DIPLOMARBEIT

Phase Transition of a Scalar Field Theory in the Early Universe

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Abstract

Measurements of the cosmic microwave background radiation show a primary inhomogeneity in the temperature distribution of the order of $\delta T/T \sim 10^{-5}$. The inflationary theory explains this inhomogeneity to be primeval quantum fluctuations expanded to galactic scales. Inflation is driven by the phase transition of a scalar field. In this work we analyze the non-equilibrium evolution of the effective scalar field mass through a phase transition in an expanding space-time background starting from an initial thermal equilibrium. The real-time formalism for a curved background metric is used to express the propagator in terms of mode functions. The one-loop mass correction is calculated from the Green function. A WKB-like approximation is applied to the resulting system of differential equations and an analytical expression for the scalar field mass is found in the high-temperature limit. Comparing this result to numerical calculations, we find that the analytical expression describes the scalar field mass pretty accurately far beyond the first classical turning point of the lowest mode function.

"And can *all* the flowers talk?"

"As well as *you* can," said the Tiger-lily. "And a great deal louder."

"It isn't manners for us to begin, you know," said the Rose,

"and I really was wondering when you'd speak!"

from Lewis Carroll, "Through the Looking-Glass"
(Alice in Wonderland II)

Contents

1 Introduction

Imagine that somebody grips you and blows you up to 10^{42} times your size within 10^{-32} seconds. Independently of how you looked like before, you would not only become really fat, but theory of inflation predicts that you would also appear to be locally flat. As incredible as it may sound, the very same thing happened to our universe right after the big bang according to the inflationary universe scenario that is being supported by more and more recent observational facts.

The COBE (Cosmic Background Explorer) satellite measured the temperature of the cosmic microwave background radiation (CMBR) to be 2.7277 ± 0.002K with a deviation from a perfect black-body radiation of less than 0.03% [1, 2]. Apart from a dipolar anisotropy of about 3mK that accounts for a relative velocity of our solar system of 370 km/s with respect to the cosmic rest frame, COBE found a primordial anisotropy in the CMBR at the level of 30μK (or $\delta T/T \simeq 10^{-5}$) on angular scales of $10°$. The photons of the CMBR last scattered when the universe was about 300,000 years old and had cooled down to a temperature of about 3000K [3]. Therefore the CMBR is a snapshot of the universe at that time.

From these data we can draw two essential conclusions: First, we have evidence that the universe was extremely smooth when the CMBR originated, since density variations imply proportional temperature variations. Second, the inhomogeneities in the CMBR of $\delta\rho/\rho \simeq 10^{-5}$ are of the right magnitude to explain the structures that we observe today, like stars, galaxies, or clusters, by gravitational action mainly of dark matter over the past 14 billion years. Dark matter is invisible matter of presently unknown nature whose presence is only known through its gravitational effects. Structure formation is in perfect accordance with the standard big bang cosmology, but new questions about why the universe was that flat in the beginning and where the small primeval inhomogeneity came from are raised. Several ideas were proposed to overcome problems about the initial state of the universe, from special initial singularities [4] to a quantum cosmological wavefunction of the universe [5] to the anthropic principle, but the inflationary solution appears to be the most promising.

The inflationary universe scenario states that our universe was inflated exponentially fast during the first 10^{-32} seconds after the big bang. The possibility of such an exponential expansion was found in the General Theory of Relativity by de Sitter [6] already in 1917, but it was not until the 1980's that Guth [7] described the basic principles of inflation: A small region of the universe is expanded exponentially to a size much bigger than the universe we can observe today. This explains the smoothness of the universe because everything stems from a tiny part of the original region. Inhomogeneities are explained by quantum fluctuations that are frozen in later as the universe continues to expand. Also, due to the increase in size, any curvature of the initial region would become small and the universe would appear to be flat. The original model was soon enhanced by other models like new inflation, chaotic inflation, hybrid inflation [8]. These models require the knowledge of elementary particle theory at very high energies.

Early stages of the evolution of the universe involve enormous energy densities and temperatures. They provide an indirect testing ground for theories that can hardly be studied in a laboratory. The Glashow-Weinberg-Salam theory of weak and electromagnetic interactions [9] proposes a phase transition at temperatures of the order of 10^{15}K corresponding to an energy density of 10^{2}GeV at which the symmetry of weak and electromagnetic interactions is restored to a single electroweak interaction. Grand unified theories (GUT) have even higher critical temperatures of $T_c \sim 10^{28}\mathrm{K} \sim 10^{15}\mathrm{GeV}$ at which the symmetry between the strong and electroweak interactions is restored [8]. These are impressive energy scales, even compared to the highest temperatures attained in a supernova explosion of about 10^{11}K. Starting from a density of at least 10^{19}GeV in the standard version of the hot universe theory [10, 11], the universe cooled off, going through a number of phase transitions and breaking the symmetry between different interactions.

In most models of unified gauge theories, the symmetry between different types of interactions is broken in a phase transition due to the appearance of a constant classical scalar field φ over all space, called Higgs field. This field acquires a non-zero vacuum expectation value below a critical temperature and generates masses for gauge bosons. Since interactions with massive particles become short-range, the symmetry between various interactions is broken [12]. The process of inflation couples to the slow-rollover of a scalar field φ from a false-vacuum state to a symmetry-broken state. Knowledge about the behavior of the scalar field during the phase transition [13] can help to sort out different inflationary models.

The new satellites MAP (to be launched in 2000) and Planck (2007) [14] will improve our knowledge of the CMBR anisotropy in the near future. Comparisons of more accurate measurements of the multipole moments of the CMBR to theoretical predictions from different inflationary models will enable us to favor one of the current inflationary and cold dark matter models in the near future [1, 15].

In the following chapters we will analyze a scalar field phase transition in an expanding background based on the work of Cooper and Mottola [16]. We will try to explain the behavior of the scalar field mass analytically and compare our approximations to numerical calculations.

Chapter 2 gives a short overview of standard big bang cosmology. In its success, this model raised new questions that led to the introduction of inflation. We will see that inflation solves several shortcomings of standard cosmology at once by an enormous exponential expansion of the universe during the first 10^{-32} seconds.

The evolution of quantum fields during such an expansion can be practically described in the real-time formalism. In chapter 3 we will show how to calculate the Green function in the real-time formalism in a flat Minkowski space-time. We will express the Green function in terms of mode functions and discuss its matrix structure.

Starting from these results, we will extend the formalism to a curved space-time background in chapter 4. We will calculate the one-loop mass correction for a scalar field theory with a $\lambda\varphi^4$ interaction term and see how to renormalize it.

Chapter 5 is dedicated to the WKB approximation. It was originally invented to solve quantum mechanical problems with an arbitrary potential, but it can be applied to any second-order differential equation, hence to mode functions. Different WKB regions are linked together by so-called connection formulae.

In Chapter 6 we will demonstrate how to calculate the one-loop resummed mass, at least in principle. We will show how to analytically approximate this complex problem of a coupled system of infinitely many differential equations under certain conditions using WKB. In particular, we will find nice results in the high-temperature limit.

Finally, chapter 7 gives a summary of numerical results obtained from computer simulations using the *Mathematica* computer program. We will compare them to the analytical approximations from the previous chapter and find that a simple formula describes the behavior of the scalar field mass pretty accurately until far beyond the first classical turning point.

Recent improvements in observational instruments allow us to gain more and more data from the far end of our universe. We can take a closer look at the big bang event than ever before, but nevertheless we need new physical models to interpret the flow of observational data. And who knows what our universe still has to tell us if we just ask the right questions?

2 The inflationary universe scenario

2.1 Standard cosmology overview and its shortcomings

Hot big bang cosmology describes our universe from a fraction of a second after the beginning, when it was a hot, smooth soup of quarks, leptons, and gauge bosons, to the present, some 14 billion years later. The big bang model has its roots in the work of Gamow and his collaborators in the 1940s, but it didn't come to broad attention until 1964 with the discovery of the cosmic microwave background radiation (CMBR). With the verification of other predictions of the hot big bang model in the 1970s it became the universally accepted standard cosmology [1, 3, 8, 17].

Standard big bang cosmology is based on a homogeneous and isotropic expanding universe. The effects of this model are confirmed by three well-established observations: The first one is the red shift of distant objects that forms the basis for Hubble's law of expansion. Since the discovery of the red shift in the 1920's, thousands of distant galaxies have been observed to obey this universal law. Secondly, there is the cosmic microwave background radiation which has been measured to be an almost perfect black body with temperature $T = 2.728 \pm 0.002K$. It is a remnant of the early hot and dense stages of evolution after the big bang. Finally, the third observation is the abundance pattern of the light elements, D, ^{3}He, ^{4}He, and ^{7}Li, which is consistent with the production process in the seconds after the big bang as predicted by primordial nucleosynthesis. (All other elements in the periodic table were created in stars and stellar explosions billions of years later.)

Being such a successful theory, standard big bang cosmology also raised a bunch of new, more profound questions: Why do we observe more matter than antimatter? Why is the universe observed isotropic and homogeneous on large scales? If the universe was smooth in the beginning as suggested by the CMBR, what caused all the structure in the universe? How much dark matter is there to hold the universe together and what is it made of? What is the big bang event itself?

Questions like these motivated the search for new fundamental concepts in cosmology that go beyond the standard big bang theory. One of these ideas that is able to explain some of the questions raised above is the theory of *inflation*. According to this theory, our universe is flat because of an enormous expansion during the first 10^{-32} seconds after the big bang that increased the size of the universe by a factor of 10^{30} to 10^{40}. Quantum-mechanical fluctuations on scales of 10^{-23} cm or smaller are responsible for density perturbations that caused all the structure that we observe today [3]. To see how the necessity for inflation arises, let us start by studying a description of a homogeneous and isotropic universe.

A description like this first came up in the 1920's when Friedmann, Robertson and Walker found an expanding solution of the universe for the General Theory of Relativity [8, 18, 19]. Setting $c = 1$, the maximally symmetric metric can be written in the form

$$ds^2 = dt^2 - a^2(t)\left[\frac{dr^2}{1-kr^2} + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\right] \tag{1}$$

where $a(t)$ is the cosmic scale factor and the constant k can be chosen to be $k = +1, -1$, or 0 for space-times of constant positive, negative, or zero spatial curvature, resulting in a closed, open, or flat Friedmann universe respectively.

The fact that we observe a homogeneous and isotropic matter and radiation distribution in our universe does by no means guarantee that the *entire* universe is smooth, but we can say that a region at least as large as our present Hubble volume (which is the volume that is in principle observable by us) is smooth. Even if our observable smooth part of the universe was surrounded by an inhomogeneous and anisotropic universe, we could deduce from causality that our region would stay smooth for a time comparable to the light-crossing time of the Hubble volume, the Hubble time, which is about 10 billion years. We can thus safely describe our local Hubble volume by the FRW-metric above.

Immediately the question arises what fraction of the universe is in causally connected. That is, for what values of (r, θ, φ) would a light signal emitted at $t = 0$ reach a comoving observer with coordinates $(r_0, \theta_0, \varphi_0)$ at, or before, time t? Since a light signal satisfies the geodesic equation $ds^2 = 0$, we can use equation (1) to calculate this. If we put the observer in the origin $r_0 = 0$ then, due to the spherical symmetry of the problem, $d\theta$ and $d\varphi$ are irrelevant and we can determine t by

$$\int_0^t \frac{dt'}{a(t')} = \int_0^{r_H} \frac{dr}{\sqrt{1-kr^2}} \tag{2}$$

The proper distance to the horizon measured at time t is given by

$$d_H(t) = \int_0^{r_H} \sqrt{g_{rr}}dr = \int_0^{r_H} \frac{a(t)}{\sqrt{1-kr^2}}dr \tag{3}$$

which is simply the scale factor $a(t)$ at time t times equation (2)

$$d_H(t) = a(t)\int_0^t \frac{dt'}{a(t')} \tag{4}$$

If $d_H(t)$ is finite then our past light cone is limited by a particle horizon at the distance d_H. The particle horizon separates the part of the universe that can have any causal effect on us from the part from which light signals can not reach us. It turns out that in standard cosmology the proper distance is finite and proportional to the time $d_H(t) \propto t$ if $t = 0$ marks the initial singularity of the big bang event.

Let us consider a physical distance $d(t) \sim 100$ Mpc. Below this size, galaxies are organized in clusters with large voids between them, but on scales bigger than this size galaxies appear to be spread uniformly in the universe and we know from measurements that the universe is uniform to about a part in 10^5 on such a scale [20, 21]. Let us see how a region with the radius $d(t)$ evolved from earlier times. At times $t' < t$, the size of this patch is given by

$$d(t') = \frac{a(t')}{a(t)} d(t) \tag{5}$$

For a matter dominated universe the scale factor $a(t)$ is proportional to $t^{2/3}$, whereas for a radiation dominated universe we have $a(t) \propto t^{1/2}$. Since the horizon size is given by $d_H(t') \propto t'$, we see that the ratio $d(t')/d_H(t')$ increases as we evolve back in time. Thus at some time in the far past, the scale $d(t')$ will become larger than the horizon $d_H(t')$ at that time. This is already the case at the time of the decoupling of matter and radiation, that is when the CMBR originated some 300,000 years after the big bang. It is difficult to explain how a region that was larger than the horizon and therefore causally disconnected at the time of decoupling can be as homogeneous and isotropic as we observe it today. One can show that the present Hubble volume consisted of no less than 10^5 causally disconnected regions at the time of recombination, which spans an angle of about $0.8°$ on the sky today. Furthermore, at the time of primordial nucleosynthesis, a minute after the big bang, today's Hubble volume consisted of about 10^{25} causally independent regions, yet the synthesis of the light elements seems to have been nearly identical in all of those regions [3, 22]. This high degree of homogeneity and isotropy on large scales represents one of the important puzzles of standard big bang cosmology and is known as the *horizon problem*. We believe that the solution to this problem is inflation. Before we dive into the theory of inflation, let us see where the scale factors for a matter or radiation dominated universe that we just used come from.

In the FRW-metric in eq. (1) we have not made any restrictions on the scale factor $a(t)$ yet, but its evolution is actually determined by the Einstein equations

$$\ddot{a} = -\frac{4\pi}{3} G(\rho + 3p)a \tag{6}$$

$$H^2 + \frac{k}{a^2} \equiv \left(\frac{\dot{a}}{a}\right)^2 + \frac{k}{a^2} = \frac{8\pi}{3} G\rho \tag{7}$$

where ρ is the energy density of matter, p is its pressure, G is the gravitational constant and $H = \frac{\dot{a}}{a}$ is the Hubble parameter [8]. These equations imply an energy conservation law, given by

$$\dot{\rho} a^3 + 3(\rho + p)a^2 \dot{a} = 0 \tag{8}$$

We now have to assume a so-called equation of state, relating the energy density ρ to the pressure p in order to find out how the universe will evolve. Choosing $p = \alpha\rho$ we find from the energy conservation law that

$$\rho \sim a^{-3(1+\alpha)} \tag{9}$$

Particularly, for non-relativistic cold matter $\alpha = 0$ and $\rho \sim a^{-3}$, and for a hot ultra-relativistic gas of noninteracting particles $\alpha = 1/3$ and the energy density evolves according to $\rho \sim a^{-4}$. For small a we can therefore neglect the k/a^2 term compared to $8\pi G\rho/3$ in equation (7) and the scale factor is given by

$$a \sim t^{\frac{2}{3(1+\alpha)}} \tag{10}$$

Thus we see that in a matter dominated universe we obtain for non-relativistic cold matter an expansion of

$$a \sim t^{2/3} \tag{11}$$

whereas in a radiation dominated universe that can be described by an ultra-relativistic gas the scale factor behaves like

$$a \sim t^{1/2} \tag{12}$$

Regardless of the model used ($k = \pm 1, 0$), the scale factor vanishes at some time $t = 0$, and the energy density of matter becomes infinitely large. This space-time singularity that represents the creation of matter, space and time was appropriately named “big bang” by Hoyle [1]. Standard big bang cosmology really is a theory about the events following this singularity up to now, but the physics near this singularity is not really addressed. A new quantum theory of gravity might enable us to ask questions about the universe “before the big bang” and inflation might shed some new light on the big bang.

2.2 Inflation

In the 1980's the standard big bang cosmology had to face many open questions: We already discussed the large scale smoothness of the universe and the horizon problem. On the other hand there is the question about the small-scale inhomogeneity: We observe stars, galaxies, clusters, voids (large regions containing almost no galaxies), and superclusters. Of course, standard cosmology can explain them by the growth of small, initial distortions in a matter-dominated universe by Jeans (or gravitational) instability. But where did these initial seeds come from? There is also a question of flatness: Today the radius of curvature for our universe is of the order of $R_{curv} \sim H_0^{-1}$, since the energy density appears to be close to the critical energy density. The radius decreases relative to the Hubble radius in a matter or radiation dominated universe and therefore at an earlier time it must have been much bigger. At the Planck time about 10^{-43} seconds after the big bang, the radius of the curvature must have been at least as huge as $R_{curv} \sim 10^{30} H^{-1}$ [3] which is a severe restriction on the initial conditions. Standard cosmology leaves unanswered questions about unwanted relics, superheavy particles produced in the early universe, that should dominate the universe, or domain walls that should be observable between different parts of the universe with independently broken symmetry [1, 3, 8]. Surprisingly, a single theory could possibly be able to answer all of these questions and that is inflation + cold dark matter [17].

The basic idea of inflation is a brief period of tremendous expansion of the scale factor by a factor of at least 10^{27} during the first 10^{-32} seconds. We do not know the precise details of this inflationary phase yet, but in most models the exponential expansion is coupled to the potential energy of a scalar field going through a phase transition. In this *inflationary phase* the universe is in an unstable vacuum-like state with high energy density. In such a state, the vacuum pressure and energy density are related by $p = -\rho$. From equation (8) we see that the vacuum energy is constant during such an inflationary expansion. A constant energy density of matter also implies according to equation (7) that the scale factor grows exponentially with

$$a(t) = \begin{cases} H^{-1} \cosh Ht & \text{for } k = +1 \text{ (closed)} \\ H^{-1} e^{Ht} & \text{for } k = 0 \text{ (flat)} \\ H^{-1} \sinh Ht & \text{for } k = -1 \text{ (open)} \end{cases} \tag{13}$$

where $H = \sqrt{\frac{8\pi}{3} G\rho}$. Actually, $H(t)$ also changes with time, but during a characteristic period of time $\Delta t = H^{-1}$ there is little change in H so that one can speak of a quasi-exponential expansion of the universe

$$a(t) \sim a_0 e^{Ht} \tag{14}$$

This is also known as the *de Sitter* expansion and was first described in 1917 by de Sitter [6], well before Friedmann developed his theory of the expanding universe. However its physical meaning as an exponentially expanding universe filled with superdense matter was not discovered until 1960's. The first truly inflationary model was developed in 1981 by Guth [7] who could solve the flatness problem, the horizon problem, and the primordial monopole problem with his theory. Based on this model, many improvements have been introduced and the "old" inflationary scenario was replaced by new concepts like the "new ", "chaotic", "natural", or "hybrid" inflationary scenario. Although these models address different technical problems regarding the scalar field and its potential, they are all motivated by the following basic ideas:

A small, subhorizon-sized region of the universe is expanded to a size much greater than the universe we can observe today. Since this region was causally connected before inflation, it is likely to be smooth in the present, and so is the small portion of it that became our observable part of the universe. This explains the smoothness of our universe and the homogeneous and isotropic nature of the CMBR. It also solves the flatness problem, because due to inflation any curvature in the original region would become small. After inflation the observable universe would appear to be flat, independent of the initial curvature.

All inflationary models state that a scalar field is responsible for this exponential expansion. It takes place during a symmetry breaking phase transition. A scalar potential is assumed that changes its minimum from $\langle\varphi\rangle = 0$ at high temperatures to $\langle\varphi\rangle = \pm\sigma \neq 0$ at lower temperatures. In the simplest case the system is 1-dimensional and the scalar field has to choose between $+\sigma$ or $-\sigma$. The initial symmetry around 0 is broken. In the 2-dimensional case there is an additional degree of freedom for the scalar field in the broken phase. The potential takes the form of a "Mexican hat".

In the *old inflationary scenario*, expansion occurs while the scalar field is trapped in a $\langle\varphi\rangle = 0$ false-vacuum state. There is a symmetry-broken global minimum of the potential at $\langle\varphi\rangle = \sigma$, but the scalar field first has to get there by tunneling. Inflation ends when the scalar field tunnels through the barrier. A successful inflation requires a small tunneling rate, thus true vacuum bubbles are rarely produced. On the other hand, energy for reheating at the end of the inflationary phase could only come from bubble collisions, that are rare due to rare bubble nucleation. The criticism about this scenario is

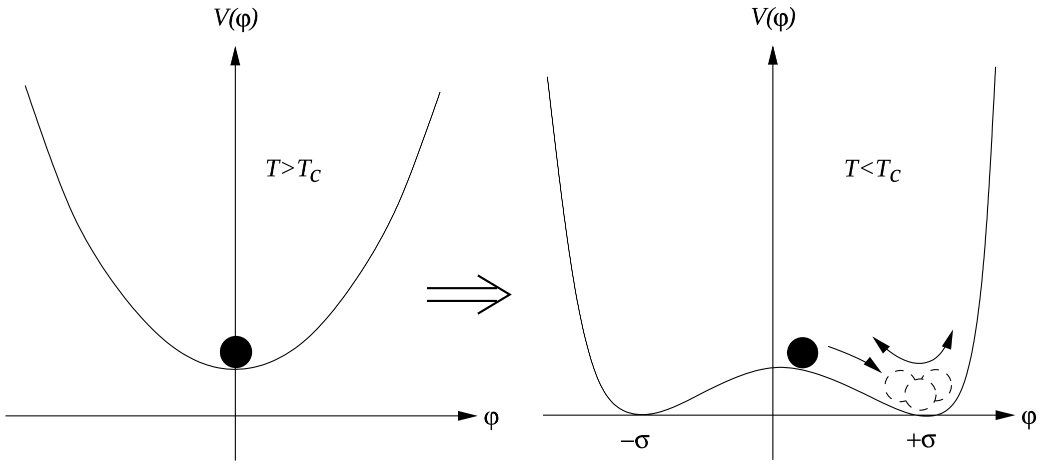


Figure 1: Schematic illustration of an inflationary potential in the new inflationary scenario.

that the phase transition would never be completed and most of the universe would continue to inflate forever [3, 23].

The *new inflationary scenario* improves the situation significantly. It is also called "slow-rollover" inflation. As this name suggests, a key feature of this theory is the slow evolution of the scalar field from the false-vacuum state to the symmetry-broken minimum of the potential as shown in Figure 1. It is during this slow rollover phase that the universe expands exponentially. This process can be compared to a ball rolling down a hill with friction, where the friction is provided here by the expansion of the universe. During the slow transition of the scalar field, the vacuum energy will dominate the energy density of the universe as soon as the temperature falls below the critical temperature of the phase transition, resulting in the de Sitter phase. When the scalar field finally arrives at the new minimum, it overshoots and begins to oscillate about the new point $\langle\varphi\rangle = \sigma$. These oscillations contain an enormous amount of vacuum energy and are damped by producing other, lighter fields or particles to which they couple. These newly created particles thermalize, a process at the end of inflation called *reheating*. It explains the tremendous heat content of the universe and finally leads to the photons in the CMBR that we can observe today. This scenario can successfully explain the cosmological problems stated above and all models of inflation today are based on the slow-rollover mechanism.

3 Real-time formalism

We want to study dynamical properties of a system at $T \neq 0$. This combines two different basic difficulties in one question: First, we want to study a finite temperature problem. For static, equilibrium systems this can be done in the imaginary-time formalism where the thermal factor $e^{-\beta H}$ is reinterpreted as a time evolution in an imaginary time direction $\beta = -it$. But second, we want to study dynamical, time-dependent questions like the behavior during a phase transition in our model. The imaginary-time formalism is not readily capable of answering such questions. Therefore a new formalism, the *real-time formalism*, is necessary to tackle this problem.

The real-time formalism answers questions about dynamical problems naturally, but it is technically far more complicated than the imaginary-time formalism. Let us therefore begin with a brief review of the imaginary-time formalism.

3.1 Imaginary-time formalism

The imaginary-time formalism basically trades time for temperature. General concepts from equilibrium statistical thermodynamics can be woven into quantum field theory in a straightforward way by the concept of analytic continuation where an imaginary time takes the role of the temperature. One can easily grasp this idea by regarding the general definition of a density matrix for a thermal equilibrium system

$$\rho(\beta) \equiv e^{-\beta H} \tag{15}$$

and compare it to the time evolution of an operator, given by

$$A(t) = e^{iHt} A(0) e^{-iHt} \tag{16}$$

One sees that both, time evolution and density matrix, contain an exponential of the Hamiltonian H and the idea of likening β to $\pm it$ seems obvious. Historically it was first noticed by F. Bloch [24].

In order to see the combination of these two concepts in detail, let us first recall how the ensemble average of an observable A is defined. The partition function of a system with the density matrix (15) is given by

$$Z(\beta) \equiv \text{Tr}\ \rho(\beta) = \text{Tr}\ e^{-\beta H} \tag{17}$$

where "Tr " denotes the trace or the sum over the expectation values in any complete basis of the physical Hilbert space. The thermal average of an observable is defined as

$$\langle A \rangle_\beta \equiv \frac{\text{Tr } \rho(\beta) A}{Z(\beta)} = \frac{\text{Tr } \left(e^{-\beta H} A\right)}{e^{-\beta H}} \tag{18}$$

so that a general thermal correlation function of two operators $A(t)$ and $B(t)$ can be rewritten in the following way (using the time evolution property of an operator eq. (16) and the cyclicity of the trace)

$$\begin{aligned} \langle A(t) B(t') \rangle_\beta &= Z^{-1}(\beta) \text{Tr } \rho(\beta) A(t) B(t') \\ &= Z^{-1}(\beta) \text{Tr } e^{-\beta H} A(t) e^{\beta H} e^{-\beta H} B(t') \\ &= Z^{-1}(\beta) \text{Tr } A(t + i\beta) e^{-\beta H} B(t') \\ &= \langle B(t') A(t + i\beta) \rangle_\beta \end{aligned} \tag{19}$$

Note that this relation holds for both, bosonic as well as fermionic operators. Relations of this type are known as the *Kubo-Martin-Schwinger (KMS) relations* [25]. In particular for the correlation function of an operator with itself we get the relation

$$\boxed{\langle A(t) A(t') \rangle_\beta = \langle A(t') A(t + i\beta) \rangle_\beta} \tag{20}$$

This will be an important result for two-point Green function $G(t, t') = \langle \varphi(t) \varphi(t') \rangle_\beta$ at finite temperature.

Without going too much into detail, the usual course in the imaginary-time formalism is as follows: Using an operational method or the path integral, one can derive cyclicity conditions for propagators from the KMS relation. Fourier transformation of the finite imaginary time interval leads to discrete frequencies, the so-called *Matsubara frequencies* ω_n that are given by

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} & \text{for bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{for fermions} \end{cases} \tag{21}$$

The momentum space Green function then becomes

$$G_\beta(\omega_n, \vec{k}) = \frac{1}{\omega_n^2 + \vec{k}^2 + m^2} \tag{22}$$

It turns out that the only difference between the zero temperature and the finite temperature field theories lies in the restriction to discrete frequencies. All Feynman diagrams for calculating higher order corrections of a theory are the same in the finite as well as in the zero temperature case. In the imaginary-time formalism the complete temperature dependence is contained in the propagator, so that calculations from the zero temperature case can be easily transfered to the finite temperature case.

The drawback of this formalism is that it is difficult to apply its results to dynamical questions. That is, questions about the system out of equilibrium where the explicit time-dependence of the system should be studied, for example when going through a phase transition. Here another formalism is more readily apt to study non-equilibrium properties - the real-time formalism. One formulation of it is the closed-time-path formalism which we now want to introduce.

3.2 Closed-time-path formalism

The closed-time-path formalism provides an integration path for the system that contains both components of interest, namely time dependence and temperature. Technically, this path in the complex time plane can be described by going from minus infinity to plus infinity being infinitesimally above the real axis and going back infinitesimally below it. To see how this path arises, we start with the *Schrödinger picture* description of a general quantum mechanical system in a mixed state described by a density matrix ρ. For a general system where we do not demand that it is in thermal equilibrium, the density matrix is given by

$$\rho(t) = \sum_n p_n \left|\psi_n(t)\right\rangle \left\langle\psi_n(t)\right| \tag{23}$$

where p_n describes the probability of finding the quantum mechanical system in the state $\left|\psi_n(t)\right\rangle$. Being a probability, it satisfies

$$\sum_n p_n = 1 \tag{24}$$

The average of an operator in this mixed state can be calculated from the trace of the density matrix and the operator and can be written as

$$\left\langle A\right\rangle (t) = \mathrm{Tr}\ \rho(t)A = \sum_n p_n \left\langle\psi_n(t)\right| A \left|\psi_n(t)\right\rangle \tag{25}$$

Note that the time dependence of the operator is entirely determined by the time evolution of the density matrix, and this itself is determined by the time evolution of the states of the system.

With an Hamiltonian H the states of the system satisfy

$$i\frac{\partial\left|\psi_n(t)\right\rangle}{\partial t} = H\left|\psi_n(t)\right\rangle \tag{26}$$

Using this equation and its hermitian conjugate, we see that the density matrix satisfies the differential equation

$$\begin{aligned} i\frac{\partial\rho(t)}{\partial t} &= \sum_n p_n \left(i\frac{\partial\left|\psi_n(t)\right\rangle}{\partial t}\right)\left\langle\psi_n(t)\right| + \sum_n p_n \left|\psi_n(t)\right\rangle \left(i\frac{\partial\left\langle\psi_n(t)\right|}{\partial t}\right) \\ &= \sum_n p_n H \left|\psi_n(t)\right\rangle\left\langle\psi_n(t)\right| - \sum_n p_n \left|\psi_n(t)\right\rangle\left\langle\psi_n(t)\right| H \\ &= [H, \rho(t)] \end{aligned} \tag{27}$$

We have assumed here that the probabilities p_n are time-independent. This actually means that we regard systems with a constant entropy

$$S = -\langle \ln p \rangle = -\sum_n p_n \ln p_n \tag{28}$$

We just have to be aware of this restriction when we interpret results. Since adiabatic evolutions arise frequently in the study of physical systems we will continue with this assumption. This means that the properties of the system should change slowly enough so that they correspond to an adiabatic evolution.

For a time-independent Hamiltonian H, the differential equation (27) can be solved for $\rho(t)$ to give

$$\rho(t) = e^{-iHt}\rho(0)e^{iHt} \tag{29}$$

We also see from eq. (27) that if the Hamiltonian commutes with the density matrix, then $\rho(t) = \rho(0)$ is constant in time and describes a system in equilibrium.

In general the system is not in equilibrium and we are interested in systems where the Hamiltonian carries an explicit time dependence. In this case we can express the density matrix through the time evolution operator

$$\rho(t) = U(t,0)\rho(0)U^\dagger(t,0) = U(t,0)\rho(0)U(0,t) \tag{30}$$

where the operator $U(t,t')$ is defined as

$$i\frac{\partial U(t,t')}{\partial t} = H(t)U(t,t') \tag{31}$$

with the condition that

$$U(t,t) = 1 \tag{32}$$

Formally the solution to this differential equation (31) can be written as a time ordered exponential

$$U(t,t') = T\left(e^{-i\int_{t'}^{t} dt'' H(t'')}\right) \tag{33}$$

which is merely a short-hand notation of Dyson's equation, an iterative solution to the corresponding integral equation (see for example Ref. [26]):

$$U(t,t') = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \ldots \mathrm{d}t_n T\left(H(t_1)\ldots H(t_n)\right) \tag{34}$$

The time evolution operator satisfies the following relations

$$\begin{aligned} U(t_1,t_2)U(t_2,t_1) &= 1 \\ U(t_1,t_2)U(t_2,t_3) &= U(t_1,t_2) \quad \text{for} \quad t_1 > t_2 > t_3 \end{aligned} \tag{35}$$

We assume that the quantum system is in thermal equilibrium for negative times so that the Hamiltonian $H(t)$ may only be time dependent for $t > 0$.

$$H(t) = \begin{cases} H_i & \text{for} \quad \mathrm{Re}\, t \leq 0 \\ H(t) & \text{for} \quad \mathrm{Re}\, t \geq 0 \end{cases} \tag{36}$$

For negative times, the system is described by a thermal density matrix with the inverse temperature β (compare with eq. (15))

$$\rho(t \leq 0) = e^{-\beta H_i} \tag{37}$$

Using the fact that the Hamiltonian is time independent for negative t, one can use the definition of the evolution operator (31) to rewrite the density matrix in another way:

$$\rho(T) = U(T - i\beta, T) \tag{38}$$

where T denotes a large negative time. This already describes the last element of the closed-time-path going down in the complex time plane by $i\beta$ at a large negative time T. Starting with the density matrix at a large negative time, we can determine the density matrix for an arbitrary time by applying the evolution operator U as we did in equation (30)

$$\begin{aligned} \rho(t) &= U(t,T)\rho(T)U(T,t) \\ &= U(t,T)U(T-i\beta,T)U(T,t) \end{aligned} \tag{39}$$

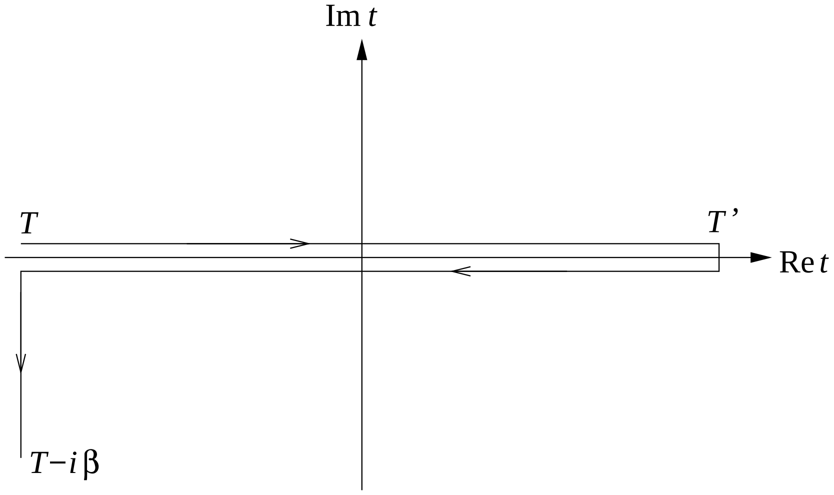
We can now calculate the expectation value of any operator. With the definition of the average of an operator (18) we can write:

$$\begin{aligned} \langle A \rangle (t) &\equiv \frac{\mathrm{Tr}\ \rho(t) A}{\mathrm{Tr}\ \rho(t)} \\ &= \frac{\mathrm{Tr}\ U(t,T)U(T-i\beta,T)U(T,t)A}{\mathrm{Tr}\ U(t,T)U(T-i\beta,T)U(T,t)} \\ &= \frac{\mathrm{Tr}\ U(T-i\beta,T)U(T,t)AU(t,T)}{\mathrm{Tr}\ U(T-i\beta,T)} \end{aligned} \tag{40}$$

This expression describes a path starting at a large negative time T and going up to the time where the operator is to be evaluated, then returning and going down by $i\beta$. To bring this expression into the standard form we have to insert yet another time point, represented by T', a large positive time. Using the property of the evolution operator in eq. (35) we can write

$$\begin{aligned} \langle A \rangle (t) &= \frac{\mathrm{Tr}\ U(T-i\beta,T)U(T,t)U(t,T')U(T',t)AU(t,T)}{\mathrm{Tr}\ U(T-i\beta,T)} \\ &= \frac{\mathrm{Tr}\ U(T-i\beta,T)U(T,T')U(T',t)AU(t,T)}{\mathrm{Tr}\ U(T-i\beta,T)U(T,T')U(T',T)} \end{aligned} \tag{41}$$

Now this is the standard form of the closed-time-path: The path in the complex time plane starts (reading the evolution operators in eq. (41) from right to left) at a large negative time T, then goes to the time t where the operator A is to be evaluated and continues to the large positive time T'. Here the path turns around and goes back to the negative time T'. The two paths are usually displaced infinitesimally from the real-time axis. Finally the last part of the path consists of going down to $T - i\beta$. In the complex time plane the path has the form



Eventually we would like to take the limits $T \to -\infty$ and $T' \to \infty$. It turns out that this limit can be taken in the path integral representation of the partition function by defining a generating functional as we will see in the following section.

3.3 Path integral formulation

We would like to rewrite the partition function (17) in the path integral representation. Path integrals were introduced by Feynman [27, 28] as a new way of describing quantum physics. Starting from probability amplitudes of particles and describing their propagation over all possible paths between the two endpoints, Feynman invented the formalism that leads to Feynman diagrams which play an important role in today's perturbation theory. This section might get a little bit technical, but the aim is to show how path integrals are introduced for the partition function in a clear way.

The trace of the partition function from equation (17) can be written by using a complete set of eigenvectors of the position operator

$$\begin{aligned} Z(\beta) &= \mathrm{Tr}\ \rho(\beta) \\ &= \sum_n p_n \langle\psi_n(t)| \, e^{-\beta H} \, |\psi_n(t)\rangle \\ &= \int \mathrm{d}q \, \langle q| \, e^{-i(-i\beta)H} \, |q\rangle \\ &= \int \mathrm{d}q F(q,-i\beta;q,0) \end{aligned} \tag{42}$$

In the last step we made use of the evolution operator

$$F(q',t';q,t) = \langle q',t'|q,t\rangle = \langle q'| \, e^{-iH(t'-t)} \, |q\rangle \tag{43}$$

that describes the probability amplitude that a particle initially at position q at a time t can be found at q' at a time t'. In our case it makes sense to introduce an imaginary time $\tau = it$ and write $F(q',t';q,t) = F(q',-i\tau';q,-i\tau)$. We will show how one can find the path integral representation for the evolution operator $F(q',-i\tau';q,-i\tau)$ and thus also see how to write the path integral for the partition function.

In a first step we divide the interval $[\tau,\tau']$ into $n+1$ subintervals of equal length

$$\varepsilon = \frac{\tau'-\tau}{n+1} \quad \text{and} \quad \tau_l = \tau + l\varepsilon \tag{44}$$

from $\tau_0 = \tau, \tau_1, \tau_2, \ldots, \tau_n, \tau_{n+1} = \tau'$ with $\varepsilon \to 0$. The exponential in (43) can be split up in a product of exponentials

$$e^{-(\tau'-\tau)H} = \prod_{l=0}^{n} e^{-(\tau_{l+1}-\tau_l)H} = \prod_{l=0}^{n} e^{-\varepsilon H} \tag{45}$$

We can now insert complete sets of eigenstates $\int dq_l \left|q_l\right\rangle \left\langle q_l\right|$ of the position operator Q at times $\tau_1, \tau_2, \ldots, \tau_n$ and get

$$\begin{aligned} F(q', -i\tau'; q, -i\tau) &= \langle q'| \prod_{l=0}^{n} e^{-\varepsilon H} |q\rangle \\ &= \int \prod_{l=1}^{n} \mathrm{d}q_l \prod_{l=0}^{n} \langle q_{l+1}| e^{-\varepsilon H} |q_l\rangle \end{aligned} \tag{46}$$

In order to calculate the matrix element in equation (46), we split up the Hamiltonian $H = P^2/(2m) + V(Q)$ in the exponential by using Trotter's (or the Lie product) theorem [29, 30]

$$\lim_{n\to\infty} \left(e^{A/n} e^{B/n}\right)^n = e^{A+B} \tag{47}$$

and write

$$\begin{aligned} \langle q_{l+1}| e^{-\varepsilon H} |q_l\rangle &= \langle q_{l+1}| \exp\left(-\varepsilon \frac{P^2}{2m}\right) \exp\left(-\varepsilon V(Q)\right) |q_l\rangle \\ &= \exp\left(-\varepsilon V(q_l)\right) \langle q_{l+1}| \exp\left(-\varepsilon \frac{P^2}{2m}\right) |q_l\rangle \end{aligned} \tag{48}$$

Here we have evaluated the potential $V(Q)$ operating on a position eigenstate $|q_l\rangle$ which simply gives the value of the potential at the position q_l. To calculate the last matrix element we now insert a complete set of eigenstates $\int dp_l \left|p_l\right\rangle \left\langle p_l\right|$ of the momentum operator P so that we get

$$\begin{aligned} \langle q_{l+1}| P^2 |q_l\rangle &= \int \mathrm{d}p_l \langle q_{l+1}| P^2 |p_l\rangle \langle p_l|q_l\rangle \\ &= \int \frac{\mathrm{d}p_l}{2\pi} p_l^2 e^{i(q_{l+1}-q_l)p_l} \end{aligned} \tag{49}$$

Now we can write $F(q', -i\tau'; q, -i\tau)$ in the form of a path integral:

$$F(q', -i\tau'; q, -i\tau) = \lim_{\varepsilon\to 0} \int \prod_{l=1}^{n} \mathrm{d}q_l \prod_{l=0}^{n} \left(\frac{\mathrm{d}p_l}{2\pi} e^{i(q_{l+1}-q_l)p_l} e^{-\varepsilon\left(\frac{p_l^2}{2m}+V(q_l)\right)}\right) \tag{50}$$

Here p_l and q_l are classical variables (numbers). Since V is a function only of q, it is possible to perform the p-integral: We first complete the square in the exponent in equation (50):

$$i\left(q_{l+1}-q_l\right)p_l-\varepsilon\frac{p_l^2}{2m}=-\frac{\varepsilon}{2m}\left(p_l+\frac{m}{\varepsilon}i\left(q_{l+1}-q_l\right)\right)^2-\frac{m}{2\varepsilon}\left(q_{l+1}-q_l\right)^2 \quad (51)$$

The integral over p_l over the first part gives a translated Gaussian integral that is equivalent to $\frac{1}{2\pi}\int \mathrm{d}p_l \exp\left(-\frac{\varepsilon}{2m}p_l^2\right)=\frac{1}{2\pi}\sqrt{\pi\left(2m/\varepsilon\right)}=\sqrt{m/\left(2\pi\varepsilon\right)}$. Equation (50) now becomes

$$\begin{aligned} F(q',-i\tau';q,-i\tau) &= \lim_{\varepsilon\to 0}\sqrt{\frac{m}{2\pi\varepsilon}}\int\prod_{l=1}^{n}\left[\sqrt{\frac{m}{2\pi\varepsilon}}\mathrm{d}q_l\right] \\ &\quad\times\exp\left[-\varepsilon\sum_{l=0}^{n}\frac{m\left(q_{l+1}-q_l\right)^2}{2\varepsilon^2}-\varepsilon\sum_{l=0}^{n}V\left(q_l\right)\right] \quad (52)\end{aligned}$$

Here we also put the product into the exponential to form sums. These Riemann sums can be converted to integrals in the limit $\varepsilon\to 0$:

$$\begin{aligned} \varepsilon\sum_{l=0}^{n}\frac{m\left(q_{l+1}-q_l\right)^2}{2\varepsilon^2} &\to \int_\tau^{\tau'}\frac{m}{2}\left(\left.\frac{\mathrm{d}q(\bar\tau)}{\mathrm{d}\bar\tau}\right|_{\bar\tau=\tau''}\right)^2\mathrm{d}\tau'' \\ \varepsilon\sum_{l=0}^{n}V\left(q_l\right) &\to \int_\tau^{\tau'}V(q(\tau''))\mathrm{d}\tau'' \quad (53)\end{aligned}$$

If we now introduce the symbol $\mathcal{D}q$ for integration over the q_l with the integration measure

$$\sqrt{\frac{m}{2\pi\varepsilon}}\prod_{l=1}^{n}\left[\sqrt{\frac{m}{2\pi\varepsilon}}\mathrm{d}q_l\right]\to\mathcal{D}q \quad (54)$$

then we can write the path integral in a compact way:

$$\begin{aligned} F(q',-i\tau';q,-i\tau) &= \int\mathcal{D}q\exp\left(-\int_\tau^{\tau'}\mathrm{d}\tau''\left(\frac{m}{2}\dot q^2(\tau'')-V(q(\tau''))\right)\right) \\ &= \int\mathcal{D}q\exp\left(-S_E(\tau'-\tau)\right) \quad (55)\end{aligned}$$

with the boundary conditions $q(\tau)=q$, $q(\tau')=q'$. $S_E(\tau'-\tau)$ is the Euclidean action

$$S_E(\tau'-\tau)=\int_\tau^{\tau'}L(q,\dot q)\mathrm{d}\tau'' \quad (56)$$

with the Lagrangian L of the particle

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q) \tag{57}$$

Note that the symbol $\mathcal{D}q$ means nothing more than is implied by equations (52) and (54).

Using this result, we can express the partition function as a path integral. Inserting equation (55) into the definition of the partition function (42) we get

$$\begin{aligned} Z(\beta) &= \int \mathrm{d}\bar{q} F(\bar{q}, -i\beta; \bar{q}, 0) \\ &= \int \mathrm{d}\bar{q} \int_{q(0)=\bar{q}}^{q(\beta)=\bar{q}} \mathcal{D}q e^{-S_E(\beta)} \end{aligned} \tag{58}$$

The first integral states that we have periodic boundary conditions for $q(\tau)$. We can finally present the usual form of the path integral for the partition function

$$\begin{aligned} Z(\beta) &= \int \mathcal{D}q(\tau) \exp\left(-\int_0^\beta \mathrm{d}\tau \left(\frac{1}{2}m\dot{q}^2(\tau) - V(q(\tau))\right)\right) \\ &= \int \mathcal{D}q e^{-S_E(\beta)} \end{aligned} \tag{59}$$

with the boundary condition $q(\beta) = q(0)$.

3.4 Propagators in the real-time formalism

The propagator $G_C(x - x') = \langle T_c (\varphi(x)\varphi(x')) \rangle$ is an interesting quantity, because as a two-point correlation function it gives basic information about a particle or field theory. We will use the path integral formulation of the partition function $Z(\beta)$ adapted for a Klein-Gordon theory as a basis and we would like to construct a generating functional $Z_\beta[j_c]$ that generates the two-point correlation function by means of functional derivatives with respect to the added sources $j_c(x)$. We will see how this approach naturally links the Green function of the Klein-Gordon operator to the two-point correlation function. Due to our closed-time-path contour C with two branches infinitesimally above and below the real axis we will see that the propagator can be naturally written as a 2×2 matrix and we will see how to write the Green functions in this matrix.

Let us start with the partition function in equation (59). Adding an external source to a real Klein-Gordon theory, we get the following generating functional:

$$Z_\beta[j_c] = \int \mathcal{D}\varphi e^{i\int_c \mathrm{d}t \int \mathrm{d}^3x(\mathcal{L}+j_c\varphi)} \tag{60}$$

with the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{m^2}{2}\varphi^2 \tag{61}$$

For simplicity we use a Lagrangian density for a flat background metric to derive the structure of the propagator in this section. We will see in the next chapter how this formalism can be extended to allow a curved space-time.

As we saw in the derivation above in equation (58), the field φ has to satisfy periodic boundary conditions. The integration path along the time-contour C is the closed-time-path described in equation (41). We will call the first part of this contour going from $-\infty$ to $+\infty$ infinitesimally above the real axis C_+, the second part of this contour returning to $-\infty$ below the real axis C_- and the final part parallel to the imaginary axis C_3.

Taking functional derivatives of the generating functional (60) automatically gives the two-point correlation function. The functional derivative is the natural generalization to continuous functions of the rule for derivatives of discrete vectors $\partial x_j/\partial x_i = \delta_{ij}$. For a path along the contour C it is defined as:

$$\begin{aligned} \frac{\delta}{\delta j_c(t,\vec{x})} j_c(t',\vec{x}') &= \delta_c(t-t')\delta^{(3)}(\vec{x}-\vec{x}') \\ \frac{\delta}{\delta j_c(t,\vec{x})} \int_c \mathrm{d}t' \int \mathrm{d}^3\vec{x}' j_c(t',\vec{x}')\varphi(t',\vec{x}') &= \varphi(t,\vec{x}) \end{aligned} \tag{62}$$

Every functional derivative with respect to a function $j_c(t,\vec{x})$ brings down a factor $i\varphi(t,\vec{x})$ from the exponential in equation (60) and we get

$$\langle T_c\left(\varphi(t,\vec{x})\varphi(t',\vec{x}')\right)\rangle = (-i)^2 \frac{1}{Z_\beta[0]} \frac{\delta^2 Z_\beta[j_c]}{\delta j_c(t,\vec{x})\delta j_c(t',\vec{x}')}\bigg|_{j_c=0} \tag{63}$$

Since we integrate over the contour C in the exponential in (60) and use sources j_c defined on this contour, we naturally get a contour-ordered propagator. This propagator can be expressed as

$$\langle T_c\left(\varphi(t,\vec{x})\varphi(t',\vec{x}')\right)\rangle = \theta_c(t-t')\left\langle\varphi(t,\vec{x})\varphi(t',\vec{x}')\right\rangle + \theta_c(t'-t)\left\langle\varphi(t',\vec{x}')\varphi(t,\vec{x})\right\rangle \tag{64}$$

where the theta function on the contour C is defined as

$$\theta_c(t-t') = \begin{cases} \theta(t-t') & t, t' \,\text{on}\, C_+ \\ \theta(t'-t) & t, t' \,\text{on}\, C_- \\ 0 & t \,\text{on}\, C_+,\, t' \,\text{on}\, C_- \\ 1 & t' \,\text{on}\, C_+,\, t \,\text{on}\, C_- \end{cases} \tag{65}$$

Here we ignore the case of a time t sitting on the third part of the contour, C_3, for reasons we will show at the end of this section. We will see that this third part C_3 only contributes to an unimportant normalization factor and can be ignored. Technically, we can think of the contour C as consisting only of the branches C_+ and C_-. As this path describes a closed contour in the complex plane, the formalism is commonly known as the closed-time-path formalism.

The definition of the theta function (65) immediately leads to the definition of the delta function on this contour:

$$\delta_c(t-t') = \frac{\mathrm{d}\theta_c(t-t')}{\mathrm{d}t} = \begin{cases} \delta(t-t') & t, t' \,\text{on}\, C_+ \\ -\delta(t-t') & t, t' \,\text{on}\, C_- \\ 0 & \text{otherwise} \end{cases} \tag{66}$$

Writing the integral over the closed-time-path contour as

$$\int_c \mathrm{d}t = \int_{-\infty}^{\infty} \mathrm{d}t_+ - \int_{-\infty}^{\infty} \mathrm{d}t_- \tag{67}$$

we see that the delta function on the contour (66) satisfies

$$\int_c \mathrm{d}t' \delta_c(t-t') f(t') = f(t) \tag{68}$$

We can evaluate the generating functional in equation (60) in a free field theory in a way that leads to Green functions. Integrating the exponent of (60) by parts we obtain

$$\int_c \mathrm{d}t \int \mathrm{d}^3x \, (\mathcal{L}_0 + j_c\varphi) = \int_c \mathrm{d}t \int \mathrm{d}^3x \left(\frac{1}{2}\varphi \left(-\partial^2 - m^2 + i\varepsilon\right)\varphi + j_c\varphi \right) \tag{69}$$

The additional term $i\varepsilon$ is a convergence factor for the functional integral. It justifies the use of Gaussian integration formulae when the exponent appears to be purely imaginary. We can complete the square by introducing a shifted field

$$\varphi'(x) \equiv \varphi(x) - i \int_c \mathrm{d}t' \int \mathrm{d}\vec{x}' G_c(t-t', \vec{x}-\vec{x}') j_c(t', \vec{x}') \tag{70}$$

where G_c is a Green function of the Klein-Gordon operator, satisfying the equation

$$\left(\partial_\mu \partial^\mu + m^2\right) G_c(t-t', \vec{x}-\vec{x}') = -\delta_c(t-t')\delta^3(\vec{x}-\vec{x}') \tag{71}$$

Substituting φ by the shifted field $\varphi' + i \int G_c j_c$ from eq. (70) in eq. (69) and applying the fact that G_c is a Green function, we get

$$\begin{aligned} &\int_c \mathrm{d}t \int \mathrm{d}^3x \, (\mathcal{L}_0 + j_c\varphi) \\ &\quad = \int_c \mathrm{d}t \int \mathrm{d}^3x \frac{1}{2}\varphi' \left(-\partial^2 - m^2 + i\varepsilon\right)\varphi' \\ &\quad - \int_c \mathrm{d}t\mathrm{d}t' \int \mathrm{d}^3x\mathrm{d}^3x' \frac{1}{2} j_c(t,\vec{x})(-i)G_c(t-t',\vec{x}-\vec{x}')j_c(t',\vec{x}') \end{aligned} \tag{72}$$

In the same manner we now change the variables in the generating functional of equation (60) from φ to φ'. As this is just a shift, the Jacobian of the transformation is 1. The result of the change of variables is

$$\begin{aligned} Z_\beta[j_c] = &\int \mathcal{D}\varphi' \exp\left[i\int_c \mathrm{d}t \int \mathrm{d}^3x \mathcal{L}_0(\varphi')\right] \\ &\times \exp\left[-\int_c \mathrm{d}t\mathrm{d}t' \int \mathrm{d}^3x\mathrm{d}^3x' \frac{1}{2} j_c(t,\vec{x})\left[-iG_c(t-t',\vec{x}-\vec{x}')\right] j_c(t',\vec{x}')\right] \end{aligned} \tag{73}$$

We see that the second exponential is independent of the field φ'. Therefore we can calculate the first path integral, which is just $Z_\beta[0]$. The generating functional of the free Klein-Gordon theory is therefore simply

$$Z_\beta[j_c] = Z_\beta[0] \exp\left[-\frac{1}{2}\int_c \mathrm{d}t\mathrm{d}t' \int \mathrm{d}^3x\mathrm{d}^3x' j_c(t,\vec{x})G_c(t-t',\vec{x}-\vec{x}')j_c(t',\vec{x}')\right] \tag{74}$$

Here it makes sense to introduce a shorthand notation combining the three spatial coordinates with the time coordinate along a contour C. We define

$$\begin{aligned} x &\equiv (t, \vec{x}) \\ \int_c \mathrm{d}^4x &\equiv \int_c \mathrm{d}t \int \mathrm{d}^3x \\ \delta_c^4(x-x') &\equiv \delta_c(t-t')\delta^3(\vec{x}-\vec{x}') \end{aligned} \tag{75}$$

Equation (74) can now be written as

$$Z_\beta[j_c] = Z_\beta[0] \exp\left[-\frac{1}{2}\int_c \mathrm{d}^4x\mathrm{d}^4x' j_c(x) G_c(x-x') j_c(x')\right] \tag{76}$$

Using this form of the generating functional for calculating the two-point function in equation (63), we get

$$\begin{aligned}
&\langle T_c\left(\varphi(x_1)\varphi(x_2)\right)\rangle \\
&\quad = -\frac{\delta}{\delta j_c(x_1)}\frac{\delta}{\delta j_c(x_2)} \exp\left[-\frac{1}{2}\int_c \mathrm{d}^4x\mathrm{d}^4x' j_c(x) G_c(x-x') j_c(x')\right]\Bigg|_{j_c=0} \\
&\quad = -\frac{\delta}{\delta j_c(x_1)}\left[-\frac{1}{2}\int_c \mathrm{d}^4x' G_c(x_2-x') j_c(x')\right. \\
&\qquad\qquad \left.-\frac{1}{2}\int_c \mathrm{d}^4x\, j_c(x) G_c(x-x_2)\right]\frac{Z_\beta[j_c]}{Z_\beta[0]}\Bigg|_{j_c=0} \\
&\quad = \frac{1}{2}G_c(x_2-x_1) + \frac{1}{2}G_c(x_1-x_2) \\
&\quad = G_c(x_1-x_2)
\end{aligned} \tag{77}$$

From the first derivative we get two identical terms. Taking the second derivative gives six terms, but only those terms survive that get rid of the $j_c(x)$ term as a factor and contain such source terms only in the exponent when we set $j_c = 0$. Obviously, the two-point correlation function is given directly by the Green function.

3.5 Calculating the real-time propagator

We just saw that the propagator, the Green function, and the two-point correlation function are in direct relationship to each other. Now we want to rewrite this quantity using mode functions so that it becomes more accessible computationally.

We start by taking the Fourier transform of the spatial coordinates of the Green function in equation (71). Inserting the spatial Fourier transforms of the Green function and the delta function, given by

$$\begin{aligned} G_c(t-t',\vec{x}-\vec{x}') &= \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{x}')} G_c(t-t',\vec{k}) \\ \delta_c(t-t')\delta^3(\vec{x}-\vec{x}') &= \delta_c(t-t') \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{x}')} \end{aligned} \tag{78}$$

into equation (71), we get

$$\left(\frac{\partial^2}{\partial t^2} + \omega_{\vec{k}}^2\right) G_c(t-t',\vec{k}) = -\delta_c(t-t') \tag{79}$$

where we use

$$\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2} \tag{80}$$

To distinguish functions and their Fourier transforms, we use the convention of calling functions in coordinate space by the arguments x and x', and their Fourier transforms in momentum space by the arguments k and k'.

Taking the same Fourier transform of equation (77) we get

$$\begin{aligned} G_c(t-t',k) &= \langle T_c \varphi(t,k)\varphi(t',k)\rangle \\ G_c^{>}(t-t',k) &\equiv \langle \varphi(t,k)\varphi(t',k)\rangle \\ G_c^{<}(t-t',k) &\equiv \langle \varphi(t',k)\varphi(t,k)\rangle \end{aligned} \tag{81}$$

Here $G_c^{>}$ and $G_c^{<}$ have been defined in such a way that the propagator can according to equation (64) be expressed as

$$G_c(t-t',k) = \theta_c(t-t')G_c^{>}(t-t',k) + \theta_c(t'-t)G_c^{<}(t-t',k) \tag{82}$$

We also see the basic property that directly follows from the definition above:

$$G_c^{>}(t-t',k) = G_c^{<}(t'-t,k) \tag{83}$$

Since the real fields $\varphi(t, k)$ propagate according to the Klein-Gordon equation

$$\left(\frac{\partial^2}{\partial t^2} + \omega_k^2\right) \varphi(t, k) = 0 \tag{84}$$

we see that the Green functions $G_c^{>,<}$ also vanish when we apply the Klein-Gordon operator to them:

$$\left(\frac{\partial^2}{\partial t^2} + \omega_k^2\right) G_c^{>,<}(t - t', k) = 0 \tag{85}$$

Inserting (82) into (79) using the property of the derivative of the delta-function $\delta'(t - t') = -\delta'(t' - t)$ we get:

$$\begin{aligned} \theta_c(t - t') \left(\partial_t^2 + \omega^2(t)\right) G_c^> + \theta_c(t' - t) \left(\partial_t^2 + \omega^2(t)\right) G_c^< + \\ +2\delta_c(t - t') \left(\partial_t G_c^> - \partial_t G_c^<\right) + \delta_c'(t - t') \left(G_c^> - G_c^<\right) \quad = \quad \delta_c(t - t') \end{aligned} \tag{86}$$

Here we omitted the arguments $(t - t', k)$ which are the same for all Green functions in eq. (86). The first two terms in this equation that contain the Klein-Gordon operator applied to the Green functions $G_c^{>,<}$ vanish as we already saw in equation (85). The other terms only give contributions for $t = t'$ and lead to the conditions

$$\left(\partial_t G_c^>(t - t', k) - \partial_t G_c^<(t - t', k)\right)\big|_{t=t'} \quad = \quad \frac{1}{2} \tag{87}$$

$$G_c^>(0, k) - G_c^<(0, k) \quad = \quad 0 \tag{88}$$

of which the latter turns out to be just a special case of eq. (83).

The solution of equation (85) for the functions $G_c^{>,<}$ can be expressed as a linear combination of *mode functions* $u_k(t)$. These mode functions appear in the Fourier decomposition of the quantum field φ at a time t

$$\varphi(t, \vec{x}) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \left(a_k u_k(t) e^{i\vec{k}\vec{x}} + a_k^\dagger u_k^*(t) e^{-i\vec{k}\vec{x}}\right) \tag{89}$$

with the ladder operators a_k and $a_k^\dagger$. They obey the canonical commutation relations

$$\begin{aligned} \left[a_k, a_{k'}^\dagger\right] \quad &= \quad (2\pi)^3 \delta^3(\vec{k} - \vec{k}') \\ \left[\frac{\partial}{\partial t}\varphi(t, \vec{x}), \varphi(t, \vec{x}')\right] \quad &= \quad -i\delta^3(\vec{x} - \vec{x}') \end{aligned} \tag{90}$$

From equations (84) and (89) we see that the mode functions u_k are homogeneous solutions to the Klein-Gordon operator

$$\left(\frac{\partial^2}{\partial t^2} + \omega_k^2\right) u_k(t) = 0 \tag{91}$$

In flat space-time the mode functions are simply given by

$$u_k(t) = \frac{1}{\sqrt{2\omega_k}} e^{-i\omega_k t} \tag{92}$$

Here we do not use this expression but we retain the general form $u_k(t)$ so that we can adapt our results more easily to the case of a curved space-time later.

Inserting (89) into equation (81) we get

$$G_c^{>,<}(t-t', \vec{x}-\vec{x}') = \left\langle \int \frac{\mathrm{d}^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{x}')} \left(\pm u_k(t) u_k^*(t') \mp u_k(t') u_k^*(t)\right) \right\rangle \tag{93}$$

where we still need to calculate the trace of the thermal average. But instead of calculating the trace directly, we will use a similar ansatz and determine the coefficients using the KMS-condition. A general ansatz for the Green function can be written as

$$G_c^{>,<}(t-t', k) = A_k^{>,<} u_k(t) u_k^*(t') + B_k^{>,<} u_k(t') u_k^*(t) \tag{94}$$

where $A_k^> = B_k^<$ and $A_k^< = B_k^>$ are constant coefficients which we now want to determine. Inserting this ansatz (94) into equation (87) we get

$$(B_k^> - A_k^>) W[u_k, u_k^*] = \frac{1}{2} \tag{95}$$

with the Wronskian $W[u, u^*] = u(t)\dot{u}^*(t) - \dot{u}(t)u^*(t)$. The Wronskian is constant over time and for all modes ω as can be easily seen by calculating its derivative $\partial_t W[u, u^*] = \dot{u}\dot{u}^* + u\ddot{u}^* - \ddot{u}u^* - \dot{u}\dot{u}^* = -\omega^2(uu^* - uu^*) = 0$ using equation (91). The value of the Wronskian can be determined by using the canonical commutation relations (90)

$$\begin{aligned}
&\left[\frac{\partial}{\partial t}\varphi(t, \vec{x}), \varphi(t, \vec{x}')\right] \\
&\quad = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \left(\dot{u}_k(t) u_k^*(t) e^{i\vec{k}(\vec{x}-\vec{x}')} - \dot{u}_k^*(t) u_k(t) e^{-i\vec{k}(\vec{x}-\vec{x}')}\right) \\
&\quad = -\int \frac{\mathrm{d}^3k}{(2\pi)^3} W[u_k(t), u_k^*(t)] e^{i\vec{k}(\vec{x}-\vec{x}')} \\
&\quad = -i\delta^3(\vec{x}-\vec{x}')
\end{aligned} \tag{96}$$

This equation is only valid if the Wronskian satisfies the normalization condition

$$W[u, u^*] = i \tag{97}$$

Immediately equation (95) gives

$$A_k^> - B_k^> = \frac{i}{2} \tag{98}$$

According to our derivation of the real-time formalism, $\omega_k(t \ll 0) = \omega_0$ is constant for large negative times. Therefore the mode functions at small times are plane wave solutions to the differential equation (91). The most general solution of this kind satisfying the Wronskian condition (97) is given by

$$u_k(t \ll 0) = \frac{\sinh \xi}{\sqrt{2\omega_0}} e^{+i(\omega_0 t + \theta_1)} + \frac{\cosh \xi}{\sqrt{2\omega_0}} e^{-i(\omega_0 t + \theta_2)} \tag{99}$$

where the parameter ξ and the phases θ_1 and θ_2 are three arbitrary real constants. Setting $\xi = 0$, the product uu^* is independent of the phases θ_1 and θ_2:

$$u_k(t) u_k^*(t') = \frac{1}{2\omega_0} e^{-i\omega_0(t-t')} \tag{100}$$

and the Green function in equation (94) can be written as

$$G_c^{>,<}(t-t', k) = \frac{1}{2\omega_0} \left(A_k^{>,<} e^{-i\omega_0(t-t')} + B_k^{>,<} e^{-i\omega_0(t'-t)} \right) \tag{101}$$

From the KMS condition (20) we directly obtain the periodicity condition

$$G_c^>(t-t', k) = G_c^<((t+i\beta) - t', k) \tag{102}$$

Inserting the Green function (101) into the periodicity condition (102) and setting $t' = t \ll 0$, we get

$$A_k^> + B_k^> = B_k^> e^{\beta\omega_0} + A_k^> e^{-\beta\omega_0} \tag{103}$$

or $A_k^> = B_k^> e^{\beta\omega_0}$. Together with equation (98) we finally get

$$\begin{aligned} A_k^> &= \frac{-i}{2(e^{-\beta\omega_0} - 1)} \\ B_k^> &= \frac{i}{2(e^{\beta\omega_0} - 1)} \end{aligned} \tag{104}$$

These parameters from the ansatz in equation (94) determine the full propagator from equation (82) to be

$$\begin{aligned} G_c(t-t', k) &= \frac{i}{2} \left[\theta_c(t-t') \left(-\frac{u_k(t)u_k^*(t')}{e^{-\beta\omega_0} - 1} + \frac{u_k(t')u_k^*(t)}{e^{\beta\omega_0} - 1} \right) \right. \\ &\quad \left. + \theta_c(t'-t) \left(\frac{u_k(t)u_k^*(t')}{e^{\beta\omega_0} - 1} - \frac{u_k(t')u_k^*(t)}{e^{-\beta\omega_0} - 1} \right) \right] \end{aligned} \tag{105}$$

One can further simplify this expression by using $\theta_c(t-t') = 1 - \theta_c(t'-t)$ and by introducing the bosonic number density

$$n(\omega_0) \equiv \frac{1}{e^{\beta\omega_0} - 1} \tag{106}$$

and obtain an equation for the propagator where ω_0 is entirely contained in the bosonic number density:

$$\boxed{\begin{aligned} G_c(t-t',k) &= \frac{i}{2}\left[\theta_c(t-t')u_k(t)u_k^*(t') + \theta_c(t'-t)u_k(t')u_k^*(t)\right. \\ &\quad \left. + n(\omega_0)\left(u_k(t)u_k^*(t') + u_k(t')u_k^*(t)\right)\right] \end{aligned}} \tag{107}$$

Note the occurrence of two different ω in this equation when we will express the mode functions $u_k(t)$ by their WKB-approximation (164): In a curved space-time $\omega = \omega_{\vec{k}}(t)$ from the mode functions will be time-dependent and will change for a specific wave vector $\vec{k}$ with the mass $m(t)$, whereas $\omega_0 = \omega_{\vec{k}}(t \ll 0)$ from the number density will be a $\vec{k}$-dependent but time-independent constant that will represent the initial conditions. In a flat space-time however, both, ω and ω_0, are the same.

Let us finally note how the Green function vanishes if one of the times t or t' lies on C_3 of the real-time path and the other on C_+ or C_-. Using equation (100) for large negative times t and t' and with $t' = T - i\sigma$ lying on C_3 we effectively get

$$\begin{aligned} &\lim_{T\to-\infty} G_c(t-T+i\sigma,\omega) \\ &\quad = \frac{i}{4\omega_0}\lim_{T\to-\infty}\left(\frac{e^{-i\omega_0(t-T+i\sigma)}}{e^{\beta\omega_0}-1} - \frac{e^{i\omega_0(t-T+i\sigma)}}{e^{-\beta\omega_0}-1}\right) \to 0 \end{aligned} \tag{108}$$

by virtue of the Riemann-Lebesgue lemma [31]. We see that the propagator cannot connect a point on C_3 with a point on C_+ or C_-. This means that the generating functional in equation (76) cannot have mixed terms combining J_3 with J_+ or J_-. The contribution to the path integral from the branch C_3 can be factorized and sources on this branch can safely be set to zero. The remaining contour which consists of the parts C_+ and C_- is really the relevant part and represents a closed path in the complex t-plane. In the next section we will see how these two branches of the closed contour naturally lead to a doubling of the degrees of freedom and to a propagator matrix.

3.6 Matrix structure for propagators

We just saw that a description of the propagator can be reduced to the two branches of the closed-time-path, namely C_+ and C_-. The resulting Green function (107) now has four possible propagator structures that depend on how the fields of the propagator are distributed to the two branches. Using the definition of the contour-theta-function (65) we can denote them as

$$\begin{aligned}
G_{++}(t-t',k) &= \frac{i}{2}\left[\theta(t-t')u_k(t)u_k^*(t') + \theta(t'-t)u_k(t')u_k^*(t)\right.\\
&\quad \left. +n(\omega_0)\left(u_k(t)u_k^*(t') + u_k(t')u_k^*(t)\right)\right]\\
G_{+-}(t-t',k) &= \frac{i}{2}\left[n(\omega_0)u_k(t)u_k^*(t') + (1+n(\omega_0))\,u_k(t')u_k^*(t)\right]\\
G_{-+}(t-t',k) &= \frac{i}{2}\left[(1+n(\omega_0))\,u_k(t)u_k^*(t') + n(\omega_0)u_k(t')u_k^*(t)\right]\\
G_{--}(t-t',k) &= \frac{i}{2}\left[\theta(t'-t)u_k(t)u_k^*(t') + \theta(t-t')u_k(t')u_k^*(t)\right.\\
&\quad \left. +n(\omega_0)\left(u_k(t)u_k^*(t') + u_k(t')u_k^*(t)\right)\right]
\end{aligned} \tag{109}$$

The subscripts for the Green functions + and − denote the branches of the contour on which the respective time coordinates reside. In terms of ensemble averages of the scalar field φ according to equations (81) and (82), the propagators take the form

$$\begin{array}{lcll}
G_{++}(t-t',k) &=& \langle T\varphi(t,k)\varphi(t',k)\rangle & t,t' \in C_+\\
G_{+-}(t-t',k) &=& \langle \varphi(t',k)\varphi(t,k)\rangle & t \in C_+, t' \in C_-\\
G_{-+}(t-t',k) &=& \langle \varphi(t,k)\varphi(t',k)\rangle & t \in C_-, t' \in C_+\\
G_{--}(t-t',k) &=& \langle T^*\varphi(t,k)\varphi(t',k)\rangle & t,t' \in C_-
\end{array} \tag{110}$$

where T^* denotes anti-time ordering.

Writing the propagator this way suggests that we can similarly define a doublet of field variables and sources as

$$\begin{aligned}
\varphi_a &= \begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix}\\
j_a &= \begin{pmatrix} j_+ \\ j_- \end{pmatrix}
\end{aligned} \tag{111}$$

where $a = +,-$; $\varphi_+, j_+ \in C_+$ and $\varphi_-, j_- \in C_-$. If we furthermore assume that the metric in this two-dimensional space is $(1,-1)$, then we can write the generating functional for the free theory in equation (76) as

$$Z_\beta[j_+,j_-] = Z_\beta[0]\exp\left[-\frac{1}{2}\int \mathrm{d}^4x\mathrm{d}^4x' j^a(x)G_{ab}(x-x')j^b(x')\right] \tag{112}$$

This would represent the generating functional corresponding to an action

$$\begin{aligned} S &= S(\varphi_+, j_+) - S(\varphi_-, j_-) \\ &= \int \mathrm{d}^4x \, (\mathcal{L}(\varphi_+, j_+) - \mathcal{L}(\varphi_-, j_-)) \end{aligned} \tag{113}$$

and the components of the propagator could be simply written as

$$G_{ab}(x, x') = (-i)^2 \frac{1}{Z_\beta[0]} \left. \frac{\delta^2 Z_\beta[j]}{\delta j^a(x) \delta j^b(x')} \right|_{j=0} \tag{114}$$

In this case we integrate time over the usual interval $-\infty \leq t \leq \infty$ instead of using the contour C. The need for a second branch C_- of the closed-time-path contour became obsolete by doubling the degrees of freedom. We can write the Green function as a 2×2 matrix

$$G = \begin{pmatrix} G_{++} & G_{+-} \\ G_{-+} & G_{--} \end{pmatrix} \tag{115}$$

One can think of this as describing the two branches of the closed-time-path contour, or, alternatively, as a matrix in the space of the doubled degrees of freedom. Not all of these components are independent of each other. In fact, from equations (109) one can see that they obey the constraint relation

$$G_{++} + G_{--} = G_{+-} + G_{-+} \tag{116}$$

4 Scalar field theory in curved space-time

4.1 Scalar field theory with a $\lambda\varphi^4$ self interaction

Scalar field theory in a background geometry with a $\lambda\varphi^4$ self interaction is a simple model of a renormalizable quantum field theory in curved space-time. It can be used for describing phase transitions characterized by a scalar order parameter like the one for the Higgs particle of the standard model of electroweak interactions. Its Lagrangian density takes the form [16]

$$\mathcal{L}[\varphi] = \frac{1}{2} g^{\mu\nu}\partial_\mu\varphi\partial_\nu\varphi - \frac{1}{2} m^2\varphi^2 - \mathcal{V}[\varphi] \tag{117}$$

$$\mathcal{V}[\varphi] = -\frac{1}{2}\left(\mu^2 + m^2\right)\varphi^2 + \frac{\lambda}{4!}\varphi^4 \tag{118}$$

where the difference to the Lagrangian in equation (61) lies in the background metric, represented by the metric tensor $g^{\mu\nu}$. The thermal mass term $-m^2\varphi^2$ is included in these equations so that we can describe the classical propagator of the theory. The action of this Lagrangian is given by

$$\mathcal{S}[\varphi] = \int \mathcal{L}[\varphi]\sqrt{-g}\, d^4x \tag{119}$$

where $g \equiv \det g$ is defined as the determinant of the metric. The square root of $(-g)$ is included in order to make the action relativistically invariant. We use the variational principle $\delta\mathcal{S}/\delta\varphi = 0$ to obtain the equation of motion for the quantum field φ. Integration by parts of the first term in (117) yields an expression that contains a derivative of the metric:

$$\underbrace{-\partial_\mu\left(\sqrt{-g}g^{\mu\nu}\partial_\nu\varphi\right) - \sqrt{-g}m^2\varphi}_{\text{free part}} + \underbrace{\sqrt{-g}\left(\mu^2 + m^2\right)\varphi + \sqrt{-g}\frac{\lambda}{3!}\varphi^3}_{\text{perturbation}} = 0 \tag{120}$$

The free part of this equation defines the propagator $G_c(x, x') = \langle T_c\varphi(x)\varphi(x')\rangle$. The other two terms are treated as a perturbation and will be taken into consideration later in the mass correction by a one-loop resummation. Let us just mention here that one-loop corrections will give an additional term $-\sqrt{-g}\delta m^2\varphi$ in the perturbation. The parameter m^2 will be chosen in the resummation such that the three mass terms cancel in the perturbation, that is $m^2 + \mu^2 - \delta m^2 = 0$, and the remaining part of the perturbation $\sqrt{-g}\lambda\varphi^3/3!$ will be proportional to λ.

The defining equation for the free propagator is:

$$\left(\partial_\mu\left(\sqrt{-g}g^{\mu\nu}\partial_\nu\right)+\sqrt{-g}m^2\right)G_c(x,x')=-\delta_c^{(4)}(x-x') \tag{121}$$

Note how this equation trivially reduces to equation (71) for the metric $g=(+,-,-,-)$. The delta function represents a short-hand version of the contour delta of the real time formalism defined in equation (75).

In the following we will assume a spatially flat universe. The metric $g(x)$ should only depend on time and not on space:

$$g(x)=g(x^0) \tag{122}$$

In this metric it is useful to apply a Fourier transformation only to the spatial part of the four-vector in order to calculate the propagator. Inserting the Fourier transformation expressions defined in the equations (78) into equation (121) and taking derivatives of the spatial part, assuming that $g^{0m}=g^{m0}=0$ for $m=1,\,2,\,3$, we finally get to the defining equation for $G_c(t-t',\vec{k})$

$$\begin{aligned}\left(\frac{\partial}{\partial x^0}\left(\sqrt{-g}g^{00}\frac{\partial}{\partial x^0}\right)+\sqrt{-g}g^{mn}(ik_m)(ik_n)+\sqrt{-g}m^2\right)G_c(t-t',\vec{k})\\=-\delta_c(t-t')\end{aligned} \tag{123}$$

The homogeneous solutions to this equation describe the mode functions $u_{\vec{k}}(t)$ and can be used to calculate the propagator.

$$\left(\frac{\partial}{\partial x^0}\left(\sqrt{-g}g^{00}\frac{\partial}{\partial x^0}\right)-\sqrt{-g}g^{mn}k_mk_n+\sqrt{-g}m^2\right)u_{\vec{k}}(t)=0 \tag{124}$$

For a time-independent metric these equations would reduce to the equations (79) and (91) that we already used in the last chapter.

4.2 Metric and Scale Factor

4.2.1 Comoving metric

The cooling of the quantum system in our model will be driven by an expansion of the whole system. There are different ways for describing an expansion. For example, one could choose a static background metric and let the particles fly apart from each other. Although this approach seems conceptually easy, the processes during the phase transitions of the early universe is far better described by an expanding metric. That means that the background itself expands according to a scale factor $a(t)$ which basically describes the large scale properties of the expanding system.

A description like this first came up in the 1920's with the solution to a homogeneous and isotropic expanding universe by Friedmann, Robertson and Walker. We already presented the Friedmann-Robertson-Walker metric in equation (1). This is an example of a *comoving metric*, because particles at rest with $d\vec{x} = 0$ have $ds^2 = dt^2$ meaning that the time coordinate t in eq. (1) is the proper time measured by an observer at rest in the comoving frame. Observers at rest in the comoving frame remain at rest and its comoving coordinates remain unchanged.

Inflation makes any universe flat, regardless of its initial properties. Therefore we can safely assume the metric of a flat universe:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = dt^2 - a^2(t) dx^2 \tag{125}$$

One can easily read off the components of the metric tensor that only has entries in the diagonal $g_{\mu\nu}(t) = \mathrm{diag}(1, -a^2(t), -a^2(t), -a^2(t))$ using $dx^0 = dt$. In the differential equation for the mode functions (124) we also need the square root of the determinant of the metric $\sqrt{-g} = a^3$ and the metric with upper indices $g^{\mu\nu} = \mathrm{diag}(1, -a^{-2}, -a^{-2}, -a^{-2})$ which satisfies $g_{\mu\nu} g^{\nu\sigma} = \delta_\mu^{\ \sigma}$, so that we finally obtain

$$\left(\frac{\partial}{\partial t} \left(a^3(t) \frac{\partial}{\partial t} \right) + a(t) \vec{k}^2 + a^3(t) m^2 \right) u_{\vec{k}}(t) = 0 \tag{126}$$

Denoting the shorthand versions of $\vec{k}^2$, $a(t)$, and $u_{\vec{k}}(t)$ as k^2, a, and u respectively and the derivation with respect to time by a dot, we find $3a^2 \dot{a} \dot{u} + a^3 \ddot{u} + ak^2 u + a^3 m^2 u = 0$. We can get rid of the $\dot{u}$-term in this equation by the transformation $u(t) = a^n(t) \tilde{u}(t)$ where $n = -3/2$. Dividing the resulting equation by $a^{-3/2}(t)$ we get:

$$\boxed{\ddot{\tilde{u}} + \left(\frac{k^2}{a^2} + m^2 - \frac{3}{4} \left(\frac{\dot{a}}{a} \right)^2 - \frac{3}{2} \frac{\ddot{a}}{a} \right) \tilde{u} = 0} \tag{127}$$

Defining the expression in the bracket to be $\omega_{\vec{k}}^2(t)$, we get a simple wave equation with $\vec{k}$- and time-dependent dispersion $\ddot{\tilde{u}} + \omega_{\vec{k}}^2(t) \tilde{u} = 0$. Unless $\omega_{\vec{k}}^2(t)$ changes too quickly, one can use the WKB-approximation to describe the behavior of the mode functions $\tilde{u}_{\vec{k}}(t) = a^{3/2}(t) u_{\vec{k}}(t)$.

4.2.2 Conformal time metric

For certain kinds of calculations it turns out that another form of the metric is more easy to handle. That is, also the time dimension will be scaled according to the scale factor. Introducing such a *conformal time*, we obtain a line element of the space-time that is conformal to Minkowski space-time. As a result one can treat space-time like an ordinary Minkowski space-time and equations get more elegant in this metric. Of course there is some additional complication when one wants to convert the results back to a metric with a non-conformal time. The line element of the conformal time metric is given by

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = a^2(\eta)\left(d\eta^2 - dx^2\right) \quad \text{with } dt = a(\eta)dx^0 = a(\eta)d\eta \tag{128}$$

The scale factor $a(\eta)$ is now a function of η and not of t. One can use the relationship between the two time-coordinates $\eta(t) = \int_{t_0}^{t} a^{-1}(t')dt'$ and use its inverse function $t(\eta)$ to finally obtain $a(\eta) = a(t(\eta))$. Also the metric is a function of the conformal time so that $g_{\mu\nu}(\eta) = \text{diag}(b^2(\eta), -b^2(\eta), -b^2(\eta), -b^2(\eta))$; $\sqrt{-g} = b^4$; and $g^{\mu\nu} = \text{diag}(b^{-2}, -b^{-2}, -b^{-2}, -b^{-2})$. In this metric equation (124) takes the form:

$$\left(\frac{\partial}{\partial\eta}\left(a^2(\eta)\frac{\partial}{\partial\eta}\right) + a^2(\eta)\vec{k}^2 + a^4(\eta)m^2\right)u_{\vec{k}}(\eta) = 0 \tag{129}$$

Defining the dot now as a derivative with respect to η, this equation becomes $2a\dot{a}\dot{u} + a^2\ddot{u} + a^2k^2u + a^4m^2u = 0$. Again, we can get rid of the term containing the first derivative $\dot{u}$ by the transformation $u(\eta) = a^n(\eta)\tilde{u}(\eta)$, now with $n = -1$. Dividing this equation by $a(\eta)$ we get:

$$\ddot{\tilde{u}} + \left(k^2 + m^2a^2 - \frac{\ddot{a}}{a}\right)\tilde{u} = 0 \tag{130}$$

4.3 Calculating the propagator

In the following we want to calculate the propagator $G_c(t-t', \vec{k})$ and express it in terms of the mode functions $u_{\vec{k}}(t)$. The steps are quite similar to the derivation of the propagator in a static background, therefore we will concentrate on the differences in the case of an expanding system. For now, we assume the comoving metric of equation (125), but the calculation is completely analogous in the case of the conformal time metric (128). Using the comoving metric (125) in (123), we get:

$$\left(3a^2\dot{a}\frac{\partial}{\partial t} + a^3\frac{\partial^2}{\partial t^2} + a\vec{k}^2 + a^3m^2\right)G_c(t-t', \vec{k}) = -\delta_c(t-t') \tag{131}$$

Similarly as in the calculation of the mode functions, one can get rid of the first-derivative term by the transformation

$$G_c(t-t',\vec{k}) = a^n(t)a^n(t')\tilde{G}_c(t-t',\vec{k}) \tag{132}$$

where $n = -3/2$. The $a^n(t')$-term in this transformation rule ensures that $\tilde{G}_c(t-t',\vec{k})$ is symmetric in t and t'. Bringing overall a-factors to the r.h.s. where $a^{-3/2}(t)$ and $a^{3/2}(t')$ cancel because of the $\delta(t-t')$-function, we finally get:

$$\begin{aligned} \left(\frac{\partial^2}{\partial t^2} + \omega_{\vec{k}}^2(t)\right)\tilde{G}_c(t-t',\vec{k}) &= -\delta_c(t-t') \\ \text{with} \quad \omega_{\vec{k}}^2(t) &= m^2 + \frac{k^2}{a^2} - \frac{3}{4}\left(\frac{\dot{a}}{a}\right)^2 - \frac{3}{2}\frac{\ddot{a}}{a} \end{aligned} \tag{133}$$

This is almost the same equation as (79). The difference lies in the fact that $\omega_{\vec{k}}(t)$ is time-dependent now and that the propagator G_c is replaced by the rescaled propagator $\tilde{G}_c$. Just as in equation (81) we define the rescaled propagator as

$$\tilde{G}_c(t-t',\vec{k}) = \left\langle T_c\tilde{\varphi}(t,\vec{k})\tilde{\varphi}(t',\vec{k})\right\rangle \tag{134}$$

where the rescaled fields $\tilde{\varphi}(t,\vec{k}) = a^{3/2}(t)\varphi(t,\vec{k})$ satisfy the homogeneous Klein-Gordon equation

$$\left(\frac{\partial^2}{\partial t^2} + \omega_{\vec{k}}^2(t)\right)\tilde{\varphi}(t,\vec{k}) = 0 \tag{135}$$

Rescaling is also necessary for the Fourier decomposition of the quantum field $\tilde{\varphi}$ as in equation (89). Here we find that the mode functions $u_{\vec{k}}$ also have to be changed by the scale factor $a(t)$ according to

$$\tilde{u}_{\vec{k}}(t) = a^{3/2}(t)u_{\vec{k}}(t) \tag{136}$$

if they should be homogeneous solutions to the Klein-Gordon equation. We already anticipated this result in the Klein Gordon equation (127) for the rescaled mode functions $\tilde{u}_{\vec{k}}$. Also the canonical commutation relations (90) should be applied to the rescaled field $\tilde{\varphi}$

$$\left[\frac{\partial}{\partial t}\tilde{\varphi}(t,\vec{x}),\tilde{\varphi}(\vec{x}',t)\right] = -i\delta^3(\vec{x}-\vec{x}') \tag{137}$$

Following the steps from equation (94) to equation (107) in exactly the same manner, only replacing the quantities G, φ, and u by their rescaled counterparts $\tilde{G}$, $\tilde{\varphi}$, and $\tilde{u}$, we finally get to the expression of the rescaled propagator. Literally going through the very same steps, writing an ansatz for $\tilde{G}^{>,<}$, finding the same Wronskian $W[\tilde{u}, \tilde{u}^*]$ from the canonical commutation relations, setting up plane wave solutions for the mode functions $\tilde{u}$ at large negative times and applying the KMS condition to the propagator we finally get

$$\begin{aligned} \tilde{G}_c(t-t',\vec{k}) &= \frac{i}{2}\Big[\theta_c(t-t')\tilde{u}_{\vec{k}}(t)\tilde{u}^*_{\vec{k}}(t') + \theta_c(t'-t)\tilde{u}_{\vec{k}}(t')\tilde{u}^*_{\vec{k}}(t) \\ &\qquad + n(\omega_0(\vec{k}))\left(\tilde{u}_{\vec{k}}(t)\tilde{u}^*_{\vec{k}}(t') + \tilde{u}_{\vec{k}}(t')\tilde{u}^*_{\vec{k}}(t)\right)\Big] \end{aligned} \tag{138}$$

The full propagator including the scale factor $a(t)$ takes the form

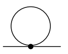
$$\begin{aligned} G_c(t-t',\vec{k}) &= \frac{1}{a^{3/2}(t)a^{3/2}(t')}\frac{i}{2}\left[\theta(t-t')\tilde{u}(t)\tilde{u}^*(t') + \theta(t'-t)\tilde{u}(t')\tilde{u}^*(t)\right. \\ &\qquad \left. + n_{\vec{k}}\left(\tilde{u}(t)\tilde{u}^*(t') + \tilde{u}(t')\tilde{u}^*(t)\right)\right] \end{aligned} \tag{139}$$

In the case of a propagator with $t = t'$ this equation simplifies to

$$\boxed{G_c(t-t,\vec{k}) = \frac{i}{2a^3(t)}(1+2n_{\vec{k}})\left|\tilde{u}_{\vec{k}}(t)\right|^2} \tag{140}$$

where $n_{\vec{k}} = \frac{1}{e^{\omega_{\vec{k}}(0)\beta}-1}$ is the thermal bosonic distribution factor.

4.4 One-loop mass correction

The mass correction to the lowest order in the $\lambda\varphi^4$-theory is given by the one-loop term. The squared mass can be expressed as $m^2 = -\mu^2 + \delta m^2$ where $\delta m^2 = -i\lambda[$  $]$. This graph can be calculated using usual Feynman rules and gives $\delta m^2(t) = -i\lambda\int d^3\vec{k}G_c(t-t,\vec{k})/(2\pi)^3$. Inserting the result from equation (140), the equation for δm^2 is given by

$$\delta m^2(t) = \frac{\lambda}{2a^3(t)}\int\frac{d^3\vec{k}}{(2\pi)^3}(1+2n_{\vec{k}})\left|\tilde{u}_{\vec{k}}(t)\right|^2 \tag{141}$$

The self-consistency relation for m^2 thus reads:

$$m^2(t) = -\mu^2 + \frac{\lambda}{2a^3(t)}\int\frac{d^3\vec{k}}{(2\pi)^3}(1+2n_{\vec{k}})\left|\tilde{u}_{\vec{k}}(t)\right|^2 \tag{142}$$

4.5 Mass renormalization

The integral for the mass correction in equation (141) turns out to be divergent. At a first glance, it does not make sense that a mass correction should be larger than the unperturbed mass itself, let alone infinitely large. Nevertheless useful information can be extracted from this equation with an appropriate renormalization scheme. Such a renormalization is mandatory to specify the meaning of the masses from the Lagrangian. It defines a new renormalized mass μ_R or a renormalized coupling constant λ_R which now appears in the equation of the Lagrangian density instead of the original bare parameters.

$$\begin{aligned} \mu^2 &= \mu_R^2 + \delta_\mu \\ \lambda &= Z(\lambda_R)\lambda_R \end{aligned} \tag{143}$$

These renormalized quantities represent the physically measured mass and the physically measured coupling constant. Infinities are incorporated in δ-terms and thus hidden from physical measurements. Nevertheless renormalization must be a consistent and well-defined procedure that ensures that one can extract physically relevant results from a theory containing unphysical divergences.

There are several techniques to regularize and renormalize a theory. For example one could introduce a cut-off $\Lambda_{\vec{k}}$ for the wave vector $\vec{k}$ that cuts off the ultraviolet part of the integral, a regime we do not have any physical knowledge about anyway [12]. In this sense the theory is renormalizable if it gives physical results that are independent of the choice of $\Lambda_{\vec{k}}$. The arbitrarily introduced cut-off constant cancels out at the end of the calculation.

Another renormalization procedure is dimensional regularization . Here one tries to find a generalization of the divergent integral from 3 spatial dimensions to d-dimensions. In certain cases this leads to a finite expression that can be calculated for a real d where an analytic continuation for $d = 3$ exists.

In the following, a way of renormalizing the mass correction integral (141) is presented that absorbs all divergences in the mass and coupling constant parameters. In the end we will get the same equations but with renormalized parameters that are finite and contain the relevant information that can be observed physically. The bare parameters are infinite and physically not accessible.

In order to handle the divergences analytically, we approximate the mode functions $\tilde{u}_{\vec{k}}(t)$ by a WKB-approximation. We will discuss the WKB approximation in detail in the next chapter, but let us anticipate some of the results. In the first region before the phase transition the WKB-approximation is given by equation (164). We already know from the discussion before equation (99) that the canonical commutation relations determine the sign in the exponent to be negative so that the mode functions in this approximation are given by

$$\tilde{u}_{\vec{k}}(t) = \frac{1}{\sqrt{2\omega_{\vec{k}}(t)}} e^{-i\int_{t_0}^{t} dt' \omega_{\vec{k}}(t')} \tag{144}$$

and the absolute square of this expression simply becomes

$$\left|\tilde{u}_{\vec{k}}(t)\right|^2 = \frac{1}{2\omega_{\vec{k}}(t)} \tag{145}$$

Approximating $\omega_{\vec{k}}(t)$ from equation (133) by $\sqrt{m^2(t) + k^2/a^2(t)}$ we can write the squared mass including the one-loop correction from equation (142) as

$$m^2(t) = -\mu^2 + \frac{\lambda}{2a^3(t)} \int \frac{d^3\vec{k}}{(2\pi)^3} \left(1 + \frac{2}{e^{\beta\sqrt{m^2(0)+\frac{k^2}{a^2(0)}}} - 1}\right) \frac{1}{2\sqrt{m^2(t) + \frac{k^2}{a^2(t)}}} \tag{146}$$

The integral turns out to have quadratic and logarithmic divergences which we will see in a moment.

Let us now introduce a change of variables for the wave vector $\vec{k}$ which does not have to do anything with the renormalization, but just makes the $a(t)$-dependence of the integral more transparent. Since the integral is spherically symmetric in $\vec{k}$, we can replace $d^3\vec{k}/(2\pi)^3$ by $4\pi k^2 dk/(2\pi)^3 = k^2 dk/2\pi^2$ and $\vec{k}$ by $k = |\vec{k}|$. Introducing a *physical wave vector*

$$\bar{k}(t) \equiv \frac{k}{a(t)} \tag{147}$$

we note that the integration boundaries 0 and ∞ do not change so that we safely can omit the t-dependence from $\bar{k}(t)$ and write:

$$m^2(t) = -\mu^2 + \frac{\lambda}{2} \int_0^\infty \frac{\bar{k}^2 d\bar{k}}{2\pi^2} \left(1 + \frac{2}{e^{\beta\sqrt{m^2(0)+\bar{k}^2\frac{a^2(t)}{a^2(0)}}} - 1}\right) \frac{1}{2\sqrt{m^2(t) + \bar{k}^2}} \tag{148}$$

Obviously the first term in the brackets contributes to the quadratically divergent part of the integral. The second term in the brackets, the distribution factor, ensures that this part of the integral falls off exponentially fast for

$\bar{k} \to \infty$ so that there is no ultraviolet problem here. It is not uncommon that the divergence in the expression for the mass correction is entirely contained in the zero temperature part and that the temperature dependent part is free from ultraviolet divergences [32]. That means that zero temperature counter terms are sufficient to renormalize the theory.

We want $m^2(t)$ to be our finite renormalized mass for which the equation above is valid. To compensate the divergent integral, its constant divergent part is included in μ^2 and the resulting finite mass is defined to be μ_R^2 as in equation (143). Given a finite $m^2(0)$, we can try to get rid of the quadratic divergence by subtracting it from the time-dependent $m^2(t)$. In order to give sense to the subtraction of two infinite quantities, we now introduce a cut-off $\Lambda_{\bar{k}}$ as the upper limit of the integrals. In the end when we have calculated the renormalized mass, we should be able to take the limit $\Lambda_{\bar{k}} \to \infty$ and obtain a finite result that is independent of this cut-off. The difference between the masses thus reads

$$\begin{aligned} m^2(t) - m^2(0) &= \frac{\lambda}{2}\int_0^{\Lambda_{\bar{k}}} \frac{\bar{k}^2 d\bar{k}}{2\pi^2}\left(\frac{1}{2\sqrt{m^2(t)+\bar{k}^2}} - \frac{1}{2\sqrt{m^2(0)+\bar{k}^2}}\right) \\ &\quad + \frac{\lambda}{2}\int_0^{\infty} \frac{\bar{k}^2 d\bar{k}}{2\pi^2} 2n(\bar{k})\left(\frac{1}{2\omega_{\bar{k}}(t)} - \frac{1}{2\omega_{\bar{k}}(0)}\right) \end{aligned} \tag{149}$$

Note that the second integral is exponentially damped because of the $n(\bar{k})$-term and is already finite without the need of regularization by a cut-off.

By forming the difference we got rid of the quadratic divergence in the first integral of equation (149), but it left over a logarithmic divergence[1]. To handle this divergence, we also need to renormalize the coupling constant λ. The theory behind the following renormalization scheme is a sum of bubbles in the scattering amplitude at large N [16, 33]. It turns out that the coupling constant can be renormalized by

$$\lambda_R = \frac{\lambda}{1+\lambda\delta_\lambda} \qquad \Longleftrightarrow \qquad \lambda = \frac{\lambda_R}{1-\lambda_R\delta_\lambda} \tag{150}$$

where

$$\delta_\lambda = \frac{1}{2}\Sigma(0) = \frac{1}{2}\int \frac{1}{4\omega_k^3(0)}\frac{\mathrm{d}^3k}{(2\pi)^3} \tag{151}$$

[1]Using $\int_0^\infty k^2 dk \frac{1}{\omega_k(t)} = \frac{1}{2}k\sqrt{m^2(t)+k^2} - \frac{1}{2}m^2(t)\log\left(k+\sqrt{m^2(t)+k^2}\right)\Big|_{k=0}^{\infty}$ the first quadratic divergent term gives a finite contribution $\frac{1}{4}\left(m^2(t)-m^2(0)\right)$ in the subtraction $m^2(t)-m^2(0)$, but the second term gives an undetermined contribution that diverges like $m^2(t)/m^2(0) \times \lim_{k\to\infty}\log(2k)$.

is the divergent part of λ that comes from the sum of bubbles at large N. Multiplying the whole equation (149) by a factor $(1 - \lambda_R \delta_\lambda)$ and adding the term $\left(m^2(t) - m^2(0)\right) \lambda_R \delta_\lambda$ on both sides of the equation we get:

$$\begin{aligned} m^2(t) - m^2(0) &= \frac{\lambda_R}{2} \int_0^{\Lambda_{\bar{k}}} \frac{\bar{k}^2 d\bar{k}}{2\pi^2} \left(\frac{1}{2\omega_{\bar{k}}(t)} - \frac{1}{2\omega_{\bar{k}}(0)} \right) \\ &+ \lambda_R \left(m^2(t) - m^2(0)\right) \delta_\lambda \\ &+ \frac{\lambda_R}{2} \int_0^{\infty} \frac{\bar{k}^2 d\bar{k}}{2\pi^2} 2n(\bar{k}) \left(\frac{1}{2\omega_{\bar{k}}(t)} - \frac{1}{2\omega_{\bar{k}}(0)} \right) \end{aligned} \tag{152}$$

Now we can integrate the formerly divergent part[2]:

$$\begin{aligned} &\lim_{\Lambda_{\bar{k}} \to \infty} \frac{\lambda_R}{2} \int_0^{\Lambda_{\bar{k}}} \frac{\bar{k}^2 d\bar{k}}{2\pi^2} \left(\frac{1}{2\omega_{\bar{k}}(t)} - \frac{1}{2\omega_{\bar{k}}(0)} + \frac{m^2(t) - m^2(0)}{4\omega_{\bar{k}}^3(0)} \right) \\ &= \frac{\lambda_R}{2} \frac{1}{2\pi^2} \frac{1}{8} \left(m^2(t) \left(\log \frac{m^2(t)}{m^2(0)} - 1 \right) + m^2(0) \right) \end{aligned} \tag{153}$$

so that we finally get

$$\begin{aligned} m^2(t) - m^2(0) &= \frac{\lambda_R}{32\pi^2} \left(m^2(t) \left(\log \frac{m^2(t)}{m^2(0)} - 1 \right) + m^2(0) \right) \\ &+ \frac{\lambda_R}{2} \int_0^{\infty} \frac{\bar{k}^2 d\bar{k}}{2\pi^2} 2n(\bar{k}) \left(\frac{1}{2\omega_{\bar{k}}(t)} - \frac{1}{2\omega_{\bar{k}}(0)} \right) \end{aligned} \tag{154}$$

The logarithmic term on the r.h.s. of this equation is of the order of $m^2(t)$, yet it is multiplied by $\lambda/32\pi^2$, a small number[3] that makes the whole term negligible. Introducing μ_R as the initial time part of this equation we can write:

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2} \int_0^{\infty} \frac{n(\bar{k})}{2\omega_{\bar{k}}(t)} \bar{k}^2 d\bar{k} \tag{155}$$

$$\mu_R^2 = -m^2(0) + \frac{\lambda_R}{2\pi^2} \int_0^{\infty} \frac{n(\bar{k})}{2\omega_{\bar{k}}(0)} \bar{k}^2 d\bar{k} \tag{156}$$

Inserting the definitions of $n(\bar{k})$ and $\omega_{\bar{k}}(t)$ we get the formula for the renormalized mass

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2} \int_0^{\infty} \frac{1}{2\sqrt{m^2(t) + \bar{k}^2}} \frac{1}{e^{\beta\sqrt{m^2(0) + \bar{k}^2 \frac{a^2(t)}{a^2(0)}}} - 1} \bar{k}^2 d\bar{k} \tag{157}$$

[2]Here we use $\int_0^{\Lambda} k^2 dk \frac{1}{\omega_k(t)} = \frac{1}{2} k\omega_k(t) - \frac{1}{2} m^2(t) \log\left(k + \omega_k(t)\right)\Big|_{k=0}^{\Lambda}$ and $\int_0^{\Lambda} k^2 dk \frac{m^2(t)}{\omega_k^3(0)} = -\frac{m^2(t)k}{2\omega_k(0)} + \frac{1}{2} m^2(t) \log\left(k + \omega_k(0)\right)\Big|_{k=0}^{\Lambda}$ so that two of the logarithmic divergent terms cancel.

[3]In our numeric simulations we used $\lambda_R < \frac{1}{100}$, an inflationary model would suggest $\lambda_R \simeq 10^{-12}$.

It is this equation that we want to analyze and try to understand analytically as much as possible.

In this section we showed how to renormalize the one-loop mass correction for a WKB-approximation before the phase transition $t < t_{TP}$. The same result also holds for times $t > t_{TP}$ after the phase transition, because the ultraviolet divergence stems from the zero temperature part which is the same in both cases. For a general mode function the squared mass can therefore be written as

$$\boxed{m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2 a^3(t)} \int_0^\infty |\tilde{u}_k(t)|^2 \frac{1}{e^{\beta\omega_k(0)} - 1} k^2 dk} \tag{158}$$

where we obtained the factor $a^3(t)$ in the denominator by changing from physical wave vectors $\bar{k}(t)$ back to time-independent wave vectors k.

The mass in equation (158) can be calculated if we know the mode functions $\tilde{u}_k(t)$. They are determined by the differential equation (127). For each mode $k \in (0, \infty)$ we get such a differential equation, which gives infinitely many of these equations that we have to solve simultaneously. One way to tackle this seemingly hopeless situation is by using the WKB approximation of the mode functions. The WKB approximation is given by a simple exponential function that can be inserted into equation (158) to give a more manageable integral.

5 WKB approximation

5.1 WKB solution and its restrictions

The WKB approximation [34] is a method for approximating the solutions to a second-order differential equation with an arbitrary potential. The basic idea behind the method is to separate the sinusoidal solution into its amplitude, its frequency and its phase. Under certain conditions these quantities can be approximated independently from the given potential and easily put together to form the solution.

WKB was first used to approximate the one-dimensional Schrödinger equation for an arbitrary potential $V(x)$ [34, 35]

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x) = E\psi(x) \tag{159}$$

This is basically the same type of equation as (127), the defining differential equation for the mode functions that are needed to calculate the propagator. Here we want to solve with respect to time instead of space and the potential becomes $\omega_{\vec{k}}^2(t) \approx -\frac{2m}{\hbar^2}(V(x) - E)$. In the following we will not worry about the exact form of $\omega_{\vec{k}}(t)$, but try to solve the equation for a general time-dependent $\omega_{\vec{k}}(t)$[4]:

$$\left(\partial_t^2 + \omega_{\vec{k}}^2(t)\right) u_{\vec{k}}(t) = 0 \tag{160}$$

If $\omega_{\vec{k}}(t) = \bar{\omega}_{\vec{k}}$ was constant in time, there would be plane wave solutions of the form $u_{\vec{k}}(t) = e^{\pm i\bar{\omega}_{\vec{k}}t}$. If $\omega_{\vec{k}}(t)$ is only slowly varying there should be solutions with a similar form (where we yet have to find out what *slowly* means). Therefore it is reasonable to try the following ansatz with real $R(t)$ and $S(t)$:

$$u_{\vec{k}}(t) = R(t)e^{iS(t)} \tag{161}$$

Inserting this in equation (160) gives:

$$\frac{d^2R(t)}{dt^2} + 2i\frac{dR(t)}{dt}\frac{dS(t)}{dt} + iR(t)\frac{d^2S(t)}{dt^2} - R(t)\left(\frac{dS(t)}{dt}\right)^2 + \omega^2(t)R(t) = 0 \tag{162}$$

This equation can be separated into an imaginary part $2\dot{R}\dot{S} + R\ddot{S} = 0$ and a real part $\ddot{R} - R\dot{S}^2 + \omega^2 R = 0$. Solving the first equation gives a condition

[4] In this chapter u takes the role of the scaled mode function $\tilde{u}$ of the previous chapters.

for R and S: Integrating $\dot{R}/R = -\frac{1}{2}\ddot{S}/\dot{S}$ and exponentiating it gives $R = c/\sqrt{\dot{S}}$. Inserting this result and its derivatives $\dot{R}/c = -\frac{1}{2}\dot{S}^{-3/2}\ddot{S}$ and $\ddot{R}/c = \frac{3}{4}\dot{S}^{-5/2}\ddot{S}^2 - \frac{1}{2}\dot{S}^{-3/2}\dddot{S}$ into the real part of equation (162) gives a differential equation for $S(t)$ (the following equation is already divided by $R(t)$):

$$\frac{3}{4}\dot{S}^{-2}\ddot{S}^2 - \frac{1}{2}\dot{S}^{-1}\dddot{S} - \dot{S}^2 + \omega^2 = 0 \tag{163}$$

Up to now everything has been exact, but this equation is really difficult to solve if we want to consider a general $\omega(t)$-function. Since we want to consider *slowly* varying functions $\omega(t)$, it is reasonable to assume that also the parameters $R(t)$ and $S(t)$ vary slowly, meaning that we neglect the second and third derivatives of $S(t)$ in equation (163). The resulting equation is simply solved by $\dot{S} = \pm\omega$ or $S(t) = \pm\int_{t_0}^{t} dt'\omega(t')$. Therefore we get the following solution in the WKB approximation:

$$\boxed{u_{\vec{k}}(t) = \frac{c_{\vec{k}}}{\sqrt{\omega_{\vec{k}}(t)}} e^{\pm i\int_{t_0}^{t} dt'\omega_{\vec{k}}(t')}} \tag{164}$$

When is this approximation valid? A criterion would be to demand that the terms in (163) containing the second and third derivatives of $S(t)$ are much smaller than ω^2:

$$\begin{aligned} \left|\tfrac{3}{4}\dot{S}^{-2}\ddot{S}^2\right| &\ll \omega^2 \quad \Rightarrow \quad |\omega^{-2}\dot{\omega}^2| \ll \omega^2 \quad \Rightarrow \quad |\dot{\omega}| \ll \omega^2 \\ \left|\tfrac{1}{2}\dot{S}^{-1}\dddot{S}\right| &\ll \omega^2 \quad \Rightarrow \quad |\omega^{-1}\ddot{\omega}| \ll \omega^2 \quad \Rightarrow \quad |\ddot{\omega}| \ll \omega^3 \end{aligned} \tag{165}$$

Using $\frac{d}{dt}\left(\frac{1}{\omega}\right) = -\frac{\dot{\omega}}{\omega^2}$ and $\frac{d^2}{dt^2}\left(\frac{1}{\omega^2}\right) = -2\frac{\ddot{\omega}}{\omega^3} + 6\left(\frac{\dot{\omega}}{\omega^2}\right)^2$ we may rewrite these two conditions as

$$\boxed{\left|\frac{d}{dt}\left(\frac{1}{\omega_{\vec{k}}(t)}\right)\right| \ll 1 \quad \text{and} \quad \left|\frac{d^2}{dt^2}\left(\frac{1}{\omega_{\vec{k}}^2(t)}\right)\right| \ll 1} \tag{166}$$

The way the WKB approximation has been derived here, there are no further restrictions on any higher derivatives of ω than its second derivative. That means that $\dddot{\omega}$ and higher derivatives of ω may have any value as long as the conditions (166) are met[5].

[5]Strictly speaking, the conditions (166) are sufficient, but not necessary for the WKB approximation to be valid. From equation (163) it follows that it is sufficient to demand that $\left|\frac{3}{4}\dot{S}^{-2}\ddot{S}^2 - \frac{1}{2}\dot{S}^{-1}\dddot{S}\right| \ll \omega^2$ or $\left|3\left(\frac{\dot{\omega}}{\omega^2}\right)^2 - 2\frac{\ddot{\omega}}{\omega^3}\right| \ll 1$. This gives somewhat milder restrictions on $\omega(t)$. In particular, one can find a solution for $\omega(t)$ where the l.h.s. of this inequality vanishes, thereby making the WKB approximation exact: Integrating the condition $\frac{\ddot{\omega}}{\dot{\omega}} = \frac{3}{2}\frac{\dot{\omega}}{\omega}$and exponentiating it results in $\omega^{-3/2}\dot{\omega} = c$ that can be integrated again to give the solution $\omega(t) = (c_1 t + c_2)^{-2}$. Using such an $\omega(t)$, WKB is no longer an approximation, but the solution (164) solves the differential equation (160) exactly.

5.2 WKB in comoving metric

Let us apply the results of the previous section to the differential equations of the mode functions in a comoving metric without or with conformal time. The solution to these equations in the WKB approximation is easily obtained, but it is the range of validity that has to be checked carefully and thoroughly.

5.2.1 Comoving metric

In the case of a comoving metric, the equation of interest is (compare to eq. (127))

$$\ddot{u}_{\vec{k}}(t) + \left(\frac{k^2}{a^2(t)} + m^2(t) - \frac{3}{4}\left(\frac{\dot{a}(t)}{a(t)}\right)^2 - \frac{3}{2}\frac{\ddot{a}(t)}{a(t)} \right) u_{\vec{k}}(t) = 0 \tag{167}$$

which is of the form of equation (160). Its solution is given by (164) and its restrictions are stated in (166).

It is interesting to see if we can convert these restrictions to somewhat more useful and manageable inequalities. Obviously if we try to apply the restrictions $\left|\frac{d}{dt}\left(\frac{1}{\omega}\right)\right| \ll 1$ and $\left|\frac{d^2}{dt^2}\left(\frac{1}{\omega^2}\right)\right| \ll 1$ to $\omega^2 = \frac{k^2}{a^2(t)} + m^2(t) - \frac{3}{4}\left(\frac{\dot{a}(t)}{a(t)}\right)^2 - \frac{3}{2}\frac{\ddot{a}(t)}{a(t)}$ for the comoving metric, we will definitely not obtain inequalities that allow a simple interpretation. Let us tackle this problem step by step. Assuming that $\dot{a}/a$ and $\ddot{a}/a$ are sufficiently small (which we yet have to check), we first want to derive the conditions for the simpler problem:

$$\ddot{\bar{u}}(t) + \bar{\omega}^2(t)\bar{u}(t) = 0 \quad \text{with} \quad \bar{\omega}(t) = \sqrt{\frac{k^2}{a^2(t)} + m^2(t)} \tag{168}$$

The first relation $|\partial_t \bar{\omega}^{-1}(t)| \ll 1$ gives:

$$\left| k^2 \frac{\dot{a}}{a^3}\frac{1}{\bar{\omega}^3} - \frac{m\dot{m}}{\bar{\omega}^3} \right| \ll 1 \tag{169}$$

This inequality is satisfied if we demand that the absolute value of each of its terms is much smaller than 1. We can therefore split up this equation to obtain:

$$\left|\frac{\dot{a}}{a}\right| \ll \bar{\omega}\left(\frac{a\bar{\omega}}{k}\right)^2 \quad \text{and} \quad \left|\frac{\dot{m}}{m}\right| \ll \bar{\omega}\left(\frac{\bar{\omega}}{m}\right)^2 \tag{170}$$

These are restrictions comparing the Hubble constant $H = \dot{a}/a$ and the relative change in the mass[6] $\dot{m}/m$ to $\bar{\omega}$ for a certain wave vector $\vec{k}$. Here we

[6]The relative change in the squared mass can be easily expressed by this, too: $\frac{dm^2(t)}{dt}/m^2(t) = 2\frac{\dot{m}}{m}$.

made use of the dimensionless terms $a\bar{\omega}/k$ and $\bar{\omega}/m$ that are both ≥ 1:

$$\frac{1}{\alpha} \equiv \frac{a\bar{\omega}}{k} = \sqrt{1 + \left(\frac{am}{k}\right)^2} \geq 1 \quad \text{and} \quad \frac{1}{\beta} \equiv \frac{\bar{\omega}}{m} = \sqrt{\left(\frac{k}{am}\right)^2 + 1} \geq 1 \quad (171)$$

The definitions of α and β will help to write the following formulae in a compact way. They are in relation to each other by $\alpha^2 + \beta^2 = 1$ which also shows that each of these real variables is ≤ 1. We see that essentially the Hubble constant and the relative change in the mass should be small compared to $\bar{\omega}$, a characteristic time-scale in the WKB approximation. The second WKB restriction $|\partial_t^2 \bar{\omega}^{-2}(t)| \ll 1$ gives:

$$\left| 8\left(\frac{H}{\bar{\omega}}\right)^2 \alpha^4 - 6\left(\frac{H}{\bar{\omega}}\right)^2 \alpha^2 - 16\frac{H}{\bar{\omega}}\alpha^2\frac{\dot{m}}{m\bar{\omega}}\beta^2 + 8\left(\frac{\dot{m}}{m\bar{\omega}}\right)^2 \beta^4 \right.$$
$$\left. -2\left(\frac{\dot{m}}{m\bar{\omega}}\right)^2 \beta^2 + 2\frac{\ddot{a}}{a\bar{\omega}^2}\alpha^2 - 2\frac{\ddot{m}}{m\bar{\omega}^2}\beta^2 \right| \ll 1 \quad (172)$$

In this sum we demand that each of the seven terms is $\ll 1$. This is automatically satisfied for the first term, using the condition of eq. (170) $H\alpha^2\bar{\omega}^{-1} \ll 1$. Unfortunately, using this condition we can not conclude that the second term also satisfies $(H\alpha/\bar{\omega})^2 \ll 1$. Squaring eq. (170), we only get $(H\alpha/\bar{\omega})^2 \ll \alpha^{-2} \geq 1$. Therefore we have to demand a stricter condition for the Hubble constant: $|H| \ll \bar{\omega}\alpha^{-1} \leq \bar{\omega}\alpha^{-2}$. This stricter condition is sufficient that the first two terms in eq. (172) are $\ll 1$. The last but one term in eq. (172) finally gives a new restriction for $\ddot{a}/a$.

In a similar manner one can set up restrictions for the derivatives of the mass. One can see that the following restrictions have to be demanded[7] so that each term in eq. (172) is $\ll 1$:

$$|H| = \left|\frac{\dot{a}}{a}\right| \ll \frac{\bar{\omega}}{4\alpha} \qquad \left|\frac{\ddot{a}}{a}\right| \ll \frac{\bar{\omega}^2}{2\alpha^2}$$
$$\left|\frac{\dot{m}}{m}\right| \ll \frac{\bar{\omega}}{4\beta} \qquad \left|\frac{\ddot{m}}{m}\right| \ll \frac{\bar{\omega}^2}{2\beta^2} \quad (173)$$

These are the loosest possible restrictions on the scale factor $a(t)$ and on the mass $m(t)$ so that the WKB approximation for (168) is valid. Again, there are no restrictions on third or higher order derivatives of $a(t)$ or $m(t)$.

[7] Strictly speaking it is only necessary to demand $|H| \ll \bar{\omega}/(\sqrt{6}\alpha)$, $|\dot{m}/m| \ll \bar{\omega}/(\sqrt{8}\beta)$ and $|H\dot{m}/m| \ll \bar{\omega}^2/(16\alpha\beta)$, but this is a playful subtlety since the l.h.s. should be much smaller than the r.h.s. anyway. =)

Now, let us take a look at the initial eq. (167) again. The condition that the terms containing derivatives of $a(t)$ should be small compared to $\bar{\omega} = k^2/a^2 + m^2$ is simply written as $|\dot{a}/a| \ll \bar{\omega}$ and $|\ddot{a}/a| \ll \bar{\omega}^2$. Since $\alpha \geq 1$ this imposes even tighter restrictions on $a(t)$ than the equations in (173). Thus we have proven that by restricting the evolution of the scale factor $a(t)$ and the mass $m(t)$ to k

$$\boxed{\begin{array}{llll} |H| = \left|\frac{\dot{a}}{a}\right| \ll \frac{\bar{\omega}}{4} & & \left|\frac{\ddot{a}}{a}\right| \ll \frac{\bar{\omega}^2}{2} \\ \left|\frac{\dot{m}}{m}\right| \ll \frac{\bar{\omega}}{4\beta} & & \left|\frac{\ddot{m}}{m}\right| \ll \frac{\bar{\omega}^2}{2\beta^2} \end{array}} \tag{174}$$

the WKB restrictions are met automatically.

This result shows that the WKB approximation is essentially valid if the second and third logarithmic derivatives of the variables involved are much smaller than $\bar{\omega}$ and $\bar{\omega}^2$ respectively. That is $|\partial_t \log a| \ll \bar{\omega}$, $|\partial_t^2 \log a| \ll \bar{\omega}^2$, $|\partial_t \log m| \ll \bar{\omega}$ and $|\partial_t^2 \log m| \ll \bar{\omega}^2$. The WKB approximation in this region breaks down if $\bar{\omega} = \sqrt{k^2/a^2 + m^2}$ gets too small when both m and k approach 0. One consequence is that even near the turning point, where $m^2 \approx 0$, there are still mode-functions with high momentum k that can still be described very well by the WKB approximation. WKB first breaks down for low momentum mode functions. We will see that these mode functions give up their sinusoidal character and start to grow exponentially. Their behavior can still be described by making use of the connection formulae and exponentially growing WKB solutions.

5.2.2 Conformal time metric

The equations for the comoving metric with conformal time are very similar to the equations for the comoving metric without conformal time. The calculations are basically the same as in the last section. The mode-functions are defined by the differential equation given in (130):

$$\ddot{u}(\eta) + \left(k^2 + m^2(\eta)a^2(\eta) - \frac{\ddot{a}(\eta)}{a(\eta)}\right) u(\eta) = 0 \tag{175}$$

Again we define a simpler differential equation by

$$\ddot{\bar{u}}(t) + \bar{\omega}^2(\eta)\bar{u}(\eta) = 0 \quad \text{with} \quad \bar{\omega}(\eta) = \sqrt{k^2 + m^2(\eta)a^2(\eta)} \tag{176}$$

and we can find conditions for $m(\eta)$ and $a(\eta)$ from the first and second derivatives of inverse powers of $\bar{\omega}(\eta)$. Introducing α and β as

$$\frac{1}{\beta} \equiv \frac{\bar{\omega}(\eta)}{ma} = \sqrt{\left(\frac{k}{am}\right)^2 + 1} \geq 1 \quad \text{and} \quad \frac{1}{\alpha} \equiv \frac{\bar{\omega}(\eta)}{k} = \sqrt{1 + \left(\frac{ma}{k}\right)^2} \geq 1 \tag{177}$$

we find from the restriction $|\partial_\eta \bar{\omega}^{-1}(\eta)| \ll 1$ that

$$\left| -\frac{H}{\bar{\omega}}\beta^2 - \frac{\dot{m}}{m\bar{\omega}}\beta^2 \right| \ll 1 \tag{178}$$

and from $\left|\partial_\eta^2 \bar{\omega}^{-2}(\eta)\right| \ll 1$ that

$$\begin{aligned} \Bigg| 8\left(\frac{H}{\bar{\omega}}\right)^2 \beta^4 - 2\left(\frac{H}{\bar{\omega}}\right)^2 \beta^2 + 16\frac{H}{\bar{\omega}}\frac{\dot{m}}{m\bar{\omega}}\beta^4 - 8\frac{H}{\bar{\omega}}\frac{\dot{m}}{m\bar{\omega}}\beta^2 \\ +8\left(\frac{\dot{m}}{m\bar{\omega}}\right)^2 \beta^4 - 2\left(\frac{\dot{m}}{m\bar{\omega}}\right)^2 \beta^2 - 2\frac{\ddot{a}}{a\bar{\omega}^2}\beta^2 - 2\frac{\ddot{m}}{m\bar{\omega}^2}\beta^2 \Bigg| \ll 1 \end{aligned} \tag{179}$$

These two restrictions for the simplified conformal differential equation are met if we demand

$$\begin{aligned} |H| = \left|\frac{\dot{a}}{a}\right| &\ll \frac{\bar{\omega}}{4\beta} & \left|\frac{\ddot{a}}{a}\right| &\ll \frac{\bar{\omega}^2}{2\beta^2} \\ \left|\frac{\dot{m}}{m}\right| &\ll \frac{\bar{\omega}}{4\beta} & \left|\frac{\ddot{m}}{m}\right| &\ll \frac{\bar{\omega}^2}{2\beta^2} \end{aligned} \tag{180}$$

which are the same equations as in the conformal case. Taking a look at the full conformal differential equation (175) again, we find that we only get a tighter restriction on $\ddot{a}$, not on $\dot{a}$. Therefore we get the following restrictions for the full conformal differential equation:

$$\begin{aligned} |H| = \left|\frac{\dot{a}}{a}\right| &\ll \frac{\bar{\omega}}{4\beta} & \left|\frac{\ddot{a}}{a}\right| &\ll \frac{\bar{\omega}^2}{2} \\ \left|\frac{\dot{m}}{m}\right| &\ll \frac{\bar{\omega}}{4\beta} & \left|\frac{\ddot{m}}{m}\right| &\ll \frac{\bar{\omega}^2}{2\beta^2} \end{aligned} \tag{181}$$

Note that β appears in three of the four inequalities on the r.h.s. whereas for the comoving metric in (174) it only appeared twice.

5.3 Special scale factors $a(t)$

The scale factor takes simple analytical forms in various theories. Here we want to apply them to the WKB conditions. From equations (11) and (12) we know that the expansion of the universe behaves like $a(t) \sim t^{1/2}$ during the radiation dominated era, and like $t^{2/3}$ in a matter dominated universe. We will treat these two cases together in the power law $a(t) \sim t^p$ with $p = \frac{1}{2}, \frac{2}{3}$. During the inflationary phase of an expanding *de Sitter* universe the scale factor grows exponentially like $a(t) \sim e^{Ht}$ with a given inflation parameter or the Hubble parameter H as we saw in equation (14).

For an exponential expansion $a(t) \sim e^{Ht}$ in a comoving metric, the conditions (174) for which the WKB approximation (164) for the differential equation (167) is valid, simply become

$$\begin{array}{ll} |H| \ll \dfrac{\bar{\omega}}{4} & \left|H^2\right| \ll \dfrac{\bar{\omega}^2}{2} \\ \left|\dfrac{\dot{m}}{m}\right| \ll \dfrac{\bar{\omega}}{4\beta} & \left|\dfrac{\ddot{m}}{m}\right| \ll \dfrac{\bar{\omega}^2}{2\beta^2} \end{array} \tag{182}$$

If all mode functions should be describable by the WKB approximation at the beginning of the inflationary phase, then these equations constrain the Hubble parameter H to

$$H \ll \frac{m(0)}{4} \tag{183}$$

In the case of a radiation or matter dominated universe with the power law $a(t) \sim (t+t_0)^p$ in a comoving metric, we get the same restrictions for derivatives of the mass and we can calculate the restrictions on the scale factor in the following way:

$$\left|\frac{p}{t+t_0}\right| \ll \frac{\bar{\omega}}{4} \qquad \left|\frac{p(p-1)}{t+t_0}\right| \ll \frac{\bar{\omega}^2}{2} \tag{184}$$

If we want to be able to describe all mode functions by a WKB approximation, at least at the beginning, then this equation puts restrictions to the choice of t_0: From $|t+t_0| \gg 4p/\bar{\omega}$ we see that restrictions come from low momentum modes k in $\bar{\omega}^2 = m^2 + k^2/a^2$ at early times t. The tightest restriction[8] on t_0 therefore reads:

$$t_0 \gg \frac{4p}{m(0)} \tag{185}$$

[8]The second restriction gives $t_0 \gg \frac{\sqrt{2p|p-1|}}{m(0)}$ which is less tight since $\frac{4p}{m(0)} > \frac{\sqrt{2p|p-1|}}{m(0)}$ for $p > \frac{1}{9}$.

To calculate the effects of the WKB restrictions in the case of a conformal time metric, we first have to transform the scale-factor dependencies from $a(t)$ to $a(\eta)$, η being the time coordinate for conformal coordinates. The transformation between t and η is given by an integration. From its definition $dt = a(\eta)d\eta$ or $d\eta = a^{-1}(t)dt$ we get a relationship between these two time coordinates:

$$\eta(t) = \int_{t_0}^{t} \frac{dt'}{a(t')} \tag{186}$$

Inverting this relation, we can obtain an expression for $t(\eta)$ and thus for $a(\eta) = a(t(\eta))$.

For the de Sitter universe with an expansion $a(t) = e^{Ht}$ we get:

$$\eta(t) = \int_{t_0}^{t} e^{-Ht'}dt' = \frac{e^{-Ht_0} - e^{-Ht}}{H} \quad \Rightarrow \quad t(\eta) = -\frac{\log\left(e^{-Ht_0} - \eta H\right)}{H} \tag{187}$$

$$a(\eta) = e^{Ht(\eta)} = \frac{1}{e^{-Ht_0} - \eta H} = \frac{1}{1 - H(\eta - \eta_0)} \tag{188}$$

using $\eta_0 \equiv \eta(t = 0) = \left(e^{-Ht_0} - 1\right)/H$. We also see that there is a maximal $\eta_{max} = \frac{1}{H} + \eta_0$. Inserting the η-dependent scale factor into the WKB restrictions (181) we get:

$$\begin{aligned} \left|\frac{H}{1 - H(\eta - \eta_0)}\right| = |Ha(\eta)| \ll \frac{\bar{\omega}}{4\beta} \qquad & \left|2H^2a^2\right| \ll \frac{\bar{\omega}^2}{2} \\ \left|\frac{\dot{m}}{m}\right| \ll \frac{\bar{\omega}}{4\beta} \qquad & \left|\frac{\ddot{m}}{m}\right| \ll \frac{\bar{\omega}^2}{2\beta^2} \end{aligned} \tag{189}$$

In the conformal time metric we have $\bar{\omega}^2 = m^2a^2 + k^2$, so on the r.h.s. of these inequalities we can replace $\bar{\omega}$ by $\bar{\omega} \approx ma$ for small k. Therefore for low momentum modes these inequalities reduce to

$$H \ll \frac{m(0)}{4} \tag{190}$$

just like in the case for the comoving metric.

Finally, let us analyze the WKB restrictions for a power law $a(t) = t^p$ in a conformal time metric:

$$\eta(t) = \int_{t_0}^{t} t'^{-p}dt' = \frac{t_0^{-p+1} - t^{-p+1}}{p-1} \quad \Rightarrow \quad t(\eta) = \sqrt[-p+1]{t_0^{-p+1} - \eta(p-1)} \tag{191}$$

$$a(\eta) = t^p(\eta) = \left(t_0^{-p+1} - \eta(p-1)\right)^{\frac{p}{-p+1}} \tag{192}$$

The WKB restrictions on the scale factor (181) become:

$$\left|na^{1-\frac{1}{p}}\right| \ll \frac{\bar{\omega}}{4\beta} \qquad \left|p(2p-1)a^{2-\frac{2}{p}}\right| \ll \frac{\bar{\omega}^2}{2} \tag{193}$$

Using $\bar{\omega} \geq ma$ again, we find $a \gg (4p/m)^p$ and $a^2 \gg (2p(2p-1)/m^2)^p$. Initially $a(\eta = 0) = t_0^p$ so that we get a restriction[9] on t_0:

$$t_0 \gg \frac{4p}{m(0)} \tag{194}$$

It is the same restriction that we also got from the calculation in the comoving metric in eq. (185).

Comparing the results from eq. (183) and (185) to (190) and (194), we see that the WKB approximation is applicable to the same extent in the case of a comoving metric without conformal time as it is in the case of a metric with conformal time. If we want all mode functions to be describable by a WKB approximation initially, there are certain restrictions to initial parameters of the scale factor: In a de Sitter universe H has to be $\ll m(0)/4$, in a matter or radiation dominated universe t_0 has to be $\gg 4p/m(0)$. Also, $|\dot{m}/m|$ should be $\ll \bar{\omega}/(4\beta)$ and $|\ddot{m}/m|$ should be $\ll \bar{\omega}^2/(2\beta^2)$ in both cases.

5.4 WKB for $\omega^2 < 0$

The WKB approximation that is used to solve eq. (160) with $\omega^2 > 0$ can also be applied to the case of $\omega^2 < 0$ in a modified version. The mode functions are no longer quasi-periodic functions, but grow or decay exponentially. The derivation in this range is similar to the case for $\omega^2 > 0$: We assume the following ansatz for $u(t)$, which differs from the original ansatz (161) only by omitting a factor i in the exponential:

$$u_{\vec{k}}(t) = R(t)e^{S(t)} \tag{195}$$

Inserting this into eq. (160), we get $\ddot{R} + 2\dot{R}\dot{S} + R\ddot{S} + R\dot{S}^2 - (-\omega^2)R = 0$. This equation does not really allow the easy separation in an imaginary and a real part. Nevertheless, we assume $2\dot{R}\dot{S} + R\ddot{S} = 0$ to get $R = c\dot{S}^{-1/2}$. Using this result, we get the equation:

$$\frac{3}{4}\dot{S}^{-2}\ddot{S}^2 - \frac{1}{2}\dot{S}^{-1}\dddot{S} + \dot{S}^2 - (-\omega^2) = 0 \tag{196}$$

[9] The second condition gives $t_0 \gg \frac{\sqrt{2p|2p-1|}}{m}$ which is less tight for $p > \frac{1}{10}$.

Again, assuming $\ddot{S}$ and $\dddot{S}$ to be small quantities in this equation compared to ω^2 we get the approximate result $\dot{S} = \pm\sqrt{-\omega^2} = \pm|\omega|$ or $S(t) = \pm\int_{t_0}^{t} dt'\,|\omega(t')|$. Inserting the results of S and R into eq. (195) we get the final result:

$$u_{\vec{k}}(t) = \frac{c_{\vec{k}}}{\sqrt{|\omega_{\vec{k}}(t)|}} e^{\pm\int_{t_0}^{t} dt'|\omega_{\vec{k}}(t')|} \tag{197}$$

The assumption above that the terms containing $\ddot{S}$ and $\dddot{S}$ in eq. (196) are small quantities compared to $|\omega|^2$ translates accordingly to

$$\left|\frac{d}{dt}\left(\frac{1}{|\omega_{\vec{k}}(t)|}\right)\right| \ll 1 \quad \text{and} \quad \left|\frac{d^2}{dt^2}\left(\frac{1}{|\omega_{\vec{k}}(t)|^2}\right)\right| \ll 1 \tag{198}$$

5.5 Connection formulae

Can one find a connection between the WKB approximation region for $\omega^2 > 0$ and $\omega^2 < 0$? WKB has to fail in the vicinity of the *classical turning point*, at which $\omega^2(t)$ changes its sign. This can be seen if we rewrite the conditions (166) and (198) for the validity of the WKB approximation:

$$\left|\frac{d}{dt}|\omega_{\vec{k}}(t)|\right| \ll |\omega_{\vec{k}}(t)|^2 \quad \text{and} \quad \left|\frac{d^2}{dt^2}|\omega_{\vec{k}}(t)|\right| \ll |\omega_{\vec{k}}(t)|^3 \tag{199}$$

Since ω vanishes at the turning point, these inequalities can not be satisfied anymore for non-vanishing derivatives of ω. But we can try a different approach near the turning point. We will see that there is an approximate solution near the turning point that links together the periodic part and the exponentially growing part of the WKB solutions.

Let us assume a turning point at $t = t_1$ such that $\omega^2(t) > 0$ for $t < t_1$ and $\omega^2(t) < 0$ for $t > t_1$. This resembles the situation of approaching a phase transition from the symmetric phase with $m^2 > 0$ before approaching it and $m^2 < 0$ upon entering further into the symmetry-broken region. At the turning point we can approximate $\omega^2(t)$ by:

$$\omega^2(t) \simeq -A(t-t_1) \quad \text{with} \quad A = -\left(\frac{d\omega^2(t)}{dt}\right)\bigg|_{t=t_1} > 0 \tag{200}$$

where the signs were chosen such that the constant A is positive. Using this approximation we rewrite the differential equation for the mode functions (160) as

$$\left(\partial_t^2 - A\,(t-t_1)\right) u(t) = 0 \tag{201}$$

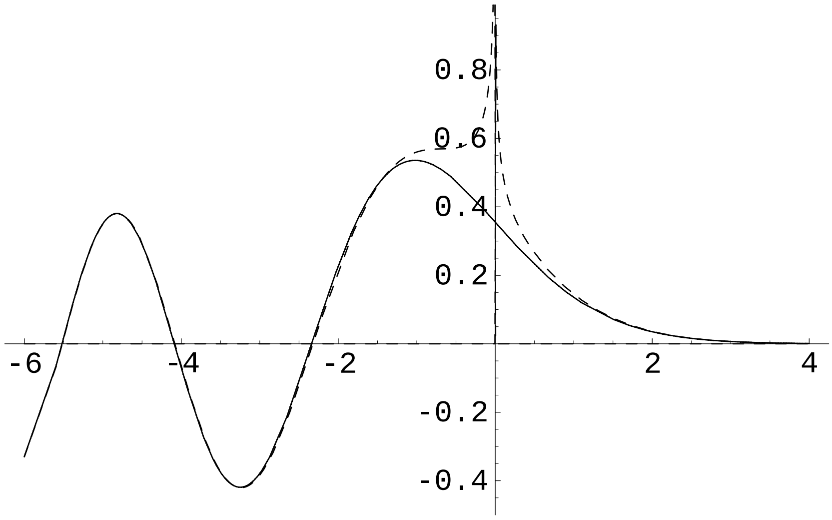


Figure 2: Airy function $\mathrm{Ai}(q)$ (solid line) and its asymptotic forms for $q \to \pm\infty$ (dashed line). Note that both asymptotic forms diverge at $q = 0$.

The general solution to this equation is a linear combination of *Airy functions* $\mathrm{Ai}(q)$ and $\mathrm{Bi}(q)$ that are solutions to the differential equation $y''(q) - qy(q) = 0$ [36].

$$u(t) = \lambda \mathrm{Ai}\left(\sqrt[3]{A}(t - t_1)\right) + \mu \mathrm{Bi}\left(\sqrt[3]{A}(t - t_1)\right) \tag{202}$$

Figure 2 shows the function $\mathrm{Ai}(q)$. It is bounded and has the asymptotic forms

$$\mathrm{Ai}(q)\big|_{q\to-\infty} \longrightarrow \frac{1}{\sqrt{\pi}} |q|^{-\frac{1}{4}} \cos\left(\frac{2}{3}|q|^{\frac{3}{2}} - \frac{\pi}{4}\right) \tag{203}$$

$$\mathrm{Ai}(q)\big|_{q\to+\infty} \longrightarrow \frac{1}{2}\frac{1}{\sqrt{\pi}} q^{-\frac{1}{4}} \exp\left(-\frac{2}{3}q^{\frac{3}{2}}\right) \tag{204}$$

Its linearly independent function $\mathrm{Bi}(q)$, plotted in Figure 3, is unbounded as $q \to \infty$ and has the asymptotic forms:

$$\mathrm{Bi}(q)\big|_{q\to-\infty} \longrightarrow -\frac{1}{\sqrt{\pi}} |q|^{-\frac{1}{4}} \cos\left(\frac{2}{3}|q|^{\frac{3}{2}} - \frac{\pi}{4}\right) \tag{205}$$

$$\mathrm{Bi}(q)\big|_{q\to+\infty} \longrightarrow \frac{1}{\sqrt{\pi}} q^{-\frac{1}{4}} \exp\left(\frac{2}{3}q^{\frac{3}{2}}\right) \tag{206}$$

Equation (202) is an accurate solution to the differential equation (160) near the turning point $t = t_1$. However, if we want to match this solution

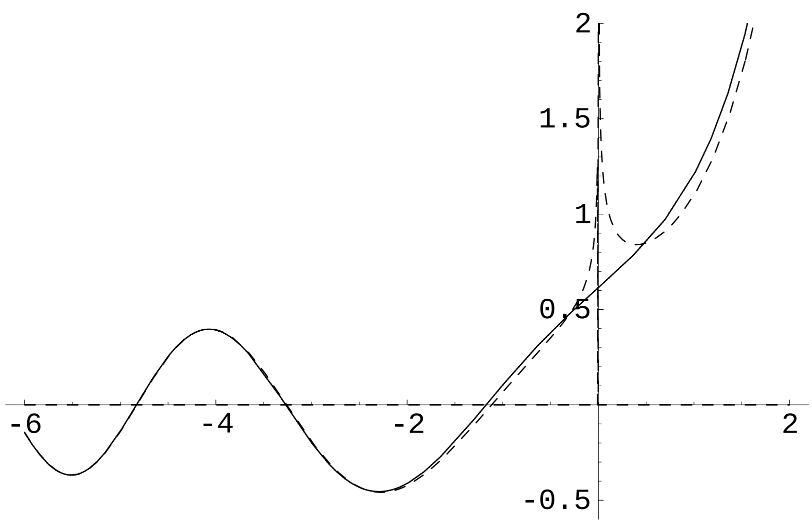


Figure 3: Airy function $\mathrm{Bi}(q)$ (solid line) and its asymptotic forms for $q \to \pm\infty$ (dashed line).

to the WKB solutions for $t \ll t_1$ and $t \gg t_1$ we have to try to transform the differential equation (160) into a differential equation of the form (201) over the whole interval $-\infty < t < \infty$, so that a solution of the form (202) becomes an approximate solution for all values of t. We do this by regarding a similar differential equation with the variable q instead of t

$$\left(\frac{d^2}{dq^2} - q\right) y(q) = 0 \tag{207}$$

where we still have to find the dependence of $q = q(t)$ on t so that this equation is approximately the transformed equation of (160) for all t. The WKB solutions for this equation with $\omega^2(q) = -q$ can be given for $q < 0$ an $q > 0$, provided that the conditions $\left|\frac{d}{dq}\left|\omega(q)\right|^{-1}\right| = \left|q^{-2}\right| \ll 1$ and $\left|\frac{d^2}{dq^2}\left|\omega(q)\right|^{-2}\right| = \left|6q^{-4}\right| \ll 1$ are met, which is satisfied for $|\pm q| \gg \sqrt[4]{6} \approx 1$. Using equations (164) and (197), the solutions in the WKB approximation are given by

$$y(q) = \begin{cases} c\left|q\right|^{-\frac{1}{4}} \exp\left(\pm i \int_0^q \sqrt{|q'|}dq'\right) & \text{for } q \ll -1 \\ cq^{-\frac{1}{4}} \exp\left(\pm \int_0^q \sqrt{q'}dq'\right) & \text{for } q \gg +1 \end{cases} \tag{208}$$

The inner integral can be evaluated to give

$$y(q) = \begin{cases} c\left|q\right|^{-\frac{1}{4}} \exp\left(\pm i\frac{2}{3}\left|q\right|^{\frac{3}{2}}\right) & \text{for } q \ll -1 \\ cq^{-\frac{1}{4}} \exp\left(\pm\frac{2}{3}q^{\frac{3}{2}}\right) & \text{for } q \gg +1 \end{cases} \tag{209}$$

A comparison with the solutions (164) and (197) for a general $\omega(t)$ replacing t_0 in the integrals by the turning point t_1 suggests that $u(t)$ can be approximated by a function $\hat{u}(t)$ with

$$\hat{u}(t) = \left(\frac{|q(t)|}{|\omega(t)|^2}\right)^{\frac{1}{4}} y\left(q(t)\right) \tag{210}$$

where

$$q(t) = \begin{cases} -\left(-\frac{3}{2}\int_{t_1}^{t}\omega(t')dt'\right)^{\frac{2}{3}} & \text{for } q(t)<0,\ \ t<t_1, \text{ and } \omega^2(t)>0 \\ \left(\frac{3}{2}\int_{t_1}^{t}|\omega(t')|\,dt'\right)^{\frac{2}{3}} & \text{for } q(t)>0,\ \ t>t_1, \text{ and } \omega^2(t)<0 \end{cases} \tag{211}$$

Near $t \simeq t_1$ we find that $q(t)$ is given by $q(t) = \left(-\frac{d}{dt}\omega^2(t)\right)^{1/3}\Big|_{t=t_1}(t-t_1) = A^{1/3}(t-t_1)$, transforming the differential equation (207) into (201). So we see that (210) is indeed an accurate solution in the vicinity of the turning point. To see how accurately $\hat{u}(t)$ approximates $u(t)$ in general, we insert (210) and (211) into the differential equation (207) to get the following exact differential equation for $\hat{u}(t)$ (see [35]):

$$\left(\frac{d^2}{dt^2} + \omega(t) + \epsilon(t)\right)\hat{u}(t) = 0 \tag{212}$$

where

$$\epsilon(t) = -\left|\frac{dq}{dt}\right|^{\frac{1}{2}} \frac{d^2}{dt^2}\left(\left|\frac{dq}{dt}\right|^{-\frac{1}{2}}\right) \tag{213}$$

Now we can say that $\hat{u}(t)$ is a good approximation of $u(t)$ if $|\epsilon(t)/\omega^2(t)| \ll 1$ which, according to [35], is a weaker condition than (166) or (198) far from the turning point.

Finally, we can join these results to get the connection formulae. Writing the general solution to the differential equation (207) as

$$y(t) = y(q(t)) = \lambda \mathrm{Ai}(q(t)) + \mu \mathrm{Bi}(q(t)) \tag{214}$$

we can use the results for $y(t)$ and $q(t)$ given by (210) and (211) and the asymptotic forms of the Airy functions (203)-(206) to connect the WKB approximations for $t \ll t_1$ and $t \gg t_1$. Setting the overall normalization constant equal to unity, we get the following asymptotic solutions for $u(t)$. When connecting the asymptotic solutions of the Airy function $\mathrm{Ai}(q)$ we get

$$\frac{1}{\sqrt{\omega(t)}}\cos\left(\int_{t_1}^{t}\omega(t')dt' + \frac{\pi}{4}\right)\Bigg|_{t\ll t_1} \longleftrightarrow \frac{1}{2}\frac{1}{\sqrt{|\omega(t)|}}\exp\left(-\int_{t_1}^{t}|\omega(t')|\,dt'\right)\Bigg|_{t\gg t_1} \tag{215}$$

and for the Airy function Bi(q) we get

$$\frac{1}{\sqrt{\omega(t)}}\sin\left(\int_{t_1}^{t}\omega(t')dt'+\frac{\pi}{4}\right)\Bigg|_{t\ll t_1}\longleftrightarrow\frac{1}{\sqrt{|\omega(t)|}}\exp\left(\int_{t_1}^{t}|\omega(t')|\,dt'\right)\Bigg|_{t\gg t_1} \tag{216}$$

These are the so-called *WKB connection formulae*, connecting two WKB solutions in the *uniform approximation* [35]. Note that there is an additional factor $\frac{1}{2}$ in the case of the Ai(q)-function that is not there for the Bi(q)-function.

It is important to know that usually in quantum mechanical problems the WKB connection formulae can only be applied in one direction. That is, assuming a decaying exponential in a region with a high potential, one can conclude that the phase of the wave-function on the other side of the turning point is determined by the connection formula for Ai(q), a cosine with a phase $\frac{\pi}{4}$. However, knowing that the solution is given by an increasing exponential on one side, one can not deduce that the sine-solution should be used on the other side of the turning point. It is not possible to imply this, because a small admixture of the exponentially decreasing solution to the increasing solution would be negligible, but that could result in an appreciable admixture of the cosine solution to the sine solution. Similarly, coming from the cosine or sine side of the turning point, one can not clearly decide between the increasing or the decreasing form of the exponential.

5.6 WKB through phase transition

With the help of the WKB connection formulae it should be possible to describe mode functions before and after a turning point. Starting from a thermal equilibrium, the turning point is being approached from a sine/cosine solution region. But in the last section we just saw that without the knowledge of the exact phase information of the incoming wave one is not able to determine whether the solution on the other side of the turning point will be exponentially increasing or decreasing or any other linear combination of these two solutions. Since WKB is only an approximation scheme, we could never determine the exact phase of the incoming solution and would never know if we had exponentially growing or decaying modes on the other side of the phase transition. To calculate the mass correction, these mode functions are summed up finally, and exponentially growing or decaying solutions would make a huge difference.

However, we are not really interested in any phase information. On a statistical basis one would assume that the solution would be exponentially growing in general if we assume an arbitrary linear combination of growing and decaying solutions. But still every exponential behavior between the two extremes seems to be possible a priori.

Yet the situation is not completely hopeless. We are really interested in expressions like the absolute square of the mode functions $u(t)u^*(t)$ and it turns out that this expression is independent of the initial phase, even after a first turning point, for complex conjugate, linearly independent, orthogonal solutions $u(t)$ and $u^*(t)$.

To see this in detail, we combine the two connection formulae (215) and (216), using $\sin(\xi+\delta) = \cos\delta\sin\xi + \sin\delta\cos\xi$ where $\xi = \int\omega + \frac{\pi}{4}$ to one connection formula with an arbitrary incoming phase δ:

$$\boxed{\begin{array}{c}\left.\frac{1}{\sqrt{\omega(t)}}\sin\left(\int_{t_1}^{t}\omega(t')dt' + \frac{\pi}{4} + \delta\right)\right|_{t\ll t_1} \longleftrightarrow \\ \left.\frac{\cos\delta}{\sqrt{\omega(t)}}\exp\left(\int_{t_1}^{t}|\omega(t')|\,dt'\right) + \frac{1}{2}\frac{\sin\delta}{\sqrt{\omega(t)}}\exp\left(-\int_{t_1}^{t}|\omega(t')|\,dt'\right)\right|_{t\gg t_1}\end{array}} \tag{217}$$

Here we assumed a turning point at $t = t_1$ such that $\omega^2(t) > 0$ for $t < t_1$ and $\omega^2(t) < 0$ for $t > t_1$. For a second turning point at $t = t_2$ with $\omega^2(t) < 0$ for $t < t_2$ and $\omega^2(t) > 0$ for $t > t_2$ one just needs to flip the connection formulae (215) and (216) so that one gets for the Airy function $\mathrm{Ai}(q)$

$$\left.\frac{1}{\sqrt{|\omega(t)|}}\exp\left(\int_{t_2}^{t}|\omega(t')|\,dt'\right)\right|_{t\ll t_2} \longleftrightarrow \left. 2\frac{1}{\sqrt{\omega(t)}}\cos\left(\int_{t_2}^{t}\omega(t')dt' - \frac{\pi}{4}\right)\right|_{t\gg t_2} \tag{218}$$

and for the Airy function $\mathrm{Bi}(q)$

$$\left.\frac{1}{\sqrt{|\omega(t)|}}\exp\left(-\int_{t_2}^{t}|\omega(t')|\,dt'\right)\right|_{t\ll t_2} \longleftrightarrow \left. -\frac{1}{\sqrt{\omega(t)}}\sin\left(\int_{t_2}^{t}\omega(t')dt' - \frac{\pi}{4}\right)\right|_{t\gg t_2} \tag{219}$$

The integrations on the l.h.s. of the last couple of equations might also be rewritten as $\int_{t_{1,2}}^{t} = -\int_{t}^{t_{1,2}}$ since $t < t_{1,2}$, but we adopt the convention that the upper integration limit represents the variable whereas the lower integration limit is a constant. The changes in the signs from the r.h.s. of equations (215) and (216) to the l.h.s. of equations (218) and (219) are due to the fact that the integral $\int|\omega|\,dt'$ which has been negative for $t_1 < t < t_2$ is now positive.

Note that the connection formulae require the exact knowledge of the turning point position since the integrals on the l.h.s. and on the r.h.s. of the formulae contain the turning point as one of their integration limits. This is of no concern in quantum mechanical applications of the WKB approximation as the turning point is explicitly given by the form of the potential. But it will pose a certain problem in our case since the quantum mechanical potential corresponds to $\omega(t)$ which in turn is calculated by a mass correction where all mode functions are summed up. So our turning point is the result of a calculation that has to use a WKB approximation in a region where this technique fails - that is in the vicinity of the turning point. Through the connection formulae we could make pretty good approximations to the left and to the right of a turning point without actually knowing what really lies in between. We just would have to know the exact position of the turning point, which we don't since WKB fails there. Yet, in the following we assume that we know $\omega(t)$ over the whole region and the positions of the two turning points and we will try to calculate how the mode functions will look after one and after two turning points without caring how they behave in between. Later we will think about how to approximate the positions of the turning points.

5.6.1 First turning point

The first turning point separates a region with positive $\omega_{\vec{k}}^2(t)$ from a region with negative $\omega_{\vec{k}}^2(t)$. In our model of an expanding system $\omega_{\vec{k}}^2(t)$ is positive for all wave vectors $\vec{k}$ at the beginning. The mode functions are given by oscillating WKB solutions in this region. Canonical commutation relations enforce that the *Wronskian* $\mathrm{W}[u,u^*] \equiv u\dot{u}^* - \dot{u}u^*$ of the mode function $u_{\vec{k}}(t)$ and its complex conjugate $u_{\vec{k}}^*(t)$ is constant. This allows only "circular polarized"[10] solutions of the form

$$\begin{aligned} u_{\vec{k}}(t) &= \frac{1}{\sqrt{\omega_{\vec{k}}(t)}} \exp\left\{ \pm i \left(\int_{t_1}^{t} \omega_{\vec{k}}(t')dt' + \varphi \right) \right\} \\ &= \frac{1}{\sqrt{\omega}} \cos\left(\int_1 \omega + \varphi \right) \pm \frac{i}{\sqrt{\omega}} \sin\left(\int_1 \omega + \varphi \right) \end{aligned} \tag{220}$$

The index "1" at the integral $\int_1$ means that the integration starts at the first turning point ($\int_1 \equiv \int_{t_1}^{t}$). The most general solution in region I to the left of

[10]Naming the solutions "circular polarized" should not imply any physical meaning, but refers to the two possible solutions for the complex mode function $u_{\vec{k}}(t)$. Note that the scalar field φ from equation (89) is real.

the first turning point is therefore

$$\begin{aligned}
u_{(I)} \equiv u_{(t \ll t_1)} &\equiv \frac{r_1}{\sqrt{}} e^{+i\left(\int_1 \omega + \varphi_1\right)} + \frac{r_2}{\sqrt{}} e^{-i\left(\int_1 \omega + \varphi_2\right)} \\
&= \frac{1}{\sqrt{}} \left[r_1 \cos\left(\int_1 \omega + \varphi_1 \right) + r_2 \cos\left(\int_1 \omega + \varphi_2 \right) \right] \\
&\quad + \frac{i}{\sqrt{}} \left[r_1 \sin\left(\int_1 \omega + \varphi_1 \right) - r_2 \sin\left(\int_1 \omega + \varphi_2 \right) \right] \qquad (221)
\end{aligned}$$

with real constants r_1, r_2, φ_1, and φ_2. Any complex part of r_1 or r_2 could be easily transfered into the phases φ_1 and φ_2. The Wronskian and the absolute square of u are given by

$$\mathrm{W}[u_{(I)}, u^*_{(I)}] = -2i(r_1^2 - r_2^2) \qquad (222)$$

$$u_{(I)} u^*_{(I)} = \frac{1}{\omega} \left[r_1^2 + r_2^2 + 2 r_1 r_2 \cos\left(\varphi_1 + \varphi_2 + 2 \int_1 \omega \right) \right] \qquad (223)$$

We see that the Wronskian is actually independent of the integral $\int_1 \omega$ and the phases φ_1 and φ_2. If we also want uu^* to be independent of the choice of initial phases and the integral, we see that either r_1 or r_2 has to vanish. That means the system starts in a purely right circular polarized or left circular polarized mode function u. The choice between left or right is fixed by the canonical commutation relations. Nevertheless, for the sake of completeness in the following all formulae are calculated for general real constants r_1 and r_2 without the constraint that one of them has to vanish.

Note that we already separated the general solution (221) into its real and its imaginary part. This allows us to independently apply the WKB connection formulae (217) to get the WKB solution in region II between the first and the second turning point. Using equation (217) with $\varphi = \frac{\pi}{4} + \delta$ and $\cos\varphi = \sin(\varphi + \frac{\pi}{2})$ we get:

$$\begin{aligned}
u_{(II)} \equiv u_{(t_1 \ll t \ll t_2)} &= \frac{1}{\sqrt{}}\left[r_1 \cos\left(\varphi_1 + \frac{\pi}{4}\right) e^{\int_1 |\omega|} + \frac{r_1}{2} \sin\left(\varphi_1 + \frac{\pi}{4}\right) e^{-\int_1 |\omega|}\right. \\
&\quad \left. + r_2 \cos\left(\varphi_2 + \frac{\pi}{4}\right) e^{\int_1 |\omega|} + \frac{r_2}{2} \sin\left(\varphi_2 + \frac{\pi}{4}\right) e^{-\int_1 |\omega|}\right] \\
&\quad + \frac{i}{\sqrt{}}\left[r_1 \cos\left(\varphi_1 - \frac{\pi}{4}\right) e^{\int_1 |\omega|} + \frac{r_1}{2} \sin\left(\varphi_1 - \frac{\pi}{4}\right) e^{-\int_1 |\omega|}\right. \\
&\quad \left. - r_2 \cos\left(\varphi_2 - \frac{\pi}{4}\right) e^{\int_1 |\omega|} - \frac{r_2}{2} \sin\left(\varphi_2 - \frac{\pi}{4}\right) e^{-\int_1 |\omega|}\right] \\
&= \frac{r_1}{\sqrt{|\omega|}}\left(e^{\int_1 |\omega|} - \frac{i}{2} e^{-\int_1 |\omega|}\right) e^{i\left(\varphi_1 + \frac{\pi}{4}\right)} \\
&\quad + \frac{r_2}{\sqrt{|\omega|}}\left(e^{\int_1 |\omega|} + \frac{i}{2} e^{-\int_1 |\omega|}\right) e^{-i\left(\varphi_2 + \frac{\pi}{4}\right)} \qquad (224)
\end{aligned}$$

This solution gives the following Wronskian and uu^* in the second region $t_1 \ll t \ll t_2$:

$$\mathrm{W}[u_{(II)}, u^*_{(II)}] = -2i(r_1^2 - r_2^2) \qquad (225)$$

$$\begin{aligned}
u_{(II)} u^*_{(II)} &= \frac{1}{|\omega|}\left\{e^{2\int_1 |\omega|}\left(r_1^2 + r_2^2 - 2 r_1 r_2 \sin(\varphi_1 + \varphi_2)\right)\right. \\
&\quad + \frac{1}{4} e^{-2\int_1 |\omega|}\left[r_1^2 + r_2^2 + 2 r_1 r_2 \sin(\varphi_1 + \varphi_2)\right. \\
&\quad \left.\left. + 2 r_1 r_2 \cos(\varphi_1 + \varphi_2)\right]\right\} \\
&= \frac{1}{|\omega|}\left[\left(r_1^2 + r_2^2\right)\left(e^{2\int_1 |\omega|} + \frac{1}{4} e^{-2\int_1 |\omega|}\right)\right. \\
&\quad - 2 r_1 r_2 \left(e^{2\int_1 |\omega|} - \frac{1}{4} e^{-2\int_1 |\omega|}\right) \sin(\varphi_1 + \varphi_2) \\
&\quad \left. + 2 r_1 r_2 \cos(\varphi_1 + \varphi_2)\right] \qquad (226)
\end{aligned}$$

We get the same Wronskian as in region I, which is very nice. If we choose $r_1 = 0$ or $r_2 = 0$ initially then the absolute square of u becomes

$$uu^* = \frac{r_1^2}{|\omega|}\left(e^{2\int_1} + \frac{1}{4} e^{-2\int_1}\right) \qquad (227)$$

which is independent of the initial phases.

A remark about the use of the connection formulae is probably necessary at this point. Usually it is assumed that the exponentially decaying solution is negligible compared to the exponentially growing solution since WKB is just an approximation anyway. We could have followed the same tactics in equation (224) and omitted all exponentially decaying factors. But then, for a merely exponentially growing solution, the Wronskian would have vanished and would no longer be the same as in region I. In order to fix that, we would have had to add a small counter-term, perpendicular to the direction of the exponentially growing mode in the complex plane. This counter-term must be proportional to an exponentially decaying mode if we want the Wronskian to be independent of the phases and of the integral over $|\omega|$. But this would just have been the exponential solution that we got from the WKB connection formulae automatically with the right factor. Therefore we can keep track of the exponentially decaying solutions as well, in order to keep the Wronskian constant over all regions.

5.6.2 Second turning point

Now we want to describe the transition through a second turning point t_2 where $\omega_{\vec{k}}^2(t)$ changes from being negative to positive. We assume that we are far enough away from the first turning point $t_2 \gg t_1$, such that the asymptotic solutions of the first and the second turning point overlap. We can match those solutions and use the connection formulae for the second turning point to get the WKB solution for $t \gg t_2$. Assuming that the mode functions in a region $t_1 \ll t \ll t_2$ can be written as in equation (224), we find the following mode function for region III, using the connection formulae (218) and (219). First we have to rewrite equation (224) such that integrations start at the second turning point, using

$$\int_1 \equiv \int_{t_1}^{t} = \int_{t_1}^{t_2} + \int_{t_2}^{t} \equiv P + \int_2 \tag{228}$$

where we defined

$$P \equiv \int_{t_1}^{t_2} \left|\omega_{\vec{k}}(t')\right| dt' > 0 \tag{229}$$

as the area of $|\omega|$ between the two turning points, and we obtain

$$\begin{aligned} u_{(II)} \;=\; & \frac{r_1}{\sqrt{|\omega|}} \left(e^{P} e^{\int_2 |\omega|} - \frac{i}{2} e^{-P} e^{-\int_2 |\omega|} \right) e^{i\left(\varphi_1 + \frac{\pi}{4}\right)} \\ & + \frac{r_2}{\sqrt{|\omega|}} \left(e^{P} e^{\int_2 |\omega|} + \frac{i}{2} e^{-P} e^{-\int_2 |\omega|} \right) e^{-i\left(\varphi_2 + \frac{\pi}{4}\right)} \end{aligned} \tag{230}$$

Now we apply the connection formulae (218) and (219) to this equation, basically converting $\exp\left(\int\right)$ into $2\cos\left(\int -\frac{\pi}{4}\right)$ and $\exp\left(-\int\right)$ into $-\sin\left(\int -\frac{\pi}{4}\right)$:

$$\begin{aligned} u_{(III)} &= \frac{r_1}{\sqrt{\omega}}\left[2e^P\cos\left(\int_2 \omega - \frac{\pi}{4}\right) + \frac{i}{2}e^{-P}\sin\left(\int_2 \omega - \frac{\pi}{4}\right)\right] e^{i\left(\varphi_1+\frac{\pi}{4}\right)} \\ &\quad + \frac{r_2}{\sqrt{\omega}}\left[2e^P\cos\left(\int_2 \omega - \frac{\pi}{4}\right) - \frac{i}{2}e^{-P}\sin\left(\int_2 \omega - \frac{\pi}{4}\right)\right] e^{-i\left(\varphi_2+\frac{\pi}{4}\right)} \\ &= \frac{r_1}{\sqrt{\omega}}\left[\cosh Q e^{i\left(\int_2\omega-\frac{\pi}{4}\right)} + \sinh Q e^{-i\left(\int_2\omega-\frac{\pi}{4}\right)}\right] e^{i\left(\varphi_1+\frac{\pi}{4}\right)} \\ &\quad + \frac{r_2}{\sqrt{\omega}}\left[\cosh Q e^{-i\left(\int_2\omega-\frac{\pi}{4}\right)} - \sinh Q e^{i\left(\int_2\omega-\frac{\pi}{4}\right)}\right] e^{-i\left(\varphi_2+\frac{\pi}{4}\right)} \end{aligned} \quad (231)$$

with $Q \equiv P + \log 2$. This solution gives the following Wronskian and uu^* in the third region with $t \gg t_2$:

$$\mathrm{W}[u_{(III)}, u^*_{(III)}] = -2i(r_1^2 - r_2^2) \quad (232)$$

$$\begin{aligned} u_{(III)}u^*_{(III)} &= \frac{1}{\omega}\Big\{\left(r_1^2 + r_2^2\right)\left[\cosh(2Q) + \sinh(2Q)\cos(2\Omega(t))\right] \\ &\quad + \frac{ir_1r_2}{2}e^{i(\varphi_1+\varphi_2)}\left(\cosh Q e^{i\Omega(t)} + \sinh Q e^{-i\Omega(t)}\right)^2 \\ &\quad - \frac{ir_1r_2}{2}e^{-i(\varphi_1+\varphi_2)}\left(\cosh Q e^{-i\Omega(t)} + \sinh Q e^{i\Omega(t)}\right)^2\Big\} \end{aligned} \quad (233)$$

with

$$\begin{aligned} Q &\equiv P + \log 2 = \int_{t_1}^{t_2} \left|\omega_{\vec{k}}(t')\right| dt' + \log 2 \\ \Omega(t) &\equiv \int_2 \omega - \frac{\pi}{4} = \int_{t_2}^{t} \omega_{\vec{k}}(t')dt' - \frac{\pi}{4} \end{aligned} \quad (234)$$

Again we find a solution with the right Wronskian. If we start with $r_2 = 0$, the expression uu^* is independent of the initial phase φ_1. Compared to region I, uu^* is basically scaled by a factor $\cosh(2P + \log 4)$ where P is the integral over $|\omega|$ between the two turning points, wiggling with an amplitude of a $\sinh(2P + \log 4)$.

Equation (231) suggests that $u_{(III)}$ can be written in the general form for $u_{(I)}$ in equation (221), consisting of a general superposition of a left and a right circular polarized function, where now both r_1 and r_2 are nonzero with nontrivial phases φ_1 and φ_2. After a third and a fourth turning point we can use the same formulae that we derived above, now for general real r_1, r_2, φ_1, and φ_2. This is as difficult as it can get, because the formulae don't get more complicated for a fifth or higher turning point.

In our derivation of the solutions of the mode functions through turning points we assumed that $t_1 \ll t_2 \ll t_3 \ll ...$ so that the asymptotic solutions that we want to link together are valid in the WKB approximation. If two turning points are too close to each other then the results above are not accurate and the growing of a mode function does not simply depend on the area of $\omega(t)$ between the two turning points. Also the connection formulae before and after a turning point do not really match in the vicinity of the turning point. At the turning point these solutions even diverge with $1/\sqrt{\omega}$ as $\omega \to 0$. There the solutions have to be expressed in terms of the Airy-functions as in eq. (202) so that the absolute square of the mode function is given by

$$u(t)u^*(t) \sim \mathrm{Ai}^2\left(\sqrt[3]{A}(t-t_1)\right) + \mathrm{Bi}^2\left(\sqrt[3]{A}(t-t_1)\right) \tag{235}$$

Unfortunately, the Wronskian $\mathrm{W}[u,u^*] \sim \mathrm{AiAi}' + \mathrm{BiBi}'$ is no longer constant, because equation (202) is only an approximation in the vicinity of the turning point. Trying to link this Airy-solution together with the trigonometric asymptotic solutions might involve even more effort than linking together two asymptotic solutions as we did so far in the connection formulae. For now, the connection formulae through two turning points should give enough possibilities to try to understand our differential equation system with the evolution of the mode functions and the mass correction with the one-loop resummation in an analytical way as far as possible.

6 Analytical description of the scalar field mass

So far we have gathered various aspects of calculating the evolution of the scalar field mass of a $\lambda\varphi^4$-theory in an expanding background: We saw how to calculate the propagator in a curved space-time, how to express it by mode functions, how to calculate the 1-loop resummed mass, how to renormalize it, and finally how to write the mode functions in the WKB approximation. In this chapter we will show how to combine these results to calculate the mass in principle as it may be done in a numerical simulation. We will also try to explain the resulting mass curve analytically by calculating low order terms of a Taylor series. A successful analytical approach might give valuable physical insight into the problem and might result in simple formulae that are easier and quicker to apply than extensive numerical simulations.

There are two important equations that define the core of the problem: One is the 1-loop resummed mass that we calculated in equation (158). The other is the differential equation (127) that determines $\tilde{u}_k(t)$ that is needed in the first equation. Emphasizing all time dependent variables rigorously, these two equations are given by

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2 a^3(t)} \int_0^\infty |\tilde{u}_k(t)|^2 \frac{1}{e^{\beta\omega_k(0)} - 1} k^2 dk \tag{236}$$

$$\ddot{\tilde{u}}_k(t) + \left(\frac{k^2}{a^2(t)} + m^2(t) - \frac{3}{4}\left(\frac{\dot{a}(t)}{a(t)}\right)^2 - \frac{3}{2}\frac{\ddot{a}(t)}{a(t)} \right) \tilde{u}_k(t) = 0 \tag{237}$$

We assume our system to start in a thermal equilibrium which constrains the initial conditions of our variables: Before the expansion starts at $t_0 = 0$ the mode functions are given by equation (144). In the flat space-time for $t < 0$ they reduce to plain wave solutions of the form (92). Immediately we get the initial conditions for the mode functions by

$$\begin{aligned} \tilde{u}_k(0) &= \frac{1}{\sqrt{2\omega_k}} \\ \dot{\tilde{u}}_k(0) &= -i\sqrt{\frac{\omega_k}{2}} \end{aligned} \tag{238}$$

In our model the scale factor $a(t)$ is arbitrary and we are free to choose any scale factor. We merely demand that the system does not expand during the thermal equilibrium stage:

$$a(t) = 1 \qquad \text{for } t \leq 0 \tag{239}$$

Finally, we also set $m^2(t) = 1$ for $t \leq 0$ and determine μ_R by the choice of the coupling constant λ_R. We reduced our physical question about the scalar field mass to the mathematical problem of solving this system of differential equations with well-defined initial conditions.

If the equations (236) and (237) were two simple, separate differential equations then we could regard the problem as solved. Unfortunately they are coupled in a non-trivial way: First, to calculate the mass, one has to solve the differential equation (237) for each mode k. Since we integrate over all modes k from 0 to ∞, we have to solve this equation for every possible wave vector k from 0 to ∞, giving an infinite magnitude of differential equations that we would have to calculate. Secondly, as if this was not enough misery, these differential equations contain the mass that we just want to calculate! We would have to know the mode functions to calculate the mass, and we would have to know the mass to solve the differential equations for the mode functions! It's like two snakes swallowing each other's tails (of which one snake has infinitely many heads!).

Luckily, there are ways out of this problem: Numerically one can introduce finite time steps and calculate the system of equations step by step. Another approach is to write down analytical solutions of the mode functions. Since the equation (237) can not be solved exactly, we will use the WKB approximation of the mode functions, paying attention to when this approximation is valid.

6.1 WKB approximation of the scalar field mass

The solution to the differential equation for the mode functions (237) can be nicely approximated by the WKB approximation. Depending on the sign of

$$\omega_k^2(t) = \frac{k^2}{a^2} + m^2(t) - \frac{3}{4}\left(\frac{\dot{a}}{a}\right)^2 - \frac{3}{2}\frac{\ddot{a}}{a} \tag{240}$$

we either get sinusoidal solutions or exponentially growing solutions. In the last chapter we denoted the region between the thermal equilibrium starting point and the first turning point by WKB I, the subsequent region with a negative ω_k^2 by WKB II, and the region after a second turning point by WKB III. The respective WKB solutions for the mode functions $u_k(t)$ and their absolute square are given in Table 1 and 2. They are essentially a summary of the results of the last chapter (equations 221, 224, and 231) for the initial conditions given in equation (238).

From Table 1 we see that both WKB I and WKB III are sinusoidal solutions, in contrary to the WKB II region which has exponentially growing

Region	$u_k(t)$
WKB I	$\frac{1}{\sqrt{2\omega_k(t)}} e^{-i\int_0^t \omega_k(t')dt'}$
WKB II	$\frac{1}{\sqrt{2\lvert\omega_k(t)\rvert}} \left(e^{\Omega_1(t)} - \frac{i}{2}e^{-\Omega_1(t)}\right) e^{i\Phi}$
WKB III	$\frac{1}{\sqrt{2\omega_k(t)}} \left[\cosh Q e^{i\Omega_2(t)} + \sinh Q e^{-i\Omega_2(t)}\right] e^{i\Phi}$

Table 1: The mode functions $u_k(t)$ in different WKB approximation regions where we used $\Omega_1(t) \equiv \int_{TP1}^t \lvert\omega_k(t')\rvert\, dt'$, $\Omega_2(t) \equiv -\frac{\pi}{4} + \int_{TP2}^t \omega_k(t')dt'$, $\Phi \equiv \frac{\pi}{4} - \int_0^{TP1} \omega_k(t')dt'$, and $Q \equiv \Omega_1(TP2) + \log 2$.

Region	$u_k(t)u_k^*(t)$
WKB I	$\frac{1}{2\omega_k(t)}$
WKB II	$\frac{1}{2\lvert\omega_k(t)\rvert} \left(e^{2\Omega_1(t)} + \frac{1}{4}e^{-2\Omega_1(t)}\right)$
WKB III	$\frac{1}{2\omega_k(t)} \left[\cosh(2Q) + \sinh(2Q)\cos(2\Omega_2(t))\right]$

Table 2: Same as Table 1 for the absolute square of the mode functions.

solutions. Yet they differ in their absolute square as we can see in Table 2: In the WKB I region $\lvert u_k(t)\rvert^2$ changes only slowly with $\omega_k(t)$, meaning that it stays constant for a constant $\omega_k(t)$. In WKB III we basically have the same result, enlarged by the factor $\cosh(2Q)$ that represents the behavior of the mode function between two turning points, but an additional wiggling with the angular frequency $2\omega_k(t)$ is superposed. Although it is not clear at this point how this wiggling will effect the mass after integrating over all wave vectors, we can already say that any wiggling in the resulting mass stems from mode functions that started wiggling in the WKB III region, meaning that these mode functions had been enlarged between two turning points.

The mode functions $u_k(t)$ go through the two turning points at different times for different k. From equation (240) we see that even if the mass $m^2(t)$ is negative, $\omega^2(t)$ can still be positive for big wave modes k. Hence, at the same time t some mode functions are described by a WKB I solution while others are described by a WKB II solution. How are the different WKB regions spread upon the mode functions? Figure 4 gives a schematic view on a possible scenario:

Up to the first turning point TP1 all mode functions can be described by WKB I solutions. They all start from the plain wave solutions of the

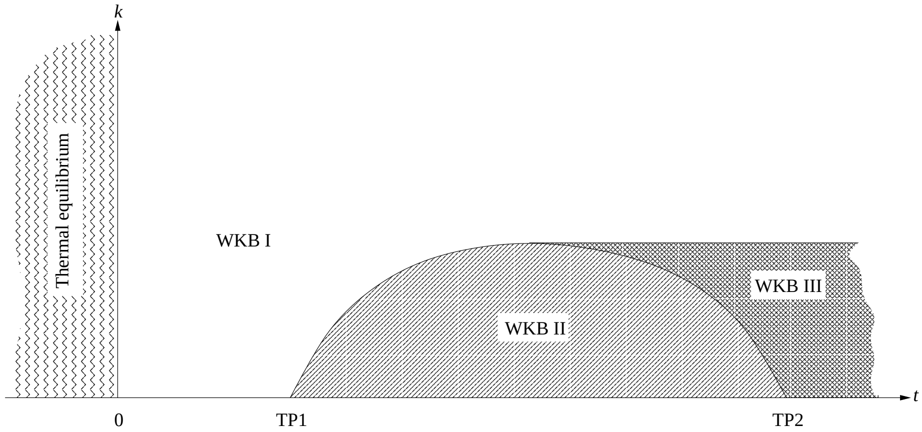


Figure 4: Schematic description of the different WKB approximation regions for the mode functions $u_k(t)$. The squared mass $m^2(t)$ becomes negative at the first turning point TP1 and gets positive at the second turning point TP2 again.

thermal equilibrium region. As the scale factor $a(t)$ grows, the mass $m^2(t)$ becomes smaller as we will see later, until it vanishes. This is where the mode function with the smallest wave vector reaches the first turning point. For $k = 0$ we already have to switch to the WKB II solution whereas modes with $k > 0$ still can be described by the WKB I solution. As $m^2(t)$ keeps falling, more and more mode functions $u_k(t)$ go through a turning point and have to be described by WKB II. If $k_{TP}(t)$ is the solution to $\omega_{k_{TP}}(t) = 0$ at some time t, then all $u_k(t)$ with $k < k_{TP}(t)$ are described by WKB II and all $u_k(t)$ with $k > k_{TP}(t)$ are described by WKB I. From equation (240) we see that the boundary $k_{TP}(t)$ between the two regions is given by $k_{TP}^2(t) = -a^2(t)m^2(t) + \frac{3}{4}\dot{a}^2(t) + \frac{3}{2}a(t)\ddot{a}(t)$.

Mode functions that enter the WKB II region start growing exponentially. They soon become the dominating contribution to the integral in equation (236) and $m^2(t)$ soon starts growing, too. As an effect, no more mode functions enter the WKB II region, but some of the mode functions go through another turning point and are now described by WKB III solutions. As the mass keeps growing with time, more and more mode functions are described by WKB III solutions, until only mode functions of type WKB I and WKB III are left.

In Figure 4 we can clearly see how the range of mode functions is split in WKB I and WKB III solutions after the phase transition. As we already noticed, only the low-momentum mode functions are responsible for any wiggling. High-momentum mode functions can be described by WKB I solutions through the whole process.

Of course this was just one possible scenario, and there could be different pictures of WKB regions, too: The mass could fall again, giving rise to entering another WKB region after the WKB III region that we would have to call WKB IV. WKB V can follow, too, but we saw in the previous chapter that yet another region WKB VI would essentially be WKB IV again. In the following, we will concentrate on the scenario as sketched above.

Let us also note that the nicely drawn boundaries in Figure 4 are far from being fine lines: Actually the regions near turning points can analytically only be described by *Airy* functions properly, and only under the assumption that we know the position of the turning point. We avoid *Airy* functions by using the *connection formulae* to link together different WKB regions as we did in the previous WKB chapter. But we do not really know the position of the turning point, since it would only follow from the knowledge of $m^2(t)$. On the contrary we can not calculate $m^2(t)$ near the turning point unless we know the position of the turning point. The situation is not really hopeless though, because we will see that we can approximate the position of the turning point pretty accurately. Using this approximated turning point, we can calculate the mode functions in adjacent WKB-regions and thus calculate the mass $m^2(t)$.

6.2 Taylor expansion of $m^2(t)$

One way to find an approximate solution to a complicated function is by calculating its Taylor expansion. In a Taylor expansion all variables are evaluated at the expansion point. This is an advantage because we would have to deal with two different masses $m^2(t)$ and $m^2(0)$ in equation (157), but with an series expansion about $t = 0$ we only need to know $m^2(0)$ and its derivatives at the origin. We won't be able to get rid of the integral, but by performing the series expansion, this integral can be expressed in terms of *Debye functions*, that only have one parameter - the temperature scaled mass βm.

Starting point for the expansion is the renormalized mass from equation (157)

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2} \int_0^\infty \frac{1}{\sqrt{m^2(t) + \bar{k}^2}} \frac{1}{e^{\beta\sqrt{m^2(0)+\bar{k}^2 \frac{a^2(t)}{a^2(0)}}} - 1} \bar{k}^2 d\bar{k} \qquad (241)$$

which we derived from the 1-loop-correction of a scalar φ^4-theory in the WKB approximation. In this form the equation is at most valid up to the first turning point. After the first turning point, the mode functions with long wavelengths start to grow exponentially, which would have to be taken into account by an exponentially growing term in uu^* like the one derived from the WKB connection formulae in eq. (224). We will see that the first couple of terms in the Taylor series expansion can describe the function $m^2(t)$ fairly well. Surprisingly, we will find that there is a simple analytical expression for the high-temperature limit for certain cases of scale factors $a(t)$ that describe the evolution of the squared mass quite well even beyond the first turning point to a certain extent. This method fails as soon as the exponential growth of long wavelength mode functions begins to dominate the integral. We would have to take the exponential growth into account to further improve the results.

Equation (241) is already expressed in terms of physical wave vectors $\bar{k}(t) = \frac{k}{a(t)}$. We can further simplify the series expansion by introducing temperature scaled masses and wave vectors:

$$\begin{aligned} \hat{m}^2(t) &\equiv \beta^2 m^2(t) \\ \hat{k} &\equiv \beta\bar{k} \\ \hat{\mu} &\equiv \beta\mu \end{aligned} \tag{242}$$

so that we get a temperature independent equation for $\hat{m}^2(t)$:

$$\hat{m}^2(t) = -\hat{\mu}_R^2 + \frac{\lambda_R}{2\pi^2}\int_0^\infty \frac{1}{\sqrt{\hat{m}^2(t)+\hat{k}^2}} \frac{1}{e^{\sqrt{\hat{m}^2(0)+\hat{k}^2\frac{a^2(t)}{a^2(0)}}}-1}\hat{k}^2 d\hat{k} \tag{243}$$

The inverse temperature $\beta = \frac{1}{T}$ that we used for rescaling the equation is the initial temperature from the thermal equilibrium that our system starts from. Since the mass $\hat{m}^2(t)$ and the scale factor $a^2(t)$ are both evaluated at 0 in this equation already, we will also expand our Taylor series about the point $t = 0$:

$$\begin{aligned} \hat{m}^2(t) &= \hat{m}^2(0) + t\,\frac{d\hat{m}^2(t)}{dt}\bigg|_{t=0} + \frac{t^2}{2}\,\frac{d^2\hat{m}^2(t)}{dt^2}\bigg|_{t=0} + \frac{t^3}{3!}\,\frac{d^3\hat{m}^2(t)}{dt^3}\bigg|_{t=0} + \ldots \\ &= \hat{m}^2(0) + t\hat{m}^{2\prime}(0) + \frac{t^2}{2}\hat{m}^{2\prime\prime}(0) + \frac{t^3}{3!}\hat{m}^{2\prime\prime\prime}(0) + \ldots \end{aligned} \tag{244}$$

It turns out that the squared mass and its derivatives at the origin can be conveniently expressed using *Debye functions* of the form

$$\boxed{\mathcal{D}_{r,s,t}(\hat{m}) \equiv \int_0^\infty \frac{1}{\left(\sqrt{\hat{k}^2+\hat{m}^2}\right)^r} \frac{\left(e^{\sqrt{\hat{k}^2+\hat{m}^2}}\right)^{s-1}}{\left(e^{\sqrt{\hat{k}^2+\hat{m}^2}}-1\right)^s}\hat{k}^t d\hat{k} \;\geq\; 0} \tag{245}$$

with positive integers r, s, and t. Note that there is no more dependence on the inverse temperature β or on the scale factor $a(t)$ in this function. It only depends on the initial mass $\hat{m}^2(0)$ and no longer on both, $\hat{m}^2(0)$ and the time dependent mass $\hat{m}^2(t)$. By construction, the Debye functions are always positive for all combinations r, s, t, and a positive initial mass $\hat{m}$. This will enable us to give rough estimates on some expressions.

For ease of notation we will use a generalization of the *Hubble parameter* $H = \frac{a'(0)}{a(0)}$ and define

$$H_2 \equiv \frac{a''(0)}{a(0)},\ H_3 \equiv \frac{a'''(0)}{a(0)},\ H_n \equiv \frac{a^{(n)}(0)}{a(0)},\ ... \tag{246}$$

We can also omit the argument in the Debye functions since it is always $\hat{m}(0)$ and define

$$\mathcal{D}_{r,s,t} \equiv \mathcal{D}_{r,s,t}\left(\hat{m}(0)\right) = \mathcal{D}_{r,s,t}\left(\beta m(0)\right) \tag{247}$$

and since all derivatives of the squared mass are evaluated at $t = 0$, we also define

$$\hat{m}_0^2 \equiv \hat{m}^2(0),\ \hat{m}_0^{2\prime} \equiv \hat{m}^{2\prime}(0),\ \hat{m}_0^{2\prime\prime} \equiv \hat{m}^{2\prime\prime}(0)\ ,\ ... \tag{248}$$

Using these definitions, the squared mass and its derivatives about 0 can be expressed entirely by the Debye functions and Hubble parameters evaluated at the origin. There is no other integral to be solved except for the one in the Debye functions. The first three terms of this kind that we need for the series expansion (244) are given by

$$\begin{aligned}
\hat{m}_0^2 &= -\hat{\mu}_R^2 + \frac{\lambda_R}{2\pi^2}\mathcal{D}_{1,1,2} \\
\hat{m}_0^{2\prime} &= \frac{\lambda_R}{2\pi^2}\left(-H\mathcal{D}_{2,2,4} - \frac{1}{2}\hat{m}_0^{2\prime}\mathcal{D}_{3,1,2}\right) \\
\hat{m}_0^{2\prime\prime} &= \frac{\lambda_R}{2\pi^2}\left[H^2\left(\mathcal{D}_{4,2,6} + 2\mathcal{D}_{3,3,6} - \mathcal{D}_{3,2,6} - \mathcal{D}_{2,2,4}\right) - H_2\mathcal{D}_{2,2,4}\right. \\
&\quad \left. + H\hat{m}_0^{2\prime}\mathcal{D}_{4,2,4} + \frac{3}{4}\left(\hat{m}_0^{2\prime}\right)^2\mathcal{D}_{5,1,2} - \frac{1}{2}\hat{m}_0^{2\prime\prime}\mathcal{D}_{3,1,2}\right]
\end{aligned} \tag{249}$$

We see that higher derivatives of the squared mass also appear on the r.h.s. of these equations. Starting with the first derivative, terms with the same derivative order as on the l.h.s. come with a factor $\frac{1}{2}\frac{\lambda_R}{2\pi^2}\mathcal{D}_{3,1,2}$ on the r.h.s. in all subsequent derivatives. Bringing these terms to the l.h.s. and dividing by

$1+\frac{1}{2}\frac{\lambda_R}{2\pi^2}\mathcal{D}_{3,1,2}$ where necessary, we finally obtain for the original mass without temperature rescaling

$$\begin{aligned}
m_0^2 &= -\mu_R^2 + \frac{1}{\beta^2}\frac{\lambda_R}{2\pi^2}\mathcal{D}_{1,1,2} \\
m_0^{2\prime} &= -\frac{1}{\beta^2}H\frac{\lambda_R}{2\pi^2}\frac{\mathcal{D}_{2,2,4}}{1+\frac{1}{2}\frac{\lambda_R}{2\pi^2}\mathcal{D}_{3,1,2}} \\
m_0^{2\prime\prime} &= \frac{1}{\beta^2}\frac{\lambda_R}{2\pi^2}\frac{1}{1+\frac{1}{2}\frac{\lambda_R}{2\pi^2}\mathcal{D}_{3,1,2}}\Big[H^2\left(\mathcal{D}_{4,2,6}+2\mathcal{D}_{3,3,6}-\mathcal{D}_{3,2,6}-\mathcal{D}_{2,2,4}\right) \\
&\quad -H_2\mathcal{D}_{2,2,4}+H\beta^2 m_0^{2\prime}\mathcal{D}_{4,2,4}+\frac{3}{4}\left(\beta^2 m_0^{2\prime}\right)^2\mathcal{D}_{5,1,2}\Big] \qquad (250)
\end{aligned}$$

Obviously higher order derivatives give rise to even longer expressions. Comparing these results to numerical results, we find that the derivatives can be described pretty accurately by these formulae.

This result also enables us to give general statements. For example, using the fact that the Debye functions are always positive, we see that the expression for the first derivative $m_0^{2\prime}$ is always negative for a positive expansion parameter $H > 0$. One can show that the term $\mathcal{D}_{4,2,6}+2\mathcal{D}_{3,3,6}-\mathcal{D}_{3,2,6}-\mathcal{D}_{2,2,4}$ in the expression for the second derivative $m_0^{2\prime\prime}$ is also always positive. Therefore $m_0^{2\prime\prime}$ is positive if $H_2 = a''(0)/a(0)$ is small enough. This is still the case in an exponentially expanding de Sitter universe where $H_2 = H^2$ as we will see in the high-temperature limit.

6.2.1 High-temperature limit

The expressions for the derivatives of the squared mass (250) can be simplified by regarding the high-temperature limit $T \gg m$, or $\hat{m} = \beta m = \frac{m}{T} \ll 1$. It turns out that the Debye functions in this limit $\mathcal{D}_{r,s,t}(\hat{m} \to 0)$ are finite if $r+s \leq t$ and that they diverge like $1/\hat{m}^{r+s-t-1}$ for $r+s > t+1$. For example the following high-temperature limits are finite and can be calculated giving nice analytical expressions:

$$\begin{aligned}
\mathcal{D}_{1,1,2}(0) &= \frac{\pi^2}{6} \\
\mathcal{D}_{2,2,4}(0) &= \mathcal{D}_{4,2,6}(0) = \mathcal{D}_{r,2,r+2}(0) = \frac{\pi^2}{3} \\
\mathcal{D}_{3,2,6}(0) &= -6\zeta(3) \\
\mathcal{D}_{3,3,6}(0) &= 3\zeta(3)+\frac{\pi^2}{2} \\
\mathcal{D}_{r,s,t}(0) &= \mathcal{D}_{r+v,s,t+v}(0) = \mathcal{D}_{0,s,t-r}(0) \quad \text{for } r+s \leq t \qquad (251)
\end{aligned}$$

The last relation shows that the finite result basically depends only on two parameters, s and $(t-r)$. Also the Debye function combination appearing in the second derivative in eq. (250) has a simple high-temperature limit:

$$\mathcal{D}_{4,2,6}(0)+2\mathcal{D}_{3,3,6}(0)-\mathcal{D}_{3,2,6}(0)-\mathcal{D}_{2,2,4}(0)=\pi^2 \tag{252}$$

The following high-temperature limits diverge, but one can calculate with which power of $\hat{m}$ they diverge and even give a general formula for these cases:

$$\begin{aligned}
\mathcal{D}_{3,1,2}(\hat{m}\to 0) &\to \frac{\pi}{4\hat{m}} \\
\mathcal{D}_{4,2,4}(\hat{m}\to 0) &\to \frac{3\pi}{16\hat{m}} \\
\mathcal{D}_{4,2,4}(\hat{m}\to 0) &\to \frac{\pi}{16\hat{m}^3} \\
\mathcal{D}_{r,s,t}(\hat{m}\to 0) &\to \frac{\Gamma\left(\frac{r+s-t-1}{2}\right)\Gamma\left(\frac{t+1}{2}\right)}{2\Gamma\left(\frac{r+s}{2}\right)}\frac{1}{\hat{m}^{r+s-t-1}} \quad \text{for}\, r+s>t+1
\end{aligned} \tag{253}$$

Using these limits we can calculate the high-temperature limit of the derivatives of the squared mass in equation (250) and get

$$\begin{aligned}
m_0^2 &= -\mu_R^2+\frac{\lambda_R}{12\beta^2} \\
m_0^{2\prime} &= -\frac{\lambda_R}{12\beta^2}\frac{2H}{1+\frac{\lambda_R}{16\pi\beta m_0}} \\
m_0^{2\prime\prime} &= \frac{1}{\beta^2}\frac{\lambda_R}{2\pi^2}\frac{H^2\pi^2-H_2\frac{\pi^2}{3}+H\beta^2 m_0^{2\prime}\frac{3\pi}{16\beta m_0}+\frac{3}{4}\left(\beta^2 m_0^{2\prime}\right)^2\frac{\pi}{16(\beta m_0)^3}}{1+\frac{\lambda_R}{16\pi\beta m_0}}
\end{aligned} \tag{254}$$

We can further simplify the last expression by omitting small terms: The two terms containing $m_0^{2\prime}$ are small compared to the other two terms in the numerator under certain conditions (e.g. $\lambda_R^2 \ll 768\pi(\beta m_0)^3$ or $\beta m_0 \gg \frac{1}{768\pi}$) that are likely in our application. These conditions also imply $\lambda_R \ll \beta m_0$ which means that we can also omit the denominator $1+\frac{\lambda_R}{16\pi\beta m_0}\approx 1$ in this approximation. Neglecting such terms for the first and second derivative as well as for higher derivatives or $m^2(t)$, we can continue the results of the high-temperature limit:

$$\begin{aligned}
m_0^2 &= -\mu_R^2 + \frac{\lambda_R}{12\beta^2} \\
m_0^{2\prime} &= -\frac{\lambda_R}{12\beta^2} 2H \\
m_0^{2\prime\prime} &= \frac{\lambda_R}{12\beta^2} \left(6H^2 - 2H_2\right) \\
m_0^{2\prime\prime\prime} &= -\frac{\lambda_R}{12\beta^2} \left(24H^3 - 18HH_2 + 2H_3\right) \\
m_0^{2\prime\prime\prime\prime} &= \frac{\lambda_R}{12\beta^2} \left(120H^4 - 144H^2H_2 + 18H_2^2 + 24HH_3 - 2H_4\right) \qquad (255)
\end{aligned}$$

We see that the scale factor $a(t)$ and its derivatives play an important role in determining the high-temperature limit: Higher order derivatives of the scale factor seem to equally well determine the derivatives of m_0^2 as lower order derivatives. It might be interesting to see whether one can find analytical expressions that represent the whole Taylor series for certain choices of the scale factor $a(t)$. Two commonly used scale factors, the *de Sitter* universe and the *power law* universe, shall be discussed in the following.

6.2.2 Analytical expression for the high-temperature limit

There might be an analytical expression for the high-temperature limit (255), but since it is not obvious to me, we first take a look at the special case of a de Sitter universe. The scale factor $a(t) = e^{Ht}$ gives:

$$H_2 = H^2,\ H_3 = H^3, ...,\ H_n = H^n, ... \qquad (256)$$

Inserting this into equations (255) we find an astonishingly easy geometric series as a result for the mass derivatives:

$$\begin{aligned}
m_0^2 &= -\mu_R^2 + \frac{\lambda_R}{12\beta^2} \\
m_0^{2\prime} &= -\frac{\lambda_R}{12\beta^2} 2H \\
m_0^{2\prime\prime} &= \frac{\lambda_R}{12\beta^2} 4H^2 \\
m_0^{2\prime\prime\prime} &= -\frac{\lambda_R}{12\beta^2} 8H^3 \\
m_0^{2\prime\prime\prime\prime} &= \frac{\lambda_R}{12\beta^2} 16H^4 \qquad (257)
\end{aligned}$$

With these derivatives a suitable analytical expression is given by an exponential function with the argument $-2Ht$. The following formula gives the same four derivatives about $t = 0$:

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{12\beta^2} e^{-2Ht} \tag{258}$$

This simple equation shows that in principle the squared mass starts at $-\mu_R^2 + \lambda_R/12\beta^2$ at $t = 0$ and falls off to $-\mu_R^2$ for $t \to \infty$. There is no growing of the mass in this simple model since we have not regarded the exponential growth of long wavelength modes yet.

Let us see whether there is such a nice analytical expression also for the case of a radiation or matter dominated universe. The scale factor is given by $a(t) = c(t + t_0)^p$ with $p = \frac{1}{2}$ for the radiation dominated universe and $p = \frac{2}{3}$ for the matter dominated universe. We shifted the scale factor compared to equations (11) and (12) by t_0 which is the time span between the big bang singularity and the beginning of our simulation. The derivatives of the scale factors are given by

$$H = \frac{p}{t_0},\ H_2 = \frac{p(p-1)}{t_0^2},\ H_3 = \frac{p(p-1)(p-2)}{t_0^3}, ..., H_n = \frac{\Gamma(p+1)}{\Gamma(p-n+1)t_0^n}, ... \tag{259}$$

Inserting them into equations (255) yields the derivatives of the squared mass for a power law scale factor. We can factor the resulting polynomials in p in such a way that it will be obvious how to continue the series of derivatives:

$$\begin{aligned}
m_0^2 &= -\mu_R^2 + \frac{\lambda_R}{12\beta^2} \\
m_0^{2\prime} &= -\frac{\lambda_R}{12\beta^2} 2p \frac{1}{t_0} \\
m_0^{2\prime\prime} &= \frac{\lambda_R}{12\beta^2} 2p(2p+1) \frac{1}{t_0^2} \\
m_0^{2\prime\prime\prime} &= -\frac{\lambda_R}{12\beta^2} 2p(2p+1)(2p+2) \frac{1}{t_0^3} \\
m_0^{2\prime\prime\prime\prime} &= \frac{\lambda_R}{12\beta^2} 2p(2p+1)(2p+2)(2p+3) \frac{1}{t_0^4}
\end{aligned} \tag{260}$$

Guessing higher order derivative terms and putting them together in a Taylor series, the proper analytical expression is given by the $-2p$ power of t. The following formula gives the same four derivatives about $t = 0$:

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{12\beta^2} \frac{t_0^{2p}}{(t + t_0)^{2p}} \tag{261}$$

Again we find that the squared mass starts at $-\mu_R^2 + \lambda_R/12\beta^2$ and falls off to $-\mu_R^2$ for large t. In the case of a radiation dominated universe with $p = 1/2$ we see that $m^2(t)$ falls off like $1/t$.

It attracts the attention that in both cases, in equations (258) and (261), the squared mass basically falls off with the squared inverse scale factor. Can one combine these two formulae in a natural way? Coming this long way, it seems ridiculously easy to write:

$$m^2(t) \approx -\mu_R^2 + \frac{\lambda_R}{12\beta^2}\left(\frac{a(0)}{a(t)}\right)^2 \tag{262}$$

This result can even be improved by noting that $m^2(0)$ is actually determined by a Debye function $\mathcal{D}_{1,1,2}(\beta m(0))$ so that the expression (262) is not really exact for $t = 0$. We can easily fix this by replacing the approximate term by $\mu_R^2 + m^2(0)$, two variables that we know from initially setting up the system, and write

$$\boxed{m^2(t) \approx -\mu_R^2 + \left(\mu_R^2 + m^2(0)\right)\left(\frac{a(0)}{a(t)}\right)^2} \tag{263}$$

Comparisons to numerical simulations show that this is a surprisingly good approximation for the squared mass up to the first turning point where $m^2(t)$ changes its sign and even beyond this point.

Can one verify this result directly by inserting it in the WKB solution in equation (241)? For the case that $\mu_R^2 = 0$ it is easy to show that the relation (263) is exact: Using $\bar{\bar{k}} \equiv \bar{k}\frac{a(t)}{a(0)} = \frac{k}{a(0)}$we insert $m^2(t) = m^2(0)\left(\frac{a(0)}{a(t)}\right)^2$ on the r.h.s. of equation (241) and find that this relation is self-consistent:

$$\begin{aligned}
m^2(t) &= \frac{\lambda_R}{2\pi^2}\int_0^\infty \frac{1}{\sqrt{\left[m^2(0)\left(\frac{a(0)}{a(t)}\right)^2\right] + \bar{k}^2}}\,\frac{1}{e^{\beta\sqrt{m^2(0)+\bar{k}^2\frac{a^2(t)}{a^2(0)}}} - 1}\bar{k}^2 d\bar{k} \\
&= \left(\frac{a(0)}{a(t)}\right)^2 \frac{\lambda_R}{2\pi^2}\int_0^\infty \frac{1}{\sqrt{m^2(0) + \bar{\bar{k}}^2}}\,\frac{1}{e^{\beta\sqrt{m^2(0)+\bar{\bar{k}}^2}} - 1}\bar{\bar{k}}^2 d\bar{\bar{k}} \\
&= \left(\frac{a(0)}{a(t)}\right)^2 m^2(0)
\end{aligned} \tag{264}$$

Also in the case of $\mu^2 \neq 0$ the analytical results are very close to the numerical results, but the reason seems to be more subtle.

6.2.3 Calculation of the turning point in the high-temperature limit

Equation (263) is a pretty good description of the time evolution of the squared mass up to the turning point. Beyond the turning point this approximation does not regard exponentially growing long wavelength modes. Yet, comparisons to numerical simulations suggest that this formula is a good approximation even after the turning point. Therefore we can get a pretty good estimation of the actual turning point by calculating the turning point of the approximation (263).

The first turning point is characterized by $m^2(t_{TP}) = 0$. Inverting the relation for the squared mass, we get:

$$t_{TP} = a^{(-1)} \left(a(0) \sqrt{1 + \left(\frac{m(0)}{\mu_R} \right)^2} \right) \tag{265}$$

where $a^{(-1)}$ denotes the inverse of the scale factor. For the de Sitter universe with $a(t) = e^{Ht}$ this relation becomes

$$t_{TP} = \frac{1}{H} \log \sqrt{1 + \left(\frac{m(0)}{\mu_R} \right)^2} \tag{266}$$

In the case of a power law scale factor $a(t) = (t + t_0)^p$ the turning point can be approximately calculated by

$$t_{TP} = t_0 \left(\left(\sqrt{1 + \left(\frac{m(0)}{\mu_R} \right)^2} \right)^{\frac{1}{p}} - 1 \right) \tag{267}$$

7 Numerical calculations

Numerical calculations are necessary whenever no analytical formulae can be found to a problem. Calculations of a scalar field theory in a curved space-time have been performed before by Boyanovsky, Cooper, Mottola, and others [16, 37, 38]. Basically they solve the pair of differential equations (236) and (237) by introducing finite time steps Δt. Using well-known integration algorithms, very accurate results can be obtained this way, but the computational effort is immense: An equation for the mode functions like eq. (237) has to be solved for every wave vector $k \in (0, \infty)$ which in principle are infinitely many differential equations, and in every time step the absolute square values of the mode functions at a time t are integrated to give the mass $m(t)$ which is used as the input mass $m(t + \Delta t)$ for the next time step.

The drawback of this procedure is that one has to specify at the beginning which discrete vectors k are being used during the numerical calculation. A different approach is to use numerical integration algorithms that independently choose how many and which discrete wave vectors have to be regarded in order to gain a certain accuracy-goal. Such algorithms are implemented in *Mathematica*, but require a slightly different approach to our problem: The differential equations (237) for mode functions $u_k(t)$ are solved adaptively in the k/t-plane for a given function $m_{[n]}(t)$. Using these mode functions, a new mass function $m_{[n+1]}(t)$ is calculated from equation (236) that in turn is used to solve for new mode functions again. This procedure is conveniently implemented in *Mathematica* and quickly converges for small times t.

7.1 Mathematica program code

A *Mathematica* program, written by Carl Woll from the University of Washington, was used in order to test analytical approximations. We pursued an iterative approach in calculating the pair of equations (236) and (237): In a first step the mass $m^2(t)$ is set constant $m^2_{[0]}(t) = 1$ for all t and the differential equations for the mode functions are calculated. Integrating over these mode functions, we obtain a new function $m^2_{[1]}(t)$ that is the first iteration. Using this function we can calculate new mode functions that produce a new mass function $m^2_{[2]}(t)$. At small times t this procedure converges quickly to the desired function $m^2(t) \simeq m^2_{[n]}(t)$.

We relied on *Mathematica*'s internal numerical calculation procedures to minimize the error. We let *Mathematica* choose the modes k and time steps Δt adaptively through its internal numeric differential equation solver. For high momentum modes, the mode functions $u_k(t)$ oscillate with a high frequency that makes numerical calculations hard. But we know from the

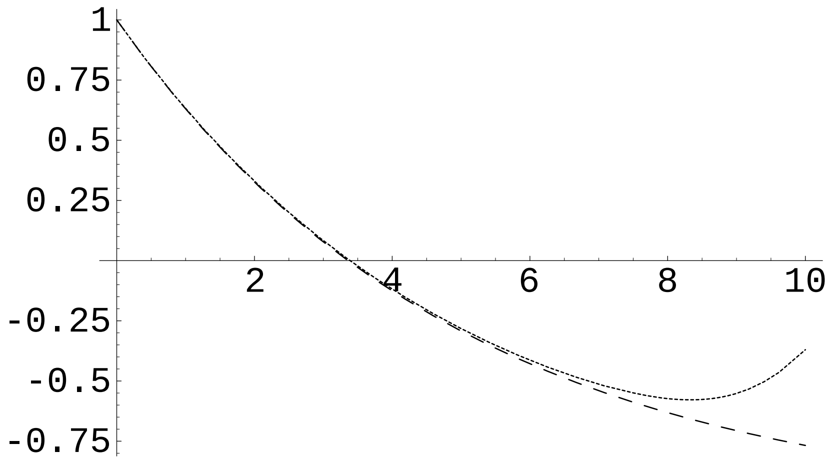


Figure 5: Numerical result (dotted line) compared to the analytical result (dashed line) for $m^2(t)$ in a de Sitter universe with the parameters $\lambda_R = 0.01$, $\beta = 0.02$, $a(t) = e^{Ht}$, $H = 0.1$, and $m(0) = 1$.

discussion about Figure 4 that high momentum modes can entirely be described by WKB I solutions. Therefore we introduced a cut-off to solve the mode functions for low and high momenta separately.

7.2 Numerical results

To test the quality of the analytical expressions from the last chapter we used toy models with simple parameters. Figure 5 shows the evolution of the mass $m^2(t)$ over time for a de Sitter universe. In our calculations the scale factor is given by an exponential expansion $a(t) = e^{Ht}$ with the Hubble constant $H = 0.1$ in arbitrary units. The renormalized coupling constant is assumed to be $\lambda_R = 0.01$ and the initial inverse temperature is given by $\beta = 0.02$. Initially we set our mass to be $m(0) = 1$. We can calculate the renormalized mass parameter μ_R from equation (250) and obtain $\mu_R^2 = 1.044$ for our initial set of parameters.

From Figure 5 we see that the mass $m(t)$ decreases as soon as the expansion starts, as we already predicted from the first derivative of $m^2(t)$ which is always negative in equation (250) for a positive Hubble parameter. The dotted line shows the numerical result from the *Mathematica* program. It crosses the t-axis at $t = \text{TP1} = 3.388$. This marks the classical turning point for the lowest mode function. The schematic Figure 4 shows how more and more mode functions with small k start to grow exponentially for $t \geq \text{TP1}$. This

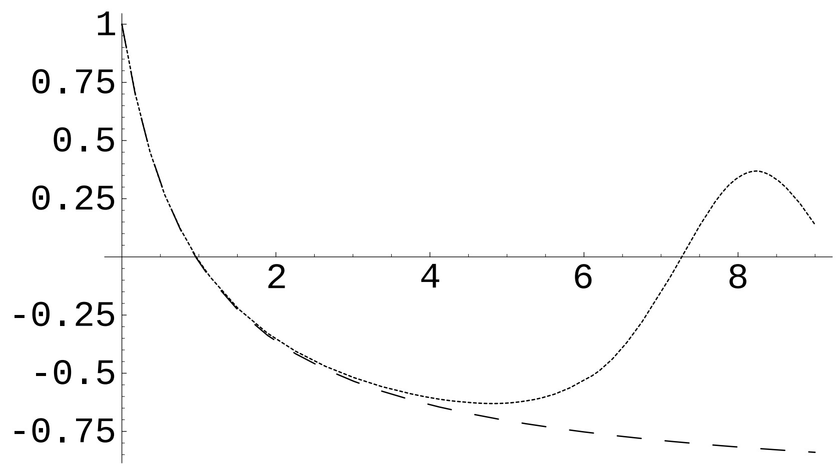


Figure 6: Numerical result (dotted line) compared to the analytical result (dashed line) for $m^2(t)$ in a radiation dominated universe with the parameters $\lambda_R = 0.01$, $\beta = 0.02$, $a(t) = \sqrt{t+1}$, and $m(0) = 1$.

contributes to the squared mass until it starts growing again after $t \approx 8.4$.

The dashed line in Figure 5 shows the high-temperature limit from equation (263). This function falls exponentially from $m^2(0) = 1$ to its asymptotic value $-\mu_R^2$. Since this analytical result does not consider the exponentially growing modes from the WKB II region in Figure 4, we find that it keeps falling even if the numerical result starts to grow again. This is no calculation error, but merely represents the fact that we have not regarded growing modes in the Taylor expansion yet.

From equation (266) we see that we can calculate the position of the first classical turning point by

$$\mathrm{TP1} \approx \frac{1}{2H} \log\left(1 + \frac{m^2(0)}{\mu_R^2}\right) \tag{268}$$

With our initial values this gives TP1 ≈ 3.358 which is pretty close to the numerical result TP1 $= 3.388$. The ability to calculate an approximate position of the turning point without knowing the exact behavior of $m^2(t)$ is necessary for implementing approximations of the growing mode functions in the WKB II region: Any application of the connection formulae depends on the knowledge of the position of the turning point.

Figure 6 shows the evolution of the mass $m^2(t)$ in the case of a radiation dominated universe with the scale factor $a(t) = \sqrt{t+1}$. The other parameters are the same as for Figure 5 with a coupling constant $\lambda_R = 0.01$ and the inverse temperature $\beta = 0.02$. Again, for the initial mass $m(0) = 1$ we obtain the same parameter $\mu_R^2 = 1.044$. From the high-temperature limit (261) with $p = 1/2$ we know that the mass falls off like $m^2(t) + \mu_R^2 \propto 1/(t+1)$. According to equation (267) the position of the classical turning point can be approximated in the high-temperature limit as

$$\mathrm{TP1} \approx t_0 \frac{m^2(0)}{\mu_R^2} \tag{269}$$

This simple equation gives TP1 ≈ 0.958 while from the numeric calculation we obtain TP1 $= 0.964$. In both models, the de Sitter universe and the radiation dominated universe, the turning points could be approximated for our choice of initial values by simple high-temperature limit formulae with an error of less than 1%. The accuracy of an approximate turning point is crucial for further analytical descriptions of the mass through WKB II and WKB III regions.

8 Summary and outlook

In this work we presented a way of describing the time evolution of a scalar field mass in an expanding background. Two approaches, an analytical approximation and a numerical calculation, were compared to each other and the limits for each approach were discussed. Scalar field systems in a curved space-time play an important role in the physical processes at the very beginning of our universe.

Studying dynamical properties of a system at finite temperature requires a special formalism. While static, equilibrium systems at finite temperature can be described in the imaginary-time formalism, it is not straightforward to answer questions about a time-dependent behavior of such a system. A new formalism, called real time formalism, can overcome this difficulty.

Starting from the Keldysh-Schwinger closed-time-path formalism in a flat space-time [32], we enhanced the real time formalism by the notion of a curved space-time. We found that the mode functions, which are solutions to the Klein-Gordon operator, are no longer simple plane wave solutions, but they depend on the time-dependent background metric in a non-trivial way. With this in mind, we showed how to derive the closed-time-path formalism for general mode functions. We calculated the Green function of the Klein-Gordon operator using canonical commutation relations for the scalar field φ and the KMS-conditions for the initial temperature of the system and we expressed the full propagator in terms of general mode functions.

This general result was applied to the metric of a Friedmann-Robertson-Walker universe with a flat space-time. This metric contains one scale factor $a(t)$ that describes the expansion of the universe. Technically it makes sense to describe the system in comoving coordinates where particles at rest expanding with the metric keep their coordinates. We also studied the consequences of introducing a conformal time $d\eta = dt/a(t)$ which makes certain equations easier as space-time is conformal to Minkowski space-time.

Using a generic scale factor $a(t)$, we rescaled quantities like the propagator, the scalar field, or the mode functions for this metric. The canonical commutation relations for the scalar field are now written in terms of the rescaled field $\tilde{\varphi}$, and the propagator $G_c(t-t', \vec{k})$ in the Fourier transformed space can be expressed using scaled mode functions $\tilde{u}_{\vec{k}}(t)$.

We calculated the mass of the scalar field to the lowest order of perturbation theory for a scalar field theory with a $\lambda\varphi^4$-interaction term. The first-order mass correction is given by the one-loop Feynman diagram which basically is an integration of the equal time propagator over all modes $\vec{k}$. The resulting equation for the mass turns out to be divergent and has to be renormalized in order to give reasonable physical results.

In essence, we followed the renormalization scheme of Cooper and Mottola [16] and introduced a renormalized mass μ_R and coupling constant λ_R. A quadratic divergence can be removed by shifting the original bare mass. An additional logarithmic divergence requires a summation of bubbles in the scattering amplitude [33]. For regularizing the integrals we introduced the cut-off $\Lambda_{\vec{k}}$ for the wave vector. The resulting equation for the mass is given by

$$m^2(t) = -\mu_R^2 + \frac{\lambda_R}{2\pi^2 a^3(t)} \int_0^\infty |\tilde{u}_k(t)|^2 \frac{1}{e^{\beta\omega_k(0)} - 1} k^2 dk$$

This equation was the starting point for further investigations. Calculating this equation numerically means quite some effort: Each mode function $\tilde{u}_k(t)$ for different k is determined by its own second-order differential equation. To make things worse, these differential equations contain the mass $m(t)$ as an argument. We would have to know $u_k(t)$ to calculate $m(t)$ and, vice versa, the knowledge of $m(t)$ is required to be able to calculate $u_k(t)$. There is no simple solution to this system of infinitely many coupled differential equations.

Therefore we asked the question whether it is possible to gain any useful information from this equation by regarding certain approximations to this system. The differential equations of the mode functions turned out to be well described in the WKB approximation. Having its roots in simple quantum mechanical applications [35], the basic idea of the WKB approximation is a separation of the sinusoidal solution into its frequency and its amplitude. The strength of this approximation lies in the fact that it generates a solution for a second-order differential equation with an arbitrary potential that only depends analytically on this potential and on the integral thereof.

The ability to apply the WKB approximation is restricted by the form of the potential. Therefore, for the comoving metric we found that WKB can only be applied to regions where

$$\frac{k^2}{a^2} + m^2 \gg 16H^2$$

Similar restrictions on $\dot{H}$, $\dot{m}$, and $\ddot{m}$ have to be met. These are severe constraints since the interesting part of the physics happens when $\bar{\omega}^2 \equiv k^2/a^2 + m^2$ becomes negative due to a negative squared mass $m^2 < 0$ in a false-vacuum state! Luckily, in the opposite case, $k^2/a^2 + m^2 \ll -16H^2$ the system can be described in the WKB approximation again. The solutions loose their sinusoidal character and are given by exponentially growing or decaying functions.

The time t at which $\bar{\omega}^2(t)$ changes from being positive to negative marks the first classical turning point. The WKB approximations are not valid in the vicinity of the turning point. Yet, WKB solutions to the left and to the right of a turning point can be linked to each other by so-called connection formulae. We derived these formulae using Airy functions that describe the linearly approximated solution near a turning point.

By repeated application of these connection formulae we showed how to trace the time evolution of the mode functions through a first and a second classical turning point. For an initially solely circular polarized state, we denoted WKB regions separated by turning points by WKB I, WKB II, and WKB III. We found that the absolute square of the mode function that we needed in order to calculate the mass integral is given in the WKB III region by

$$|u_k(t)|^2 \approx \frac{1}{2\omega_k(t)} \left[\cosh\left(2Q\right) + \sinh\left(2Q\right)\cos\left(2\Omega_2(t)\right)\right]$$

We saw that the solution in the WKB I region $|u|^2 \approx (2\omega)^{-1}$ is not only enhanced in the WKB III region by a factor $\cosh 2Q$ that essentially depends on the area of $\bar{\omega}$ in the WKB II region between the two turning points; the formerly constant solution also starts to wiggle with an $\bar{\omega}$-dependent frequency. Thus we could demonstrate that any wiggling in the resulting mass after going through a phase transition stems from low momentum modes with small k.

We then calculated the Taylor expansion of the mass integral for the WKB I region. The main difficulty was the appearance of two different masses $m(t)$ and $m(0)$ in the integral that prohibited the use of a Mellin transform. Using generalized Debye functions, we calculated the first couple of terms of the Taylor series for the mass. Especially we saw that the first derivative of the mass has the opposite sign of the Hubble parameter which proves that the mass starts decreasing in an expanding universe.

In the high-temperature limit $\beta m \ll 1$ we found an analytical expression representing the terms of a Taylor series. For an arbitrary scale factor we found that

$$m^2(t) \approx -\mu_R^2 + \left(\mu_R^2 + m^2(0)\right)\left(\frac{a(0)}{a(t)}\right)^2$$

Although this approximation is only valid in the WKB I region, comparisons to numerical calculations show that it is astonishingly accurate even far beyond the first turning point in the WKB II region. This enables us to approximate the position of the first turning point TP1 by inverting the relation $m^2(\text{TP1}) = 0$.

Extensions to the work presented here could include regarding the exponential growth of low momentum mode functions in an analytical approximation. This problem involves finding a suitable approximation to how different mode functions pass the turning point at different times.

Another interesting idea would be to study the next order of the mass perturbation. Once the mode functions are calculated for a one-loop mass correction, this information could be used to calculate the next order Feynman diagram, the so-called sunset diagram, and to see whether the first-order approximation is a good one.

Our methods of finding analytical expressions that describe the mass evolution of scalar fields might help to deepen the understanding of the process of phase transitions. A deeper knowledge of the underlying physics could complement existing results from numerical calculations. It could ultimately lead to valuable criteria that might be able to differentiate between current theories of inflation.

We are lucky that we will not be blown up to ultra galactic scales within hyper-short times because we do not have the necessary super-high energy density. But who knows what other strange concepts wait hidden in the universe just to be explored by creatures that formerly originated from quantum fluctuations of a tiny, tiny patch.

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