its behavior in the neighborhood of $t = x$. To make this idea explicit, we write $t = x + \xi$, $\xi \in [0, \infty]$ and obtain

$$I(x) \sim \int_0^\infty \mathrm{d}\xi\; e^{-x^4 - 4x^3\xi}, \tag{244}$$

where $\mathcal{O}(\xi^2)$ and higher terms in the exponent where neglected. We integrate over ξ and find

$$I(x) \sim \frac{1}{4x^3} e^{-x^4}. \tag{245}$$

To improve on this result, we note that it implies that the integral $I(x)$ is determined by a *derivative* of $\ln(e^{-t^4})$ at $t = x$. We therefore re-write the integral

$$I(x) = -\int_x^\infty \mathrm{d}t\; \frac{1}{4t^3}\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-t^4}\right), \tag{246}$$

integrate by parts and find

$$I(x) = \frac{1}{4x^3} e^{-x^4} - \frac{3}{4}\int_x^\infty \frac{\mathrm{d}t}{t^4}\; e^{-t^4}. \tag{247}$$

To continue expanding in $1/x$, we have to repeat what we just did for the second integral on the right hand side of the above equation. We write

$$\int_x^\infty \frac{\mathrm{d}t}{t^4}\, e^{-t^4} = -\int_x^\infty \frac{\mathrm{d}t}{4t^7}\, \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-t^4}\right) = \frac{1}{4x^7} e^{-x^4} - \frac{7}{4}\int_x^\infty \frac{\mathrm{d}t}{t^8}\, e^{-t^4}. \tag{248}$$

Repeating this several times, we find

$$I(x) \sim \frac{1}{4x^3} e^{-x^4} \left\{ 1 - \frac{3}{4x^4} + \frac{3\cdot 7}{(4x^4)^2} - \frac{3\cdot 7\cdot 11}{(4x^4)^3} + \ldots \right\}. \tag{249}$$

The series is not convergent but is asymptotic. Nevertheless, it describes the integral $I(x)$ very well; indeed, even for values of x as small as $x \sim 1.5$, three terms of the expansion describe the result with the precision that is better than a percent. For larger values of x or on account of more terms in the series, the result is even more accurate.

Sometimes it is not obvious how integration by parts can be applied to a given integral; in such cases rewriting an integral before integrating by parts may help. As an example, consider

$$I(x) = \int_0^x \mathrm{d}t\; t^{-1/2} e^{-t}. \tag{250}$$

We are interested in the behavior of this integral in the limit $x \to \infty$. It is not very useful to integrate e^{-t} by parts since, if we do that, we will have to evaluate the integrand at $t = 0$ where the integrand diverges. Instead, we first re-write the integral

$$I(x) = \int_0^\infty \mathrm{d}t\; t^{-1/2} e^{-t} - \int_x^\infty \mathrm{d}t\; t^{-1/2} e^{-t}. \tag{251}$$

The first integral is equal to $\Gamma(1/2) = \sqrt{\pi}$. The second one can be asymptotically expanded using integration by parts

$$\begin{aligned} \int_x^\infty \mathrm{d}t\; t^{-1/2} e^{-t} &= -\int_x^\infty \mathrm{d}t\; t^{-1/2} \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-t}\right) = x^{-1/2} e^{-x} - \frac{1}{2}\int_x^\infty \mathrm{d}t\; t^{-3/2}\, e^{-t} \\ &\sim x^{-1/2} e^{-x} - \frac{1}{2} x^{-3/2} e^{-x}. \end{aligned} \tag{252}$$

Hence, we find

$$I(x) \sim \sqrt{\pi} - x^{-1/2} e^{-x} + \frac{1}{2} x^{-3/2} e^{-x}. \tag{253}$$

It is straightforward to calculate more terms in the expansion by repetitive application of integration by parts.

Laplace integrals and Laplace method: An important class of integrals that we will discuss now are the so-called *Laplace integrals* defined as

$$I(x) = \int_a^b \mathrm{d}t \; f(t) \; e^{x\phi(t)}. \tag{254}$$

We assume that $f(t)$ and $\phi(t)$ are real-valued continuous functions.

We will be interested in understanding the behavior of such integrals in the limit $x \to \infty$. As the first step, we can apply the integration-by-parts technology once again. Indeed, by writing

$$I(x) = \int_a^b \mathrm{d}t \, \frac{f(t)}{x\phi'(t)} \frac{\mathrm{d}}{\mathrm{d}t} \left[e^{x\phi(t)} \right], \tag{255}$$

and integrating by parts, we obtain

$$I(x) = \frac{f(t)}{x\phi'(t)} e^{x\phi(t)} \bigg|_a^b - \int_a^b \mathrm{d}t \, \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{f(t)}{x\phi'(t)} \right] \; e^{x\phi(t)}. \tag{256}$$

Repeating the above procedure one more time, we obtain

$$I(x) \sim \frac{f(t)}{x\phi'(t)} e^{x\phi(t)} \bigg|_a^b - \frac{1}{x^2\phi'(t)} \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{f(t)}{\phi'(t)} \right] e^{x\phi(t)} \bigg|_a^b + \mathcal{O}(x^{-3}). \tag{257}$$

Hence, we obtained an expansion of $I(x)$ in $1/x$. Then, depending on the relation between $\phi(a)$ and $\phi(b)$ etc., a simpler version of the asymptotic approximation to $I(x)$ can, in principle, be derived from the above equation.

However, the above approach has limitations because $1/\phi'(t)$ appears in the integrand. Therefore, if there is a point t in the interval $t \in [a, b]$ where $\phi'(t) = 0$, the above calculation becomes dubious. This case is addressed with the help of the so-called Laplace method.

The method is based on the following observation. Suppose that the function $\phi(t)$ has a *maximum* at the point $t = c$, $c \in [a, b]$. Then, $\phi'(c) = 0$, the above discussion is not applicable and a different approach is required. To describe it, we note that if $f(c) \neq 0$ or otherwise pathologically small, the leading contribution to $I(x)$ in the limit $x \to \infty$ comes from the immediate neighborhood of $t = c$ since $e^{x\phi(c)}$, for large x, is exponentially large compared to a value of $e^{x\phi(t)}$ for any other point $t \in [a, b]$. Hence, we can approximate $I(x)$ by $I(x, \epsilon)$ where $0 < \epsilon \ll 1$ and

$$I(x,\epsilon) = \int_{c-\epsilon}^{c+\epsilon} \mathrm{d}t\ f(t)e^{x\phi(t)}, \tag{258}$$

if $a < c < b$,

$$I(x,\epsilon) = \int_{b-\epsilon}^{b} \mathrm{d}t\ f(t)e^{x\phi(t)}, \tag{259}$$

if $c = b$ and

$$I(x,\epsilon) = \int_{a}^{a+\epsilon} \mathrm{d}t\ f(t)e^{x\phi(t)}, \tag{260}$$

if $c = a$.

The important result that we want to explain is that the above formulas provide a starting point for obtaining the asymptotic expansion of $I(x)$ and that, in spite of their appearance, they are *independent of* ϵ. We will consider the case $c = a$.

We write

$$I(x) = I(x,\epsilon) + \delta I(x,\epsilon), \tag{261}$$

where

$$I(x,\epsilon) = \int_{a}^{a+\epsilon} \mathrm{d}t\ f(t)\ e^{x\phi(t)}, \qquad \delta I(x,\epsilon) = \int_{a+\epsilon}^{b} \mathrm{d}t\ f(t)\ e^{x\phi(t)}. \tag{262}$$

To simplify the notation, we denote values of functions and their derivatives at a particular point $x = d$ as follows

$$\varphi(d) = \varphi_d, \quad \frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\Big|_{x=d} = \varphi'_d, \quad \frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\Big|_{x=d} = \varphi''_d, \quad \text{etc.} \tag{263}$$

We consider $I(x,\epsilon)$ and take ϵ small so that we can approximate functions

$\phi(t)$ and $f(t)$ by Taylor series. The leading term reads

$$\begin{aligned} I(x,\epsilon) &\sim \int\limits_a^{a+\epsilon} \mathrm{d}t\ f_a e^{x\phi_a + x\phi_a'(t-a)} = f_a e^{x\phi_a} \int\limits_a^{a+\epsilon} \mathrm{d}t\ e^{x\phi_a'(t-a)} \\ &= f_a e^{x\phi_a} \int\limits_0^{\epsilon} \mathrm{d}\xi\ e^{x\phi_a'\xi} = \frac{f_a e^{x\phi_a}}{x|\phi_a'|} \left(1 - e^{-x|\phi_a'|\epsilon}\right). \end{aligned} \tag{264}$$

We can choose ϵ in such a way that two conditions are satisfied

$$\epsilon \ll (b-a), \qquad 1 \ll \epsilon x |\phi_a'|. \tag{265}$$

These conditions are compatible because we are interested in the limit $x \to \infty$. Given the second condition, we observe that the second term on the r.h.s. in Eq.(264) is exponentially suppressed[6] and, therefore, can be dropped. The same line of reasoning allows us to drop $\delta I(x,\epsilon)$ in Eq.(261). Indeed, since

$$\frac{\delta I(x,\epsilon)}{I(x,\epsilon)} \sim e^{x\epsilon\phi_a'}, \tag{266}$$

$\delta I(x,\epsilon)$ is also exponentially suppressed compared to such terms in the expansion of $I(x)$ that are suppressed by powers of $1/x$. We conclude (c.f. Eq.(264)) that the leading term in the asymptotic expansion of the integral $I(x)$ for large values of x reads

$$I(x) \sim \frac{f_a e^{x\phi_a}}{x|\phi_a'|}. \tag{267}$$

We can improve this estimate by accounting for more terms in the Taylor expansion of the functions $f(t)$ and $\phi(t)$. We write

$$\begin{aligned} I(x,\epsilon) &\sim \int\limits_a^{a+\epsilon} \mathrm{d}t\ \left(f_a + f_a'(t-a) + \frac{1}{2} f_a''(t-a)^2\right) e^{x\phi_a + x\phi_a'(t-a)} \left(1 + \frac{x\phi_a''}{2}(t-a)^2\right) \\ &= e^{x\phi_a} \int\limits_0^{\infty} \mathrm{d}\xi\ \left(f_a + f_a'\xi + f_a \frac{x\phi_a''}{2}\xi^2\right) e^{x\phi_a'\xi} = \frac{f_a e^{x\phi_a}}{x|\phi_a'|} \left(1 + \frac{1}{x|\phi_a'|}\left(\frac{f_a'}{f_a} + \frac{\phi_a''}{|\phi_a'|}\right)\right). \end{aligned} \tag{268}$$

[6] Since the maximal value of $\phi(x)$ on the interval $x \in [a,b]$ occurs at the point $x = a$, the derivative of the function $\phi(x)$ at $x = a$ is negative, i.e. $\phi_a' < 0$.

Note that in deriving this result, we have neglected all terms which are suppressed by $e^{-\epsilon x|\phi_a'|}$; the practical way of doing this is to extend the ξ integration boundary to $+\infty$. Obviously, we do not need to re-consider $\delta I(x,\epsilon)$ since it is always exponentially suppressed relative to power-suppressed terms retained in Eq.(268).

There is a particular case of this general result that is known as the *Watson's lemma*. It applies to the asymptotic behavior of the integrals with $\phi(t) = t$, i.e.

$$I(x) = \int\limits_0^b {\rm d}t\ f(t)\ e^{-xt}, \quad b > 0. \tag{269}$$

We are interested in the behavior of this integral in the limit $x \to \infty$. Suppose that $f(t)$ can be represented by asymptotic series at $t \sim 0$

$$f(t) \sim t^\alpha \sum_{n=0}^{N} a_n t^{\beta n}, \tag{270}$$

where $\alpha > -1$ and $\beta > 0$. Then,

$$I(x) \sim \sum_{n=0}^{\infty} \frac{a_n \Gamma(\alpha + \beta n + 1)}{x^{\alpha+\beta n+1}}. \tag{271}$$

Again, with exponential accuracy, the results is independent of the upper integration boundary since we neglect all terms that are exponentially small.

To give an example of a situation where the Watson's lemma can be applied, consider the following integral

$$I(x) = \int\limits_0^{\pi/2} {\rm d}s\ e^{-x\sin^2 s}. \tag{272}$$

The integral is not in the form of Eq.(269); we can, however, transform it to the right form by changing variables $s \to t$ where

$$t = \sin^2 s. \tag{273}$$

Then $t \in [0,1]$ and

$$ {\rm d}s = \frac{{\rm d}t}{2\sqrt{t(1-t)}}. \tag{274}$$

Hence, $I(x)$ becomes

$$I(x) = \int\limits_0^1 {\rm d}t\ f(t) e^{-xt}, \tag{275}$$

where

$$f(t) = \frac{1}{2}\, t^{-1/2}(1-t)^{-1/2} = \frac{1}{2} t^{-1/2} \sum_{n=0}^{\infty} \frac{\Gamma(n+1/2) t^n}{n! \Gamma(1/2)}. \tag{276}$$

To apply the Watson lemma, we need a_n, α and β. We read them off from the above equation

$$\alpha = -1/2, \quad \beta = 1, \quad a_n = \frac{1}{2} \frac{\Gamma(n+1/2)}{n! \Gamma(1/2)}. \tag{277}$$

Hence,

$$I(x) \sim \frac{1}{2} \sum_{n=0}^{\infty} \frac{[\Gamma(n+1/2)]^2}{n!\ \Gamma(1/2)\ x^{n+1/2}}. \tag{278}$$

The above formulas are valid if the maximum of the function ϕ occurs at the boundary of the interval $[a, b]$. We will now move to the case when the maximum occurs in the interior of an interval $[a, b]$. The logic of the calculation is nearly identical but there are some differences in details.

We consider an integral

$$I(x) = \int\limits_a^b \mathrm{d}t\ f(t)\ e^{x\phi(t)}, \tag{279}$$

and assume that the function $\phi(t)$ for $t \in [a, b]$ reaches the maximum at the point $t = c \in [a, b]$. We are interested in the asymptotic behavior of $I(x)$ as $x \to \infty$.

We write

$$I(x) = I(x, \epsilon) + \delta I(x, \epsilon), \tag{280}$$

where

$$I(x, \epsilon) = \int\limits_{c-\epsilon}^{c+\epsilon} \mathrm{d}t\ f(t)\ e^{x\phi(t)}, \quad \delta I(x, \epsilon) = \int\limits_a^{c-\epsilon} \mathrm{d}t\ f(t)\ e^{x\phi(t)} + \int\limits_{c+\epsilon}^{b} \mathrm{d}t\ f(t)\ e^{x\phi(t)}. \tag{281}$$

We take ϵ to be small, so that the functions $f(t)$ and $\phi(t)$ can be expanded in Taylor series around $t = c$. The leading term reads

$$I(x, \epsilon) \sim f_c \int\limits_{c-\epsilon}^{c+\epsilon} \mathrm{d}t\ e^{x\phi_c + x\phi'_c(t-c) + \frac{1}{2}x\phi''_c(t-c)^2}. \tag{282}$$

We write $t - c = \xi$ and use the fact that $\phi'_c = 0$ and $\phi''_c < 0$ since c is the maximum. It follows

$$I(x, \epsilon) \sim f_c \; e^{x\phi_c} \int\limits_{-\epsilon}^{+\epsilon} \mathrm{d}\xi \; e^{-\frac{1}{2}x|\phi''_c|\xi^2}. \tag{283}$$

If we choose ϵ such that

$$\epsilon \ll |b-a|, \qquad 1 \ll x|\phi''_c|\epsilon^2, \tag{284}$$

where the possibility to do that follows from the fact that we consider $x \to \infty$ limit, we can extend integration boundaries in Eq.(283) to infinity without changing power-suppressed terms.

The simplest way to see this is to change variable $\xi \to \mu$ where $\xi = \mu/\sqrt{x|\phi''_c|}$. We then find

$$I(x, \epsilon) \sim \frac{f_c \; e^{x\phi_c}}{\sqrt{|x\phi''_c|}} \int\limits_{-\epsilon\sqrt{x|\phi''_c|}}^{+\epsilon\sqrt{x|\phi''_c|}} \mathrm{d}\mu \; e^{-\mu^2/2} \sim \frac{f_c \; e^{x\phi_c}}{\sqrt{|x\phi''_c|}} \int\limits_{-\infty}^{\infty} \mathrm{d}\mu \; e^{-\mu^2/2} \sim \frac{f_c \; e^{x\phi_c}\sqrt{2\pi}}{\sqrt{|x\phi''_c|}}. \tag{285}$$

Similar to examples discussed earlier, we can also discard $\delta I(x, \epsilon)$ contribution to the integral $I(x)$ since they are exponentially suppressed

$$\frac{\delta I(x, \epsilon)}{I(x, \epsilon)} \sim e^{-1/2\epsilon^2|\phi''_c|x} \ll 1. \tag{286}$$

We can improve the description of the asymptotic behavior of the integral $I(x)$ by computing power-suppressed terms in the asymptotic expansion. To this end, we expand $f(t)$ and $\phi(t)$ into series. We should be careful with these expansions since the function ϕ has a prefactor x in front of it. Suppose we aim at finding $1/x$ corrections to Eq.(285). Since each power of ξ in the integrand leads to $1/\sqrt{x}$ suppression in the integral (since the integration region is $\xi \sim 1/\sqrt{x}$), we need to expand the function $f(t)$ through the second order and the function $\phi(t)$ through the fourth order around $t = c$. When $e^{x\phi(t)}$ is expanded, we need to account for $(\phi'''_c)^3$ contribution since it also delivers the $1/x$ correction. Hence, we write

$$\begin{aligned} I(x, \epsilon) \sim e^{x\phi_c} \int\limits_{-\epsilon}^{\epsilon} \mathrm{d}\xi \; e^{-1/2x|\phi''_c|\xi^2} & \left(f_c + f'_c\xi + \frac{1}{2}f''_c\xi^2 + ..\right) \\ & \times \left(1 + \frac{1}{6}x\phi'''_c\xi^3 + \frac{1}{72}x^2(\phi'''_c)^2\xi^6 + \frac{1}{24}x\phi''''_c\xi^4 + ..\right). \end{aligned} \tag{287}$$

Since all odd terms integrate to zero, we find

$$I(x,\epsilon) \sim f_c e^{x\phi_c} \int\limits_{-\epsilon}^{\epsilon} \mathrm{d}\xi\; e^{-1/2|\phi_c''|\xi^2} \left(1 + \frac{f_c''}{2f_c}\xi^2 + \frac{f_c'}{f_c}\frac{x\phi_c'''\xi^4}{6} + \frac{x^2(\phi_c''')^2\xi^6}{72} + \frac{x\phi_c''''\xi^4}{24} + \cdots\right). \tag{288}$$

The relevant integrals can be computed using the following formula

$$\int\limits_{-\epsilon}^{\epsilon} \mathrm{d}\xi\; \xi^{2n} e^{-1/2x|\phi_c''|\xi^2} = \int\limits_{-\epsilon\sqrt{x|\phi_c''|/2}}^{\epsilon\sqrt{x|\phi_c''|/2}} \frac{\mathrm{d}\mu\; \mu^{2n} e^{-\mu^2}}{|x\phi_c''/2|^{n+1/2}} \to \int\limits_{-\infty}^{\infty} \frac{\mathrm{d}\mu\; \mu^{2n} e^{-\mu^2}}{|x\phi_c''/2|^{n+1/2}} = \frac{\Gamma(n+1/2)}{|x\phi_c''/2|^{n+1/2}}. \tag{289}$$

Finally, using this result and discarding contributions $\delta I(x,\epsilon)$ because of their exponential suppression, we obtain the final result

$$I(x) \sim f_c e^{x\phi_c}\sqrt{\frac{2\pi}{x|\phi_c''|}}\left[1 + \frac{1}{x|\phi_c''|}\left(\frac{f_c''}{2f_c|\phi_c''|} + \frac{f_c'\phi_c'''}{2|\phi_c''|^2 f_c} + \frac{\phi_c''''}{8f_c|\phi_c''|^2} + \frac{5}{24}\frac{(\phi_c''')^2}{f_c|\phi_c''|^3}\right)\right]. \tag{290}$$

Let us consider a few examples that do not directly fall into classes of integrals that we just discussed but that can be dealt with using similar logic. We will begin with the modified Bessel function. The modified Bessel function $I_n(x)$ has the following integral representation

$$I_n(x) = \frac{1}{\pi}\int\limits_0^{\pi} e^{x\cos t}\cos(nt)\,\mathrm{d}t. \tag{291}$$

We are interested in the behavior of $I_n(x)$ in the limit $x \to \infty$. According to our classification of Laplace integrals $\phi(t) = \cos(t)$. Considering the interval $t \in [0,\pi]$, we observe that the maximum of the function $\phi(t)$ occurs at $t = 0$. An interesting aspect of this integral, however, is that $\phi'_{t=0} = 0$ so we cannot apply formulas that we derived at the beginning of our discussion of Laplace integrals. Instead, we have to expand to second order and beyond keeping quadratic terms $\mathcal{O}(t^2)$ in the exponent. We find

$$\cos(t) \sim 1 - \frac{t^2}{2} + \frac{t^4}{24}, \quad \cos(nt) \sim 1 - \frac{n^2t^2}{2} + \frac{n^4t^4}{24}, \tag{292}$$

so that

$$I_n(x) \sim \frac{e^x}{\pi}\int_0^\infty \mathrm{d}t\ e^{-xt^2/2}\left(1 - \frac{n^2t^2}{2} + \frac{xt^4}{24}\right)$$
$$= \frac{e^x}{\pi}\sqrt{\frac{2}{x}}\int_0^\infty \mathrm{d}\xi\ e^{-\xi^2}\ \left(1 - \frac{1}{x}\left(n^2 - \frac{1}{6}\right)\xi^2\right) = \frac{e^x}{\sqrt{2\pi x}}\left(1 - \frac{1}{2x}\left(n^2 - \frac{1}{6}\right)\right). \tag{293}$$

The second example we want to consider refers to the Stirling's formula for $n!$ at large n. To be slightly more general, we will derive the asymptotic behavior of the Gamma-function and use the fact that $n! = \Gamma(n+1)$. The Gamma function is defined as

$$\Gamma(z) = \int_0^\infty \mathrm{d}t\ t^{z-1}e^{-t}. \tag{294}$$

We are interested in the asymptotic behavior of $\Gamma(z)$ at $z \to \infty$. To write $\Gamma(z)$ in a form that is consistent with Laplace integral, we change variables $t = sz$, use the fact that $t^z = e^{z\ln t} = e^{z\ln s + z\ln z} = z^z e^{z\ln s}$ and write

$$\Gamma(z) = z^z\int_0^\infty \frac{\mathrm{d}s}{s}\ e^{z(\ln s - s)}. \tag{295}$$

The function $\phi(s) = \ln(s) - s$ equals to $-\infty$ at $s = 0$ and $s = \infty$. Moreover,

$$\phi'(s) = 1/s - 1, \tag{296}$$

so that $\phi(s)$ reaches the maximum at $s = 1$. Expanding around $s = 1$, we find

$$\phi(s) \approx -1 - \frac{(s-1)^2}{2} + \mathcal{O}\left((1-s)^3\right). \tag{297}$$

We introduce $\xi = (s-1)$, extend the integration region to $-\infty < \xi < +\infty$ and obtain

$$\Gamma(z) \sim z^z e^{-z}\int_{-\infty}^\infty \mathrm{d}\xi\ e^{-z\xi^2/2} \sim \sqrt{\frac{2\pi}{z}}z^z e^{-z}, \tag{298}$$

We can use this result to re-derive the Stirling formula that gives the behavior of $n!$ at large n. To this end, we write

$$n! = \Gamma(n+1) = n\Gamma(n) \sim (2\pi n)^{1/2}\ n^n\ e^{-n}, \tag{299}$$

where in the last step we used Eq.(298).

6 Asymptotic expansion of complex-valued integrals: integration by parts and the method of stationary phase

An immediate generalization of the Laplace-type integrals that we studied in the previous lecture are integrals that contain a *complex-valued* function $\phi(t)$ in the exponent. We will assume that the second function that appeared in the definition of a Laplace integral, $f(t)$, is real since this assumption does not restrict what we do in any way (if $f(t)$ is complex-valued, the problem simply splits into two problems).

As the first step we will assume that the function in the exponent is pure imaginary and consider the following integrals

$$I(x) = \int_a^b \mathrm{d}t\; f(t)\; e^{ix\phi(t)}. \tag{300}$$

We would be typically interested in the behavior of such integrals as $x \to \infty$.

Similar to Laplace integrals discussed earlier, there is a variety of cases to consider; the simplest ones are cases where integration by parts can be used. We will start with an example.

Consider the following integral

$$I(x) = \int_0^1 \mathrm{d}t\; \frac{e^{ixt}}{1+t}. \tag{301}$$

We are interested in the behavior of this integral in the $x \to \infty$ limit. We would like to expand this integral in powers of $1/x$. To construct an expansion, we write

$$I(x) = \int_0^1 \mathrm{d}t\; \frac{1}{1+t}\,\frac{1}{ix}\,\frac{\mathrm{d}}{\mathrm{d}t}\left[e^{ixt}\right]. \tag{302}$$

Integrating by parts, we obtain

$$I(x) = \frac{1}{ix}\frac{1}{1+t}e^{ixt}\Big|_{t=0}^{t=1} + \frac{1}{ix}\int_0^1 \frac{\mathrm{d}t}{(1+t)^2}e^{ixt}. \tag{303}$$

The central point is that the second term on the r.h.s. of Eq.(303) is smaller than the first one. To prove this, we apply integration by parts one more time

$$\begin{aligned}\frac{1}{ix}\int\limits_0^1 \frac{\mathrm{d}t\; e^{ixt}}{(1+t)^2} &= \frac{1}{(ix)^2}\int\limits_0^1 \frac{\mathrm{d}t}{(1+t)^2}\frac{\mathrm{d}}{\mathrm{d}t}\left[e^{ixt}\right] \\ &= \frac{e^{ixt}}{(ix)^2}\frac{1}{(1+t)^2}\Big|_{t=0}^{t=1} + \frac{2}{(ix)^2}\int\limits_0^1 \frac{\mathrm{d}t\; e^{ixt}}{(1+t)^3}.\end{aligned} \tag{304}$$

Since the r.h.s. of the above equation scales as $1/x^2$, we conclude that in the r.h.s. of Eq.(303), the second term is negligible compared to the first one. Hence,

$$I(x) \sim \frac{1}{ix}\left(\frac{e^{ix}}{2} - 1\right). \tag{305}$$

This result implies that, if integration by parts is applicable, the boundary terms vanish more slowly than the remaining integral. Although we demonstrated this by repeated application of integration by parts, this fact is a consequence of the so-called Riemann-Lebesgue lemma. This lemma states that

$$\int\limits_a^b \mathrm{d}t\; f(t)e^{i\phi(t)x} \to 0, \tag{306}$$

as $x \to \infty$. The condition for this is that the integral $\int\limits_a^b \mathrm{d}t\; |f(t)|$ exists. Hence, in Eq.(303), the integral over t is suppressed compared to the boundary terms.

Although Eq.(306) can be rigorously proven, it can also be intuitively understood. The $x \to \infty$ limit implies that $e^{i\phi(t)x}$ oscillates strongly, whereas the function $f(t)$ changes quite slow, in comparison. As the result, contributions from adjacent sub-intervals nearly cancel *except* in regions where oscillations do not happen. Such regions are characterized by a vanishing derivative of the function ϕ; this gives rise to the name of one of the methods to compute them – the *stationary phase* approximation.

To what extent this cancellation actually happens and how the integral in Eq.(306) approaches zero depends on the details of the problem. If $\phi'(t)$ does not vanish anywhere on the interval $[a, b]$, the integral vanishes as $1/x$; this follows from a straightforward generalization of the integration-by-parts discussion.

However, similar to our discussion of real-valued integrals in the previous lecture, integration by parts does not work if the derivative of the function

$\phi(t)$ vanishes in the interval $t \in [a, b]$. We will suppose that this happens at the boundary point $x = a$. We then write

$$I(x) = \int\limits_a^{a+\epsilon} \mathrm{d}t\ f(t)\ e^{i\phi(t)x} + \int\limits_{a+\epsilon}^{b} \mathrm{d}t\ f(t)\ e^{i\phi(t)x}. \tag{307}$$

Consider the first term and assume that the first $p-1$ derivatives of the function $\phi(t)$ vanish, $p > 1$. Then

$$\int\limits_a^{a+\epsilon} \mathrm{d}t\ f(t)\ e^{i\phi(t)x} \sim \int\limits_0^{\epsilon} \mathrm{d}\xi\ f_a\ e^{ix\phi_a + ix\phi_a^{(p)}/p!\xi^p} = e^{ix\phi_a} f_a \int\limits_0^{\epsilon} \mathrm{d}\xi\ e^{i\Omega\,\xi^p}, \tag{308}$$

where $\xi = t - a$ and $\Omega = x\phi_a^{(p)}/p! \to \infty$. Let us assume that $\phi_a^{(p)} > 0$. We change variables $\xi = (\mu/\Omega)^{1/p}$ and find

$$\int\limits_0^{\epsilon} \mathrm{d}\xi\ e^{i\Omega\xi^p} = \frac{1}{p\ \Omega^{1/p}} \int\limits_0^{\epsilon^p\Omega} \mathrm{d}\mu\ \mu^{1/p-1} e^{i\mu}. \tag{309}$$

We choose ϵ such that $\epsilon^p\Omega = \epsilon^p x\phi_a^{(p)}/p! \gg 1$. This allows us to extend the upper integration boundary in the above integral to infinity. Then, we use Cauchy's theorem and write the required integral as an integral over the positive imaginary axis. We find

$$\int\limits_0^{\infty} \mathrm{d}\mu \mu^{1/p-1} e^{i\mu} = e^{i\pi/(2p)}\Gamma(1/p). \tag{310}$$

This result implies the following asymptotic behavior of the integral $I(x)$ at $x = \infty$

$$I(x) \sim e^{i(x\phi_a + \pi/(2p))}\frac{f_a}{p}\,\Gamma\left(\frac{1}{p}\right)\left[\frac{p!}{x\phi_a^{(p)}}\right]^{1/p}, \qquad \phi_a^{(p)} > 0. \tag{311}$$

We note that if $\phi_a^{(p)} < 0$, the above formula will slightly change. In this case, we will perform the rescaling in Eq.(309) with the absolute value of $|\phi_a^{(p)}|$; this will leave us with the *complex conjugated* version of Eq.(310). Hence, for $\phi_a^{(p)} < 0$, we obtain

$$I(x) \sim e^{i(x\phi_a - \pi/(2p))}\frac{f_a}{p}\,\Gamma\left(\frac{1}{p}\right)\left[\frac{p!}{x|\phi_a^{(p)}|}\right]^{1/p}, \qquad \phi_a^{(p)} < 0. \tag{312}$$

It remains to explain why the upper integration boundary in Eq.(309) can be extended to infinity and why the second integral in Eq.(307) is irrelevant for the leading $x \to \infty$ asymptotic behavior of $I(x)$.

Let us start with the second question. Since on the interval $t \in [a+\epsilon, b]$ the first derivative of the function $\phi(t)$ does not vanish, we can use integration by parts to estimate the contribution of this interval to the integral $I(x)$. We find

$$I(a+\epsilon, x) = \int\limits_{a+\epsilon}^{b} \mathrm{d}t \; e^{ix\phi(t)} \sim \frac{f_a}{x\phi'_{a+\epsilon}} \sim \frac{f_a p!}{px\phi_a^{(p)}\epsilon^{p-1}} \sim \frac{f_a\epsilon}{\epsilon^p p\Omega}, \tag{313}$$

where we used an estimate of the derivative of the function ϕ at $a+\epsilon$, $\phi'_{a+\epsilon} \sim p\phi_a^{(p)}/p!\epsilon^{p-1}$. We can now compare $I(x)$ in Eq.(311) and $I(a+\epsilon, x)$ in Eq.(313). Taking the ratio of relevant factors, we obtain

$$\frac{I(a+\epsilon, x)}{I(x)} \sim \frac{\epsilon}{\epsilon^p\Omega\left[\frac{p!}{x\phi_a^{(p)}}\right]^{1/p}} \sim \frac{\epsilon}{\epsilon^p\Omega\left[\frac{\epsilon^p}{\epsilon^p\Omega}\right]^{1/p}} \sim (\epsilon^p\Omega)^{1/p-1} \ll 1, \tag{314}$$

since ϵ is chosen in such a way that $\epsilon^p\Omega$ is very large and $1/p-1$ is negative.

A similar estimate works for terms neglected in Eq.(309) when the upper integration boundary was taken to infinity. To show this, we note that the lower integration boundary is irrelevant for understanding how an integral depends on the upper integration boundary. Hence, we can conveniently change the lower integration boundary and consider the following integral

$$\int\limits_{1}^{\epsilon^p\Omega} \mathrm{d}\mu \; \mu^{1/p-1} e^{i\mu}, \tag{315}$$

for which integration by parts computation can be applied. We write

$$\int\limits_{1}^{\epsilon^p\Omega} \mathrm{d}\mu \; \mu^{1/p-1} e^{i\mu} = \int\limits_{1}^{\infty} \mathrm{d}\mu \; \mu^{1/p-1} e^{i\mu} - \int\limits_{\epsilon^p\Omega}^{\infty} \mathrm{d}\mu \; \mu^{1/p-1} e^{i\mu}. \tag{316}$$

We then apply integration by parts to the second integral neglecting the contributions from the upper integration boundary and find

$$\int\limits_{\epsilon^p\Omega}^{\infty} \mathrm{d}\mu \; \mu^{1/p-1} e^{i\mu} \sim c_2 \left(\epsilon^p\Omega\right)^{1/p-1}. \tag{317}$$

Hence, we obtain

$$\int_1^{\epsilon^p\Omega} d\mu\, \mu^{1/p-1} e^{i\mu} = c_1 + c_2 \left(\epsilon^p\Omega\right)^{1/p-1}, \tag{318}$$

where the constant c_1 corresponds to the $\epsilon^p\Omega \to \infty$ limit. The second term in the above equation is the neglected contribution which is sub-leading, similar to Eq.(314). Hence, Eq.(311) indeed describes the leading asymptotic behavior of the integral $I(x)$ at $x = \infty$.

We will consider a few simple examples where the results Eqs.(311,312) can be applied. We begin with the integral

$$I(x) = \int_0^{\pi/2} dt\, e^{ix\cos t}, \tag{319}$$

and consider its behavior as $x \to \infty$. First, we note that $\phi(t) = \cos t$ and $\phi'(t) = 0$ at $t = 0$. Then we write $\cos t \sim 1 - \frac{t^2}{2}$, so that $\phi_0 = 1$, $p = 2$, $\phi_0^{(p)} = -1$. Then, using Eq.(312), we find

$$I(x) \sim e^{ix - i\pi/4} \left[\frac{2}{x}\right]^{1/2} \frac{\Gamma(1/2)}{2} \sim \sqrt{\frac{\pi}{2x}} e^{i(x-\pi/4)}. \tag{320}$$

As another example, we consider the following integral

$$I(x) = \int_0^1 dt\, e^{ix(t-\sin t)}. \tag{321}$$

We are interested in the behavior of $I(x)$ in the limit $x \to \infty$. We find $\phi(t) = t - \sin t$, $\phi'(t) = 1 - \cos t$ and $\phi'(t) = 0$ if $t = 0$. Expanding $\phi(t)$ at $t = 0$, we find $\phi(t) \sim t^3/3!$. We conclude that $\phi_0 = 0$, $\phi_0^{(3)} = 1$, $p = 3$. Hence, we conclude that

$$I(x) \sim \frac{e^{i\pi/6}}{3} \Gamma\left(\frac{1}{3}\right) \left(\frac{6}{x}\right)^{1/3}, \tag{322}$$

as $x \to \infty$.

7 The steepest-descent method

The *steepest-descent method* is a generalization of the stationary-phase method discussed in the previous lecture. It is used to calculate integrals of the following type

$$I(x) = \int_C \mathrm{d}t\; h(t) e^{x\rho(t)}, \tag{323}$$

in the limit $x \to \infty$. The integration is performed in the complex plane of a variable t along the contour C. The functions $h(t)$ and $\rho(t)$ are analytic on C. The idea of the method is to use analyticity of the integrand to express $I(x)$ as an integral along a *new* contour C_1 such that $\rho(t)$ has a constant imaginary part on C_1. To see why this helps, imagine that this has been accomplished. Then, $\rho(t) = \phi(t) + i\psi$ and the integral becomes

$$I(x) = e^{i\psi} \int_{C_1} \mathrm{d}t\; h(t) e^{x\phi(t)}. \tag{324}$$

Hence, in spite of the fact that the integration is performed along a complex path, the argument of the exponential function is real and the analysis of this integral can be performed using the Laplace method discussed in the previous lecture.

We will consider a few examples to get a sense of how this works. Consider

$$I(x) = \int_0^1 \mathrm{d}t \ln t\; e^{ixt}. \tag{325}$$

We are interested in the behavior of this integral in the limit $x \to +\infty$. To find it, we view $I(x)$ as an integral in the complex plane ($t \to z$) along the positive real axis. Since $\ln(z)$ is an analytic function in the complex plane with a cut along the *negative* real axis, we can use the Cauchy theorem to write (c.f. Fig. 1)

$$\int_{C_1} \mathrm{d}z \ln z\; e^{ixz} + \int_{C_2} \mathrm{d}z \ln z\; e^{ixz} + \int_{C_3} \mathrm{d}z \ln z\; e^{ixz} = 0, \tag{326}$$

where the three contours are 1) $C_1 : z = x, x \in [0,1]$; 2) $C_2 : z = 1 + iy, y \in [0, +\infty]$; 3) $C_3 : z = is,\ s \in [+\infty, 0]$. The integral along C_1 is the original integral $I(x)$. It follows that

$$I(x) = -\int_{C_2} \mathrm{d}z \ln z\; e^{ixz} - \int_{C_3} \mathrm{d}z \ln z\; e^{ixz}. \tag{327}$$

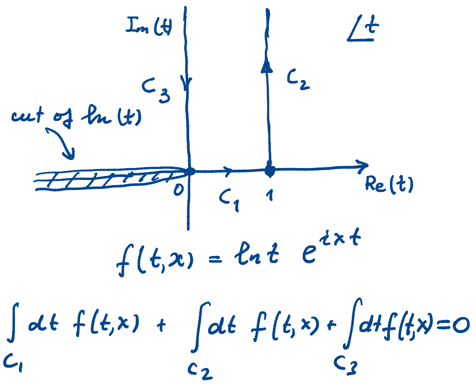

Figure 3: Contour choice for the integral in Eq.(325).

Let us start with the last integral on the r.h.s. of Eq.(327) since it can be calculated exactly. It reads

$$\int\limits_{C_3} \mathrm{d}z \ln z\, e^{ixz} = -i \int\limits_0^\infty \mathrm{d}s\;\ln(is) e^{-xs} = -\frac{i}{x}\int\limits_0^\infty \mathrm{d}\xi\, \left(\frac{i\pi}{2} - \ln(x) + \ln(\xi)\right) e^{-\xi}$$
$$= -\frac{i}{x}\left(\frac{i\pi}{2} - \ln(x) - \gamma_E\right), \tag{328}$$

where γ_E is the Euler constant and we used $\xi = xs$.

The first integral on the r.h.s. of Eq.(327) reads

$$\int\limits_{C_2} \mathrm{d}z \ln z\, e^{ixz} = i e^{ix}\int\limits_0^\infty \mathrm{d}y\;\ln(1+iy) e^{-xy}. \tag{329}$$

Since

$$\ln(1+iy) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} i^n}{n} y^n, \tag{330}$$

we find

$$\int\limits_{C_2} \mathrm{d}z \ln z\, e^{ixz} \sim i e^{ix} \sum_{n=1}^{\infty} \frac{(-1)^{n+1} i^n \Gamma(n+1)}{n} x^{-n-1}. \tag{331}$$

The complete result for the asymptotic expansion of $I(x)$ at $x = \infty$ reads

$$I(x) \sim \frac{i}{x}\left(\frac{i\pi}{2} - \ln(x) - \gamma_E\right) - e^{ix}\sum_{n=1}^{\infty} \frac{(-i)^{n+1}\Gamma(n+1)}{n x^{n+1}}. \tag{332}$$

As another example, consider the following integral

$$I(x) = \int_0^1 \mathrm{d}t e^{ixt^2}. \tag{333}$$

We are interested in its asymptotic behavior for $x \to \infty$. Similar to the previous case, we will have to extend the calculation of this integral into the complex plane, to obtain integrals which converge rapidly. Recall that we would like to do that in such a way that the argument of the exponential function has constant imaginary part along the integration contour. Hence, we write $t = z = u + iv$ and compute

$$it^2 = i(u^2 - v^2) - 2uv. \tag{334}$$

Therefore, for the rapid convergence, we would like to choose the integration contour in such a way that

$$\mathrm{Im}(it^2) = u^2 - v^2 = \mathrm{const}, \quad \mathrm{Re}(it^2) = -2uv < 0. \tag{335}$$

The second condition ensures that the integrand is exponentially suppressed on the integration path.

Consider the two boundary points of the integral, $t = 0$ and $t = 1$. The selected contours should run through them, see Fig. 4.

We begin with the analysis of the point $t = 0$. Since at $t = 0$, $it^2 = 0$, the contour that runs through the the point $t = 0$ and has constant imaginary part satisfies

$$u^2 - v^2 = 0, \quad \Rightarrow \quad u = v > 0. \tag{336}$$

Note that the the choice of $u = v$, as opposed to the $u = -v$ solution, is due to the condition $uv > 0$, c.f. Eq.(335). Hence, we can parameterize the integration contour as follows

$$t = \frac{1+i}{\sqrt{2}} s = e^{i\pi/4}\, s, \tag{337}$$

where $0 < s < \infty$ is the real parameter that measures the distance to the origin along the integration contour.

The second boundary is at $t = 1$ where $it^2 = i$. Hence, for the second contour, we need to choose

$$u^2 - v^2 = 1 \quad \to \quad u = \sqrt{v^2 + 1}. \tag{338}$$

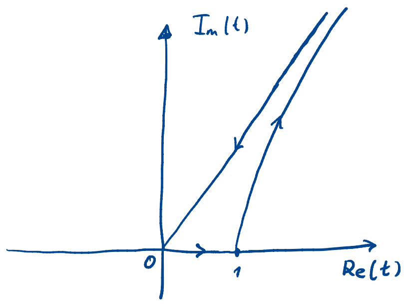

Figure 4: Contour choice for the integral in Eq.(342).

Therefore, along this contour $t = \sqrt{v^2+1} + iv$ and $it^2 = i - 2v\sqrt{1+v^2}$. Motivated by that, we introduce a new variable s defined as

$$it^2 = i - s. \tag{339}$$

It follows that

$$t = \sqrt{1+is}, \tag{340}$$

and

$$\mathrm{d}t = \frac{i}{2(1+is)^{1/2}}\,\mathrm{d}s. \tag{341}$$

Hence, using Cauchy theorem (i.e. absence of singularities inside the integration contour, cf. Fig.2) we find

$$I(x) = e^{i\pi/4}\int_0^\infty \mathrm{d}s e^{-xs^2} - \frac{ie^{ix}}{2}\int_0^\infty \frac{\mathrm{d}s}{(1+is)^{1/2}} e^{-xs}. \tag{342}$$

Asymptotic expansion of these integrals is now easily performed. To compute the first integral, we change integration variables $s \to \xi/\sqrt{x}$, use the well-known result for the Gaussian integral

$$\int_0^\infty \mathrm{d}\xi\; e^{-\xi^2} = \frac{\sqrt{\pi}}{2}, \tag{343}$$

and find

$$e^{i\pi/4}\int_0^\infty \mathrm{d}s e^{-xs^2} = \frac{e^{i\pi/4}}{2}\sqrt{\frac{\pi}{x}}. \tag{344}$$

The second integral in Eq.(342) is more difficult to compute. Nevertheless, we can expand the square root in Taylor series around $s = 0$ since the exponential function cuts off the integral at $s \sim 1/x$. We find

$$\frac{i}{2}\int_0^\infty \frac{\mathrm{d}s}{(1+is)^{1/2}} e^{-xs} = \frac{i}{2}\sum_{n=0}^{\infty}\int_0^\infty \mathrm{d}s e^{-xs} \frac{\Gamma\left(n+\frac{1}{2}\right)(-is)^n}{\Gamma\left(\frac{1}{2}\right) n!}. \tag{345}$$

Using

$$\int_0^\infty \mathrm{d}s\, s^n e^{-xs} = \Gamma(n+1)\, x^{-n-1}, \tag{346}$$

we obtain the result

$$\frac{i}{2}\int_0^\infty \frac{\mathrm{d}s}{(1+is)^{1/2}} e^{-xs} = \frac{i}{2}\sum_{n=0}^{\infty} \frac{\Gamma(n+1)\,\Gamma\left(n+\frac{1}{2}\right)(-i)^n}{\Gamma\left(\frac{1}{2}\right) n!\, x^{n+1}}. \tag{347}$$

Finally, putting the two parts together we find

$$I(x) \sim \frac{e^{i\pi/4}}{2}\sqrt{\frac{\pi}{x}} + \frac{e^{ix}}{2}\sum_{n=0}^{\infty}\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}\left(\frac{-i}{x}\right)^{n+1}. \tag{348}$$

Having considered the two examples, we can discuss the problem in a more formal way and briefly talk about the general theory behind the steepest-descent method in the complex plane. The complex plane can be described by a variable $z = u + iv$, where u and v are real and imaginary parts of z. For any function of two variables $f(u, v)$ and any point in the (u, v) plane we can define a gradient vector $\vec{\nabla} f = (\partial_u f, \partial_v f)$. The rate of change of the function $f(u, v)$ at a point (u, v) along the path characterized by a unit vector $\vec{n}$, is given by $\vec{n} \cdot \vec{\nabla} f$. Since

$$\vec{n} \cdot \vec{\nabla} f = |\vec{\nabla} f| \cos\alpha, \tag{349}$$

where α is the angle between $\vec{n}$ and $\vec{\nabla} f$, the maximal change occurs in the direction of the vector $\vec{\nabla} f$ itself ($\alpha = 0$).

Suppose we need to integrate a function $e^{x\rho(z)}$ over z along some contour in the complex z-plane. The function ρ is written as $\rho = \phi + i\psi$. Then

$$e^{x\rho(z)} = e^{ix\psi(u,v)} e^{x\phi(u,v)}. \tag{350}$$

The steepest-descent contour is defined as a contour whose tangent is parallel to $\vec{\nabla} e^{x\phi(u,v)} = e^{x\phi(u,v)}\, \vec{\nabla}\phi \sim \vec{\nabla}\phi$; hence, the steepest-descent contour is a contour along which the function $e^{x\phi}$ changes most rapidly.

However, if the original function $\rho(z)$ is *analytic* along the integration contour, $\vec{\nabla}\phi$ and $\vec{\nabla}\psi$ *are not independent*. Indeed, analytic functions satisfy

$$\frac{\partial \rho}{\partial \bar{z}} = 0. \tag{351}$$

Separating real and imaginary parts in this equation, we obtain

$$\frac{\partial \phi}{\partial u} = \frac{\partial \psi}{\partial v}, \quad \frac{\partial \phi}{\partial v} = -\frac{\partial \psi}{\partial u}. \tag{352}$$

These equations imply

$$\vec{\nabla}\phi \cdot \vec{\nabla}\psi = \frac{\partial \phi}{\partial u}\frac{\partial \psi}{\partial u} + \frac{\partial \phi}{\partial v}\frac{\partial \psi}{\partial v} = -\frac{\partial \phi}{\partial u}\frac{\partial \phi}{\partial v} + \frac{\partial \phi}{\partial v}\frac{\partial \phi}{\partial u} = 0. \tag{353}$$

It follows that the steepest-descent contour is aligned with the direction along which the function ψ – the imaginary part of the function ρ – does not change. Hence, *steepest-descent contours are stationary-phase contours.*

We will now articulate why the knowledge of a steepest-descent contour is important. Consider a point $z_0 = (u_0, v_0)$ and an integration contour characterized by a vector $\vec{n}$ passing through this point. Then, parameterizing the contour by $s\vec{n}$ we find

$$e^{x\phi} \approx e^{x\phi_0} e^{xs|\vec{\nabla}\phi_0| \cos\alpha}, \tag{354}$$

where α is the angle between $\vec{\nabla}\phi$ and $\vec{n}$. It follows that if the integration contour can be deformed in the direction $-\vec{\nabla}\phi_0$, the integration will converge very rapidly in the $x \to \infty$ limit.

Similar to cases discussed earlier, the relative importance of different parts of the integration contour is determined by maxima of the function ϕ and there are several options. The function ϕ can be maximal either at the integration boundaries or somewhere along the integration contour.

This latter case is somewhat peculiar since analytic functions *can not have true local maxima or minima*. This feature is a consequence of the fact that both functions ϕ and ψ satisfy Laplace equations

$$\nabla^2\phi = 0, \quad \nabla^2\psi = 0. \tag{355}$$

Therefore if, say, $\partial_u^2\phi < 0$, then $\partial_v^2\phi > 0$. The first condition means that the function decreases in the u direction, while the second condition implies that the function increases in the v direction. This situation is referred to as a "saddle point" and the integration contour should, in general, be deformed in such a way that it passes through the saddle point along the direction of the fastest descent, avoiding directions of the fastest ascent.

We will consider an example now. The Bessel function $J_0(x)$ obeys the following representation

$$J_0(x) = \int\limits_{-\pi/2}^{\pi/2} \cos(x\cos\theta)\frac{d\theta}{\pi}. \tag{356}$$

We are interested in the behavior of $J_0(x)$ at large x. To determine it, we will try to write an integral representation for $J_0(x)$ in the complex plane choosing integration contour(s) in such a way that taking the $x \to \infty$ limit becomes straightforward.

We can change variables $\theta = it$, use the fact that $\cos\theta = \cos it = \cosh t$ and write

$$J_0(x) = \mathrm{Re}\left[\frac{1}{i\pi}\int\limits_{-i\pi/2}^{i\pi/2} dt\ e^{ix\cosh t}\right]. \tag{357}$$

We would like to modify the above equation by introducing an integration over a particular contour that we will refer to as C. We write

$$J_0(x) = \mathrm{Re}\left[\frac{1}{i\pi}\int\limits_{C} dt\ e^{ix\cosh t}\right]. \tag{358}$$

The contour C is given by a union of three intervals $[-\infty - i\pi/2, -i\pi/2] \cup [-i\pi/2, i\pi/2] \cup [i\pi/2, i\pi/2+\infty]$, The first and the last segments are contours that run parallel to the real axis. The equivalence of Eq.(357) and Eq.(358) is not immediately obvious, but it follows from the fact that integrals over the added segments vanish. To see why, consider one of them

$$\mathrm{Re}\left[\frac{1}{i\pi}\int\limits_{i\pi/2}^{i\pi/2+\infty} dt\ e^{ix\cosh t}\right]. \tag{359}$$

To parameterize the integration variable along the contour, we write $t = i\pi/2 + y$, $0 < y < \infty$ and obtain

$$\mathrm{Re}\left[\frac{1}{i\pi}\int\limits_{0}^{\infty} dy\ e^{ix\cosh(i\pi/2+y)}\right] = \mathrm{Re}\left[\frac{1}{i\pi}\int\limits_{0}^{\infty} dy\ e^{-x\sinh(y)}\right] = 0. \tag{360}$$

The last step follows from the fact that the integral in brackets is real; this implies that its product with $1/(i\pi)$ is purely imaginary.

We will now use representation Eq.(358) to compute the asymptotic expansion of the Bessel function $J_0(x)$ for $x \to \infty$. To this end, we note that there is a contour of a constant phase that connects the points $-\infty - i\pi/2$ and $+\infty + i\pi/2$ that passes through the origin. To find it, we write $z = u + iv$ and compute

$$i \cosh z = i \cos v \cosh u - \sin v \sinh u. \tag{361}$$

If we choose the contour to pass through $u = 0, v = 0$, the constant phase contour satisfies

$$\cos v \cosh u = 1. \tag{362}$$

We can show that the maximum of the function $\sin v \sinh u$ on the contour described by Eq.(362) occurs at $u = v = 0$. To prove this, we use Eq.(362) and find that along the contour

$$\frac{\mathrm{d}u}{\mathrm{d}v} = \frac{\sin v}{\cos v} \frac{\cosh u}{\sinh u}. \tag{363}$$

It follows

$$\frac{\mathrm{d} \sin v \sinh u}{\mathrm{d}v} = \cos v \sinh u + \frac{\sin^2 v \cosh^2 u}{\cos v \ \sinh u}. \tag{364}$$

We use $\sin^2 v = 1 - \cos v^2$ and Eq.(362) to eliminate $\cos v$ and $\sin v$ from the above equation and obtain

$$\frac{\mathrm{d} \sin v \sinh u}{\mathrm{d}v} = \sinh(u) \frac{1 + \cosh^2 u}{\cosh u}. \tag{365}$$

It follows from Eq.(365) that the derivative of the real part of $i \cosh(t)$ only vanishes at the point $z = (u, v) = (0, 0)$ and nowhere else on the integration contour described by Eq.(362). The point $z = 0$ is a saddle point as can be seen by expanding $i \cosh(t)$ in small u and v. Then

$$i \cosh t = i \cos v \cosh u - \sin v \sinh u \approx i + i \frac{(u^2 - v^2)}{2} - vu. \tag{366}$$

The contours of constant phase require $u^2 = v^2$, so that $v = \pm u$. The curves of steepest descent correspond to $v = u$ and the curves of steepest ascent to $v = -u$.

Hence, to parameterize the steepest-descent path in the neighborhood of $t = 0$, we write $t = e^{i\pi/4} s$, extend the integral over s to $\pm\infty$ and obtain

$$J_0(x) \sim \mathrm{Re} \left[\frac{e^{i(x+\pi/4)}}{i\pi} \int\limits_{-\infty}^{\infty} \mathrm{d}s \ e^{-xs^2/2} \right] = \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi}{4}\right). \tag{367}$$

Finally, we note that it is possible to compute more terms in the asymptotic expansion of $J_0(x)$ at $x = \infty$ following the approach described above.

8 Perturbation theory

We will discuss and illustrate general features of perturbation theory. A standard way in which perturbation theory appears in a physics problem is that there is a small parameter in the problem that prevents us from solving it exactly. However, if the small parameter is set to zero, the problem becomes solvable. We then develop methods that allow us to solve the original problem approximately by systematically expanding in the small parameter.

It is possible to think about perturbation theory in a broader sense, simply as a way to approximately solve complicated problems even when no obvious small parameter is present. In this case, we have to introduce an auxiliary small parameter into the problem, find solutions in dependence of this "small" parameter and, finally, set the value of this parameter to what it appears to be in the original problem.

Let us consider a few simple examples. We are interested in solving the following cubic equation.

$$x^3 - 4.001x + 0.002 = 0. \tag{368}$$

There is no small parameter here but we can introduce one by writing

$$x^3 - (4+\epsilon)x + 2\epsilon = 0. \tag{369}$$

The original problem, i.e. Eq.(368) is recovered if we choose $\epsilon = 10^{-3}$.

It is obvious that roots of Eq.(369) are functions of ϵ. We write

$$x(\epsilon) = a_0 + a_1\epsilon + a_2\epsilon^2 + \ldots, \tag{370}$$

substitute Eq.(370) to Eq.(369) and find the following result

$$\sum_{i=0}^{\infty} f_i(a_0, \ldots, a_i)\epsilon^i = 0. \tag{371}$$

Since ϵ is a parameter, Eq.(371) is only satisfied if all coefficients vanish independently of each other. Hence, instead of a single equation Eq.(369), we obtain an infinite sequence of equations

$$f_0(a_0) = 0, \quad f_1(a_0, a_1) = 0, \quad f_2(a_0, a_1, a_2) = 0, \cdots f_i(a_0, \ldots, a_i) = 0. \tag{372}$$

Inspecting the arguments of the functions f_i, it should become clear that we can solve these equations iteratively, starting with f_0 to determine a_0 and then continuing step by step to find the remaining coefficients a_i. Each of these steps is obviously simpler than solving the original third-order equation since we only have to solve one simple equation at a time.

We start with f_0. It reads

$$f_0 = a_0(a_0^2 - 4) = 0. \tag{373}$$

It follows that $a_0 = \pm 2, 0$ are three possible solutions.

We will consider $a_0 = -2$ for concreteness. Computing $f_1(-2, a_1)$, we find the following equation

$$f_1(-2, a_1) = 4 + 8a_1 = 0, \tag{374}$$

so that $a_1 = -1/2$. Computing $f_2(-2, -1/2, a_2)$, we find

$$(-1 + 8a_2) = 0, \tag{375}$$

which implies that $a_2 = 1/8$. Hence, one of the roots reads

$$x(\epsilon) \sim -2 - \frac{1}{2}\epsilon + \frac{1}{8}\epsilon^2 + \mathcal{O}(\epsilon^3), \tag{376}$$

which, for $\epsilon = 10^{-3}$, evaluates to -2.000499875. This is very close to the right answer -2.0004998751; the difference is consistent with $\mathcal{O}(\epsilon^3) \sim 10^{-9}$ which is the expected magnitude of the neglected terms.

We can do a similar exercise for $a_0 = 0$. We obtain

$$x(\epsilon) \sim \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2 + \frac{1}{16}\epsilon^3. \tag{377}$$

This evaluates to $x = 0.00049987506250$ which, again, agrees very well with the exact result 0.00049987506249.

This example illustrates three steps of a perturbative analysis of a problem: 1) convert the original problem into a perturbative problem by introducing a would-be small parameter; the perturbative problem should be easily solvable if the small parameter is set to zero; 2) assume that the answer is given by a series in the small parameter, and solve iteratively a sequence of simpler problems to find coefficients of the series; 3) recover the answer to the original problem by summing up – to the extent possible – the perturbative series for the required value of the small parameter.

We turn to another example that shows how a problem can be turned into a perturbative one in the context of solving differential equations. Consider a second order differential equation

$$y'' = f(x)y, \tag{378}$$

with the boundary conditions

$$y(0) = 1, \quad y'(0) = 1. \tag{379}$$

The function $f(x)$ is arbitrary; Eq.(378) should remind us about the Schrödinger equation for an arbitrary potential. Let us turn Eq.(378) into a perturbative problem by re-writing it as follows

$$y'' = \epsilon f(x) y. \tag{380}$$

If we set $\epsilon \to 0$, the equation becomes $y_0'' = 0$. It has two solutions $y_0(x) = a$ and $y_0(x) = bx$. We can satisfy the boundary conditions in Eq.(378) by choosing $y_0(x) = 1 + x$. Then, we write $y(x)$ as series in ϵ

$$y(x) = \sum_{n=0}^{\infty} \epsilon^n y_n(x), \tag{381}$$

substitute this series into into Eq.(380) and derive an equation for the coefficients of the series in Eq.(381). The result reads

$$y_n''(x) = f(x)\; y_{n-1}(x). \tag{382}$$

Since we satisfied the boundary conditions for the full solution $y(x)$ by an appropriate choice of $y_0(x)$, the boundary conditions for $y_n(x)$, $n > 0$, read $y_n(0) = 0$ and $y_n'(0) = 0$. The solution to Eq.(382) that satisfies these boundary conditions reads

$$y_n(x) = \int\limits_0^x \mathrm{d}t \int\limits_0^t \mathrm{d}s\; f(s) y_{n-1}(s). \tag{383}$$

Hence, the complete solution of the original differential equation is written as follows

$$\begin{aligned} y(x,\epsilon) &= 1 + x + \epsilon \int\limits_0^x \mathrm{d}t_1 \int\limits_0^t \mathrm{d}s_1\; f(s_1)(1+s_1) \\ &+ \epsilon^2 \int\limits_0^x \mathrm{d}t_2 \int\limits_0^{t_2} \mathrm{d}s_2\; f(s_2) \int\limits_0^{s_2} \mathrm{d}t_1 \int\limits_0^{t_1} \mathrm{d}s_1\; f(s_1)(1+s_1) + \ldots \end{aligned} \tag{384}$$

We can estimate if this series converges. Let us suppose that the function $|f(x)|$ is bounded from above on the interval $[0, x]$, $|f(x)| < K$. Then, the

$\mathcal{O}(\epsilon^n)$ contribution to Eq.(384) can be estimated from above by replacing $f(s_i)$ with K in Eq.(384). Integrating $(1+s_1)$ n times, we find

$$
\begin{aligned}
y_n(x) &< \epsilon^n K^n \left[\frac{x^{2n+1}}{(2n+1)!} + \frac{x^{2n}}{(2n)!}\right] = \epsilon^n K^n \frac{x^{2n}}{(2n)!}\left(1 + \frac{x}{2n+1}\right) \\
&< \epsilon^n K^n \frac{x^{2n}}{(2n)!}\left(1+x\right).
\end{aligned}
\tag{385}
$$

Hence,

$$
y(x,\epsilon) < (1+x)\cosh(\sqrt{\epsilon K}x). \tag{386}
$$

We find that the series solution Eq.(384) converges absolutely for all values of ϵ including $\epsilon = 1$ provided that $|f(x)|$ is bounded from above on the interval $[0,x]$. It is also clear from Eq.(386) that the quality of the approximate solution is controlled by the parameter $\sqrt{K}x = \sqrt{|\max[f(x)]|}x$. If this parameter is small, a few terms in Eq.(384) are sufficient to obtain an accurate description of the solution at $\epsilon = 1$ for all $x \in [0,x]$.

The construction of solutions by means of perturbative expansion that we described assumes that a Taylor expansion in a small parameter actually exists. If this is indeed the case, the procedure is referred to as "regular" perturbation theory. There are also cases when this is not the case; this means that either series does not have a form of a Taylor series (cf. Frobenius series in a local analysis of differential equations) or they do not converge (c.f. irregular singular points in local analysis of differential equations). In both cases one talks about "singular" perturbation theory.

Let us consider a few examples. Consider the following equation

$$
\epsilon^2 x^6 - \epsilon x^4 - x^3 + 8 = 0. \tag{387}
$$

We would like to find roots of this equation for small values of ϵ. We notice that if $\epsilon = 0$, the equation becomes

$$
x^3 = 8, \tag{388}
$$

so that the solutions are $x = 2, 2e^{i\phi}, 2e^{2i\phi}$, where $\phi = 2\pi/3$. We note, however, that the original equation Eq.(387) is a sixth order differential equation whereas Eq.(388) is a third order differential equation. This implies that when we set $\epsilon = 0$ in the original equation Eq.(387) *three roots of the original equation disappear*. This dramatic change in the number of solutions of the equation, that occurs when the small parameter is set to zero, implies that we deal with singular perturbation theory in this case.

Before we discuss the fate of the "disappeared" solutions, we will show that for the three solutions of Eq.(388) we can construct solutions that are valid also at finite ϵ by applying regular perturbative expansion. To this end, we write

$$x(\epsilon) = \sum_{n=0}^{\infty} a_0 \epsilon^n, \tag{389}$$

and find the following equations for various orders in the ϵ-expansion

$$8 - a_0^3 = 0, \quad a_0^2(3a_1 + a_0^2) = 0, \quad a_0(a_0^5 - 4a_0^2 a_1 - 3a_1^2 - 3a_0 a_2) = 0, \ \ldots. \tag{390}$$

Solving them for $a_0 = 2$ as an example, we find

$$x(\epsilon) = 2 - \frac{4}{3}\epsilon + 8\epsilon^2 - \frac{2864}{81}\epsilon^3 + \mathcal{O}(\epsilon^4). \tag{391}$$

For $\epsilon = 0.01$, $x(\epsilon) = 1.9874313$ whereas the exact solution is 1.9874334... A similar analysis can be applied to the other two $\mathcal{O}(\epsilon^0)$ solutions of Eq.(388).

We will now try to understand what has happened with the three solutions of Eq.(387) that disappeared from Eq.(388). The hypothesis that we have is that these solutions have such a dependence on ϵ that in the limit $\epsilon \to 0$ they move to infinity. The reason they are not visible in Eq.(388) is that Eq.(388) is computed under the implicit assumption that $x(\epsilon)$ stays finite when ϵ is taken to zero.

To see what happens if this assumption is violated, we write $x = y/\epsilon^\alpha$, where $\alpha > 0$. We will be looking for solutions where $y \sim \mathcal{O}(1)$.

Substituting this into Eq.(387) and multiplying the whole equation with $\epsilon^{6\alpha-2}$, we find

$$y^6 - \epsilon^{2\alpha-1}y^4 - \epsilon^{3\alpha-2}y^3 + 8\epsilon^{6\alpha-2} = 0. \tag{392}$$

We need to find the value of α that enables the construction of the solution of this equation with $y \sim \mathcal{O}(1)$. Upon some reflection, it is possible to see that the only possible choice is $\alpha = 2/3$. Then Eq.(392) becomes

$$y^6 - \epsilon^{1/3}y^4 - y^3 + \epsilon^2 8 = 0. \tag{393}$$

Taking $\epsilon \to 0$, we obtain the leading equation

$$y^3(y^3 - 1) = 0, \tag{394}$$

which, besides the trivial solution $y = 0$, contains three non-trivial solutions $y = 1, y = e^{i2\pi/3}, y = e^{i4\pi/3}$. These are exactly the three solutions that we were missing! The three $y = 0$ solutions are the ones that we found earlier.

The fact that they correspond to zero simply means that they *do not* contain terms that are proportional to $y/\epsilon^{2/3}$.

It follows from Eq.(393) that ϵ-dependent corrections to Eq.(394) scale as $\epsilon^{1/3}$. Hence, to develop a perturbative expansion, we write

$$x(\epsilon) = \epsilon^{-2/3} \sum_{n=0}^{\infty} a_n \epsilon^{n/3}. \tag{395}$$

For $a_0 = 1$, the first few terms read

$$x(\epsilon) = \epsilon^{-2/3} \left(1 + \frac{\epsilon^{1/3}}{3} - \frac{\epsilon}{81} + ... \right). \tag{396}$$

One can perform a similar analysis to determine corrections to other $\mathcal{O}(\epsilon^0)$ solutions of Eq.(394) following what we just discussed.

Another interesting example of singular perturbation theory concerns the following differential equation

$$\epsilon y'' - y' = 0, \tag{397}$$

with the boundary conditions $y(0) = 0$ and $y(1) = 1$. We would like to determine the solution of Eq.(397) using perturbation theory in ϵ. We will attempt to obtain the leading term in the ϵ-expansion of $y(x)$ by setting ϵ to zero in Eq.(397). We obtain

$$y' = 0, \tag{398}$$

as the zeroth-order equation; its solution is $y = \text{const}$ and it is not possible to satisfy the two boundary conditions $y(0) = 0$ and $y(1) = 1$ that we would like to impose on the solution of Eq.(397).

To understand what is going on, we solve Eq.(397) exactly. We easily find

$$y(x, \epsilon) = \frac{e^{x/\epsilon} - 1}{e^{1/\epsilon} - 1}. \tag{399}$$

This solution is quite spectacular (c.f. Fig. 9). For small ϵ, it is zero everywhere except in a small neighborhood of $x = 1$. This small $(1 - x) \sim \mathcal{O}(\epsilon)$ region is called "boundary layer". Outside of the boundary layer, the solution is indeed the $\epsilon \to 0$ limit of the equation Eq.(397) and the *left* boundary condition $y(0) = 0$ applies. We will discuss the construction of the solution in the full region in a separate lecture dedicated to boundary layer problems.

We will continue with the discussion of perturbative methods that can be used to solve an eigenvalue problem of the Schrödinger equation. This

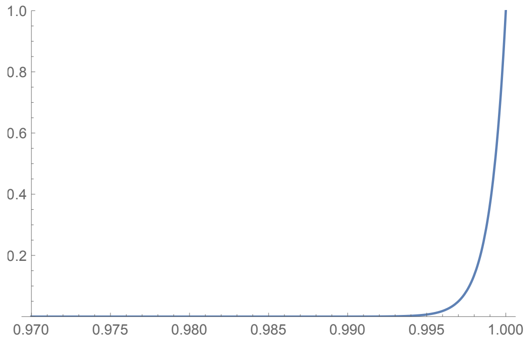

Figure 5: Solution to Eq.(397) for $\epsilon = 10^{-3}$.

is a known topic that is covered in Quantum Mechanics courses but we will discuss it for completeness. Consider the Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) + W(x) - E\right] \Psi = 0. \tag{400}$$

We assume that $V(x)$ and $W(x)$ become infinite at $|x| \to \infty$. We are interested in solutions that vanish at $|x| \to \infty$; we also know that this should be possible to achieve for certain values of the parameter E that we will refer to as "energy eigenvalues".

Note that we have split the potential in Eq.(400) into two functions $V(x)$ and $W(x)$; we assume that we can find solutions to Eq.(400) with $W(x) = 0$. Hence, we turn the problem of solving Eq.(400) with specific boundary conditions into a perturbative one by introducing a parameter ϵ as follows

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) + \epsilon W(x) - E\right] \Psi = 0. \tag{401}$$

We are interested in finding Ψ and E that appear in Eq.(401) as series in the parameter ϵ. We write

$$\Psi(x,\epsilon) = \sum_{n=0}^{\infty} \epsilon^n \Psi_n(x), \quad E = \sum_{n=0}^{\infty} \epsilon^n E_n. \tag{402}$$

To proceed further, we substitute Eq.(402) into Eq.(401), collect contributions proportional to ϵ^n and equate them to zero. We obtain

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) \Psi_n(x) + W(x)\Psi_{n-1} = \sum_{m=0}^{n} E_m \Psi_{n-m}(x). \tag{403}$$

Eq.(403) is somewhat peculiar since it contains both the unknown wave function Ψ_n and the unknown energy E_n. To disentangle them, we write $\Psi_n(x) = \Psi_0(x)F_n(x)$, $F_0(x) = 1$. We then substitute this ansatz into Eq.(403) and find

$$-2\Psi_0' F_n' - \Psi_0 F_n'' = -\Psi_0 \left(W F_{n-1} - \sum_{m=1}^{n} E_m F_{n-m} \right). \tag{404}$$

Multiplying with Ψ_0, we find

$$\frac{\mathrm{d}}{\mathrm{d}x} \left[\Psi_0^2 F_n'(x) \right] = \Psi_0^2(x) \left(W(x) F_{n-1}(x) - \sum_{m=1}^{n} E_m F_{n-m}(x) \right). \tag{405}$$

We can now integrate both sides of this equation over x, from $x = -\infty$ to $x = +\infty$. The integral of the left hand side vanishes, thanks to the boundary conditions. Hence, we obtain

$$E_n = \frac{\int\limits_{-\infty}^{+\infty} \mathrm{d}x\ \Psi_0^2(x) \left(W(x) F_{n-1}(x) - \sum\limits_{m=1}^{n-1} E_m F_{n-m}(x) \right)}{\int\limits_{-\infty}^{\infty} \mathrm{d}x\ \Psi_0^2(x)}. \tag{406}$$

If we use conventional quantum mechanical normalization for bound states $\int \Psi_0(x)^2 = 1$, the denominator in the above equation becomes one.

To find the function $\Psi_n(x) = \Psi_0(x)F_n(x)$ we integrate Eq.(405) twice and find

$$\Psi_n(x) = \Psi_0(x) \int\limits_a^x \frac{\mathrm{d}t}{\Psi_0^2(t)} \int\limits_{-\infty}^{t} \mathrm{d}s \Psi_0(s) \left(W(s)\Psi_{n-1}(s) - \sum_{m=0}^{n} E_m \Psi_{n-m}(s) \right). \tag{407}$$

Note that the quantity a that appears on the r.h.s. of the above equation fixes the normalization of $\Psi_n(x)$ in such a way that $\Psi_n(a) = 0$.

Next, we will discuss the concept of "asymptotic matching". The idea here is to find an approximate solution to, say, a differential equation using *different* perturbative expansions in two overlapping regions. Requiring that the two solutions coincide in the overlapping region, we obtain a solution that is valid in the union of the two regions. The concept of "asymptotic matching" is also very useful for the computation of integrals that depend on a small parameter; we will discuss an example at the end of the lecture.

We will introduce the concept of asymptotic matching by considering the following differential equation

$$y' + \left(\epsilon x^2 + 1 + \frac{1}{x^2}\right) y = 0. \tag{408}$$

We consider the interval $x \in [1, \infty]$ and use $y(1) = 1$ as the boundary condition. The parameter ϵ is considered to be small.

The interval $[1, \infty]$ is naturally divided into two intervals. Indeed, if $x \ll 1/\sqrt{\epsilon}$, the term ϵx^2 is much smaller than 1 and $1/x^2$ and we can neglect it in comparison. We denote the solution valid in the interval $[1, x_b]$ such that $x_b \ll \sqrt{1/\epsilon}$ as $y_1(x)$, write the simplified version of Eq.(408) and solve it

$$y_1' + \left(1 + \frac{1}{x^2}\right) y_1 = 0 \quad \to \quad y_1 = e^{-x+1/x}. \tag{409}$$

We note that this solution is consistent with the boundary condition $y(1) = 1$.

If, on the other hand, $\epsilon x^2 \sim 1$ then $1/x^2 \sim \epsilon$ and, therefore, it is small. In this case, we can neglect $1/x^2$, while keeping ϵx^2 and 1 in the second term on the l.h.s. of Eq.(408). We denote the corresponding solution as $y_2(x)$, write a simplified version of Eq.(408) and solve it

$$y_2' + \left(\epsilon x^2 + 1\right) y_2 = 0, \quad y_2 = c e^{-\epsilon x^3/3 - x}. \tag{410}$$

Here, c is the unknown integration constant.

However, this constant can be fixed because there exist values of x for which both both solutions, y_1 and y_2 are valid. To see this, we split the interval $[1, \infty]$ into two intervals $[1, \delta]$ and $[\delta, \infty]$. We require that $y_1(x)$ is valid on the first interval and $y_2(x)$ on the second. This requires that δ satisfies the two equalities

$$\delta \epsilon^2 \ll 1, \quad \text{and} \quad \frac{1}{\delta^2} \ll 1. \tag{411}$$

Both of these inequalities are satisfied if we choose δ from the following interval

$$1 \ll \delta \ll \frac{1}{\sqrt{\epsilon}}. \tag{412}$$

Since we are interested in $\epsilon \to 0$, this interval is clearly not empty.

For a given δ, the two solutions $y_1(x)$ and $y_2(x)$ should match at $x = \delta$. Given the constraints on δ, $y(x)$ for $x = \delta$ simplify as follows

$$y_1(x) = e^{-x+1/x} \to e^{-x}, \quad y_2(x) = c e^{-\epsilon x^3/3 - x} \to c e^{-x}. \tag{413}$$

Since $y_1(\delta)$ should be equal to $y_2(\delta)$, we find $c = 1$. This gives us the approximate solution on the full interval $x \in [1, \infty]$. It reads

$$y(x) = \begin{cases} e^{-x+1/x}, & x \ll \epsilon^{-1/2}; \\ e^{-x-\epsilon^2 x^3/3}, & x \gg 1. \end{cases} \tag{414}$$

The concept of asymptotic matching is often used for the evaluation of integrals. To see how this works, consider the following example. Suppose we want to compute an integral

$$F(\epsilon) = \int_0^\infty \mathrm{d}t \; e^{-t-\epsilon/t}, \tag{415}$$

in the limit $\epsilon \to 0$. We can easily compute the leading behavior by setting ϵ to zero and evaluating the integral. We find $F(0) = 1$. The question is how to find sub-leading terms in the expansion of $F(\epsilon)$.

The idea is as follows. We introduce a parameter δ and write

$$F(\epsilon) = \int_0^\delta \mathrm{d}t \; e^{-t-\epsilon/t} + \int_\delta^\infty \mathrm{d}t \; e^{-t-\epsilon/t}. \tag{416}$$

In the first integral, we would like to expand e^{-t} in a Taylor series; this is possible if $\delta \ll 1$. In the second integral, we would like to expand $e^{-\epsilon/t}$ in series in $1/t$. This is possible if $\epsilon/\delta \ll 1$. Hence, choosing δ such that

$$\epsilon \ll \delta \ll 1, \tag{417}$$

we obtain the overlapping interval where both expansions are possible. Hence, we find the following representations for the two integrals

$$\begin{aligned} I_1 &= \int_0^\delta e^{-t-\epsilon/t}\mathrm{d}t = \sum_{n=0}^\infty \int_0^\delta \frac{(-t)^n}{n!} e^{-\epsilon/t}\mathrm{d}t = \sum_{n=0}^\infty \int_0^{\delta/\epsilon} \epsilon^n \frac{(-\xi)^n}{n!} e^{-1/\xi}\mathrm{d}\xi \\ &= \sum_{n=0}^\infty \frac{(-1)^n \epsilon^{n+1}}{n!} \int_{\epsilon/\delta}^\infty \xi^{-n-2} e^{-\xi}\mathrm{d}\xi, \end{aligned} \tag{418}$$

and

$$I_2 = \int_\delta^\infty e^{-t-\epsilon/t}\mathrm{d}t = \sum_{n=0}^\infty \frac{(-\epsilon)^n}{n!} \int_\delta^\infty \mathrm{d}t \; t^{-n} e^{-t} \; \mathrm{d}t. \tag{419}$$

We notice the following: the remaining integral in I_2 is independent of ϵ and only depends on δ. Hence, if we are interested in the computation of the original integral to a particular order in ϵ, it is quite clear where to truncate the series that appears in I_2. Suppose we work to *first* order in ϵ. Then,

$$I_2 \sim \int_\delta^\infty \mathrm{d}t\ e^{-t}\left(1-\frac{\epsilon}{t}\right). \tag{420}$$

The first relevant integral reads

$$\int_\delta^\infty \mathrm{d}t\ e^{-t} = 1 - \int_0^\delta \mathrm{d}t\ e^{-t} \sim 1-\delta+\mathcal{O}(\delta^2). \tag{421}$$

The second integral is easy to compute if we integrate by parts once[7]

$$\begin{aligned}\int_\delta^\infty \mathrm{d}t\ e^{-t}\ \frac{\epsilon}{t} &= \epsilon\left(\ln t e^{-t}\Big|_\delta^\infty + \int_\delta^\infty \mathrm{d}t\ \ln(t)e^{-t}\right)\\ &= \epsilon\left(-\ln\delta\ e^{-\delta} + \int_0^\infty \mathrm{d}t\ \ln(t)e^{-t} - \int_0^\delta \mathrm{d}t\ \ln(t)e^{-t}\right)\\ &= \epsilon\left(-\ln\delta-\gamma_E+\delta\right)+\mathcal{O}(\epsilon\delta^2).\end{aligned} \tag{422}$$

Hence, we find

$$I_2 = 1-\delta-\epsilon\left(-\ln\delta-\gamma_E+\delta\right)+\mathcal{O}(\delta^2,\epsilon\delta^2). \tag{423}$$

Calculation of I_1 is more complicated because the integrals there still depend on ϵ. It is, however, easy to understand this dependence. Indeed, the strongest dependence comes from the lower integration boundary. Since ϵ/δ is small, $e^{-\xi}$ there is close to one, so that

$$\epsilon^{n+1}\int_{\epsilon/\delta}^\infty e^{-\xi}\xi^{-n-2}\ \mathrm{d}\xi \sim \epsilon^{n+1}\frac{\delta^{n+1}}{\epsilon^{n+1}} \sim \delta^{n+1}. \tag{424}$$

Hence, we conclude that the n-th term in the series that contributes to I_1 contains terms $\mathcal{O}(\delta^{n+1})$, $\mathcal{O}(\delta^n\epsilon)$, $\ldots\mathcal{O}(\epsilon^{n+1})$. Hence, to compute terms up

[7] We require $\int_0^\infty \ln t\ e^{-t}\ \mathrm{d}t = -\gamma_E$.

to $\mathcal{O}(\epsilon^0\delta)$ we need to study the $n=0$ contribution to I_1 and if we want to compute all terms up to $\mathcal{O}(\epsilon\delta)$ we also require the $n=1$ contribution.

Upon accounting for these two terms, we find

$$I_1 = \epsilon \int_{\epsilon/\delta}^{\infty} \mathrm{d}\xi\, \xi^{-2} e^{-\xi} - \epsilon^2 \int_{\epsilon/\delta}^{\infty} \mathrm{d}\xi\, \xi^{-3} e^{-\xi} + \cdots \tag{425}$$

We start with the first integral in Eq.(425). Repeatedly integrating by parts, we find

$$\begin{aligned} \epsilon \int_{\epsilon/\delta}^{\infty} \mathrm{d}\xi\, \xi^{-2} e^{-\xi} =& \epsilon \left(\frac{\delta}{\epsilon} e^{-\epsilon/\delta} + \ln \frac{\epsilon}{\delta} e^{-\epsilon/\delta} + \gamma_E - \frac{\epsilon}{\delta}\left(1 - \ln \frac{\epsilon}{\delta}\right)\right) \\ &\approx \delta - \epsilon + \epsilon \ln \frac{\epsilon}{\delta} + \gamma_E \epsilon.. \end{aligned} \tag{426}$$

We compute the second term in Eq.(425) in a similar manner. The result reads

$$\begin{aligned} &\epsilon^2 \int_{\epsilon/\delta}^{\infty} \mathrm{d}\xi\, \xi^{-3} e^{-\xi} = \epsilon^2 \left(-\frac{e^{-\xi}}{2\xi^2}\bigg|_{\epsilon/\delta}^{\infty} + \frac{e^{-\xi}}{2\xi}\bigg|_{\epsilon/\delta}^{\infty} - \frac{1}{2}\int_{\epsilon/\delta}^{\infty} \frac{\mathrm{d}\xi}{\xi}\, e^{-\xi} \right) \\ &\approx -\epsilon\delta + \mathcal{O}(\delta^2, \epsilon^2). \end{aligned} \tag{427}$$

Combining results for I_1 and I_2 we obtain $F(\epsilon)$ to first order in ϵ

$$\begin{aligned} F(\epsilon) &\sim 1 - \delta - \epsilon(-\ln\delta - \gamma_E + \delta) + \delta - \epsilon + \epsilon \ln \frac{\epsilon}{\delta} \\ &+ \gamma\epsilon + \epsilon\delta + \mathcal{O}(\epsilon^2, \delta^2) \\ &\sim 1 + \epsilon(\ln\epsilon + 2\gamma_E - 1) + \mathcal{O}(\epsilon^2). \end{aligned} \tag{428}$$

We emphasize that we were supposed to include all the terms in our computation that scale as $\mathcal{O}(\delta)$, $\mathcal{O}(\epsilon)$ and $\mathcal{O}(\epsilon\delta)$ and we clearly see from Eq.(428) that the dependence on the auxiliary parameter δ cancels out through this order, as expected.

9 Summation of series

We have seen in many examples that solutions to various problems can be written in the form of series. Sometimes we know all terms in the series and sometimes just the first few. To turn series into numbers, we need to understand how to sum them up in a way that, ideally, requires a minimal number of terms in the series for arriving at a meaningful result.

However, there are plenty of cases when series converge slowly, if at all. A very simple example is

$$S(x) = \sum_{k=0}^{\infty} (-x)^k = 1/(1+x). \tag{429}$$

For $x = 0.9$, the sum of first fifty terms in the series, gives only the first two digits of the result, already the third digit is incorrect ($S_{50}(0.9) = 0.5288$ vs. $S(0.9) = 0.5263$). An interesting question is if we can do better.

To find an answer to this question, consider generic series

$$S = \sum_{n=0}^{\infty} a_n, \tag{430}$$

and define N-th partial sum as

$$S_N = \sum_{n=0}^{N} a_n. \tag{431}$$

Then,

$$S = S_N + R_N, \tag{432}$$

where R_N is called the *remainder*. Our goal is to deduce S from S_N; clearly, R_N controls how successful we will be in doing that.

In the example Eq.(429), we can easily compute the remainder

$$R_N = \sum_{n=N+1}^{\infty} (-x)^n = \frac{(-x)^{N+1}}{1+x}. \tag{433}$$

We now see that for positive x and, especially, for x close to 1, the remainder has oscillatory behavior and that oscillations around the right value of the sum S are significant until large values of N. Indeed, if we would like R_N to disappear (decay) on its own for $x \sim 1 - \epsilon$, $\epsilon \to 0$, we require values of $N \gg 1/\epsilon$, as can be seen from this estimate

$$x^N \sim e^{N \ln x} = e^{N \ln(1-\epsilon)} \sim e^{-\epsilon N}, \quad N \gg \epsilon^{-1}. \tag{434}$$

This result can be confirmed by numerical tests – for $x = 0.99$ we need 400 terms to be within 2% of the correct result and for $x = 0.999$ we need to 4000 terms to achieve similar accuracy.

If the remainder of the series can be made smaller in a *systematic way*, the convergence rate is improved. To see how this can be done, we consider an ansatz

$$S_N \sim S + \alpha q^N, \tag{435}$$

for the N-th partial sum. Here α and q are parameters and we assume that $|q| < 1$. In practice, it is quite rare that the above form is exact and there can be multiple remainders of the above form. However, we can imagine that this procedure works iteratively and that by writing Eq.(435) we will be removing a remainder with the largest value of q.

In case when the remainder of the series has the form shown in Eq.(435), the accelerated convergence is accomplished through the *Shanks transformation*. Indeed, in case there is a single remainder, the partial sum is determined by only (!) three parameters S, α and q and we can fix them from any three consecutive terms in series. Indeed, consider

$$S_{N+1} = S + \alpha q^{N+1}, \;\; S_N = S + \alpha q^N, \quad S_{N-1} = S + \alpha q^{N-1}. \tag{436}$$

We then write

$$S_{N+1} - S = q(S_N - S), \quad (S_{N-1} - S) = q^{-1}(S_N - S), \tag{437}$$

and upon multiplying the two equations and expressing S through $S_{N\pm1}, S_N$, we find

$$S = \frac{S_{N+1}S_{N-1} - S_N^2}{S_{N+1} + S_{N-1} - 2S_N}. \tag{438}$$

We note that for the series in Eq.(429) the remainder of the series has indeed the form shown in Eq.(435), see Eq.(433); hence, Eq.(438) should give the exact result for the series Eq.(429). It is easy to check explicitly that it does, indeed.

In a general case, the formula in Eq.(438) is not exact and we can view it as a transformation that maps original series into *another* series that (hopefully) converges faster than the original one because the remainder with the largest q has been removed. Therefore, to make use of the Shanks transformation in such cases, we interpret Eq.(438) as the definition of the N-th term of a new series $\tilde{S}_N$ and then we apply Shanks transformation to a new series.

Consider the following sum as an example

$$S = \sum_{k=0}^{\infty} (-1)^k \left(1 - \frac{1}{2^{k+1}}\right) z^k, \tag{439}$$

and take $z = 0.99$. The series converges very slowly. The first few terms for partial sums S_N are

$$0.5, -0.2425, 0.615088, -0.294568, 0.63601, -0.300121, 0.63400, -0.294421$$

for values of N from 0 to 7. The correct result is 0.1680644 and it is next to impossible to guess it from the above numbers.

However, consider the Shanks transformation and define

$$\tilde{S}_N = \frac{S_{N+1} S_{N-1} - S_N^2}{S_{N+1} + S_{N-1} - 2S_N}. \tag{440}$$

We compute $\tilde{S}_N$ for N from one to six and find

$$\{\tilde{S}_N\} = \{0.1555452, 0.17366, 0.165431, 0.169337, 0.167442, 0.168371, \ldots\}. \tag{441}$$

We see that the Shanks transformation changes the situation dramatically and that six first terms of the new series are close to the right answer 0.1680644.

To improve the convergence further, we can apply the Shanks transformation to the Shanks-transformed partial sum sequence Eq.(441). We will call the resulting sequence $\tilde{\tilde{S}}_N$. The result reads

$$\tilde{\tilde{S}}_N = \{0.168001, 0.16808, 0.168061, 0.168065\}. \tag{442}$$

Obviously, by a repeated application of the Shanks transformation, we are able to obtain a very accurate prediction for the sum Eq.(439). In fact, it is important to realize that we used the explicit knowledge of just *seven* first terms in the series Eq.(439) to arrive at the result Eq.(442). However, if we do this naively and just sum up seven terms of the original series, we will get $S = 0.63400$ which is a factor three larger than the exact result. By using the same seven terms in the context of Shanks transformations we obtain the result for S that is accurate to 0.01 percent.

We can try to understand why the Shanks transformation is so effective in improving the convergence of the series in Eq.(439). To this end, we compute the N-th partial sum and find

$$\begin{aligned} S_N &= \sum_{k=0}^{N} (-1)^k \left(1 - \frac{1}{2^{k+1}}\right) z^k = \frac{\left(1 - (-z)^{N+1}\right)}{1+z} - \frac{\left(1 - \left(-\frac{z}{2}\right)^{N+1}\right)}{2+z} \\ &= \frac{1}{(1+z)(2+z)} - \frac{(-z)^{N+1}}{1+z} + \frac{\left(-\frac{z}{2}\right)^{N+1}}{2+z}. \end{aligned} \tag{443}$$

The first term on the r.h.s. of Eq.(443) corresponds to true value of the series Eq.(439). The other two terms on the r.h.s. of Eq.(443) describe two transients that decay as $(-z)^N$ and as $(-z/2)^N$, respectively. Note that for $z = 0.99$, the $(z/2)^N \ll z^N$ for $N \geq 1$.

We now use Eq.(438) to compute the Shanks-transformed series. We obtain

$$\tilde{S}_N = \frac{1}{(1+z)(2+z)} + \frac{(-z/2)^{N+2}}{(1+z)(2+z)(1+z-(2+z)/2^{2+N})}. \tag{444}$$

A comparison of Eq.(443) and Eq.(444) shows that in the Shanks-transformed partial sums, at large values of N, the remainder $\mathcal{O}((-z)^N)$ disappeared and the only remainder that remains is $\mathcal{O}((-z/2)^N)$. Hence, by applying the Shanks transformation we gained a factor 2^N in the convergence rate. If we apply the Shanks transformation one more time, we will remove $\mathcal{O}((-z/2)^{N+1})$ transient and will be left with $\mathcal{O}((-z/4)^N)$, gaining another factor 2^N in the convergence speed.

It is not always easy to understand why the convergence of a particular series is improved when the Shanks transformation is used and to estimate the improvement in the convergence rate. An interesting series that illustrates this point is

$$S = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} = \ln 2 = 0.693147. \tag{445}$$

This series converges rather slowly. In fact, the first hundred terms of the series give a precision of about a percent; the first thousand – 0.1 percent etc. If we apply the Shanks transformation, we obtain partial sums

$$\tilde{S}_2 = 0.7, \quad \tilde{S}_3 = 0.6905, \quad \tilde{S}_{10} = 0.693254, \quad \tilde{S}_{100} = 0.693147... \tag{446}$$

In fact, $\tilde{S}_{100}$ agrees with the exact result $\ln 2 = 0.693147$ to 10^{-5} percent – to be compared with one percent if terms in the series Eq.(445) are summed up naively.

It is interesting to understand why the convergence improves for the series in Eq.(445). Similar to the previous case, we need to compare remainders of the original series and the Shanks-transformed series but it is clearly less straightforward to do so for the series Eq.(445). To accomplish this, we introduce an auxiliary parameter z and write the remainder of the series as

$$R_N(z) = \sum_{k=N+1}^{\infty} \frac{(-1)^{k+1} z^k}{k}. \tag{447}$$

We cannot sum this series directly, but we can write a differential equation for it. We compute the derivative of $R_N(z)$ w.r.t. z and find

$$\frac{\mathrm{d}R_N(z)}{\mathrm{d}z} = (-1)^N z^N \sum_{k=0}^{\infty} (-z)^k = (-1)^N \frac{z^N}{1+z}. \tag{448}$$

We integrate over z using the boundary condition $R_N(0) = 0$ and obtain

$$R_N(z) = (-1)^N \int_0^z \frac{u^N}{1+u}\,\mathrm{d}u. \tag{449}$$

We are interested in the behavior of $R_N(z)$ in the $z \to 1$ limit for large values of N. To this end, we set $z \to 1$, change variables $u \to 1-\xi$ and write

$$R_N(1) = (-1)^N \int_0^1 \mathrm{d}\xi\, \frac{(1-\xi)^N}{2-\xi}. \tag{450}$$

To understand the behavior of this integral in the $N \to \infty$ limit, we write

$$\begin{aligned}
&(1-\xi)^N = e^{N\ln(1-\xi)} = e^{-N\xi}\left(1 - \frac{N}{2}\xi^2 - \frac{N}{3}\xi^3 + \ldots\right), \\
&\frac{1}{2-\xi} \sim \frac{1}{2} + \frac{\xi}{4} + \ldots
\end{aligned} \tag{451}$$

Using these results in the expression for $R_N(1)$ and extending the integration boundary to infinity (which is allowed since such an extension only introduces exponentially suppressed terms), we obtain

$$\begin{aligned}
R_N(1) = (-1)^N \int_0^1 \mathrm{d}\xi \frac{(1-\xi)^N}{2-\xi} &\sim (-1)^N \int_0^\infty \mathrm{d}\xi\; e^{-N\xi}\left(\frac{1}{2} + \frac{\xi}{4} - \frac{N\xi^2}{4} + ..\right) \\
&\sim (-1)^N \left(\frac{1}{2N} - \frac{1}{4N^2} + \mathcal{O}(N^{-3})\right).
\end{aligned} \tag{452}$$

Hence, we see that R_N decreases as $1/N$ which is the reason for the slow convergence of the original series Eq.(445).

To understand the consequences of the Shanks transformation, we substitute $\tilde{S}_N = S - R_N$ into Eq.(438) and find

$$\tilde{S}_N = S + \frac{R_{N+1}R_{N-1} - R_N^2}{2R_N - R_{N+1} - R_{N-1}}. \tag{453}$$

To simplify this expression further, we use Eq.(447) to write

$$R_{N+1} = R_N + \frac{(-1)^{N+1} z^{N+1}}{N+1}, \quad R_{N-1} = R_N - \frac{(-1)^N z^N}{N}. \tag{454}$$

Substituting these expressions into Eq.(453) we obtain

$$\tilde{S}_N = S + \Delta_N, \tag{455}$$

where

$$\Delta_N(z) = -R_N(z) + \frac{(-1)^N z^{1+N}}{1 + N(1+z)} \tag{456}$$

is a remainder of Shanks-improved series.

We can now evaluate the asymptotic behavior of Δ_N for $z = 1$ and large values of N. The asymptotic behavior of $R_N(1)$ has already been computed in Eq.(452). We use it to find

$$\begin{aligned} \Delta_N(1) &\sim (-1)^N \left(-\frac{1}{2N} + \frac{1}{4N^2} + \frac{1}{1+2N} \right) \\ &\sim (-1)^N \left(-\frac{1}{2N} + \frac{1}{4N^2} + \frac{1}{2N} - \frac{1}{4N^2} + \cdots \right) \sim \mathcal{O}(N^{-3}). \end{aligned} \tag{457}$$

Hence, the improvement in convergence of the Shanks-transformed series *relative* to the original ones is governed by a factor $(2N)^{-2}$ in this case.

Another useful trick that allows acceleration of slowly convergent series is known as *Richardson extrapolation*. The idea is very simple. Suppose that, for large values of N, a partial sum of the series can be written as follows

$$S_N = \sum_{n=0}^{N} a_n \sim S + Q_1 N^{-1} + Q_2 N^{-2} + Q_3 N^{-3} + \ldots. \tag{458}$$

It is clear that the convergence of the series can be drastically improved if we can determine and remove as many terms beyond S on the right hand side of Eq.(458) as possible. This can be done iteratively, starting with the first, $\mathcal{O}(N^{-1})$ term. Discarding Q_2, Q_3 etc., we write

$$S_N = S + \frac{Q_1}{N}, \quad S_{N+1} = S + \frac{Q_1}{N+1}. \tag{459}$$

Hence, we use

$$NS_N = SN + Q_1, \tag{460}$$

and a similar equation for S_{N+1} to find

$$S = (N+1)S_{N+1} - NS_N. \tag{461}$$

To get a better approximation, we account for all terms on the r.h.s. of Eq.(458) that decrease slower than $1/N^3$ and write

$$S_N = S + \frac{Q_1}{N} + \frac{Q_2}{N^2}. \tag{462}$$

We multiply both sides of this equation with N^2 and obtain

$$N^2 S_N = N^2 S + NQ_1 + Q_2 \rightarrow N^2(S_N - S) = NQ_1 + Q_2. \tag{463}$$

To proceed further, we denote the l.h.s. of the above equation by $F(N) = N^2(S_N - S)$ and find

$$F(N+2) - F(N+1) = F(N+1) - F(N), \tag{464}$$

since both sides of this equation give Q_1. Solving Eq.(464) for S, we obtain

$$S = \frac{(N+2)^2 S_{N+2} - 2(N+1)^2 S_{N+1} + N^2 S_N}{2}. \tag{465}$$

It is quite clear that one can keep including more and more power-suppressed terms in the right hand side of Eq.(458) and keep deriving equations for S similar to Eqs.(461) and Eq.(465) in each case. It is interesting and perhaps not obvious that one can write down a closed formula for S under the assumption that all terms up to $\mathcal{O}(1/N^n)$ are included on the r.h.s. of Eq.(458). The formula that expresses S in terms of partial sums $S_N, S_{N+1}, S_{N+2}, ..., S_{N+n}$, reads

$$S = \sum_{k=0}^{n} \frac{S_{N+k}\,(N+k)^n(-1)^{k+n}}{k!(n-k)!}. \tag{466}$$

The proof of this formula is based on the following identity

$$1 = \sum_{k=0}^{n} \frac{(N+k)^n(-1)^{k+n}}{k!(n-k)!}, \tag{467}$$

which by itself is quite peculiar. To prove Eq.(467), we proceed by writing

$$(N+k)^n = \sum_{i=0}^{n} \frac{n!\;N^{n-i}k^i}{i!(n-i)!}. \tag{468}$$

We use this result in Eq.(467) and find that the following identity should hold

$$1 \stackrel{?}{=} \sum_{i=0}^{n} \frac{n!\ N^{n-i}}{i!(n-i)!} F(i,n), \tag{469}$$

where $F(i,n)$ is defined as follows

$$F(i,n) = \sum_{k=0}^{n} \frac{k^i (-1)^{k+n}}{k!(n-k)!}. \tag{470}$$

We will now show that the majority of $F(i,n)$'s vanish. Consider first $F(0,n)$. It reads

$$\begin{aligned} F(0,n) &= \sum_{k=0}^{n} \frac{(-1)^{k+n}}{k!(n-k)!} = \frac{1}{n!} \sum_{k=0}^{n} \frac{(-1)^{k+n} n! (1)^{n-k}}{k!(n-k)!} \\ &= \frac{1}{n!} (-1)^n (1-1)^n = 0, \end{aligned} \tag{471}$$

where we made use of binomial formula to sum up the series. Similarly,

$$\begin{aligned} F(1,n) &= \sum_{k=0}^{n} \frac{k(-1)^{k+n}}{k!(n-k)!} = \sum_{k=1}^{n} \frac{(-1)^{k+n}}{(k-1)!(n-k)!} \\ &= \sum_{j=0}^{n-1} \frac{(-1)^{j+n+1}}{j!(n-1-j)!} \sim F(0,n-1) = 0. \end{aligned} \tag{472}$$

Repeating this calculation for other $F(i,n)$'s, it is easy to convince oneself that they all vanish except for $F(n,n)$ which is equal to 1. Then, the r.h.s. of Eq.(469) turns into

$$\sum_{i=0}^{n} \frac{n!\ N^{n-i}}{i!(n-i)!} \delta_{in} = 1, \tag{473}$$

which proves Eq.(467).

We will use Eq.(467) to prove Eq.(466). To this end, we write

$$S_{N+k}(N+k)^n = S(N+k)^n + \sum_{i=1}^{n} Q_i (N+k)^{n-i}, \tag{474}$$

where quantities Q_i appear in Eq.(458). We multiply both sides of the above equation with $(-1)^{k+n}/k!/(n-k)!$ and sum over k from $k=0$ to $k=n$.

We find

$$\sum_{k=0}^{n} \frac{S_{N+k}(N+k)^n(-1)^{k+n}}{k!(n-k)!} = S \sum_{k=0}^{n} \frac{(N+k)^n(-1)^{k+n}}{k!(n-k)!}$$
$$+ \sum_{i=1}^{n} \mathcal{O}_i \sum_{k=0}^{n} \frac{(N+k)^{n-i}(-1)^{k+n}}{k!(n-k)!} = S + \sum_{i=1}^{n} \mathcal{O}_i \sum_{k=0}^{n} \frac{(N+k)^{n-i}(-1)^{k+n}}{k!(n-k)!} = S, \tag{475}$$

where we have used Eq.(467) and the equation

$$\sum_{k=0}^{n} \frac{(N+k)^{n-i}(-1)^{k+n}}{k!(n-k)!} = 0, \quad i \geq 1, \tag{476}$$

that can be proven in the same way as Eq.(467).

To see how Richardson's extrapolation improves convergence, consider the following series

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} = 1.6449340668482262. \tag{477}$$

Summing up the first ten terms of the series, we obtain 1.54977; this is a six percent deviation from the exact result. On the other hand, using Richardson's extrapolation formula Eq.(466) with $N = 0$ and $n = 10$, we obtain $S = 1.6449340662$ which agrees with the exact result to about ten (!) significant digits. This is an amazing improvement – especially if one recognizes that we have used the same amount of information about the series in both cases.

We will now turn to the question of how to sum *divergent* series. This, of course, is an ill-posed question since divergent series by definition do not allow one to get a unique answer. It is therefore important to either know where divergent series come from and what they mean *or* follow well-defined rules to deal with them. We have seen the appearance of such series in the context of *asymptotic* series where such series gave us an approximate description of complicated functions.

There exist different "rules" or prescriptions that allow one to sum up evidently divergent series. For example, consider *divergent* series

$$S = \sum_{n=0}^{\infty} a_n. \tag{478}$$

However, suppose that the coefficients a_n are such that we can define a function $f(x)$

$$f(x) = \sum_{n=0}^{\infty} a_n x^n, \tag{479}$$

for $|x| < 1$; in other words we assume that the series in Eq.(479) converges. We then define the series in Eq.(478) through the following formula[8]

$$S = \lim_{x \to 1^-} f(x). \tag{480}$$

The reason that S in the above formula is not the same as in Eq.(478) is that for divergent series

$$S = \lim_{x \to 1^-} f(x) = \lim_{x \to 1^-} \sum_{n=0}^{\infty} a_n x^n \neq \sum_{n=0}^{\infty} a_n. \tag{481}$$

It is this interchange of the order in which the limit and sum are calculated that makes all the difference. Of course, at this point this is just a prescription and nothing else.

To see how this works in practice, consider the series

$$S = \sum_{n=0}^{\infty} (-1)^n. \tag{482}$$

The series is just

$$S = 1 - 1 + 1 - 1 + 1 - 1 + \cdots \tag{483}$$

and so obviously has no limit. However,

$$f(x) = \sum_{n=0}^{\infty} (-1)^n x^n = \frac{1}{1+x}. \tag{484}$$

Hence,

$$S = \lim_{x \to 1} f(x) = \frac{1}{2}. \tag{485}$$

We may be dissatisfied with the above prescription since it looks completely ad hoc. Perhaps we can see that it is indeed ad hoc if we come up with another prescription, compute the same series and get a totally different results. To check this, let us try another prescription, the so-called *Borel*

[8]This summation method is due to Euler.

summation formula. It works as follows. Similar to the previous case, we consider a divergent series

$$S = \sum_{n=0}^{\infty} a_n. \tag{486}$$

We use it to construct a function

$$\phi(x) = \sum_{n=0}^{\infty} \frac{a_n x^n}{n!}. \tag{487}$$

We assume that it exists. We define

$$B(x) = \int\limits_0^{\infty} \mathrm{d}t \; e^{-t} \phi(xt). \tag{488}$$

To compute the integral, we replace $\phi(x)$ with its series representation Eq.(487) and find

$$B(x) = \lim \sum_{n=0}^{\infty} \frac{a_n}{n!} x^n \int\limits_0^{\infty} \mathrm{d}t \; e^{-t} t^n \sim \sum_{n=0}^{\infty} a_n x^n. \tag{489}$$

Finally, although, strictly speaking the function $B(x)$ is only asymptotic to the series $\sum\limits_{n=0}^{\infty} a_n x^n$ for $x \to 0$, we can also *define* the *Borel sum* of the series $\sum\limits_{n=0}^{\infty} a_n$ as $B(1)$. Hence,

$$\sum_{n=0}^{\infty} a_n = \int\limits_0^{\infty} \mathrm{d}t \; e^{-t} \phi(t). \tag{490}$$

To illustrate how the Borel summation works, consider the same divergent series Eq.(483). The function $\phi(t)$ reads

$$\phi(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^n}{n!} = e^{-t}. \tag{491}$$

Then,

$$S = \int\limits_0^{\infty} \mathrm{d}t \; e^{-t} \phi(t) = \int\limits_0^{\infty} \mathrm{d}t \; e^{-2t} = \frac{1}{2}. \tag{492}$$

It is interesting that the Borel sum of the series Eq.(483) and the Euler sum of the same series gave *identical results* in spite of the fact that both of these summation prescriptions look quite arbitrary. We will return to the discussion of this observation shortly.

Borel summation is more powerful than the Euler summation in the sense that it can be used to sum up series with factorially-growing terms. As an example, consider

$$S = \sum_{n=0}^{\infty} (-1)^n n!. \tag{493}$$

We write

$$S = \int_0^\infty {\rm d}t \; e^{-t} \sum_{n=0}^{\infty} (-1)^n t^n = \int_0^\infty \frac{{\rm d}t}{1+t} \; e^{-t} = 0.596347, \tag{494}$$

where the last integral is computed numerically.

We now go back to the question of why Euler and Borel summation rules gave the same results for the series Eq.(483). To this end, we will introduce axioms that define summation process and allow us to compute series. These axiom are not random – they are identical to what is expected from the convergent series *except* that we should give up on *the commutativity and associativity within infinite sums*; in other words, one can not change the order in which summation is performed in the infinite series and one can not combine the various terms either.

To present the axioms, let us introduce the following notation

$$\sum_{i=1}^{\infty} a_i = S(a_1 + a_2 + a_3 + \cdots + a_n \cdots). \tag{495}$$

The order in which a_i's appear in the argument of S is important and cannot be changed.

The first requirement that S should satisfy reads

$$S(a_1 + a_2 + a_3 + \cdots) = a_1 + S(a_2 + a_3 + \cdots) \tag{496}$$

We also impose the linearity requirement

$$S\left(\sum_n (\alpha a_n + \beta b_n)\right) = \alpha S\left(\sum a_n\right) + \beta S\left(\sum b_n\right). \tag{497}$$

Note that it follows from this rule that

$$S(0+0+0+0+...) = 0, \tag{498}$$

since

$$S(\alpha 0+\alpha 0+\alpha 0+\cdots) = S(0+0+0+0+\cdots) = \alpha S(0+0+0+0+\cdots), \quad (499)$$

for any α.

The two summation rules Eqs.(496,497) are sufficient to compute the sum Eq.(483). Indeed,

$$\begin{aligned} &S(1-1+1-1+1+\cdots) = 1 + S(-1+1-1+1+\cdots) \\ &= 1 + S((-1)(1-1+1-1+\cdots)). \end{aligned} \quad (500)$$

Hence,

$$S(1-1+1-1+1+\cdots) = 1 - S(1-1+1-1+1+\cdots), \quad (501)$$

which implies that

$$S(1-1+1-1+1-1+\cdots) = \frac{1}{2}. \quad (502)$$

We see that the result of the calculation agrees with both Euler and Borel summation prescriptions since both of these summation prescriptions respect the summations axioms Eqs.(496,497).

Let us discuss another example. Consider a summation sequence

$$R = S(1+0-1+1+0-1+1+0-1+\cdots). \quad (503)$$

To compute the sum following the Euler summation rule, we introduce a function

$$\begin{aligned} f(x) &= 1 + 0 - x^2 + x^3 + 0 - x^5 + x^6 + 0 - x^6 + \cdots \\ &= 1 + x^3 + x^6 + x^9 + \ldots - (x^2 + x^5 + x^8 + \ldots) \\ &= \frac{1}{1-x^3} - \frac{x^2}{1-x^3} = \frac{1-x^2}{1-x^3}, \end{aligned} \quad (504)$$

and compute the limit

$$R = \lim_{x \to 1^-} f(x) = \frac{2}{3}. \quad (505)$$

To show how the same result follows from the two conditions that we just mentioned, we write three equations

$$\begin{aligned} R &= S(1+0-1+1+0-1..), \\ R &= 1 + S(0-1+1+0-1..), \\ R &= 1 + S(-1+1+0-1+1..). \end{aligned} \quad (506)$$

Adding the three equations and using Eq.(497) "backwards",we obtain

$$3R = 2 + S(0+0+0+0+0...) = 2. \quad (507)$$

It follows that $S = 2/3$ in agreement with the Euler summation formula.

10 Pade approximations and continued fractions

Another important method of improving convergence of (potentially divergent) series is the Pade approximation. This method is often applied when a few terms in the series expansion are known and one attempts to deduce the sum (or the function that the sum represents) from just a few terms in the series. It works in the following way. Consider the series

$$\sum_{n=0}^{\infty} a_n z^n. \tag{508}$$

We can approximate these series by a sequence of rational functions called Pade approximants. They read

$$P_M^N(z) = \frac{\sum\limits_{n=0}^{N} A_n z^n}{\sum\limits_{m=0}^{M} B_m z^m}. \tag{509}$$

The values of N and M are a matter of choice.

For a given N and M, the rational function in Eq.(509) contains $N+M+1$ unknown coefficients since we can choose $B_0 = 1$ without loss of generality. These $N+M+1$ unknown quantities can be fixed by considering the first $N+M+1$ terms in Eq.(508) and Taylor-expanding the Pade approximants at small z.

To see how this works, consider diagonal Pade approximant $P_1^1(z)$. Then, there are three unknowns (A_0, A_1, B_1) and we find

$$a_0 + a_1 z + a_2 z^2 = A_0 + (A_1 - A_0 B_1) z + (-A_1 B_1 + A_0 B_1^2) z^2. \tag{510}$$

Eq.(510) contains three equations, one for each power of z. The equations look complicated (except that $A_0 = a_0$ is simple, obviously) but it is useful to start solving equations starting from the one that originates from matching the coefficients of highest powers of z. It reads

$$a_2 = -A_1 B_1 + A_0 B_1^2. \tag{511}$$

We can rewrite the r.h.s. as

$$(-A_1 B_1 + A_0 B_1^2) = -B_1 (A_1 - A_0 B_1) = -B_1 a_1, \tag{512}$$

where the last step follows from the requirement that $\mathcal{O}(z)$ contributions to Eq.(510) agree on both sides of that equation. Eq.(512) then implies

$$B_1 = -a_2/a_1. \tag{513}$$

Matching the coefficients of $\mathcal{O}(z^1)$ terms in Eq.(510) finally gives

$$A_1 = a_1 + a_0 B_1 = a_1 - a_0 a_2/a_1. \tag{514}$$

Hence, $P_1^1(x)$ reads

$$P_1^1(x) = \frac{a_0 + (a_1^2 - a_0 a_2)/a_1 x}{1 - a_2/a_1 x}. \tag{515}$$

To see why this representation is interesting, consider the function $\log(1+x)/x$. Its Taylor expansion reads

$$\frac{\log(1+x)}{x} \approx 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{4} + \ldots \tag{516}$$

We take the first three terms of this expansion and construct the Pade approximant $P_1^1(x)$. Using Eq.(515), we find

$$P_1^1(x) = \frac{1 + \frac{x}{6}}{1 + \frac{2x}{3}}. \tag{517}$$

In Fig. 9 we compare the Taylor series of the function $\log(1+x)/x$ Eq.(516), the Pade approximant $P_1^1(x)$ Eq.(517) and the function $\log(1+x)/x$. We see that the Taylor series starts deviating from the function at around $x = 0.5$; this is a consequence of the fact that $|x| = 1$ is the radius of convergence of the Taylor expansion of $1/x \log(1+x)$ in the complex plane.

On the contrary, the simplest Pade approximation stays very close to the original function all the way up to $x = 3$; at $x = 3$, the difference between $P_1^1(x)$ and the correct result is only about eight percent. Although what we just discussed is one specific example, the fact of the matter is that Pade approximations work remarkably well in many cases where they can be compared with exact results.

We will discuss a few general things about Pade approximations. First, the way we determined the coefficients of the Pade approximant in the above example is not very transparent and, definitely, not efficient in more complex cases. A better way is to rewrite Eqs.(508,509) as follows

$$\left(\sum_{n=0}^{N+M} a_n z^n \right) \left(\sum_{m=0}^{M} B_m z^m \right) + \mathcal{O}\left(z^{N+M+1}\right) = \sum_{n=0}^{N} A_n z^n. \tag{518}$$

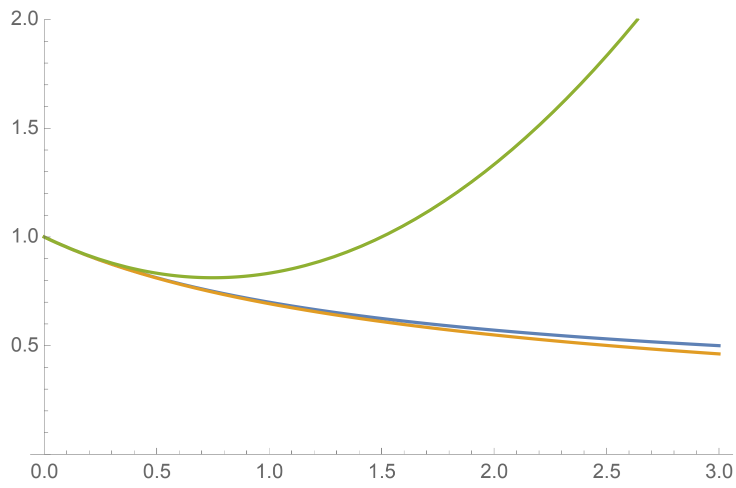

Figure 6: Taylor expansion (green) and Pade $P_1^1(x)$ approximant (blue) in comparison to the function $\log(1+x)/x$ (orange).

where the last term on the left hand side indicates that we do not fully control terms proportional to z^{N+M+1} and higher powers. We rewrite the left-hand side of Eq.(518) as follows

$$\begin{aligned}
&\left(\sum_{n=0}^{N+M} a_n z^n\right)\left(\sum_{m=0}^{M} B_m z^m\right) + \mathcal{O}\left(z^{N+M+1}\right) \\
&= \sum_{n=0}^{N+M}\sum_{m=0}^{M} z^{n+m} a_n B_m + \mathcal{O}\left(z^{N+M+1}\right) \\
&= \sum_{k=0}^{N+M} z^k \sum_{m=0}^{k} a_{k-m} B_m + \mathcal{O}\left(z^{N+M+1}\right).
\end{aligned} \tag{519}$$

An important feature of this sum is that powers of z appear there that exceed powers of z that appear on the right hand side of Eq.(518). Hence, we write

$$\sum_{k=0}^{N} z^k \sum_{m=0}^{k} a_{k-m} B_m + \sum_{k=N+1}^{N+M} z^k \sum_{m=0}^{k} a_{k-m} B_m = \sum_{n=0}^{N} A_n z^n. \tag{520}$$

Eq.(520) implies that two sets of equations should hold simultaneously

$$\begin{aligned}
&\sum_{m=0}^{k} a_{k-m} B_m = A_k, \quad k \in [0, 1, 2, .., N], \\
&\sum_{m=1}^{k} a_{k-m} B_m = -a_k, \quad k \in [N+1, ..., N+M].
\end{aligned} \tag{521}$$

The M latter equations only involve B coefficients and can be solved independently of the former equations that also involve A coefficients. In fact, these equations can be conveniently written in a matrix form

$$\hat{\alpha} \begin{pmatrix} B_1 \\ B_2 \\ .. \\ B_M \end{pmatrix} = - \begin{pmatrix} a_{N+1} \\ a_{N+2} \\ .. \\ a_{N+M} \end{pmatrix} \tag{522}$$

where the entries of the $M \times M$ matrix $\hat{\alpha}$ are

$$\hat{\alpha}_{ij} = a_{N+i-j}. \tag{523}$$

Once all the B-coefficients are determined, the A-coefficients are found from Eq.(521) in a straightforward way.

We will use this technique to construct a Pade approximant starting from the asymptotic expansion of the Gamma function $\Gamma(x)$ at large x. The asymptotic expansion reads

$$\Gamma_{\rm AS}(x) = \left(\frac{x}{e}\right)^x \sqrt{\frac{2\pi}{x}} \left(1 + \frac{1}{12x} + \frac{1}{288x^2} - \frac{139}{51840x^3}\right). \tag{524}$$

We may turn the asymptotic series into a Pade approximant. To this end, we denote $1/x = \epsilon$ and write a P_1^2 Pade approximant

$$1 + \frac{1}{12}\epsilon + \frac{1}{288}\epsilon^2 - \frac{139}{51840}\epsilon^3 = \frac{1 + a_1\epsilon + a_2\epsilon^2}{1 + b_1\epsilon}. \tag{525}$$

Upon multiplying both sides of this equation with $1 + b_1\epsilon$, we find

$$\left(1 + \frac{1}{12}\epsilon + \frac{1}{288}\epsilon^2 - \frac{139}{51840}\epsilon^3\right)(1 + b_1\epsilon) + \mathcal{O}(\epsilon^4) = 1 + a_1\epsilon + a_2\epsilon^2. \tag{526}$$

The $\mathcal{O}(\epsilon^4)$ term and higher powers of ϵ on the left hand side can not be determined; they exceed the accuracy that we work with. The $\mathcal{O}(\epsilon^3)$ term on the l.h.s. has no counter-part on the r.h.s.; it reads

$$-\frac{139}{51840} + \frac{b_1}{288} = 0, \tag{527}$$

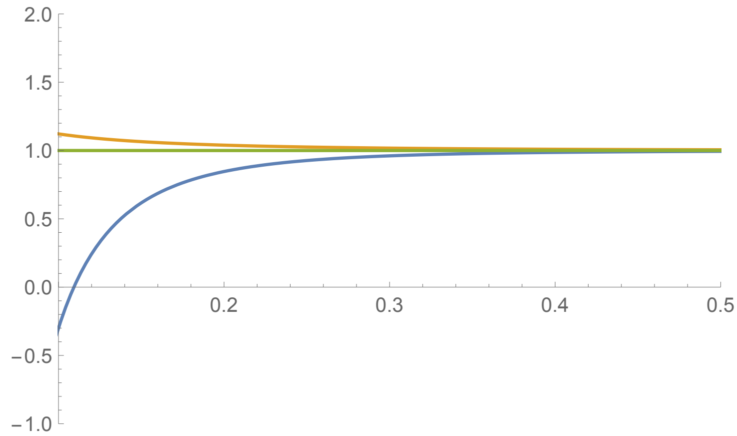

Figure 7: Comparison of the Pade approximation for the Gamma-function Eq.(529) with the asymptotic expansion Eq.(524). We plot $\Gamma_{\rm AS}(x)/\Gamma(x)$ (blue) and $\Gamma_P(x)/\Gamma(x)$ (orange).

and allows us to find $b_1 = 139/180$. Once b_1 is fixed, the left hand side of Eq.(526) is fully determined; expanding it through $\mathcal{O}(\epsilon^2)$ and equating powers of ϵ that appear on the left and the right hand sides, we find

$$P_1^2(x) = \frac{1 + \frac{77}{90x} + \frac{293}{4320x^2}}{1 + \frac{139}{180x}}. \tag{528}$$

We then write a Pade-improved formula for the asymptotically-expanded Gamma function

$$\Gamma_P(x) = \left(\frac{x}{e}\right)^x \sqrt{\frac{2\pi}{x}} P_1^2(x). \tag{529}$$

In Fig. 2 we compare how well $\Gamma_{\rm AS}(x)$ and $\Gamma_P(x)$ describe $\Gamma(x)$. First, we note that the expansion $\Gamma_{AS}(x)$ is constructed for $x \to \infty$, so it is amazing to see that it works very well all the way down to $x \sim 0.4$. For smaller values of x, the plain asymptotic expansion starts deviating from the true value significantly, but the Pade-improved function $\Gamma_P(x)$ stays within ten percent of the "true" Gamma function even for values of x as low as $x \sim 0.1$.

There are many other examples that demonstrate that Pade approximations work remarkably well and allow one to extend the region of applicability of asymptotic expansions. However, it is not always clear *why* this happens. In fact, there are two questions that have to be addressed. The first one is – do sequences of Pade approximations actually converge? The second question is – if sequences of Pade approximations do converge, do they converge to those functions that are intended to be represented by the original series?

The second question is even more complex if we consider complex-valued series since in this case functions that we obtain may require additional definitions (e.g. cuts in the complex plane), not apparent in original series, to become single-valued . It then becomes important to clarify to which branch of a multi-valued function a sequence of Pade approximants converges.

We will not discuss these questions with any degree of rigor. Below, I will describe how convergence of Pade sequences can be studied; then, I will discuss an example where a convergence of a particular Pade sequence can be proven. The question of whether the limit of a particular Pade sequence corresponds to a function that is supposed to be represented by the original series is only proven for one class of series/functions known as Stieltjes series/functions.

To discuss convergence of Pade sequences, we begin with the introduction of yet another way to provide approximate representations of series or functions – the so-called *continued fractions*. A continued fraction is defined as follows

$$F_N(z) = \cfrac{c_0}{1+\cfrac{c_1 z}{1+\cfrac{c_2 z}{1+\ddots+\cfrac{c_{N-1}z}{1+c_N z}}}}\;. \tag{530}$$

Suppose we want to construct a continued fraction representation of a function $f(z)$ that possesses a Taylor expansion at $z=0$

$$f(z) = \sum_{i=0}^{\infty} a_i z^i. \tag{531}$$

To construct its continued fraction representation, we employ the following identity

$$f(z) = \frac{f(0)}{1+zf_1(z)}, \tag{532}$$

where

$$f_1(z) = \frac{f(0)-f(z)}{zf(z)}. \tag{533}$$

To see why Eq.(532) is useful, we compute denominator of the r.h.s. of Eq.(532) to order $\mathcal{O}(z)$. This requires $f_1(0)$ which, on account of Eq.(531), evaluates to $f_1(0) = -a_1/a_0$. Hence, we find

$$f(z) \sim \frac{a_0}{1-za_1/a_0}. \tag{534}$$

Upon Taylor expansion in z, we recover the first two terms of the original series Eq.(531).

To proceed further, we return to Eq.(531) and iterate. We find

$$f(z) = c\frac{f(0)}{1+\frac{zf_1(0)}{1+zf_2(z)}}, \tag{535}$$

where

$$f_2(z) = \frac{f_1(0) - f_1(z)}{zf_1(z)}. \tag{536}$$

Yet another iteration gives the following result

$$f(z) = \frac{f(0)}{1+\frac{zf_1(0)}{1+\frac{zf_2(0)}{1+zf_3(z)}}}, \tag{537}$$

where

$$f_3(z) = \frac{f_2(0) - f_2(z)}{zf_2(z)}. \tag{538}$$

It is quite obvious how this continues. In fact, truncating iterations after N steps, we find

$$f(z) \sim F_N(z) = \frac{f(0)}{1+\frac{f_1(0)z}{1+\frac{f_2(0)z}{1+\ddots+\frac{f_{N-1}(0)z}{1+f_N(0)z}}}}, \tag{539}$$

where

$$f_i(z) = \frac{f_{i-1}(0) - f_{i-1}(z)}{zf_{i-1}(z)}, \tag{540}$$

and

$$f_i(0) = -\left.\frac{\mathrm{d}\ln f_{i-1}(z)}{\mathrm{d}z}\right|_{z=0}. \tag{541}$$

We can use these formulas to compute coefficients of continued fractions using the Taylor series representation of the function $f(z)$, Eq.(531). We obtain

$$c_1 = f_1(0) = -\frac{a_1}{a_0}, \quad c_2 = f_2(0) = \frac{a_1^2 - a_0 a_2}{a_0 a_1}, \quad c_3 = f_3(0) = \frac{a_0(a_2^2 - a_1 a_3)}{a_1(a_0 a_2 - a_1^2)}, \tag{542}$$

etc. We observe that, in order to compute the coefficient c_p in the continued fraction F_N, we only need to know $p+1$ terms $(a_0, a_1, ..., a_p)$ of the Taylor expansion of the function $f(z)$ at $z = 0$.

A continued fraction representation of a function is intimately related to a particular sequence of the Pade approximants. To establish this relation, we prove that $F_N(z)$ is the ratio of two polynomials of degree $M = N/2$, if N is even, and the ratio of degree $M = (N-1)/2$ and degree $M+1$ polynomials if N is odd. The proof proceeds by induction. The $N = 0$ and $N = 1$ cases are trivial to verify. Then, we assume that the above assertion is valid for $N = 2M$. Then, if we consider $N = 2M+1$, we find

$$F_{2M+1}(z, c_0, \ldots, c_{2M+1}) = \frac{c_0}{1 + zF_{2M}(z, c_1, \ldots, c_{2M+1})}. \tag{543}$$

Since, by assumption, F_{2M} can be written as the ratio of two degree M polynomials, we immediately conclude that, indeed, F_{2M+1} is written as the ratio of degree M and degree $M+1$ polynomials.

A similar line of reasoning shows that – for even N – $F_N(z)$ is the ratio of two degree $N/2$ polynomials. Since Pade approximations are ratios of polynomials and since coefficients of these polynomials are uniquely reconstructed from the original series once degrees of these polynomials are fixed, we conclude that the continued fraction $F_N(z)$ is one of the two Pade approximants $P_M^M(z)$ or $P_{M+1}^M(z)$, depending on whether N is even or odd.

To prove the convergence of the sequence of Pade approximants, we will consider $F_N(z)$ and investigate its $N \to \infty$ limit. Suppose that the coefficients $\{c_p\}$ of the continued fraction are known. We can write $F_N(z)$ as the ratio of two polynomials

$$F_N(z) = \frac{R_N(z)}{S_N(z)}. \tag{544}$$

A simple but important observation is that the functions $R_N(z)$ and $S_N(z)$ satisfy a recurrence relation

$$\begin{aligned} R_{N+1} &= R_N + c_{N+1} z R_{N-1}, \\ S_{N+1} &= S_N + c_{N+1} z S_{N-1}. \end{aligned} \tag{545}$$

This assertion is proved by induction. We assume that the above equations are valid for R_N, S_N and we prove them for R_{N+1}, S_{N+1}. To this end, we note that, as follows from the definition of continued fraction, we can obtain F_{N+1} from F_N if in F_N we replace c_N with $c_N/(1+c_{N+1}z)$. Hence,

$$
\begin{aligned}
F_{N+1} &= \frac{R_{N+1}}{S_{N+1}} = \left.\frac{R_N}{S_N}\right|_{c_N \to c_N/(1+c_{N+1}z)} = \frac{R_{N-1} + \frac{c_N z}{1+c_{N+1}z} R_{N-2}}{S_{N-1} + \frac{c_N z}{1+c_{N+1}z} R_{N-2}} \\
&= \frac{R_{N-1}(1+c_{N+1}z) + c_N z R_{N-2}}{S_{N-1}(1+c_{N+1}z) + c_N z R_{N-2}} = \frac{R_N + c_{N+1} z R_{N-1}}{S_N + c_{N+1} z S_{N-1}},
\end{aligned}
\tag{546}
$$

and this proves relations in Eq.(545). The third and fifth steps in the above derivation follow from the inductive assumption.

The reason Eq.(545) is useful is that it allows us to discuss the behavior of the continued fraction F_N as a function of N. Indeed, it is straightforward to use Eq.(545) to prove that

$$
R_{N+1}S_N - R_N S_{N+1} = -c_{N+1} z \left(R_N S_{N-1} - R_{N-1} S_N \right). \tag{547}
$$

This is a recurrence relation for $G_{N+1} = R_{N+1}S_N - R_N S_{N+1}$. The boundary condition for G_N is $G_1 = R_1 S_0 - R_0 S_1 = c_0 - c_0(1 + c_1 z) = -c_0 c_1 z$. Hence, we find

$$
R_N S_{N-1} - R_{N-1} S_N = c_0 c_1 c_2 \ldots c_N (-z)^N. \tag{548}
$$

We now divide this equation by $S_N S_{N-1}$ and obtain

$$
F_N(z) - F_{N-1}(z) = \frac{c_0 c_1 c_2 \ldots c_N (-z)^N}{S_N(z) S_{N-1}(z)}. \tag{549}
$$

The above equation is the basis for the analysis of the behavior of $F_N(z)$ in the limit $N \to \infty$ and for understanding of convergence properties of the continuous fractions and the Pade approximants. Apart from knowing the coefficients of the continued fractions, we also need to know $S_N(z)$. All these quantities are not universal and need to be investigated for each case separately.

We will consider a very simple example where such an analysis can be carried out explicitly. Recall the recursive construction of the continued series that we discussed; it was based on using the identity

$$
f(z) = \frac{f(0)}{1 + z f_1(z)}, \tag{550}
$$

where $f_1(z)$ is related to $f(z)$ in a particular way, c.f. Eq.(533). Suppose $f_1(z) = f(z)$. If so, all continuous fractions coefficients c_p are given by $f(0)$.

Does such a function exist? We take Eq.(550), substitute $f_1(z) \to f(z)$ and solve the quadratic equation to find

$$f(z) = \frac{1}{2z}\left(\pm\sqrt{1+4f(0)z} - 1\right). \tag{551}$$

We choose the positive sign in front of the square root to ensure that $f(z)$ is Taylor expandable at $z = 0$. Taking also $f(0) = 1/4$, for simplicity, we finally find

$$f(z) = \frac{1}{2z}\left(\sqrt{z+1} - 1\right). \tag{552}$$

All coefficients of the continued fraction representation of this function are identical, $c_p = 1/4$.

We can now use Eqs.(545) to determine S_N. The recurrence relation for S_N reads

$$S_{N+1} = S_N + \frac{z}{4}S_{N-1}. \tag{553}$$

To solve this recurrence relation, we make an ansatz $S_N = A\lambda^N$ and find an equation for λ

$$\lambda = 1 + \frac{z}{4\lambda}. \tag{554}$$

We solve this quadratic equation and find

$$\lambda_\pm = \frac{1 \pm \sqrt{1+z}}{2}. \tag{555}$$

The general solution is

$$S_N(z) = A_+(z)\lambda_+^N + A_-(z)\lambda_-^N. \tag{556}$$

We determine $A_\pm(z)$ by matching $S_N(z)$ to $S_0(z) = 1$ and $S_1(z) = 1 + z/4$. We find

$$S_N(z) = \frac{1}{\sqrt{1+z}}\left[\left(\frac{1+\sqrt{1+z}}{2}\right)^{N+2} - \left(\frac{1-\sqrt{1+z}}{2}\right)^{N+2}\right]. \tag{557}$$

Since for $z > -1$, $\sqrt{1+z}+1 > \sqrt{1+z}-1$ we can neglect the second term as compared to the first term in the $N \to \infty$ limit in the above equation.

Hence, we use Eq.(549) and find an asymptotic relation between F_N's

$$F_N(z) - F_{N-1}(z) \sim \frac{-2(1+z)}{z(1+\sqrt{1+z})}\left(\frac{1-\sqrt{1+z}}{1+\sqrt{1+z}}\right)^{N+1}. \tag{558}$$

We can solve this relation by writing

$$F_N(z) \sim A(z) + X(z) \left(\frac{1 - \sqrt{1+z}}{1 + \sqrt{1+z}} \right)^{N+2}, \tag{559}$$

where $A(z)$ is not determined at this point. It is easy to see that Eq.(558) implies

$$X(z) = \frac{\sqrt{1+z}}{z}. \tag{560}$$

Hence,

$$\lim_{N\to\infty} F_N(z) \to A(z). \tag{561}$$

One needs to do more work to find the function $A(z)$ and we are not going to do it here. Nevertheless, our discussion shows that a sequence of Pade approximants $P_1^0(z), P_1^1(z), P_2^1(z), \ldots, P_N^N(z), \ldots$ does converge to a limit as $N \to \infty$. The convergence is not uniform and depends on the value of z.

11 Boundary layer theory

The boundary layer theory applies when a *small* parameter multiplies the *highest* derivative in a differential equation. An obvious example is the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\Psi(x) = E\Psi(x). \tag{562}$$

The Planck constant $\hbar$ is small and we can think about constructing an expansion of the solutions to the Schrödinger equation in $\hbar$. The way to do this is known as the WKB (Wentzel-Kramers-Brillouin) approximation; among other things, it gives the Bohr-Sommerfeld quantization conditions for energy levels of the discrete spectrum.

The WKB method is relatively complex. The reason for that are problems that we encountered when we talked about perturbation theory. There we saw that if, by setting the small parameter to zero, we abruptly change the structure of the equation that we are trying to solve, the perturbative expansion becomes singular, most likely. The boundary layer theory allows one to avoid such problems when dealing with differential equations.

The idea of the boundary layer theory can be illustrated by studying the following differential equation

$$\epsilon y'' + (1+\epsilon)y' + y = 0. \tag{563}$$

We would like to find solution to Eq.(563) subject to boundary conditions $y(0) = 0$ and $y(1) = 1$.

Although this is not the point of the exercise, we can solve this equation exactly by introducing a function $w = y' + y$. Then Eq.(563) becomes

$$\epsilon w' + w = 0, \tag{564}$$

so that

$$w = C_0 e^{-x/\epsilon}. \tag{565}$$

Using this expression for w, we obtain a linear inhomogeneous differential equation

$$y + y' = C_0 e^{-x/\epsilon}. \tag{566}$$

The solution to this equation is

$$y = C_1 e^{-x} + C_2 e^{-x/\epsilon}, \tag{567}$$

where C_2 is a function of C_0 and ϵ whose explicit form we do not need. We now match Eq.(567) to the boundary conditions and obtain

$$y = \frac{e^{-x} - e^{-x/\epsilon}}{e^{-1} - e^{-1/\epsilon}}. \tag{568}$$

If we now take ϵ to be small, we see that on an interval $\epsilon \ll x \ll 1$, the solution is approximated by $y(x) \sim e^{1-x}$. However, for $x \sim \epsilon$ the solution changes and becomes $y(x) \sim e\left(1 - e^{-x/\epsilon}\right)$.

We would like to understand how these approximate solutions can be deduced from the original equation Eq. (563). To this end, we note that on the interval $\epsilon \ll x \ll 1$

$$y'' \sim y' \sim y. \tag{569}$$

This simply follows from the fact that $y' \sim y/x \sim y$ if x and y are both order one quantities.

Eq.(569) can be immediately used to discard $\epsilon y''$ and $\epsilon y'$ term in the original differential equation Eq.(563); we find

$$y' + y = 0. \tag{570}$$

We solve it to obtain

$$y(x) \sim e^{1-x}, \tag{571}$$

where the integration constant is determined by the "right" boundary condition $y(1) = 1$.

If we extrapolate the above solution to $x \sim \epsilon$ we find $y(\epsilon) \sim 1$. On the other hand, the "left" boundary condition $y(0) = 0$ should force a change from the above solution to the one that is consistent with the boundary condition. This implies that the function $y(x)$ should change very fast on the interval $0 < x \lesssim \epsilon$. This rapid change implies that on that interval

$$y' \sim \frac{1}{\epsilon}, \quad y'' \sim \frac{1}{\epsilon^2}, \quad y \sim 1. \tag{572}$$

It follows that the differential equation Eq.(563) on the interval $0 < x \lesssim \epsilon$ can be approximated by

$$\epsilon y'' + y' = 0. \tag{573}$$

The solution of this equation is

$$y' = Ce^{-x/\epsilon}. \tag{574}$$

Integrating one more time, we obtain

$$y(x) \approx C(1 - e^{-x/\epsilon}), \tag{575}$$

where we took into account the "left" boundary condition $y(0) = 1$.

The constant C can be obtained from the requirement that the left and the right solutions to the differential equation shown in Eqs.(571,575), respectively, match in the overlap region.

To establish that the overlap region exists, we take $x \sim \delta$ and choose $\epsilon \ll \delta \ll 1$. Then, we reconsider estimates that led to Eq. (573. We find

$$\epsilon y'' \sim \frac{\epsilon}{\delta^2}, \quad (1+\epsilon)y' \sim \frac{1}{\delta}, \quad y \sim 1. \tag{576}$$

Hence, under our assumption,

$$\epsilon y'' \ll y', \quad y \ll y' \tag{577}$$

in that region. The differential equation becomes

$$y' = 0, \tag{578}$$

which appears in a contradiction with the assumption that the $y' \sim 1/\delta$ in the leading term. However, the above equation tells us that the *large* $\sim 1/\delta$ derivative of $y(x)$ in this x-region is absent and the correct scaling is then $y' \sim 1$. And this scaling immediately implies that for small values of $x \sim \delta$, the function is approximately a constant. Inspecting the two approximate solutions that we have constructed, we indeed find that for values of x in the region $\epsilon \ll x \ll 1$, both solutions asymptote to a constant and by adjusting C in Eq. (575) we ensure that this constant is the same.

We can also argue in a slightly different way. Consider $\epsilon \ll x \sim \delta \ll 1$. For such values of x, the "right" solution is valid, it is given by Eq. (571) and it is, essentially, a constant

$$y(\delta) = e + \mathcal{O}(\delta). \tag{579}$$

For the "left" solution, taking $x \gg \epsilon$ also gives the constant solution $y(x) = C$. However, the question is if we can take this limit $x \gg \epsilon$ in the solution of Eq. (575). To understand this, we note that the scaling of derivatives $y' \sim 1/\epsilon$ that we assumed in deriving the left solution is accurate up to $\mathcal{O}(1)$ terms that we neglected. Hence, our solution should be valid as long as

$$y'(x) \sim \frac{1}{\epsilon} e^{-x/\epsilon} \gg 1. \tag{580}$$

This equation is satisfied for

$$x \ll \epsilon \ln \frac{1}{\epsilon}. \tag{581}$$

Since $\epsilon \to 0$, we can simultaneously have

$$\epsilon \ll x \sim \delta \ll \epsilon \ln \frac{1}{\epsilon}, \tag{582}$$

and in this region the "left solution" is indeed a constant but, also, the right solution is applicable.

Hence, the complete solution can be written as

$$y(x) = \begin{cases} e\left(1 - e^{-x/\epsilon}\right), & 0 < x \lesssim \delta \\ ee^{-x}, & \delta \lesssim x < 1, \end{cases} \tag{583}$$

where $\epsilon \ll \delta \ll \epsilon \ln \epsilon^{-1} \ll 1$. The small region around $x = 0$ where the solution changes quite rapidly from $y \sim \mathcal{O}(1)$ to $y \sim \mathcal{O}(0)$ is the boundary layer. One can check that this solution Eq.(583) agrees with the exact one, Eq.(567), provided that both in the boundary layer and in the bulk, we work to leading orders in the respective small parameter.

The above procedure can be extended to obtain solutions to differential equations with a boundary layer to higher orders in the small parameters. We will illustrate how to do this with a more complicated example. Consider the following differential equation

$$\epsilon y'' + (1 + x)y' + y = 0, \tag{584}$$

with the boundary conditions $y(0) = 1$ and $y(1) = 1$.

We begin with "right" solution, valid for $x \sim 1$. In this case the term $\epsilon y''$ in Eq.(584) can be treated as a perturbation. Then, we write

$$y(x) = \sum_{n=0}^{\infty} \epsilon^n y_n(x), \tag{585}$$

substitute the ansatz into the equation Eq.(584) and obtain

$$(1 + x)y_n' + y_n = -y_{n-1}''. \tag{586}$$

We set $y_{-1}(x)$ to zero, for obvious reasons.

We can rewrite the above equation as follows

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1 + x)y_n\right) = -y_{n-1}''. \tag{587}$$

Hence,

$$y_n(x) = \frac{c_n}{1 + x} - \frac{y_{n-1}'(x)}{1 + x}, \tag{588}$$

where c_n is the integration constant. Since the boundary condition $y(1) = 1$ implies that $y_0(1) = 1$ and $y_{n>0}(1) = 0$, we choose $c_0 = 2$ and $c_{n>0} = y'_{n-1}(1)$. Hence, we obtain

$$\begin{aligned} y_0 &= \frac{2}{1+x}, \\ y_1(x) &= -\frac{1}{2}\frac{1}{1+x} + 2\frac{1}{(1+x)^3}, \\ y_2(x) &= -\frac{1}{4}\frac{1}{1+x} - \frac{1}{2}\frac{1}{(1+x)^3} + \frac{6}{(1+x)^5}. \end{aligned} \tag{589}$$

To find the "left" solution as an expansion in ϵ, we introduce a new variable ξ such that $x = \epsilon\xi$. Hence, $x \sim \epsilon$ corresponds to $\xi \sim 1$. Furthermore, we denote $y(x) = Y(\xi)$, rewrite the differential equation Eq.(584) using the variable ξ and obtain

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}\xi^2} + \frac{\mathrm{d}Y}{\mathrm{d}\xi} = -\epsilon\left(\xi\frac{\mathrm{d}Y}{\mathrm{d}\xi} + Y\right). \tag{590}$$

Next, we write

$$Y(\xi) = \sum_{n=0}^{\infty} \epsilon^n Y_n(\xi). \tag{591}$$

Substituting Eq.(591) to Eq.(590), we obtain

$$\frac{\mathrm{d}^2 Y_n}{\mathrm{d}\xi^2} + \frac{\mathrm{d}Y_n}{\mathrm{d}\xi} = -\left(\xi\frac{\mathrm{d}Y_{n-1}}{\mathrm{d}\xi} + Y_{n-1}\right). \tag{592}$$

We can rewrite this equation as follows

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{\mathrm{d}Y_n}{\mathrm{d}\xi} + Y_n\right] = -\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\xi Y_{n-1}\right], \tag{593}$$

which allows us to immediately integrate it. We find

$$\frac{\mathrm{d}Y_n}{\mathrm{d}\xi} + Y_n = A_n - \xi Y_{n-1}, \tag{594}$$

where A_n is the integration constant.

To solve the above equation, we make an ansatz

$$Y_n = F_n(\xi)e^{-\xi}, \tag{595}$$

use it in Eq.(594) and find

$$\frac{\mathrm{d}F_n}{\mathrm{d}\xi} = \left(A_n - \xi Y_{n-1}(\xi)\right)e^{\xi}. \tag{596}$$

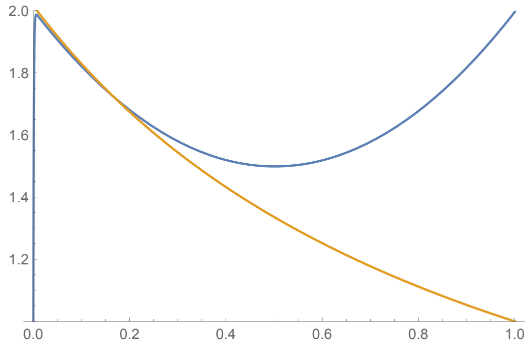

Figure 8: Two solutions of the differential equation Eq.(584) for $\epsilon = 10^{-3}$. The orange one is $y(x)$. The blue one is $Y(\xi)$. The region where the two solutions match is clearly visible. The blue solution becomes increasingly inaccurate for larger values of x. However, a combination of blue and orange remains a perfect approximation to the correct solution for all values of x.

We integrate this equation and add a solution of the homogeneous part of the differential equation Eq.(594) to satisfy the boundary condition at $\xi = 0$. We obtain

$$Y_n(\xi) = \delta_{n0} e^{-\xi} + e^{-\xi} \int\limits_0^{\xi} \mathrm{d}\mu \left(A_n - \mu Y_{n-1}(\mu)\right) e^{\mu}. \tag{597}$$

We find

$$\begin{aligned} Y_0(\xi) &= A_0 + e^{-\xi}\left(1 - A_0\right), \\ Y_1(\xi) &= A_0(1-\xi) + A_1 + e^{-\xi}\left(-A_0 - A_1 - \frac{\xi^2}{2} + \frac{A_0\xi^2}{2}\right), \\ Y_2(\xi) &= 3A_0\left(1 - \xi + \frac{\xi^2}{3}\right) + A_1(1-\xi) + A_2 \\ &\quad + e^{-\xi}\left(-3A_0 - A_1 - A_2 + \frac{A_0\xi^2}{2} + \frac{A_1\xi^2}{2} + \frac{\xi^4}{8} - \frac{A_0\xi^4}{8}\right). \end{aligned} \tag{598}$$

The constants A_0, A_1, A_2 etc. have to be determined by matching the solutions in Eq.(589) and the solutions in Eq.(598). To understand where the solutions can be matched, we note that Eq.(598) provides a valid solution to differential equation for values of ξ that are large provided only that $x \ll 1$. Similarly, Eq.(589) is valid all the way to small values of x. Hence, we if we take $\epsilon \ll x \ll 1$ we can match the solutions. We note that for such values of x all exponential terms in Eq.(598) drop out and only parts of the solutions which are represented by powers of ξ and x will have to be matched.

We then find

$$\lim_{\xi \to \infty} Y_0(\xi) \to A_0, \quad \lim_{x \to 0} y(x) \to 2, \quad \Rightarrow A_0 = 2. \tag{599}$$

The second term involves matching to first power in ϵ and first power in $x \ll 1$. Expanding Eq.(589) we find

$$y(x) = y_0(x) + \epsilon y_1(x) \approx 2 - 2x + \frac{3}{2}\epsilon. \tag{600}$$

At the same time, Eq.(598) gives

$$Y_0(\xi) + \epsilon Y_1(\xi) \approx 2 + 2\epsilon \left(1 - \frac{x}{\epsilon}\right) + \epsilon A_1 = 2 - 2x + \epsilon(2 + A_1). \tag{601}$$

It follows that $A_1 = -1/2$.

Finally, we perform the matching to $\mathcal{O}(x^2, \epsilon^2, x\epsilon)$. We write $y(x) = y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2(x)$ and expand through terms $\mathcal{O}(x^2, \epsilon^2, x\epsilon)$. We find

$$y(x) \approx 2 - 2x + 2x^2 + \epsilon\left(\frac{3}{2} - \frac{11}{2}x\right) + \frac{21}{4}\epsilon^2 + \ldots \tag{602}$$

We have to match Eq.(602) to $Y(\xi) = Y_0(\xi) + \epsilon Y_1(\xi) + \epsilon^2 Y_2(\xi)$ computed in the $\xi \to \infty$ limit. We find

$$\begin{aligned} Y(\xi) &\approx 2 + \epsilon\left[2\left(1 - \frac{\xi}{\epsilon}\right) - \frac{1}{2}\right] + \epsilon^2\left[6\left(1 - \frac{\xi}{\epsilon} + \frac{x^2}{3\epsilon^2}\right) - \frac{1}{2}\left(1 - \frac{\xi}{\epsilon}\right) + A_2\right] \\ &= 2 - 2x + 2x^2 + \epsilon\left(\frac{3}{2} - \frac{11}{2}x\right) + \epsilon^2\left(\frac{11}{2} + A_2\right). \end{aligned} \tag{603}$$

Comparison of Eq.(602) and Eq.(603) shows that $A_2 = -1/4$. Finally, having determined the three constants $A_{0,1,2}$, we can use them in Eq.(598) to provide fully determined solutions in the boundary layer $x \sim 0$ that also match the solutions in the bulk region. The two solutions are shown in Fig. 8 where also the quality of their matching can be seen.

In the example that we have just discussed, matching of inner and outer solutions was happening for values of x that were comparable to ϵ. Although the boundary layer region must be small and its smallness should be controlled by the small parameter, the exact relation between the size of the region and the small parameter depends on the equation that we are trying to solve. To see this, consider the following equation

$$\epsilon y'' - x^2 y' - y = 0, \tag{604}$$

with the boundary conditions $y(0) = y(1) = 1$. We will start by setting $\epsilon = 0$ and solving equation Eq.(604) in that approximation. We find

$$\frac{\mathrm{d}y}{y} = -\frac{\mathrm{d}x}{x^2}. \tag{605}$$

Upon integration, we obtain

$$\ln \frac{y}{C} = \frac{1}{x}. \tag{606}$$

We conclude that

$$y = Ce^{1/x}. \tag{607}$$

However, we will show that this solution *does not* provide a valid approximation of the solution at large values of x for Eq. (604).

It is clear that the solution Eq. (607) cannot satisfy the boundary condition $y(0) = 1$ for any choice of C. Hence, there must be a boundary layer around $x = 0$. To find the size of this region, we introduce a new variable $x = \delta\xi$ and re-write the differential equation as

$$\frac{\epsilon}{\delta^2}\frac{\mathrm{d}^2y}{\mathrm{d}\xi^2} - \delta\, \xi^2 \frac{\mathrm{d}y}{\mathrm{d}\xi} - y = 0. \tag{608}$$

If two out of three terms were to balance each other, three possibilities should be considered

$$1)\quad 1 \ll \frac{\epsilon}{\delta^2} \sim \delta; \qquad 2)\quad \delta \ll \frac{\epsilon}{\delta^2} \sim 1, \qquad \text{and} \qquad 3)\quad \delta \sim 1. \tag{609}$$

The first condition implies $\delta \sim \epsilon^{1/3}$ so that $\delta \ll 1$ for $\epsilon \ll 1$ and there is an inconsistency. The second condition implies $\delta \sim \epsilon^{1/2} \ll 1$. The third implies that the last two terms in Eq.(608) balance and this approximation we already considered in Eqs.(605,607).

Hence, the only possibility is $\delta \sim \epsilon^{1/2}$ which means that the first term and the last term in Eq.(607) balance. The approximate equation reads

$$\epsilon y'' = y. \tag{610}$$

The solution that satisfies the boundary condition at $x = 0$ is then

$$y(x) = B_1 e^{x/\sqrt{\epsilon}} + (1 - B_1)\, e^{-x/\sqrt{\epsilon}} \tag{611}$$

To match solutions in Eq.(607) and Eq.(611), we need to remove the increasing exponential in Eq.(611). This implies $B_1 = 0$. Then, Eq.(611) becomes exponentially suppressed at large x and we can only match it to

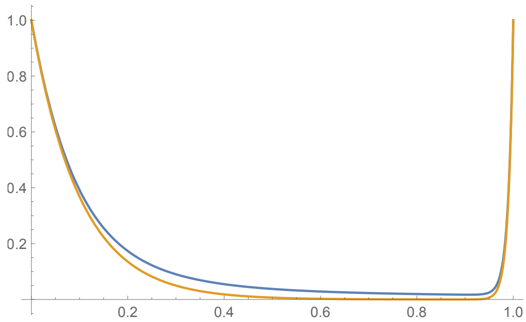

Figure 9: Exact (orange) and approximate (blue) solutions of the differential equation Eq.(604) for $\epsilon = 10^{-2}$ For the approximate solution, we used $y(x) = e^{-x/\sqrt{\epsilon}} + e^{-(1-x)/\epsilon}$.

Eq.(607) if $C = 0$. However, if $C = 0$, the outer solution becomes $y(x) = 0$ and this solution can not satisfy the boundary condition $y = 1$ at $x = 1$! This implies that we need yet another boundary layer at around $x = 1$.

This layer is easy to find. We write $x = (1 - z\delta)$, so that the equation becomes

$$\frac{\epsilon}{\delta^2}\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + \frac{(1-z\delta)^2}{\delta}\frac{\mathrm{d}y}{\mathrm{d}z} - y = 0. \tag{612}$$

Taking $\delta \sim \epsilon$, we find that the first two terms in the above equation should balance. The approximate equation therefore reads

$$\frac{\mathrm{d}^2 y}{\mathrm{d}z^2} + \frac{\mathrm{d}y}{\mathrm{d}z} = 0. \tag{613}$$

Its solution is simple to find. We obtain

$$y(z) = A + Be^{-z} = A + Be^{-(1-x)/\epsilon}. \tag{614}$$

The boundary condition $y = 1$ at $x = 1$ implies $A + B = 1$, so that

$$y(x) = A + (1 - A)e^{-(1-x)/\epsilon}. \tag{615}$$

As we move away from $x = 1$, the solution Eq.(615) becomes just a constant A so that we need to put it to zero, to match the solution from the other side. Hence, the complete solution is

Hence, the full solution of the differential equation that we constructed becomes

$$y(x) = \begin{cases} e^{-x/\sqrt{\epsilon}}, & 0 \le x \lesssim \delta \\ e^{-(1-x)/\epsilon}, & \delta \lesssim x \le 1 \end{cases} \tag{616}$$

The exact value of δ is not important as both solution decrease exponentially and are tiny for values of x that are away from the boundaries.

We compare numerical solution of the differential equation and the approximate solution for $\epsilon = 10^{-2}$ in Fig. 2; the agreement between the two is quite impressive and can be further improved by computing $\mathcal{O}(\epsilon)$ corrections to the leading approximation.

12 The WKB method

The so-called WKB (Wentzel-Kramers-Brillouin) method is a way to solve linear differential equations approximately in cases when the highest derivative term is multiplied by a small parameter. We have discussed a similar situation when talking about the boundary layer problem but the WKB approximation is more powerful since it can capture solutions that are singular at the whole interval and not just in the boundary regions.

The fact that such cases exist can be illustrated with the very simple example. Consider the differential equation

$$\epsilon^2 y''(x) + y(x) = 0, \tag{617}$$

with the boundary conditions $y(0) = 0$, $y(1) = 1$. We solve it to find

$$y(x) = \frac{\sin\left(\frac{x}{\epsilon}\right)}{\sin\left(\frac{1}{\epsilon}\right)}. \tag{618}$$

This is an oscillatory solution and the limit $\epsilon \to 0$ is singular *everywhere*. Note also that a similar equation with the opposite sign in front of $y(x)$ in Eq.(617), i.e.

$$\epsilon^2 y''(x) - y(x) = 0 \tag{619}$$

and the above boundary conditions, has the solution

$$y(x) = \frac{\sinh\left(\frac{x}{\epsilon}\right)}{\sinh\left(\frac{1}{\epsilon}\right)} \sim e^{-(1-x)/\epsilon}. \tag{620}$$

This solution is of the type that can be obtained using boundary layer methods. The WKB approximation is a formalism that allows one to treat *both* of these cases in a uniform fashion.

A typical differential equation that can be analyzed using the WKB method reads

$$\epsilon^2 \frac{\mathrm{d}^2 y(x)}{\mathrm{d}x^2} - Q(x) y(x) = 0, \qquad \epsilon \ll 1. \tag{621}$$

The main idea is to choose a particular ansatz for the function $y(x)$; in a certain sense this (exponential) ansatz is very similar to what we did to understand the behavior of differential equations at irregular singular points. We write

$$y(x) = e^{\frac{1}{\delta}\sum\limits_{n=0}^{\infty} \delta^n S_n(x)}. \tag{622}$$

At this point, the parameter δ is arbitrary but it is understood that $\delta \to 0$ if $\epsilon \to 0$. We will establish the relation between ϵ and δ shortly.

We substitute Eq.(622) into Eq.(621) and find

$$\frac{\epsilon^2}{\delta}\sum \delta^n S_n''(x) + \frac{\epsilon^2}{\delta^2}\left(\sum \delta^n S_n'(x)\right)^2 = Q(x). \tag{623}$$

We can develop a systematic expansion of this equation in a small parameter if we choose $\delta = \epsilon$. Indeed, the leading approximation then corresponds to the situation where the second term in Eq.(623) balances the term on the right-hand side of that equation and other contributions provide small perturbations. The first few terms of such an expansion read

$$\begin{aligned}
&(S_0'(x))^2 = Q(x),\\
&S_0'' + 2S_0'S_1' = 0,\\
&S_1'' + 2S_0'S_2' + (S_1')^2 = 0.
\end{aligned} \tag{624}$$

We can solve these equations iteratively. The first one gives $S_0' = \pm\sqrt{Q(x)}$, so that

$$S_0 = \pm \int^x \sqrt{Q(\xi)}\mathrm{d}\xi. \tag{625}$$

The second equation is straightforward to solve. We write

$$S_1' = -\frac{S_0''}{2S_0'} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\ln S_0' = -\frac{1}{4}\frac{\mathrm{d}}{\mathrm{d}x}\ln\left((S_0')^2\right). \tag{626}$$

It follows

$$S_1(x) = C_1 + \ln\left(Q^{-1/4}(x)\right). \tag{627}$$

Hence, a general solution of the differential equation Eq.(621) can be written as a linear combination of two independent solutions

$$y(x) = \frac{C_1}{Q^{1/4}}\exp\left[\frac{1}{\epsilon}\int^x \mathrm{d}\xi\sqrt{Q(\xi)}\right] + \frac{C_2}{Q^{1/4}}\exp\left[-\frac{1}{\epsilon}\int^x \mathrm{d}\xi\sqrt{Q(\xi)}\right]. \tag{628}$$

It is clear that if $Q(x) > 0$, we have exponentially growing and exponentially decaying solutions and if $Q(x)$ is negative, we have oscillating solutions.

The expansion that we have constructed involves, roughly, $\sqrt{Q(x)}x/\epsilon$ as the leading term and $\ln Q(x)$ as the subleading one. If $Q(x)$ is small, the first term may be not larger than the second so that the approximation then breaks down. In quantum mechanics, $\epsilon = \hbar$ and $Q(x) = 2m(V(x) - E)$, so that $Q(x) = 0$ if $E = V(x)$; this is the equation for a *classical turning point*.

Let us denote a turning point as x_0, i.e. $Q(x_0) = 0$. For the sake of definiteness, we will assume that $Q(x) > 0$ for $x > x_0$ and $Q(x) < 0$ for $x < x_0$. We consider a non-degenerate case $Q'(x_0) \neq 0$. Close to the turning point, we can write $Q(x) \sim Q_0 + (x - x_0)Q_1$, $Q_1 > 0$, and we can choose both normalization and coordinates in such a way that $Q_0 = 0$ and $x_0 = 0$.

The problem that we now discuss is as follows. As we explained, the solutions shown in Eq.(628) are valid to the left and to the right of the turning point. However, in the vicinity of the turning point the approximations that led to them are invalid and the solutions cannot be used. Hence, in order to connect the solutions on both sides of the turning point, we need to investigate the differential equation Eq.(621) in the vicinity of the turning point expanding in $x - x_0$.

Owing to our choice of the normalization and the coordinate system $Q_0 = 0$, $x_0 = 0$, we re-write Eq.(621) as

$$\epsilon^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - Q_1 x y = 0. \tag{629}$$

To simplify it further, we change variables $x \to \xi$, where $x = (\epsilon^2/Q_1)^{1/3}\xi$, and obtain

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\xi^2} - \xi y = 0. \tag{630}$$

This equation is the so-called Airy equation and its solutions are well-known (not surprisingly, they are called Airy functions).

Airy equation Eq.(630) has two canonical solution $\mathrm{Ai}(\xi)$ and $\mathrm{Bi}(\xi)$. They have the following asymptotic properties

$$\begin{aligned}
\mathrm{Ai}(\xi) &\sim \begin{cases} \frac{1}{2\sqrt{\pi}\xi^{1/4}} e^{-2\xi^{3/2}/3}, & \xi \to +\infty, \\ \frac{1}{\sqrt{\pi}(-\xi)^{1/4}} \sin\left(\frac{2(-\xi)^{3/2}}{3} + \frac{\pi}{4}\right), & \xi \to -\infty, \end{cases} \\
\mathrm{Bi}(\xi) &\sim \begin{cases} \frac{1}{\sqrt{\pi}\xi^{1/4}} e^{2\xi^{3/2}/3}, & \xi \to +\infty, \\ \frac{1}{\sqrt{\pi}(-\xi)^{1/4}} \cos\left(\frac{2(-\xi)^{3/2}}{3} + \frac{\pi}{4}\right). & \xi \to -\infty. \end{cases}
\end{aligned} \tag{631}$$

The general solution of the Airy equation is given by a linear combination of two solutions

$$y(\xi) = C_a \mathrm{Ai}(\xi) + C_b \mathrm{Bi}(\xi). \tag{632}$$

Our goal now is to match the solutions of the Airy equations, obtained in an approximation of small x and the solutions of the original equation Eq.(621) constructed in the WKB approximation, c.f. Eq.(628). We will do that assuming that the boundary conditions are similar to the ones in quantum mechanics, namely that in the limit $x \to +\infty$, the solution $y(x)$ can only have the exponentially decreasing component. For $x > x_0$, we therefore choose

$$y_I(x) = \frac{C_+}{[Q(x)]^{1/4}} \exp\left[-\frac{1}{\epsilon}\int_0^x d\xi \sqrt{Q(\xi)}\right]. \tag{633}$$

Note that we have chosen the lower-integration boundary at $x = 0$; this choice is arbitrary, but it uniquely defines the meaning of the constant C_+.

As we discussed earlier, the solution $y_I(x)$ is valid for values of x that satisfy the following inequality

$$\frac{Q_1^{1/2} x^{3/2}}{\epsilon} \gg 1. \tag{634}$$

We rewrite this inequality as

$$\left(\frac{\epsilon^2}{Q_1}\right)^{1/3} \ll x. \tag{635}$$

Since $\epsilon \to 0$, this condition can be satisfied simultaneously with the condition $x \ll 1$. This second condition, however, makes the solution in terms of Airy functions applicable *independent* of any other approximation. Hence, assuming that

$$\left(\frac{\epsilon^2}{Q_1}\right)^{1/3} \ll x \ll 1, \tag{636}$$

we can use $Q(x) = Q_1 x$ in Eq.(633) to find an approximate form of the solution in the region where *both* the WKB approximation and the solution in terms of Airy functions is applicable.

The WKB solution to the right of the turning point for x's in the range described by Eq.(636) reads

$$y_I(x) \sim \frac{C_+}{Q_1^{1/4}} x^{-1/4} \exp\left[-\frac{2Q^{1/2}x^{3/2}}{3\epsilon}\right], \quad x \ll 1. \tag{637}$$

It is easy to see that this solution matches *one* of the two asymptotic solutions of Airy functions in Eq.(631). Denoting the solution in the region around the turning point as y_{II}, we find

$$y_{II}(x) \sim 2C_+\sqrt{\pi}\,(Q_1\epsilon)^{-1/6} A_i\left[\left(\frac{Q_1}{\epsilon^2}\right)^{1/3} x\right]. \tag{638}$$

This solution continues across the turning point $x = x_0 = 0$ from positive to negative values of x. It is clear that if we consider the region of *negative* x that satisfies

$$\left(\frac{\epsilon^2}{Q_1}\right)^{1/3} \ll |x| \ll 1, \tag{639}$$

we should again be able to match the solution of the Airy equation Eq.(638) to the solution of the WKB equation for negative x. The asymptotic form of $y_{II}(x)$ for $\xi \to -\infty$ is obtained from Eq.(631). It reads

$$y_{II}(x) \sim \frac{2C_+}{Q_1^{1/4}|x|^{1/4}} \sin\left(\frac{2Q^{1/2}|x|^{3/2}}{3\epsilon} + \frac{\pi}{4}\right). \tag{640}$$

We now take the WKB solution in Eq.(628) and compute the result for negative x that satisfies Eq.(639), setting the lower integration boundary to $\xi = 0$. We use $(-1)^{1/2} = i$ and $(-1)^{1/4} = e^{i\pi/4}$) and find

$$y_{III}(x) \sim \frac{C_1}{Q_1^{1/4}|x|^{1/4}} e^{-i\phi - i\pi/4} + \frac{C_2}{Q_1^{1/4}|x|^{1/4}} e^{i\phi - i\pi/4}, \tag{641}$$

where $\phi = \frac{2Q^{1/2}|x|^{3/2}}{3\epsilon}$. We then match it to the solution in Eq.(640) by choosing $C_1 = C_+ i$ and $C_2 = C_+$. The complete solution in region III ($x < 0$, far from the turning point) is then

$$\begin{aligned} y_{III}(x) &= \frac{2C_+}{|Q(x)|^{1/4}} \sin\left[-\frac{1}{\epsilon}\int\limits_0^x \mathrm{d}\xi\, \sqrt{|Q(\xi)|} + \frac{\pi}{4}\right] \\ &= \frac{2C_+}{|Q(x)|^{1/4}} \cos\left[\frac{1}{\epsilon}\int\limits_0^x \mathrm{d}\xi\, \sqrt{|Q(\xi)|} + \frac{\pi}{4}\right]. \end{aligned} \tag{642}$$

The two solutions $y_I(x)$ and $y_{III}(x)$ provide the WKB solution of Eq.(628) for all values of x subject to the boundary condition $y(x) \to 0$ as $x \to \infty$. This solution is not valid in the vicinity of the turning point where $|x| < (\epsilon^2/Q_1)^{1/3}$ that becomes smaller and smaller as $\epsilon \to 0$. The regions of positive and negative x are connected by the solution valid under the condition $x \to 0$ which is provided by Airy functions.

It is quite natural to assume that one does not remember the asymptotic behavior of Airy functions. Can one still find a relationship between solutions to the left and to the right of a turning point? The answer to this question is, actually, positive. To explain how this can be done, consider extending the differential equation Eq.(628) to the *complex plane*. The WKB solutions are still given by formulas in Eq.(628) except that now all variables should be considered to be complex. We will also take $Q(x)$ to be $Q(z) = Q_1 z$ to study the vicinity of the turning point. The general solution reads

$$y(z) = C_1 y_+(z) + C_2 y_-(z), \tag{643}$$

where

$$y_\pm(z) = \frac{1}{Q_1^{1/4} z^{1/4}} \exp\left[\pm \frac{2\sqrt{Q_1} z^{3/2}}{3\epsilon}\right] \tag{644}$$

As it appears, this function has a branch cut at $z = 0$; this means we need to define how $\sqrt{z}$ and its powers are to be understood. We will make this cut along the *negative* real semi-axis. This implies that, for computing square roots etc., the proper parameterization of z is

$$z = |z| e^{i\phi}, \quad \text{with} \quad -\pi < \phi < \pi. \tag{645}$$

We now write the solutions $y_\pm(z)$ using the representation of z in Eq.(644). We obtain

$$y_\pm \sim \exp\left[\pm \frac{2\sqrt{Q_1}|z|^{3/2}}{3\epsilon} \cos\left(\frac{3\phi}{2}\right) + \ldots\right], \tag{646}$$

where ellipses stand for the imaginary part.

The result shown in Eq.(648) is quite instructive. Indeed, on the real axis for positive values of z, the solution y_+ is exponentially large and the solution y_- is exponentially small. However, as Eq.(648) shows, the role of large and small changes as we move *around the turning point in the complex plane*. Indeed, since $\cos 3\phi/2$ changes the sign as ϕ changes, we find that in the region $-\pi/3 < \phi < \pi/3$, the solution y_+ is much larger than y_-, but for $\pi/3 < \phi < \pi$ and $-\pi < \phi < -\pi/3$, y_+ is much smaller than y_-.

We are interested in the solution of the differential equation that equals the exponentially small solution $y_-(x)$ on the positive real axis; since the WKB approximation has power accuracy, it means that if we start with $y_-(z)$ at $\phi = 0$, we will still have $y_-(z)$ when we come to $\phi = \pm\pi/3$. However, once we move past $\pi/3$, we can not guarantee that y_- remains y_- since the solution y_+ is exponentially suppressed there (in other words, an exponentially small solution can be generated out of nothing within the WKB approximation). Hence, in the regions $\pi/3 < \phi < \pi$ and $-\pi < \phi < -\pi/3$ we should allow for two solutions

$$\begin{aligned} y_a(z) &= y_-(z) + a y_+(z), \qquad \pi/3 < \phi < \pi, \\ y_b(z) &= y_-(z) + b y_+(z), \qquad -\pi < \phi < -\frac{\pi}{3}. \end{aligned} \tag{647}$$

We can now compute the two solutions at (just above and just below) the cut. The key point now is that one should get *the same* because the point $z = 0$ is *not* a singular point of the differential equation and so the cut should not be needed. Hence, we impose the following requirement

$$y_-(|z|e^{i\pi}) + a y_+(|z|e^{i\pi}) = y_-(|z|e^{-i\pi}) + b y_+(|z|e^{-i\pi}). \tag{648}$$

We use the explicit representation of the functions $y_\pm$ to compute a relation between the various entries in Eq.(648). We obtain

$$\begin{aligned} y_\pm(|z|e^{-i\pi}) &= \frac{e^{i\pi/4}}{Q_1^{1/4}|z|^{1/4}} \exp\left[\pm i \frac{2\sqrt{Q_1}|z|^{3/2}}{3\epsilon}\right], \\ y_\pm(|z|e^{i\pi}) &= \frac{e^{-i\pi/4}}{Q_1^{1/4}|z|^{1/4}} \exp\left[\mp i \frac{2\sqrt{Q_1}|z|^{3/2}}{3\epsilon}\right]. \end{aligned} \tag{649}$$

This implies

$$y_+(|z|e^{-i\pi}) = i y_-(|z|e^{i\pi}), \qquad y_-(|z|e^{-i\pi}) = i y_+(|z|e^{i\pi}). \tag{650}$$

We use these results in Eq.(648) and find

$$a = i, \qquad b = -i. \tag{651}$$

Hence, the solution on the negative real axis reads

$$y_{II}(z) = \frac{2}{Q^{1/4} z^{1/4}} \cos\left(\frac{2\sqrt{Q}|z|^{3/2}}{3\epsilon} - \frac{\pi}{4}\right) = \frac{2}{Q^{1/4} z^{1/4}} \sin\left(\frac{2\sqrt{Q}|z|^{3/2}}{3\epsilon} + \frac{\pi}{4}\right). \tag{652}$$

This is the same result that we obtained in Eq.(640) using the asymptotic behavior of the Airy function.

We will now translate what we discussed to Quantum Mechanics; we will see that translation will leave to interesting consequences.

In this case, the equation that we would like to solve is the Schrödinger equation that we write in the following way

$$\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x) - 2m(V(x) - E)\Psi(x) = 0. \tag{653}$$

It follow that we can use the formulas that we derived above provided that we identify $\epsilon \to \hbar$ and $2m(V(x) - E) = Q(x)$.

We will consider a situation where $V(x) < E$ for $a < x < b$, so that a and b are the two classic turning points. We would like to solve the Schroödinger equation for standard boundary conditions $\Psi(x) \to 0$ for $x \to \pm\infty$. We now split the x axis into three regions 1) $x < b$, 2) $a < x < b$ 3) $x > b$.

Consider the right turning point $x = b$. For $x > b$ the solution is

$$\Psi_3(x) = \frac{C_3}{[Q(x)]^{1/4}} \exp\left[-\frac{1}{\hbar}\int_b^x \mathrm{d}\xi\ \sqrt{Q(\xi)}\right], \quad x > b. \tag{654}$$

We know that if we continue the result to $x < b$, $\Psi_3(x)$ matches the following approximate solution of the Schrödinger equation

$$\Psi_2(x) = \frac{2C_3}{[|Q(x)|]^{1/4}} \sin\left[-\frac{1}{\hbar}\int_b^x \mathrm{d}\xi\ \sqrt{|Q(\xi)|} + \frac{\pi}{4}\right], \quad a < x < b. \tag{655}$$

We can investigate the impace of the second turning point at $x = a$. Since in this case the classically-forbidden region is at $x < a$, we can make use of the above results if we write $x = a - y$ with $y > 0$ in the forbidden region. Then, in terms of y

$$\Psi_1(y) = \frac{C_1}{[Q(a-y)]^{1/4}} \exp\left[-\frac{1}{\hbar}\int_0^y \mathrm{d}\mu\ \sqrt{Q(a-\mu)}\right], \quad y > 0. \tag{656}$$

We can now go back to x and $\xi = a - \mu$. We obtain

$$\Psi_1(x) = \frac{C_1}{[Q(x)]^{1/4}} \exp\left[\frac{1}{\hbar}\int_a^x \mathrm{d}\xi\ \sqrt{Q(\xi)}\right], \quad x < a. \tag{657}$$

We can also continue to $x > a$ using $\Psi_1(y)$ written in terms of y. We find an alternative representation for the wave function in the region $a < x < b$. We find

$$\Psi_2 = \frac{2C_1}{[Q(a-y)]^{1/4}} \sin\left[-\frac{1}{\hbar}\int_0^y \mathrm{d}\mu\ \sqrt{Q(a-\mu)} + \frac{\pi}{4}\right], \quad y < 0, \tag{658}$$

which we again express in terms of x

$$\Psi_2 = \frac{2C_1}{[Q(x)]^{1/4}} \sin\left[\frac{1}{\hbar}\int_a^x \mathrm{d}\xi\ \sqrt{|Q(\xi)|} + \frac{\pi}{4}\right], \quad a < x < b. \tag{659}$$

We now have two expressions for $\Psi_2(x)$ in the allowed region $a < x < b$, Eq. (655) and Eq. (659). Requiring that they actually coincide, we obtain the following equation

$$\int_a^b \mathrm{d}x \, \sqrt{2m(E - V(x))} = \pi\hbar \left(n + \frac{1}{2} \right) , \tag{660}$$

where n is integer. Note that this is a condition on the *allowed* values of the energy E, i.e. a quantization condition. This quantization condition is the Bohr-Sommerfeld quantization condition from the early years of quantum mechanics. Finally, since $\sqrt{2m(E - V(x))} = p(x)$ is the canonical mometum, the above equation reads

$$\int_a^b p(x) \mathrm{d}x = \pi\hbar \left(n + \frac{1}{2} \right) . \tag{661}$$

In classical mechanics $\int_a^b p(x)\mathrm{d}x$ is related to

13 Resonance and secular behavior in non-linear differential equations

In this lecture we will talk about small oscillations in classical mechanics. Small (harmonic) oscillations are described by the differential equation

$$\ddot{y} + \omega^2 y = 0, \tag{662}$$

where $\ddot{y} = \mathrm{d}^2 y/\mathrm{d}t^2$. The solution to Eq.(662) is well-known

$$y(t) = a\cos(\omega t + \phi), \tag{663}$$

where a and ϕ are two parameters to be fixed using initial conditions.

In case there is an external harmonic force acting on an oscillator, the equation of motion reads

$$\ddot{y} + \omega^2 y = f_0 \cos \Omega t. \tag{664}$$

The solution of this equation is

$$y(t) = a\cos(\omega t + \phi) + \frac{f_0}{\omega^2 - \Omega^2}\cos\Omega t. \tag{665}$$

The oscillation amplitude $y(t)$ is bounded for all $\Omega \neq \omega$. However, in case $\Omega = \omega$, the solution changes and becomes

$$y(t) = \tilde{a}\cos(\omega t + \tilde{\phi}) + \frac{f_0 t}{2\omega}\sin\omega t. \tag{666}$$

Note that the amplitude of the second term on the r.h.s. is unbounded as $t \to \infty$. Terms that exhibit such a growing amplitude are called *secular* terms and their appearance in solutions to equations that describe oscillations subject to an external *resonance* force is natural because there is energy transfer from the external force to the system.

Next, consider a generalization of Eq.(662) that describes small oscillations subject to a non-linear pertubation

$$\ddot{y} + \omega^2 y = -\epsilon y^3. \tag{667}$$

We assume that the parameter ϵ is small.

It is tempting to solve Eq.(667) by developing a perturbation theory in ϵ. This amounts to writing

$$y(t) = \sum_{n=0}^{\infty} \epsilon^n y_n(t), \tag{668}$$

and then using this representation of $y(t)$ to solve Eq.(667) order by order in ϵ. We will work through order $\mathcal{O}(\epsilon)$ in the perturbative expansion. We find two equations

$$\begin{aligned} \ddot{y}_0 + \omega^2 y_0 &= 0, \\ \ddot{y}_1 + \omega^2 y_1 &= -y_0^3. \end{aligned} \tag{669}$$

The general solution of the first equation reads

$$y_0(t) = a\cos(\omega t + \beta). \tag{670}$$

For simplicity, we impose the boundary conditions $y(0) = a$ and $\dot{y}(0) = 0$; we find $\beta = 0$. The second equation we have to solve reads

$$\ddot{y}_1 + \omega^2 y_1 = -a^3 \cos^3 \omega t. \tag{671}$$

Since

$$\cos^3 \omega t = \frac{3}{4}\cos\omega t + \frac{1}{4}\cos 3\omega t, \tag{672}$$

we obtain

$$\ddot{y}_1 + \omega^2 y_1 = -a^3\left(\frac{3}{4}\cos\omega t + \frac{1}{4}\cos 3\omega t\right). \tag{673}$$

We require the solution to this equation subject to boundary conditions $y_1(0) = 0$, $\dot{y}_1(0) = 0$. We observe that Eq.(673) is equivalent to Eq.(664) with $\Omega = 3\omega$ and $\Omega = \omega$. This implies that $y_1(t)$ is a combination of the solutions shown in Eq.(665) and Eq.(666). We find

$$y_1(t) = -\frac{3a^3 t}{8\omega}\sin(\omega t) - \frac{a^3}{32\omega^2}\cos\omega t + \frac{a^3}{32\omega^2}\cos(3\omega t), \tag{674}$$

where we have fixed all the boundary condition by requiring that $y_1(0) = 0$ and $\dot{y}_1(0) = 0$.

Hence, we obtain the solution to the original equation Eq.(667) valid through first order in ϵ

$$y(t) = a\left(1 - \frac{\epsilon a^2}{32\omega^2}\right)\cos\omega t + \frac{a^3\epsilon}{32\omega^2}\cos(3\omega t) - \frac{3a^3 t\epsilon}{8\omega}\sin(\omega t) + \mathcal{O}(\epsilon^2). \tag{675}$$

From this solution, it is easy to see that perturbation theory is somewhat pathological. Indeed, the last term in Eq.(675) is secular. This implies that as long as $a^3 t\epsilon/\omega \ll 1$, the perturbation theory works fine but as time increases, we are bound to reach a moment when

$$a^2 t\epsilon/\omega \gg 1, \tag{676}$$

after which the correction becomes *larger* than the leading order solution.

Moreover, Eq.(675) predicts that the amplitude of oscillations keeps increasing and this does not make much sense physically. In fact, it is very easy to prove that any solution to Eq.(667) *is bounded*. This is accomplished by calculating the total energy stored in the mechanical system. To this end, we multiply Eq.(667) with $\dot{y}$, use

$$\dot{y}\ddot{y} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left[\dot{y}^2\right], \quad \dot{y}y^n = \frac{1}{n+1}\frac{\mathrm{d}}{\mathrm{d}t}\left[y^{n+1}\right], \tag{677}$$

integrate over t and find

$$\frac{\dot{y}^2}{2} + \frac{\omega^2 y^2}{2} + \frac{\epsilon y^4}{4} = C. \tag{678}$$

The constant C is easily computed from the boundary condition at $t = 0$. Since $\dot{y}(0) = 0$, we find

$$C = \frac{\omega^2 y^2}{2} + \frac{\epsilon y^4}{4} = \frac{\omega^2 a^2}{2} + \frac{\epsilon a^4}{4}. \tag{679}$$

Since $\dot{y}^2/2$ is positive definite,

$$\frac{\omega^2 y^2}{2} + \frac{\epsilon y^4}{4} < C, \tag{680}$$

and we conclude that $y(t)$ is *bounded from above*.

We can reconcile this observation with the fact that the perturbative solution Eq.(675) does exhibit unbounded growth at $t \to \infty$ by arguing that higher terms in the perturbative expansion in ϵ will correct the behavior of the leading order term. Indeed, if two terms in a would-be expansion

$$1 - \epsilon t \tag{681}$$

get supplemented by

$$1 - \epsilon t + \frac{\epsilon^2 t^2}{2} - \frac{\epsilon^3 t^3}{3!} + \cdots - \frac{\epsilon^n t^n}{n!} + \cdots, \tag{682}$$

the series sums up to $e^{-\epsilon t}$ which is bounded for all t. We expect something similar to happen to the series in Eq.(668).

To show that this is actually the case, we will analyze the *most secular terms* in the perturbative expansion. Such terms should contain one power of t for one power of ϵ so that n-th term in the series behaves as

$$a_n \epsilon^n t^n e^{i\omega t} + a_n^* \epsilon^n t^n e^{-i\omega t}. \tag{683}$$

We will use induction to prove that the coefficients a_n are given by the following formula

$$a_n = \frac{a}{2}\frac{1}{n!}\left(\frac{3ia^2}{8\omega}\right)^n. \tag{684}$$

However, before we do that, we need to understand how to extract the most secular terms from the following equation

$$\ddot{y}_{n+1} + \omega^2 y_{n+1} = c_n t^n e^{i\omega t}. \tag{685}$$

To do that, we write $y_{n+1} = f(t)e^{i\omega t}$, substitute this expression into Eq.(685) and find

$$\ddot{f} + 2i\omega\dot{f} = c_n t^n. \tag{686}$$

We write $f = \sum\limits_{k=0}^{n+1} b_k t^k$, substitute this ansatz into the above equation and find

$$b_{n+1} = \frac{c_n}{2i\omega(n+1)} \tag{687}$$

Hence, we can write

$$y_{n+1} = \frac{c_n t^{n+1}}{2i\omega(n+1)} e^{i\omega t} + \tilde{y}_{n+1}(t), \tag{688}$$

where the first term describes the leading secular term in the solution $y(t)$ and $\tilde{y}(t)$ describes subleading secular terms.

We return to the differential equation Eq.(667). We solve it using the perturbative expansion Eq.(668). To find the leading secular contribution in the equation for $y_{n+1}(t)$, we first determine contributions of order ϵ^{n+1} on the right-hand side. We find

$$\ddot{y}_{n+1} + \omega^2 y_{n+1} = -\sum_{j+k+l=n} y_j y_k y_l. \tag{689}$$

To find the most secular contributions, we make an inductive assumption that for $j \le n$ such terms follow from Eq.(684) and read

$$y_j = \frac{a}{2}\frac{1}{j!}\left(\frac{3a^2}{8\omega}\right)^j \left[(it)^j e^{i\omega t} + (-it)^j e^{-i\omega t}\right]. \tag{690}$$

Collecting terms that produce $e^{i\omega t}$ on the r.h.s. of Eq.(689), we obtain

$$\begin{aligned} -\sum_{j+k+l=n} y_j y_k y_l &\Rightarrow -\frac{a^3}{8}\left(\frac{3a^2}{8\omega}\right)^n t^n e^{i\omega t} \sum_{j+k+l=n} \frac{i^{j+k-l} + i^{-j+k+l} + i^{j-k+l}}{j!\,k!\,l!} \\ &= -\frac{a^3}{8}\left(\frac{3ia^2}{8\omega}\right)^n t^n e^{i\omega t} \sum_{j+k+l=n} \frac{(-1)^l + (-1)^j + (-1)^k}{j!\,k!\,l!}. \end{aligned} \tag{691}$$

To compute the last sum, we note that we can relate it to the n-th term in the expansion of the function $e^x = e^x e^x e^{-x}$ in powers of x. Indeed,

$$e^x e^x e^{-x} = e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \sum_{n=0}^{\infty} x^n \sum_{j+k+l=n} \frac{(-1)^l}{j!\ k!\ l!}. \tag{692}$$

Hence, we conclude that

$$\sum_{j+k+l=n} \frac{(-1)^l + (-1)^j + (-1)^k}{j!\ k!\ l!} = \frac{3}{n!}. \tag{693}$$

Therefore,

$$\ddot{y}_{n+1} + \omega^2 y_{n+1} = -\frac{3a^3}{8n!}\left(\frac{3ia^2}{8\omega}\right)^n t^n e^{i\omega t} + \text{c.c.} \tag{694}$$

Upon comparing the r.h.s. of this equation with Eq.(685), we find

$$c_n = -\frac{3a^3}{8n!}\left(\frac{3ia^2}{8\omega}\right)^n. \tag{695}$$

This gives

$$y_{n+1} = \frac{c_n t^{n+1}}{2i\omega(n+1)} e^{i\omega t} + \text{c.c.} = \frac{a}{2(n+1)!}\left(\frac{3ia^2}{8\omega}\right)^{n+1} t^{n+1} e^{i\omega t} + \text{c.c.}\ . \tag{696}$$

This result is consistent with our assumption about the most secular coefficients in Eq.(684); this completes the inductive proof.

It is now straightforward to sum up the most secular contributions to $y(t)$. We find

$$y(t) = \sum_{n=0}^{\infty} \frac{\epsilon^n a}{2n!}\left(\frac{3ia^2}{8\omega}\right)^n t^n e^{i\omega t} + \text{c.c.} = \frac{a}{2} e^{i\omega t + 3ia^2\epsilon t/(8\omega)} + \text{c.c.} = a\cos\omega_1 t, \tag{697}$$

with

$$\omega_1 = \omega + \frac{3a^2\epsilon}{8\omega}. \tag{698}$$

Hence, we conclude that the sum of the most secular terms in the perturbative expansion of Eq.(667) produces a *shift in the frequency of oscillations* in spite of the fact that solutions at any given order in perturbation theory appear to be unbounded.

We would like to understand how to extend these calculations to enable dealing with all secular terms and not only the most singular ones. in other words, we would like to find a way to construct a systematic expansion of non-linear equations in ϵ. The method that allows us to do that is known as *multi-scale analysis*. The idea behind it is as follows. As we have seen from the above example, the differential equation implies that, in addition to an obvious time scale $t \sim 1/\omega$, there is another time scale $t \sim \omega/(\epsilon a^2)$, where naive perturbation theory breaks down. It is convenient to *formally* treat the two time scales separately by describing them using two *different* variables. The removal of secular terms from the solution allows us to determine the dependence of the solution depends on the variable that describes larger time scale.

Following what we have just described, we introduce a new variable $\tau = \epsilon t$ and formally write

$$y(t) = Y(t, \tau). \tag{699}$$

The derivative w.r.t. t reads

$$\frac{\mathrm{d}}{\mathrm{d}t} Y(t, \tau) = \frac{\partial Y}{\partial t} + \frac{\partial Y}{\partial \tau} \frac{\mathrm{d}\tau}{\mathrm{d}t} \tag{700}$$

Since $\tau = \epsilon t$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} Y(t, \tau) = \frac{\partial Y}{\partial t} + \epsilon \frac{\partial Y}{\partial \tau} \tag{701}$$

The second derivative is computed in an analogous way; we find

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} Y(t, \tau) = \frac{\partial^2 Y}{\partial t^2} + 2\epsilon \frac{\partial^2 Y}{\partial t \partial \tau} + \epsilon^2 \frac{\partial^2 Y}{\partial \tau^2}. \tag{702}$$

We now write an expansion of $y(t)$ in powers of ϵ. Then

$$y(t) = Y_0(t, \tau) + \epsilon Y_1(\tau) + \mathcal{O}(\epsilon^2). \tag{703}$$

Note that there is a hidden dependence on ϵ in e.g. Y_0 through its dependence on τ.

Substituting Eq.(703) into Eq.(667) and using Eq.(702) to express the time derivative through derivatives w.r.t. t and τ, we find for the two first terms in the ϵ-expansion.

$$\begin{aligned} &\frac{\partial^2 Y_0}{\partial t^2} + \omega^2 Y_0(t, \tau) = 0, \\ &\frac{\partial^2 Y_1}{\partial t^2} + \omega^2 Y_1(t, \tau) + 2 \frac{\partial^2 Y_0}{\partial t \partial \tau} = -Y_0^3. \end{aligned} \tag{704}$$

The general solution of the first equation is straightforward. We find

$$Y_0 = A_0(\tau) e^{i\omega t} + A_0^*(\tau) e^{-i\omega t}. \tag{705}$$

We note that at this point the function $A_0(\tau)$ is not determined.

We consider the second equation in Eq.(704). Using Y_0 from Eq.(705) and focusing on the secular terms, we find

$$\frac{\partial^2 Y_1}{\partial t^2} + \omega^2 Y_1(t,\tau) + F(\tau)e^{i\omega t} + F^*(\tau)e^{-i\omega t} = \ldots, \tag{706}$$

where

$$F(\tau) = 2i\omega \frac{\partial A_0(\tau)}{\partial \tau} + 3A_0^2 A_0^*, \tag{707}$$

and the ellipsis stands for non-secular terms. If $F(\tau) \neq 0$, the equation for A_0 contains secular terms and the oscillation amplitude exhibits unbounded growth. We can avoid this by *requiring* that $F(\tau) = 0$. This condition gives us a differential equation for A_0. It reads

$$2i\omega \frac{\partial A_0(\tau)}{\partial \tau} + 3A_0^2 A_0^* = 0. \tag{708}$$

To solve this equation, we write

$$A_0(\tau) = R_0(\tau)e^{i\theta_0(\tau)}. \tag{709}$$

Substituting the ansatz Eq.(709) into Eq.(708) and separating real and imaginary parts, we obtain two equations that read

$$\frac{\partial R_0(\tau)}{\partial \tau} = 0, \quad -2\omega \frac{\partial \theta_0(\tau)}{\partial \tau} + 3R_0^2 = 0. \tag{710}$$

Accounting for the boundary conditions, we conclude that

$$R_0 = \frac{a}{2}, \quad \theta_0 = \frac{3a^2\tau}{8\omega}. \tag{711}$$

Hence,

$$Y_0(t,\tau) = a\cos\left(\omega t + \frac{3a^2\tau}{8\omega}\right), \tag{712}$$

and we have reproduced our previous result. This analysis can be continued also in higher orders of the expansion in ϵ.

As another example of an application of multi-scale analysis, we consider the so-called *Rayleigh oscillator*

$$\ddot{y} + \omega^2 y = \epsilon\left(\dot{y} - \frac{1}{3}\dot{y}^3\right). \tag{713}$$

We will consider the following boundary conditions

$$y(0) = 0, \quad \dot{y}(0) = 2v. \tag{714}$$

Similar to the previous case, we write

$$y(t) = Y_0(t, \tau) + \epsilon\, Y_1(t, \tau), \tag{715}$$

and expand the Rayleigh equation to first order in ϵ. We find

$$\begin{aligned} &\frac{\partial^2 Y_0}{\partial t^2} + \omega^2 Y_0(t, \tau) = 0, \\ &\frac{\partial^2 Y_1}{\partial t^2} + \omega^2 Y_1(t, \tau) + 2\frac{\partial^2 Y_0}{\partial t \partial \tau} = \frac{\partial Y_0}{\partial t} - \frac{1}{3}\left(\frac{\partial Y_0}{\partial t}\right)^3. \end{aligned} \tag{716}$$

The solution to the first equation is

$$Y(t, \tau) = A_0(\tau) e^{i\omega t} + A_0^*(\tau) e^{-i\omega t} \tag{717}$$

Next, we investigate the second equation in Eq.(716) to find the secular terms. We obtain

$$\frac{\partial^2 Y_1}{\partial t^2} + \omega^2 Y_1(t, \tau) + F(\tau) e^{i\omega t} + F^*(\tau) e^{-i\omega t} = \ldots, \tag{718}$$

where

$$F(\tau) = 2i\omega \frac{\partial A_0(\tau)}{\partial \tau} - i\omega A_0 + i\omega^3 A_0^2 A_0^*. \tag{719}$$

Requiring that there are no secular terms in Eq.(718), we obtain

$$\frac{\partial A_0(\tau)}{\partial \tau} = \frac{1}{2} A_0 \left(1 - |A_0|^2\right). \tag{720}$$

Writing $A_0(\tau) = R_0(\tau) e^{i\theta_0(\tau)}$, we obtain two equations for the real and imaginary parts

$$2\frac{\mathrm{d}R_0}{\mathrm{d}\tau} = R_0(1 - R_0^2), \qquad \frac{\mathrm{d}\theta_0}{\mathrm{d}\tau} = 0. \tag{721}$$

The solutions to these equations are

$$\theta_0 = \theta_0(0), \quad R_0(\tau) = \frac{R_0(0)}{\sqrt{e^{-\tau} + R_0^2(0)(1 - e^{-\tau})}}. \tag{722}$$

The constants of integration $\theta_0(0)$ and $R_0(0)$ are chosen in such a way that the boundary conditions Eq.(714) are satisfied. We finally obtain

$$y(t) = \frac{2v}{\omega} \frac{\sin \omega t}{\sqrt{e^{-\tau} + \left(\frac{v}{\omega}\right)^2 (1 - e^{-\tau})}}, \quad \tau = \epsilon t. \tag{723}$$

Note that the solution to the Rayleigh equation in Eq.(723) has a peculiar asymptotic behavior in the limit $t \to \infty$. Indeed, since in this limit $e^{-\tau} \to 0$, we find

$$y(t)|_{t\to\infty} \to 2\sin(\omega t), \tag{724}$$

regardless of the initial conditions. The asymptotic solution at $t = \infty$ is called the "limit cycle".

14 Parametric excitations in differential equations. Stability.

Consider a pendulum whose pivot point performs vertical oscillations; we discussed this mechanical system in the first lecture. It was shown there that it can be described by means of a differential equation with a time-dependent frequency

$$y'' + \omega^2 (1 + \kappa \cos \gamma t)\, y = 0. \tag{725}$$

We will first discuss general features of solutions to Eq.(725). An important observation is that if $y(t)$ is the solution to Eq.(725) then $y(t+T)$ where $T = 2\pi/\gamma$ is also a solution. To prove this, write

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\, y(t+T) + \omega^2 (1 + \kappa \cos \gamma t)\, y(t+T), \tag{726}$$

and replace t with τ where $t = \tau - T$. Since $\cos \gamma t = \cos(\gamma(\tau - T)) = \cos \gamma \tau$, Eq.(726) becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\, y(\tau) + \omega^2 (1 + \kappa \cos \gamma \tau)\, y(\tau), \tag{727}$$

which is zero according to Eq.(725).

Consider now two independent solutions of Eq.(725); we will call them $y_1(t)$ and $y_2(t)$. We will imagine that the two solutions are chosen in such a way that their Wronskian

$$W(t) = y_1' y_2 - y_2' y_1 \tag{728}$$

equals to one, $W(t) = 1$. Since $y_{1,2}(t+T)$ are solutions to Eq.(725) they can be written as linear combinations of $y_{1,2}(t)$ with time-independent coefficients. We find

$$\left(\begin{array}{c} y_1(t+T) \\ y_2(t+T) \end{array} \right) = \left(\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array} \right) \left(\begin{array}{c} y_1(t) \\ y_2(t) \end{array} \right). \tag{729}$$

Let us call the matrix in the above equation $\hat{A}$, i.e.

$$\hat{A} = \left(\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array} \right). \tag{730}$$

Its transpose $\hat{A}^T$ possesses eigenvectors and eigenvalues; we will call them $\vec{\epsilon}_{1,2}$ and $\lambda_{1,2}$ so that

$$\hat{A}^T \vec{\epsilon}_\sigma = \lambda_\sigma \vec{\epsilon}_\sigma, \quad \sigma = 1, 2. \tag{731}$$

Now, consider the solution to Eq.(725) defined as follows

$$\tilde{y}_i(t) = \vec{\epsilon}_i \cdot \vec{y}(t). \tag{732}$$

Then,

$$\tilde{y}_\sigma(t+T) = \vec{\epsilon}_\sigma \cdot \vec{y}(t+T) = \vec{\epsilon}_{\sigma,k}\, A_{ki}\, y_i(t) = A^T_{ik}\vec{\epsilon}_{\sigma,k}\, y_i(t) = \lambda_\sigma \tilde{y}_\sigma(t). \tag{733}$$

Therefore,

$$\tilde{y}_\sigma(t+nT) = \lambda_\sigma^n\, \tilde{y}_\sigma(t). \tag{734}$$

We can re-write this equation as follows

$$\tilde{y}_\sigma(t) = e^{t/T \ln \lambda_\sigma} f_\sigma(t), \tag{735}$$

where $f_\sigma(t)$ is a T-periodic function $f_\sigma(t+T) = f_\sigma(t)$. It follows from this representation that if $\ln \lambda_\sigma > 0$, the solution y_σ is *unstable* since it grows exponentially with time. If, on the other hand, $\ln \lambda_\sigma < 0$, the solution is said to be stable. Negative values of λ_σ lead to complex values of $\ln \lambda_\sigma$ which implies that the solutions oscillate.

Existence of stable and unstable solutions depends on parameters that appear in Eq.(725).[9] We will write this equation in the following way

$$y'' + (a^2 + 2\epsilon \cos t) y = 0, \tag{736}$$

where $a^2 = \omega^2/\gamma^2$ and $\epsilon = \kappa\omega^2/(2\gamma^2)$. We will consider ϵ to be small. Our goal will be to find regions in the (a, ϵ) plane that correspond to different (stable, unstable) types of solutions.

Let us look for the solutions to Eq.(736) using regular perturbation theory in ϵ. We write

$$y = \sum_{n=0}^{\infty} \epsilon^n y_n(t). \tag{737}$$

Substituting this expression into Eq.(736), we obtain

$$\begin{aligned} y_0'' + a^2 y_0 &= 0, \\ y_1'' + a^2 y_1 &= -2 y_0 \cos t, \\ y_2'' + a^2 y_2 &= -2 y_1 \cos t. \end{aligned} \tag{738}$$

The solution to the first equation in Eq.(738) reads

$$y_0 = A_0\, e^{iat} + \text{c.c.}\ . \tag{739}$$

[9] This equation is known as the Mathieu equation.

Note that since the problem is symmetric with respect to a transformation $a \to -a$, we can choose a to be positive.

The second equation in Eq.(738) can be written in the following way

$$y_1'' + a^2 y_1 = -A_0 \; e^{i(a+1)t} - A_0 \; e^{i(a-1)t} + \text{c.c.} \; . \tag{740}$$

It is clear that secular terms can appear in $y_1(t)$ if

$$a \pm 1 = -a. \tag{741}$$

The solution to these equations, subject to the condition $a > 0$ is $a = 1/2$; this means that secular (growing) terms in the solution of the Mathieu equation appear if $a^2 = 1/4$.

More instabilities can appear in higher orders in the expansion in ϵ. Indeed, suppose that $a \neq 1/2$ so that equation for $y_1(t)$ does not contain secular terms. According to Eq.(740), the solution to $y_1(t)$ contains harmonic functions with frequencies $a \pm 1$. Consider the equation for $y_2(t)$. The right hand side of the equation for $y_2(t)$ is proportional to $\cos t \; y_1(t)$; hence, it will contain harmonic functions with frequencies

$$a + 2, a, a - 2. \tag{742}$$

The case of a will require the standard treatment of secular terms; however, we also observe that secular solutions appear for

$$a \pm 2 = \mp a. \tag{743}$$

The solution to these equation that satisfies the $a > 0$ condition is

$$a = 1, \tag{744}$$

so that, obviously, $a^2 = 1$. After some reflection, it should be clear that if we continue to consider higher and higher orders in perturbation theory, we will find that secular terms appear at frequencies $n^2 a^2/4$, where $n = 1, 2, 3, \ldots$. However, if we assume $a \neq 2n$, no secular terms appear and solutions are stable.

What happens to the solutions in cases when the frequencies are close to one of the unstable points $a^2 = n^2/4$? To study this question, we take $n = 1$ and write $a^2 = 1/4 + \epsilon a_1$; the Matthieu equation reads

$$\frac{\mathrm{d}^2 y(t)}{\mathrm{d}t^2} + \left[\frac{1}{4} + \epsilon \left(a_1 + 2 \cos t \right) \right] y(t) = 0. \tag{745}$$

Since we expect that naive perturbation theory does not work, we use multi-scale expansion method. Similar to what we did in the previous lecture, we introduce a new time variable τ and we assume $\tau = \epsilon t$. We write

$$y(t) = Y_0(t,\tau) + \epsilon Y_1(t,\tau) + \dots \,. \tag{746}$$

From the previous lecture we recall

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} Y(t,\tau) = \frac{\partial^2 Y}{\partial t^2} + 2\epsilon \frac{\partial^2 Y}{\partial t \partial \tau} + \epsilon^2 \frac{\partial^2 Y}{\partial \tau^2}. \tag{747}$$

Hence, through order $\mathcal{O}(\epsilon)$, we have to satisfy two equations

$$\begin{aligned} &\frac{\partial^2 Y_0}{\partial t^2} + \frac{1}{4} Y_0 = 0, \\ &\frac{\partial^2 Y_1}{\partial t^2} + \frac{1}{4} Y_1 = -(a_1 + 2\cos t) Y_0 - 2\frac{\partial^2 Y_0}{\partial t \partial \tau}. \end{aligned} \tag{748}$$

We solve the first of the above equations and find

$$Y_0(t,\tau) = A_0(\tau) e^{it/2} + A_0^*(\tau) e^{-it/2}. \tag{749}$$

At order $\mathcal{O}(\epsilon)$, the equation becomes

$$\frac{\partial^2}{\partial t^2} Y_1 + \frac{1}{4} Y_1 = -(a_1 + 2\cos t) Y_0(t) - i \left(\frac{\partial A_0(\tau)}{\partial \tau} e^{it/2} - \frac{\partial A_0^*(\tau)}{\partial \tau} e^{-it/2} \right). \tag{750}$$

We now collect secular terms on the right hand side and obtain the following equation

$$-a_1 A_0 - i \frac{\partial A_0(\tau)}{\partial \tau} - A_0^* = 0. \tag{751}$$

To solve this equation, we separate real and imaginary parts

$$A_0 = A_0^R + i A_0^I. \tag{752}$$

Substituting this expression into Eq.(751) we find

$$\begin{aligned} \frac{\partial A_0^R(\tau)}{\partial \tau} &= (1 - a_1) A_0^I, \\ \frac{\partial A_0^I(\tau)}{\partial \tau} &= (1 + a_1) A_0^R. \end{aligned} \tag{753}$$

Combining the two equations, we find a second-order differential equation

$$\left[\frac{\partial^2}{\partial \tau^2} - (1 - a_1^2) \right] A_0^R(\tau) = 0. \tag{754}$$

It follows that if $|a_1| > 1$, the solution is oscillatory. It reads

$$A_0^R(\tau) = \alpha \cos \omega_1 \tau + \beta \sin \omega_1 \tau, \tag{755}$$

where $\omega_1 \sim \sqrt{a_1^2 - 1}$. If, on the other hand, $|a_1| < 1$, there are exponentially increasing and decreasing solutions

$$A_0^R(\tau) = \alpha e^{\pm\sqrt{1-a_1^2}\tau}. \tag{756}$$

The transition from stable to unstable solutions occurs at $|a_1| = 1$. This implies that stability bounds of the solutions are described by following equation.

$$a^2 = \frac{1}{4} \pm \epsilon + \mathcal{O}(\epsilon^2). \tag{757}$$

We will extend this analysis to *one higher order in the ϵ expansion* using multi-scale analysis. For this, we will assume that

$$a^2 = \frac{1}{4} + \epsilon + a_2\epsilon^2, \tag{758}$$

and study the consequences. Note that we should not try to connect what we do below to an earlier analysis since if we truncate a^2 in Eq.(758) at order $\mathcal{O}(\epsilon)$, we will be right on the line in the (a^2, ϵ)-plane that separates stable and unstable solutions and on that line the previous solution is secular. This means that if we are interested in finding solutions for such a value of a^2 we will have to discuss the relevant time scales one more time.

It is then easy to see that for $|a_1| \approx 1$, the relevant scale changes. Indeed, let us write Eq.(758) as $a^2 = 1/4 + \epsilon(1 + a_2\epsilon)$ and interpret $1 + a_2\epsilon$ as an "ϵ-dependent" a_1. We now substitute it into in Eq.(756) and find

$$\alpha e^{\pm\sqrt{1-a_1^2}\tau} \to \alpha e^{\pm\sqrt{-2a_2\epsilon}\epsilon t} \sim e^{\pm\sqrt{-2a_2}\epsilon^{3/2} t}. \tag{759}$$

This suggests that, in case when $a_1 \sim 1 + \mathcal{O}(\epsilon)$, the scale $\tau = \epsilon t$ disappears from the problem and the *new scale* $\sigma = \epsilon^{3/2} t$ appears.

We now repeat the analysis of the differential equation using a different scaling relation between regular time t and large time σ. The expansion of the solution of the differential equation in small parameter reads

$$y = Y_0(t, \sigma) + \epsilon^{1/2} Y_1(t, \sigma) + \epsilon Y_2(t, \sigma) + \epsilon^{3/2} Y_3(t, \sigma) + \epsilon^2 Y_4(t, \sigma) + \mathcal{O}(\epsilon^{5/2}). \tag{760}$$

The second time derivative evaluates to

$$\frac{d^2 y(t,\sigma)}{dt^2} = \frac{\partial^2 y}{\partial t^2} + 2\epsilon^{3/2}\frac{\partial^2 y}{\partial t \partial \sigma} + \epsilon^3 \frac{\partial^2 y}{\partial \sigma^2}. \tag{761}$$

Substituting Eq.(760) in Eq.(761), we obtain an expansion of the time derivative

$$\frac{d^2 Y}{dt^2} = \frac{\partial^2 Y_0}{\partial t^2} + \epsilon^{1/2}\frac{\partial^2 Y_1}{\partial t^2} + \epsilon\frac{\partial^2 Y_2}{\partial t^2} + \epsilon^{3/2}\left(\frac{\partial^2 Y_3}{\partial t^2} + 2\frac{\partial^2 Y_0}{\partial t \partial \sigma}\right) + \epsilon^2\left(\frac{\partial^2 Y_4}{\partial t^2} + 2\frac{\partial^2 Y_1}{\partial t \partial \sigma}\right) + \cdots . \tag{762}$$

We now substitute the time derivative from Eq.(762) and the expansions of $y(t)$ and a in powers of ϵ Eqs.(760,758), respectively, into the Mathieu equation Eq.(736). Since terms proportional to different powers of ϵ should vanish independently of it other, we obtain a system of coupled differential equations. It reads

$$\begin{aligned}
\epsilon^0 : &\quad \frac{\partial^2 Y_0}{\partial t^2} + \frac{1}{4}Y_0 = 0, \\
\epsilon^{1/2} : &\quad \frac{\partial^2 Y_1}{\partial t^2} + \frac{1}{4}Y_1 = 0, \\
\epsilon : &\quad \frac{\partial^2 Y_2}{\partial t^2} + \frac{1}{4}Y_2 = -(1+2\cos t)Y_0, \\
\epsilon^{3/2} : &\quad \frac{\partial^2 Y_3}{\partial t^2} + \frac{1}{4}Y_3 = -(1+2\cos t)Y_1 - 2\frac{\partial^2 Y_0}{\partial t \partial \sigma}, \\
\epsilon^2 : &\quad \frac{\partial^2 Y_4}{\partial t^2} + \frac{1}{4}Y_4 = -(1+2\cos t)Y_2 - 2\frac{\partial^2 Y_1}{\partial t \partial \sigma} - a_2 Y_0.
\end{aligned} \tag{763}$$

We now solve these equations one after the other, making sure that no secular terms appear in the solutions. We then find

$$Y_0 = A_0(\sigma)e^{it/2} + \text{c.c.}\,, \quad Y_1 = A_1(\sigma)e^{it/2} + \text{c.c.}\,. \tag{764}$$

With these results, the equation for Y_2 becomes

$$\frac{\partial^2 Y_2}{\partial t^2} + \frac{1}{4}Y_2 = -(A_0 + A_0^*)e^{it/2} - A_0 e^{i3t/2} + \text{c.c.}\,. \tag{765}$$

The secular term is removed from this equation if

$$A_0 + A_0^* = 0. \tag{766}$$

Hence, we choose $A_0 = iB_0$ with B_0 real, and find for Y_2

$$Y_2 = A_2(\sigma)e^{it/2} + \frac{1}{2}\,A_0(\sigma)e^{3it/2} + \text{c.c.}. \tag{767}$$

In Eq.(767) $A_2(\sigma)e^{it/2}$ is the solution of the homogeneous part of the equation Eq.(765).

We continue with the equation for Y_3. It reads

$$\frac{\partial^2 Y_3}{\partial t^2}+\frac{1}{4}Y_3=-(A_1+A_1^*+i\frac{\mathrm{d}A_0}{\mathrm{d}\sigma})e^{it/2}-A_1e^{i3t/2}+\text{c.c.}\,. \tag{768}$$

Secular terms are absent provided that

$$-i\frac{\mathrm{d}A_0}{\mathrm{d}\sigma}=A_1+A_1^*. \tag{769}$$

We continue with the equation for Y_4; it reads

$$\begin{aligned}\frac{\partial^2 Y_4}{\partial t^2}+\frac{Y_4}{4}&=-(A_2+A_2^*)e^{it/2}-\frac{A_0}{2}e^{i3t/2}-A_2e^{i3t/2}\\&-\frac{A_0}{2}e^{i5t/2}-\frac{A_0}{2}e^{it/2}-i\frac{\mathrm{d}A_1}{\mathrm{d}\sigma}e^{it/2}-a_1A_0e^{it/2}+\text{c.c.}.\end{aligned} \tag{770}$$

Collecting the secular terms, we obtain the following equation

$$-i\frac{\mathrm{d}A_1}{\mathrm{d}\sigma}=A_2+A_2^*+\left(\frac{1}{2}+a_2\right)A_0. \tag{771}$$

To proceed further, we apply complex conjugation to Eq.(771) and obtain

$$i\frac{\mathrm{d}A_1^*}{\mathrm{d}\sigma}=A_2+A_2^*-\left(\frac{1}{2}+a_2\right)A_0, \tag{772}$$

where we used the fact that $A_0^*=-A_0$. Subtracting Eq.(772) from Eq.(771), we find

$$-i\frac{\mathrm{d}(A_1+A_1^*)}{\mathrm{d}\sigma}=(1+2a_2)\,A_0. \tag{773}$$

We now use Eq.(769) to eliminate $A_1+A_1^*$ from the above equation and find

$$-\frac{\mathrm{d}^2A_0}{\mathrm{d}\sigma^2}=(1+2a_2)\,A_0. \tag{774}$$

Hence, if $a_2<-1/2$, the solutions are unstable; they are stable otherwise. We conclude that the curve in the (a^2,ϵ) plane that separates stable and unstable regions in the vicinity of $a^2=1/4$ is given by

$$a^2=\frac{1}{4}+\epsilon-\frac{1}{2}\epsilon^2+\mathcal{O}(\epsilon^3). \tag{775}$$

15 Inverted pendulum

In the very first lecture and in the previous lecture we talked about a pendulum whose pivot oscillates. We will again talk about this problem and analyze it from a somewhat different perspective, making use of what we have learned so far.

We will study a pendulum of length l with the mass m attached to its end point; the pendulum's pivot moves up and down with an amplitude $a \cos \gamma t$. We choose the angle θ to describe the position of the pendulum and construct the Lagrange function in the standard way. First, we write the coordinates of the mass as

$$x = l \sin\theta, \quad y = -l\cos\theta + a\cos\gamma t. \tag{776}$$

Then we compute derivatives

$$\dot{x} = l\dot{\theta}\ \cos\theta, \quad \dot{y} = l\dot{\theta}\sin\theta - a\gamma\sin\gamma t. \tag{777}$$

Substituting these expressions into the Lagrange function

$$L = \frac{m\dot{x}^2}{2} + \frac{m\dot{y}^2}{2} - mg(a\cos\gamma t - l\cos\theta), \tag{778}$$

and discarding θ-independent terms, we find

$$L = \frac{ml^2\dot{\theta}^2}{2} - mla\gamma\dot{\theta}\sin\theta\sin\gamma t + mgl\cos\theta. \tag{779}$$

It is convenient to rewrite the second term as

$$\begin{aligned} &- mla\gamma\dot{\theta}\sin\theta\sin\gamma t = mla\gamma\frac{\mathrm{d}\cos\theta}{\mathrm{d}t}\sin\gamma t \\ &= mla\gamma\frac{\mathrm{d}\cos\theta\sin\gamma t}{\mathrm{d}t} - mla\gamma^2\cos\theta\cos\gamma t. \end{aligned} \tag{780}$$

Since the first term in the last equation in Eq.(780) is a total derivative, it does not contribute to the equations of motion and can be omitted from the Lagrangian. Hence, the Lagrangian reads

$$L = \frac{ml^2\dot{\theta}^2}{2} - ma\gamma^2 l\cos(\gamma t)\ \cos\theta + mgl\ \cos\theta. \tag{781}$$

The Euler-Lagrange equation of motion then easily follows

$$ml^2\ddot{\theta} = ma\gamma^2 l\cos(\gamma t)\ \sin\theta - mgl\ \sin\theta. \tag{782}$$

We denote $g/l = \omega^2$ and find

$$\ddot{\theta} + \left(\omega^2 - \frac{a}{l}\gamma^2 \cos\gamma t\right)\sin\theta = 0. \tag{783}$$

Since we cannot solve Eq.(783) exactly, we will consider the following situation: the amplitude of oscillations a is small compared to the length of the pendulum l, i.e. $a/l \ll 1$, but the frequency of pivot oscillations is much higher than the natural frequency of the pendulum $\omega/\gamma \ll 1$. Note that under these conditions, it is not possible to neglect any of the terms in Eq.(783).

To proceed further, we change variables $t \to x/\gamma$ and find

$$\gamma^2 \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} + \left(\omega^2 - \frac{a}{l}\gamma^2 \cos x\right)\sin\theta = 0 \;\Rightarrow\; \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} + \left(\frac{\omega^2}{\gamma^2} - \frac{a}{l}\cos x\right)\sin\theta = 0. \tag{784}$$

It follows from the above equation that we need to decide on the hierarchy of two small parameters ω/γ and a/l. We will assume that they satisfy the following relation

$$\frac{a}{l} \sim \frac{\omega}{\gamma} \sim \epsilon \ll 1. \tag{785}$$

Then, writing $\omega^2/\gamma^2 = \epsilon^2\kappa^2$ and $a/l = \alpha\epsilon$, we obtain an equation that we will work with

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} + \left(\epsilon^2\kappa^2 - \epsilon\alpha\cos x\right)\sin\theta = 0. \tag{786}$$

To get an idea of how to approach solving this equation, let us consider the case of small oscillations. Then $\sin\theta \sim \theta$. We then imagine that the pendulum oscillates with its natural frequency ω and, at the same time, trembles around its smooth trajectory with the frequency γ. The solution then may look as follows

$$\theta \sim (1 + \beta\cos\gamma t)\cos\omega t. \tag{787}$$

Hence, we expect that the solution depends on the two time scales $\gamma t = x$ and $\omega t = \tau$. The relation between τ and x is

$$\tau = \frac{\omega}{\gamma}x = \epsilon\kappa x. \tag{788}$$

Following the discussion of multi-scale problems in preceding lectures, we assume that $\theta = \theta(x,\tau)$ and write

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = \frac{\partial^2\theta}{\partial x^2} + 2\epsilon\kappa\frac{\partial^2\theta}{\partial x\partial\tau} + \epsilon^2\kappa^2\frac{\partial^2\theta}{\partial\tau^2}. \tag{789}$$

We also write $\theta(x,\tau)$ as a series in ϵ

$$\theta(x,\tau) = \sum_{n=0}^{\infty} \epsilon^n \theta_n(x,\tau). \tag{790}$$

We now replace $\sin\theta$ with θ in Eq.(786), make use of Eqs.(789,790) there and collect powers of ϵ. We then obtain an infinite set of differential equations that the functions θ_n should satisfy. Through order $\mathcal{O}(\epsilon^2)$ these equations read

$$\begin{aligned}
&\frac{\partial^2\theta_0}{\partial x^2} = 0,\\
&\frac{\partial^2\theta_1}{\partial x^2} + 2\kappa\frac{\partial^2\theta_0}{\partial x\partial\tau} - \alpha\cos x\theta_0 = 0,\\
&\frac{\partial^2\theta_2}{\partial x^2} + 2\kappa\frac{\partial^2\theta_1}{\partial x\partial\tau} + \kappa^2\frac{\partial^2\theta_0}{\partial\tau^2} + \kappa^2\theta_0 - \alpha\cos x\theta_1 = 0.
\end{aligned} \tag{791}$$

We solve these equations one by one. The solution of the first equation in Eq.(791) is

$$\theta_0 = A_{10}(\tau)x + A_0(\tau). \tag{792}$$

Since exact solutions of the original differential equation should be periodic in x, we set $A_{10}(\tau) = 0$ so that

$$\theta_0 = A_0(\tau). \tag{793}$$

The second equation in Eq.(791) becomes

$$\frac{\partial^2\theta_1}{\partial x^2} - \alpha\cos xA_0(\tau) = 0. \tag{794}$$

The solution that is periodic in x reads

$$\theta_1 = -\alpha\cos xA_0(\tau) + A_1(\tau). \tag{795}$$

The last equation in Eq.(791) becomes

$$\begin{aligned}
&\frac{\partial^2\theta_2}{\partial x^2} + 2\alpha\kappa\sin x\frac{\partial A_0}{\partial\tau} + \kappa^2\,\frac{\partial^2 A_0(\tau)}{\partial\tau^2}\\
&+\kappa^2 A_0 + \alpha^2\cos^2 xA_0(\tau) - \alpha\cos xA_1(\tau) = 0.
\end{aligned} \tag{796}$$

We write $\cos^2 x = (1+\cos(2x))/2$ and obtain

$$\begin{aligned}
&\frac{\partial^2\theta_2}{\partial x^2} + 2\alpha\kappa\sin x\frac{\partial A_0}{\partial\tau} + \frac{\alpha^2\cos 2x}{2}A_0(\tau) - \alpha\cos xA_1(\tau)\\
&+\kappa^2\frac{\partial^2 A_0(\tau)}{\partial\tau^2} + \left(\kappa^2 + \frac{\alpha^2}{2}\right)A_0 = 0.
\end{aligned} \tag{797}$$

The part of the equation that is independent of $\cos(nx)$ and $\sin(nx)$, where n is a non-vanishing integer, has to vanish since, otherwise, θ_2 will contain terms that grow with x quadratically. This implies that the function $A_0(\tau)$ must satisfy the following equation

$$\kappa^2 \frac{\partial^2 A_0(\tau)}{\partial \tau^2} + \left(\kappa^2 + \frac{\alpha^2}{2}\right) A_0 = 0. \tag{798}$$

Solving it, we obtain

$$A_0(\tau) = a_0 \cos(\nu\tau + \phi) \tag{799}$$

where ϕ is a constant phase and

$$\nu^2 = 1 + \frac{\alpha^2}{2\kappa^2} = 1 + \frac{a^2\gamma^2}{2l^2\omega^2}, \tag{800}$$

Using $\tau = \omega t$, we find

$$A_0 = a_0 \cos(\Omega t + \phi), \tag{801}$$

where

$$\Omega^2 = \omega^2 + \frac{a^2\gamma^2}{2l^2}. \tag{802}$$

Hence, combining solutions for θ_0 and θ_1, we obtain

$$\theta \approx \left(1 - \frac{a}{l}\cos\gamma t\right)\cos(\Omega t + \phi) + \epsilon A_1(\tau). \tag{803}$$

The function $A_1(\tau)$ remains undetermined (we need to expand the original equation to $\mathcal{O}(\epsilon^3)$ to find it). However, even without A_1 we see that the dependence of θ on the time t and the shifted frequency of oscillations Ω agrees with what we have derived in the first lecture using somewhat different considerations.

We will now generalize the calculation described above in that we will *not make the assumption that the angle θ is small*. All other assumptions about how small or large various parameters are, as well as Eq.(790), remain valid. The change, however, occurs at the level of differential equations that we need to solve, Eq.(791), since the substitution $\sin\theta \to \theta$ is not valid anymore. We find

$$\begin{aligned}
&\frac{\partial^2\theta_0}{\partial x^2} = 0, \\
&\frac{\partial^2\theta_1}{\partial x^2} + 2\kappa\frac{\partial^2\theta_0}{\partial x\partial\tau} - \alpha\cos x\sin(\theta_0) = 0, \\
&\frac{\partial^2\theta_2}{\partial x^2} + 2\kappa\frac{\partial^2\theta_1}{\partial x\partial\tau} + \kappa^2\frac{\partial^2\theta_0}{\partial\tau^2} + \kappa^2\sin(\theta_0) - \alpha\cos x\cos(\theta_0)\theta_1 = 0.
\end{aligned} \tag{804}$$

We construct solutions to Eq.(804) following the discussion of the small-angle case. This gives

$$\begin{aligned}\theta_0(x,\tau) &= A_0(\tau),\\ \theta_1(x,\tau) &= -\alpha\cos x\ \sin(A_0(\tau)) + A_1(\tau).\end{aligned} \tag{805}$$

Similar to the small-angle case, we use the above solutions in the last equation in Eq.(804) and determine that θ_2 does not grow as $\mathcal{O}(x^2)$ provided that the following condition is fulfilled

$$\kappa^2\frac{\partial^2 A_0}{\partial\tau^2} + \kappa^2\sin A_0 + \frac{\alpha^2}{2}\cos A_0\sin A_0 = 0. \tag{806}$$

Eq.(806) defines the leading order (i.e. $\theta_0(x,\tau) = A_0(\tau)$) trajectory of slow (i.e. x-independent) oscillations. If we interpret Eq.(806) as a typical Euler-Lagrange equation, write $A_0 = \theta$ and replace τ with ωt, Eq.(806) becomes

$$\frac{\partial^2\theta}{\partial t^2} = f(\theta), \tag{807}$$

where

$$f(\theta) = -\omega^2\sin(\theta) - \frac{\alpha^2\omega^2}{2\kappa^2}\cos(\theta)\sin(\theta) \tag{808}$$

is the "effective" force that acts on a pendulum. Since

$$f(\theta) = -\frac{\partial U}{\partial\theta}, \tag{809}$$

where $U(\theta)$ is an "effective" potential energy for slow oscillations. We can compute the potential energy by integrating $f(\theta)$. We find

$$U(\theta) = -\omega^2\cos(\theta) - \frac{\alpha^2\omega^2}{8\kappa^2}\cos(2\theta). \tag{810}$$

Note that this "effective" potential energy contains a term that is just the usual potential energy of the pendulum in the gravitational field and the other term that describes an average effect of fast oscillations on slow oscillations. It is important that fast oscillations do not explicitly appear in the expression for the potential energy; one usually says that they have been "integrated out". These concepts of "effective interactions" and degrees of freedom "integrated out" are very popular in theoretical physics under the name of "effective field theories". This example is a simple mechanical analogy of techniques widely used in theoretical particle physics and quantum field theory.

Since we have the potential energy, we can study different types of motion of a pendulum without explicitly solving equations of motion. For example, we can investigate the various minima of the potential $U(\theta)$. Consider, e.g. $\theta = 0$. We use $\cos\theta \approx 1 - \theta^2/2$ and write

$$U(\theta) - U(0) \approx \left(\omega^2 + \frac{\alpha^2\omega^2}{2\kappa^2}\right)\frac{\theta^2}{2}. \tag{811}$$

Hence, $\theta = 0$ is the minimum of the potential for all values of parameters.

Another interesting point is $\theta = \pi$. We write $\theta = \pi - f$, assume $|f| \ll 1$ and expand the trigonometric functions

$$\begin{aligned} \cos\theta &= \cos(\pi - f) = -1 + \frac{f^2}{2}, \\ \cos 2\theta &= \cos(2\pi - 2f) = \cos(2f) = 1 - 4\frac{f^2}{2}. \end{aligned} \tag{812}$$

Hence, we find

$$U(\pi - f) - U(\pi) \approx \left(-\omega^2 + \frac{\alpha^2\omega^2}{2\kappa^2}\right)\frac{f^2}{2}. \tag{813}$$

If the coefficient of $f^2/2$ on the r.h.s. of the above equation is positive, the point $\theta = \pi$ is a point of a stable equilibrium; if the coefficient is negative, it is an unstable equilibrium point. The condition for the point $\theta = \pi$ to become a point of stable equilibrium is

$$\frac{\alpha^2\omega^2}{2\kappa^2} > \omega^2 \quad \Rightarrow \quad \frac{a^2}{l^2}\gamma^2 > \omega^2. \tag{814}$$

If this condition is satisfied, the pendulum can turn upside down and stay like that for an infinitely long time.

16 Anharmonic oscillator

In this lecture, we will discuss an anharmonic oscillator (recall that we briefly talked about it in the first lecture). An anharmonic oscillator is described by the following Hamiltonian

$$H = \frac{p^2}{2} + V(x) = \frac{p^2}{2} + \frac{\omega^2 x^2}{2} + \lambda x^4 = H_0 + \lambda x^4. \tag{815}$$

In Eq.(815), H_0 is the Hamiltonian function of the *harmonic* oscillator $H_0 = p^2/2 + \omega^2 x^2/2$. Since $\lim_{|x|\to\infty} V(x) = \infty$, the anharmonic oscillator possesses discrete energy levels; the continuous energy spectrum is absent.

We would like to compute the energy of the ground state of the anharmonic oscillator. We can do so by solving the Schrödinger equation

$$H\psi = E\psi, \tag{816}$$

with the boundary condition $\lim_{|x|\to\infty} \psi(x) \to 0$ and taking the lowest energy solution.

It should not come as a big surprise that Eq.(816) cannot be solved analytically for any $\lambda \neq 0$. We can try to make headway by solving Eq.(816) in perturbation theory, treating λ as a small parameter. We learn how to do this in Quantum Mechanics classes. The solution involves using eigenfunctions of the harmonic oscillator Hamiltonian H_0 and computing corrections to its ground state energy.

To this end, we write

$$E(\lambda) = E_0^{(0)} + \sum_n \lambda^n E_n, \tag{817}$$

where $E_0^{(0)} = \omega/2$. The first and second corrections to the ground state energy $E_{1,2}$ read

$$E_1 \sim \langle 0|x^4|0\rangle, \tag{818}$$

and

$$E_2 \sim \sum_{k\neq 0}^{\infty} \frac{\langle 0|x^4|k\rangle\langle k|x^4|0\rangle}{E_0^{(0)} - E_k^{(0)}}, \tag{819}$$

where $E_k^{(0)}$ are energy eigenvalues of the Hamiltonian H_0.

It is clear that computing corrections E_n to the ground state energy in Eq.(817) within this framework is very difficult. Fortunately, there is an alternative (better) way to do that, as we now explain. To this end, consider the Schrödinger equation that describes the anharmonic oscillator

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\omega^2 x^2}{2} + \lambda x^4\right]\psi(x) = E\psi(x). \tag{820}$$

We can simplify the equation by writing $x = \xi/\sqrt{\omega}$. The above equation becomes

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \frac{\xi^2}{2} + \left(\frac{\lambda}{\omega^3}\right)\xi^4\right]\psi(x) = \frac{E}{\omega}\psi(x). \tag{821}$$

It follows that we can write an expansion of the ground state energy in powers of λ isolating all dimensionfull quantities. We obtain

$$E = \omega \sum_{n=0}^{\infty} \left(\frac{\lambda}{\omega^3}\right)^n A_n. \tag{822}$$

The expansion coefficients A_n in Eq.(822) are just numbers.

We will solve Eq.(821) to determine the coefficients A_n; for ease of notation, we will re-write Eq.(821) using $\xi \to x$, $E/\omega \to E$, $\lambda/\omega^3 \to \lambda$. It becomes the old Schrödinger equation again

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{x^2}{2} + \lambda x^4\right]\psi(x) = E\psi(x). \tag{823}$$

To establish an efficient way to solve Eq.(823), we expand the wave function $\psi(x)$ in powers of λ

$$\psi(x) = \sum_{n=0}^{\infty} \lambda^n e^{-x^2/2} B_n(x). \tag{824}$$

In Eq.(824), we have factored out the ground-state wave function of a harmonic oscillator $e^{-x^2/2}$. The functions $B_n(x)$ are polynomials since the function $\psi(x)$ should be normalizable and vanish at $|x| \to \infty$.

To use the expansion Eq.(824) in Eq.(823), we need to compute $\mathrm{d}^2\psi/\mathrm{d}x^2$. It reads

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \sum_{n=0}^{\infty} \lambda^n e^{-x^2/2}\left[x^2 B_n(x) - 2x\frac{\mathrm{d}B_n(x)}{\mathrm{d}x} - B_n(x) + \frac{\mathrm{d}^2 B_n(x)}{\mathrm{d}x^2}\right]. \tag{825}$$

We substitute Eq.(825) into Eq.(823), collect the relevant terms and obtain a differential equation for $B_n(x)$

$$-\frac{1}{2}\frac{\mathrm{d}^2 B_n(x)}{\mathrm{d}x^2} + x\frac{\mathrm{d}B_n(x)}{\mathrm{d}x} + x^4 B_{n-1}(x) = \sum_{m=0}^{n-1} A_{n-m} B_m(x). \tag{826}$$

In deriving Eq.(826), we used the fact that $A_0 = 1/2$, the ground state energy of the harmonic oscillator.

It is easy to see that we can choose $B_0(x) = 1$. This choice is consistent with the fact that $\psi \sim e^{-x^2/2}$ is the wave function of the ground state of the *harmonic* oscillator.

Consider the $n = 1$ case. The differential equation becomes

$$-\frac{1}{2}\frac{\mathrm{d}^2 B_1(x)}{\mathrm{d}x^2} + x\frac{\mathrm{d}B_1(x)}{\mathrm{d}x} + x^4 B_0(x) = A_1 B_0(x). \tag{827}$$

It is easy to see that $B_1(x)$ is a polynomial in x^2 of degree four. We write

$$B_1(x) = B_{1,2}(x^2)^2 + B_{1,1}(x^2). \tag{828}$$

Substituting this ansatz into Eq.(827), we find

$$(4B_{1,2} + 1)x^4 + (-6B_{1,2} + 2B_{1,1})x^2 - B_{1,1} - A_1 = 0. \tag{829}$$

This immediately implies

$$B_{1,2} = -\frac{1}{4}, \quad B_{1,1} = -\frac{3}{4}, \quad A_1 = \frac{3}{4}. \tag{830}$$

Hence, we have found the $B_1(x)$ polynomial

$$B_1(x) = -\frac{1}{4}x^4 - \frac{3}{4}x^2, \tag{831}$$

and the first correction to the energy of the ground state $A_1 = 3/4$.

Consider the $n = 2$ case. The equation reads

$$-\frac{1}{2}\frac{\mathrm{d}^2 B_2(x)}{\mathrm{d}x^2} + x\frac{\mathrm{d}B_2(x)}{\mathrm{d}x} + \lambda x^4 B_1(x) = A_2 B_0(x) + A_1 B_1(x). \tag{832}$$

The highest power of x among known terms comes from the term $x^4 B_1(x) \sim x^8$. It is also clear that $B_2(x)$ is a polynomial in x^2. Hence, we make the following ansatz

$$B_2(x) = B_{2,4}(x^2)^4 + B_{2,3}(x^2)^3 + B_{2,2}(x^2)^2 + B_{2,1}x^2. \tag{833}$$

Using this expression in Eq.(832) and collecting terms with identical powers of x, we find

$$B_{2,4} = \frac{1}{32}, \quad B_{2,3} = \frac{13}{48}, \quad B_{2,2} = \frac{31}{32}, \quad B_{21} = \frac{21}{8}. \tag{834}$$

Also,

$$A_2 = -B_{2,1} = -\frac{21}{8}. \tag{835}$$

It becomes clear how to generalize these computations to obtain coefficients A_n for arbitrary n. Indeed, for any n, $B_n(x)$ is a polynomial in x^2 of degree $2n$. We write

$$B_n(x) = \sum_{i=1}^{2n} B_{n,i} (x^2)^i. \tag{836}$$

Substituting this expression into Eq.(826), we find the following results

$$\begin{aligned} &2iB_{n,i} = (i+1)(2i+1)B_{n,i+1} - B_{n-1,i-2} + \sum_{m=1}^{n-1} A_{n-m} B_{m,i}, \\ &A_n = -B_{n,1}. \end{aligned} \tag{837}$$

The above equations can be used to *recursively* find polynomials $B_n(x)$ and in this way compute large number of corrections to the ground state energy level A_n. The whole procedure is infinitely easier and faster as compared to conventional perturbative computations. One finds

$$\begin{aligned} &A_1 = \frac{3}{4}, \quad A_2 = -\frac{21}{8}, \quad A_3 = \frac{333}{16}, \quad A_4 = -\frac{30\ 885}{128}, \\ &A_5 = \frac{916\ 731}{256}, \quad A_6 = -\frac{65\ 518\ 401}{1\ 024}, \quad \dots \quad A_9 = \frac{54\ 626\ 982\ 511\ 455}{65\ 536}. \end{aligned} \tag{838}$$

As we already mentioned in the first lecture, the coefficients A_n of the perturbative expansion of the ground state energy of an anharmonic oscillator in λ exhibit a very strong growth. By fitting the coefficients A_n, one finds

$$\lim_{n\to\infty} A_n \sim (-1)^n 3^n \Gamma(n+1/2) \frac{\sqrt{6}}{\pi^{3/2}}. \tag{839}$$

Although there exist important power corrections ($1/n$ etc.) to A_n, we will assume that Eq.(839) is valid for all values of n. Then, the energy of the ground state reads

$$E(\lambda) = \sum_{n=0}^{\infty} A_n \lambda^n = \frac{\sqrt{6}}{\pi^{3/2}} \sum_{n=0}^{\infty} \Gamma\left(n+\frac{1}{2}\right) (-3\lambda)^n. \tag{840}$$

We note that since $\Gamma(n+1/2) > (n-1)!$, the radius of convergence of the series in Eq.(840) is *zero*; the series is asymptotic. To make sense out of

Eq.(840), we need to make use of what we learned about the summation of divergent series. One of the ways to sum the divergent series was the Borel method which boils down to the following steps. We write

$$\Gamma(n+1/2) = \int_0^\infty \mathrm{d}t \; t^{n-1/2} e^{-t}, \tag{841}$$

and use this expression in series Eq.(840). We change the order of integration and summation. We find

$$E(\lambda) = \frac{\sqrt{6}}{\pi^{3/2}} \int_0^\infty \mathrm{d}t \; t^{-1/2} e^{-t} \sum_{n=0}^\infty (-3t\lambda)^n = \frac{\sqrt{6}}{\pi^{3/2}} \int_0^\infty \frac{\mathrm{d}t \; e^{-t}}{t^{1/2}(1+3t\lambda)}. \tag{842}$$

To proceed further, it is convenient to change variables $t = \xi^2$. We obtain

$$E(\lambda) = \frac{2\sqrt{6}}{\pi^{3/2}} \int_0^\infty \frac{\mathrm{d}\xi \; e^{-\xi^2}}{(1+3\lambda\xi^2)}. \tag{843}$$

The above result gives us a function $E(\lambda)$ whose asymptotic expansion coincides with the asymptotic expansion of the ground state of an anharmonic oscillator at small values of λ. We will interpret this function as the ground state energy of the anharmonic oscillator.

We can express $E(\lambda)$ in Eq.(843) through special functions. To this end, we change variables $\xi = x/\sqrt{3\lambda}$ and obtain

$$E(\lambda) = \frac{2^{3/2}}{\pi^{3/2}\sqrt{\lambda}} \int_0^\infty \frac{\mathrm{d}x \; e^{-x^2/(3\lambda)}}{(1+x^2)} = \frac{2^{3/2}}{\pi^{3/2}\sqrt{\lambda}} G\left(\frac{1}{3\lambda}\right), \tag{844}$$

where the function $G(\eta)$ reads

$$G(\eta) = \int_0^\infty \frac{\mathrm{d}x \; e^{-\eta x^2}}{(1+x^2)}. \tag{845}$$

To compute $G(\eta)$, it is convenient to derive a differential equation that this function satisfies. To this end, consider the derivative of $G(\eta)$ w.r.t. η. We find

$$-\frac{\mathrm{d}G(\eta)}{\mathrm{d}\eta} = \int_0^\infty \frac{\mathrm{d}x \; x^2 e^{-\eta x^2}}{(1+x^2)} = -G(\eta) + \frac{\sqrt{\pi}}{2\eta^{1/2}}. \tag{846}$$

It is straightforward to solve this differential equation. One finds

$$G(\eta) = e^{\eta}\left[C - \frac{\sqrt{\pi}}{2}\int\limits_0^{\eta}\frac{d\xi}{\xi^{1/2}}e^{-\xi}\right], \tag{847}$$

where C is the integration constant. To find it, we note that Eq.(845) implies that $G(0) = \pi/2$. It follows from Eq.(847) that $C = \pi/2$ leading to

$$G(\eta) = e^{\eta}\frac{\pi}{2}\left[1 - \frac{1}{\sqrt{\pi}}\int\limits_0^{\eta}\frac{d\xi}{\xi^{1/2}}e^{-\xi}\right] = e^{\eta}\frac{\pi}{2}\left[1 - \frac{2}{\sqrt{\pi}}\int\limits_0^{\sqrt{\eta}}dt e^{-t^2}\right] = \frac{\pi e^{\eta}}{2}\mathrm{Erfc}\left(\sqrt{\eta}\right), \tag{848}$$

In Eq.(848), Erfc(x) is the so-called *complementary error function*. Hence, the ground state energy of an anharmonic oscillator evaluates to[10]

$$E(\lambda) = \frac{2^{3/2}}{\pi^{3/2}\sqrt{\lambda}}G\left(\frac{1}{3\lambda}\right) = \sqrt{\frac{2}{\pi\lambda}}\, e^{1/(3\lambda)}\mathrm{Erfc}\left(\frac{1}{\sqrt{3\lambda}}\right). \tag{849}$$

We can use the above formula to determine the ground state energy at large values of λ. In that case, $\mathrm{Erfc}(1/\sqrt{3\lambda}) \to 0$ and $e^{1/(3\lambda)} \to 1$. Hence, we find

$$E(\lambda)|_{\lambda\gg 1} \sim \sqrt{\frac{2}{\pi\lambda}}. \tag{850}$$

Thus, the perturbative expansion supplemented with a way to re-sum the asymptotic series allows us to determine the bound state energy for *large* values of the coupling constant λ that is clearly beyond the realm of applications of conventional perturbation theory.

We now go back to Eq.(843) where $E(\lambda)$ is written as a one-dimensional integral. It is easy to see from that formula that for *negative* values of λ, the integrand has a pole at $x = x^* = 1/\sqrt{3|\lambda|}$. To understand what the position of the pole tells us, we need to regularize the singularity. To this end, we add an infinitesimal imaginary part to the constant λ and write $\lambda = -|\lambda| \pm i\epsilon$. Then

$$E(\lambda) = \frac{2\sqrt{6}}{\pi^{3/2}}\int\limits_0^{\infty}\frac{dx\; e^{-x^2}}{1 - 3x^2|\lambda| \pm i\epsilon} \tag{851}$$

Using

$$\frac{1}{x - a \pm i\epsilon} = \mathcal{P}\left[\frac{1}{x-a}\right] \mp i\pi\delta(x-a), \tag{852}$$

[10] In the approximation that large-n asymptotic formulas for A_n's are used as if they were exact.

we see that for negative values of λ, $E(\lambda)$ develops an imaginary part that evaluates to

$$\mathrm{Im}\,[E(\lambda \pm i\epsilon)] = \mp \frac{2\sqrt{6}}{\pi^{1/2}}\theta(-\lambda) \int\limits_0^\infty \mathrm{d}x\; e^{-x^2}\delta(1-3x^2|\lambda|) = \mp\theta(-\lambda)\frac{\sqrt{6}}{\pi^{1/2}}\frac{1}{\sqrt{3|\lambda|}}e^{-1/(3|\lambda|)}. \tag{853}$$

How can we understand the fact that the energy of the ground state develops an imaginary part? In general, if a quantum state has a complex energy, e.g. $E - i\Gamma/2$, it is metastable. To see this we write the wave function

$$\psi(t) \sim e^{-i(E-i\Gamma/2)t} \sim e^{-iEt-\Gamma/2t}, \tag{854}$$

and compute the probability that a physical system is in a state $|\psi\rangle$

$$|\psi(t)|^2 \sim e^{-\Gamma t}. \tag{855}$$

The time-dependence of the probability to find a quantum system in a particular state indicates that Γ is indeed the life-time of the quantum state.

The anharmonic oscillator has the following potential energy

$$V(x) = \frac{x^2}{2} + \lambda x^4, \tag{856}$$

which, for negative values of λ, becomes unbounded from below

$$V(x) = \frac{x^2}{2} - |\lambda| x^4. \tag{857}$$

Because of that, the ground state becomes metastable. We can compute its lifetime in the *quasi-classical* approximation. The lifetime is proportional to the probability to tunnel through a barrier. The corresponding formula is

$$\Gamma \sim e^{-2\int\limits_a^b \mathrm{d}x \bar{p}(x)}, \tag{858}$$

where $\bar{p}(x) = \sqrt{|2(E - V(x))|}$ and the interval $x \in [a, b]$ is forbidden classically. In our case $E = 0$ since we are in the ground state. Then

$$\int\limits_a^b \mathrm{d}x \bar{p}(x) = \int\limits_a^b \mathrm{d}x \sqrt{x^2(1-2|\lambda|x^2)} = \sqrt{2|\lambda|}\int\limits_0^{x_*} \mathrm{d}x\sqrt{x^2(x_*^2 - x^2)} = \sqrt{2|\lambda|}x_*^3 \int\limits_0^1 \mathrm{d}\xi \xi\sqrt{1-\xi^2}, \tag{859}$$

where $x_* = \sqrt{1/(2|\lambda|)}$. Since

$$\int_0^1 \mathrm{d}\xi\, \xi\, \sqrt{1-\xi^2} = \frac{1}{3}, \tag{860}$$

we find

$$\int_a^b \mathrm{d}x \bar{p}(x) = \frac{1}{3}\sqrt{2|\lambda|}x_*^3 = \frac{1}{6|\lambda|}, \tag{861}$$

so that

$$\Gamma \sim e^{-2\int_a^b \mathrm{d}x \bar{p}(x)} = e^{-1/(3\lambda)}. \tag{862}$$

We see that up to a pre-factor, the decay width of the vacuum Γ indeed matches the result in Eq.(853). We will not discuss the calculation of the pre-factor of the decay width Γ in the semi-classical approximation but merely state that it matches that in Eq.(853).

We are now in a position to understand the deep connection between the *instability* of the ground state of the anharmonic oscillator at *negative* values of λ and the *factorial growth* of the coefficients of the perturbative expansion of the ground state energy for *positive* values of λ. The key idea is to write a *dispersion relation* for the vacuum energy $E(\lambda)$ with respect to the coupling constant

$$E(\lambda) = \frac{1}{\pi}\int_{-\infty}^{0} \frac{\mathrm{d}\lambda' \, \mathrm{Im}E(\lambda')}{\lambda' - \lambda - i0}. \tag{863}$$

The dispersion relation follows from the assumption that $E(\lambda)$ is an analytic function in the *complex* λ-plane with a cut along negative real axis. Cauchy theorem and deformation of the contour leads to Eq.(863).

As we discussed, the imaginary part of $E(\lambda)$ can be computed in the quasi-classical approximation. The result is given in Eq.(853).[11] We use it to rewrite Eq.(863)

$$E(\lambda) = -\frac{\sqrt{6}}{\pi^{3/2}}\int_{-\infty}^{0} \frac{\mathrm{d}\lambda'}{\lambda' - \lambda - i0}\, \frac{1}{\sqrt{3|\lambda'|}} e^{-1/(3|\lambda'|)}. \tag{864}$$

It is now easy to see that if we change integration variable according to the following formula

$$\lambda' = -\frac{1}{3x^2}, \tag{865}$$

[11] We need to take the expression with the minus sign to be consistent with $E \to E - i\Gamma/2$ and $\Gamma > 0$.

we obtain the result for $E(\lambda)$ shown in Eq.(843). A naive expansion of this equation in powers of λ leads to an asymptotic series for $E(\lambda)$ with coefficients that exhibit factorial growth; this is what we observe when doing conventional perturbation theory.

Hence, we conclude that the factorial growth of the coefficients of the perturbative expansion of the ground state energy of an anharmonic oscillator in powers of λ is directly connected to the instability of the ground state energy at negative values of λ. The connection arises through a dispersion relation for $E(\lambda)$ in λ. The ground state energy $E(\lambda)$ develops an imaginary part for negative values of λ that can be predicted using quasi-classical methods.