QUANTUM DESCRIPTION OF THE UNIVERSE CLOSE TO BIG BANG

Master’s thesis

2014 Fridrich Valach
QUANTUM DESCRIPTION OF THE UNIVERSE CLOSE TO BIG BANG

Master’s thesis

Study programme: Theoretical physics
Branch of study: 1160 Physics
Supervisor: Vladimír Balek, doc. RNDr., CSc.

Bratislava, 2014
Fridrich Valach
**Name and Surname:** Bc. Fridrich Valach  
**Study programme:** Theoretical Physics (Single degree study, master II. deg., full time form)  
**Field of Study:** 4.1.1. Physics  
**Type of Thesis:** Diploma Thesis  
**Language of Thesis:** English  
**Secondary language:** Slovak  

**Title:** Quantum description of the universe close to Big Bang  
**Aim:** To investigate solutions of Wheeler-DeWitt equation in minisuperspace, describing creation of the universe from "nothing", with logarithmic asymptotics for the radius of the universe approaching zero.  

**Literature:**  

**Annotation:** For a universe created from "nothing" there should exist a one-parametric class of solutions, so far not considered in the literature, with the asymptotics for the radius approaching zero proportional to the logarithm of the radius. In the thesis properties of these solutions should be investigated and subtleties of the method used in their derivation should be discussed, first in the quantum-mechanical problem of a particle tunneling from a potential well in two dimensions and then in the cosmological setting, as a tool for the description of the initial stage of the evolution of the universe.  

**Keywords:** Wheeler-DeWitt equation, tunneling, creation of the universe from "nothing"  

**Supervisor:** doc. RNDr. Vladimír Balek, CSc.  
**Department:** FMFI.KTFDF - Department of Theoretical Physics and Didactics of Physics  
**Head of department:** doc. RNDr. Tomáš Blažek, PhD.  

**Assigned:** 27.11.2012  
**Approved:** 28.11.2012 prof. RNDr. Melánia Babincová, CSc.  
Guarantor of Study Programme
Acknowledgement

I would like to thank my supervisor doc. RNDr. Vladimír Balek, CSc. for his guidance, help, kindness, patience and also for the choice of this interesting topic. I am also deeply indebted to my family for their invaluable support.
Abstract

In the thesis we study WKB solutions of the Wheeler–DeWitt equation describing creation of the universe from “nothing”. This was studied by Vilenkin in 1986. Motivated by his paper, we consider the case of a two-dimensional minisuperspace for a closed FLRW universe containing scalar field with quadratic potential. There is a close resemblance between our problem and the problem of tunnelling into a potential well in the two-dimensional quantum mechanics. The tunnelling from a potential well was investigated by Banks, Bender and Wu in 1973. We first adjust their technique to our problem and then use the resemblance of the quantum mechanical and quantum cosmological problems to explore the latter, as proposed by Balek in 2014. In particular, we construct a class of solutions so far not considered in the literature. These solutions arise when we require an asymptotic behaviour different from that of Vilenkin.

Keywords: 2D tunnelling, Wheeler–DeWitt equation, scalar field, minisuperspace, creation of the universe from “nothing”
Abstrakt


Klúčové slová: tunnelovanie v dvoch rozmeroch, Wheelerova–DeWittova rovnica, skalárne pole, minisuperpriestor, vznik vesmíru z „ničoho“
The thesis is devoted to quantum cosmology. I have chosen the topic, because it belongs to the field of quantum gravity, the centre of attention of many theoretical physicist today. This theory is not yet complete, which allows anybody working in it to develop his own ideas and approaches. On the other hand, it is generally believed that finding a satisfactory and well-defined theory of quantum gravity would be a major leap forward in theoretical physics.

Understanding of the thesis requires the knowledge of quantum mechanics. In addition, in section 4.1 we use some basic concepts from general relativity as well as the Lagrangian and Hamiltonian formalism.
Contents

1 Quantum-mechanical tunnelling 11
    1.1 WKB approximation ........................................... 11
    1.2 Matching the solutions ........................................ 14
    1.3 2D tunnelling outwards ....................................... 18

2 Modification of the problem 27
    2.1 2D tunnelling inwards ........................................ 27
    2.2 Outside the barrier ........................................... 31
    2.3 Some pictures .................................................. 33

3 In polar coordinates 40

4 Tunnelling in cosmology 45
    4.1 Wheeler–DeWitt equation ..................................... 45
    4.2 Vilenkin’s solution ........................................... 48
    4.3 Alternative solutions ......................................... 51

A Associated Legendre functions 58
Introduction

From the birth of quantum theory and general theory of relativity there have been many attempts to unify them, or to find a more general theory from which they would arise as respective limits. Over years most efforts have formed several “streams” [12]. One significant line of research, often called covariant approach, is covered by string theory. In this work we focus on another approach, called canonical. It uses the procedure of canonical quantisation, which is applied to Hamiltonian formulation of general relativity [7] (for that formulation see also [11]). The result is the Wheeler–DeWitt equation, which is in general a (functional) differential equation acting on a functional defined on the space of all possible three-geometries. This functional is referred to as the wavefunction of the universe.

It turned out, however, that the Wheeler-DeWitt equation is ill-defined in the general case. A resolution of the problem came only with loop quantum gravity, 20 years after the moment the equation was first written down [12]. Nevertheless, different versions of the equation, restricted to some special cases of three-geometries, are consistent and have been intensively studied (see for example [7], [13], [14], [15]; for more recent see [3], [5]). This will be also the focus of our thesis. More specifically, we will investigate the case of a closed FLRW universe with spatially homogeneous scalar field with quadratic potential. The classical state of the universe is at any moment given by two parameters – radius of the universe and value of the scalar field. Hence, the wavefunctional is reduced to a wavefunction dependent on just two variables. The corresponding Wheeler–DeWitt equation has a form very similar to the time-independent Schrödinger equation in two dimensions. Because of this, we can employ techniques known from ordinary quantum mechanics – in the first part of our thesis we describe in detail the methods adopted from this theory which we will later use in the quantum cosmological problem. Let us emphasise that all the work will be done in the WKB approximation, which is a reasonable framework for discussing the physical implications of solutions of the Wheeler–DeWitt equation (see for example [6]).

We start with a brief outline of the basic principles and results of the WKB approximation in quantum mechanics [10], [9] and then we proceed to describe an approach to the problem of a particle tunnelling outwards from a non-rotationally
symmetric potential well in two dimensions, as proposed in [4] (see also [5] and [3]). In the second chapter, we modify the method so that instead of a particle escaping from the well, we examine an incoming beam of particles tunnelling through the barrier to the inside of the well [3]. We describe in detail the known procedures, at some point including our own arguments. The latter is done mainly at the point where we deal with the separation constant (analysis around formula (1.62) and similar ones in the following chapters), when constructing the incoming wave corresponding to the tunnelling solution (section 2.2), and when finding a necessary condition for the solution to be well-behaved (section 2.3). As a result, we arrive at a one-parametric class of solutions for the problem considered.

In the short third chapter we obtain solutions of the same problem after performing a similar procedure as in previous chapters, but in polar coordinates (it is again done along the lines of [3]). This is an important midpoint on the way to quantum cosmology, because the Wheeler–DeWitt equation has almost the same form as Schrödinger equation in polar coordinates, the differences being only the reverse sign of the kinetic term for scalar field and the value of energy.

In the last chapter, we turn our attention to the Wheeler–DeWitt equation itself. After constructing it, we describe the approach of Vilenkin [14], who examined the case of a universe tunnelling from zero radius into the domain of finite-sized universes. This is called “creation of the universe from nothing”. It is important for us that Vilenkin in [14] uses a condition that the dependence of the wavefunction on the value of the scalar field vanishes as the radius of the universe approaches zero. Motivated by [8], in the last section of the chapter 4 we restrict ourselves to a particular choice of the ordering parameter\(^1\), and we formulate our alternative condition, which together with the techniques from previous chapters yields a new one-parametric class of solutions\(^2\).

Finally, we devoted the Appendix to formulae concerning the associated Legendre functions, as we need these throughout the computations.

---

\(^1\)This parameter represents the ambiguity in the ordering of non-commuting operators, arising during the quantisation process.

\(^2\)The reverse sign in the Wheeler–DeWitt equation implies that despite the fact that we probe the case of tunnelling outwards, we obtain the whole class of solutions as in the quantum mechanical tunnelling inwards.
Chapter 1

Quantum-mechanical tunnelling

1.1 WKB approximation

One of the most widely used approaches to semiclassical approximation of quantum mechanics is based on works of Wentzel, Kramers and Brillouin (thus the abbreviation WKB) and goes as follows [10, p. 232]:

The main idea is that a situation can be called semiclassical when the corresponding de Broglie wavelength is much shorter than a characteristic length associated with the problem, i.e. a typical scale on which the potential changes. Moreover, the de Broglie wavelength itself varies on this scale and thus we are lead to another equivalent formulation of the condition of semiclassicity

\[ \Delta \lambda |_{\lambda} \ll \lambda, \quad (1.1) \]

where \( \Delta \lambda |_{\lambda} \) is the change of \( \lambda \) on the distance of \( \lambda \).

We now rewrite the condition in terms of “more useful” variables. From

\[ \lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(E - V(x))}}, \quad (1.2) \]

where \( h \) is the Planck constant, \( p \) the momentum of the particle, \( m \) its mass, \( E \) its energy and \( V \) the potential, we have

\[ \left| \Delta \lambda |_{\lambda} \right| \approx \left| \frac{d\lambda}{dx} \right| \lambda = \left| \frac{h}{\sqrt{8m(E - V)^3}} \frac{dV}{dx} \right| \lambda = \frac{hm}{p^3} \left| \frac{dV}{dx} \right| \lambda. \quad (1.3) \]

Thus, the equivalent formulation of the condition is

\[ \frac{hm}{p^3} \left| \frac{dV}{dx} \right| \ll 1. \quad (1.4) \]
Now we turn our attention to the one dimensional time-independent Schrödinger equation and to its solution, the wavefunction $\Psi(x)$. For a free particle, we have $\Psi = A e^{i p x / \hbar}$, where $\hbar$ is the reduced Planck constant. Because the potential in our case varies very slowly, the solution should resemble the one of a free particle. Therefore we write

$$\Psi = A e^{i S(x) / \hbar}$$

(1.5)

and expect the coefficient $A$ to be almost constant. After passing to exactly constant $A$ and inserting this into the Schrödinger equation we obtain

$$-i \hbar \frac{d^2 S}{dx^2} + \left( \frac{dS}{dx} \right)^2 = p^2.$$

(1.6)

Now we perform the crucial step: we expand the $S$ function into the Taylor series in $\hbar$. One motivation is that the (reduced) Planck constant in some way characterises the quantum world (e.g. through the uncertainty principle) and “the smaller the constant, the smaller the quantum effects”. Considering this, it seems natural that when investigating the semiclassical effects, we write such an expansion and then consider only first few terms in it. However, there is an alternative point of view, which we adopt here. In this approach, we write the expansion (which should of course exist for every well behaved function) and then we inspect the terms one by one and see whether we can use the condition (1.4) to cut off the series.

When we put

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2} S_2(x) + \ldots$$

(1.7)

into (1.6) and collect together the terms of the same order we have equations

$$\left( \frac{dS_0}{dx} \right)^2 = p^2$$

(1.8)

$$\frac{dS_0}{dx} \frac{dS_1}{dx} - i \frac{d^2 S_0}{dx^2} = 0$$

(1.9)

$$\frac{dS_0}{dx} \frac{dS_2}{dx} + \left( \frac{dS_1}{dx} \right)^2 - i \frac{d^2 S_1}{dx^2} = 0$$

(1.10)

$$\vdots$$

From (1.8) we immediately have

$$S_0(x) = \pm \int p(x) dx.$$  

(1.11)

The equation (1.9) implies

$$\frac{dS_1}{dx} = \frac{i}{2p} \frac{dp}{dx}.$$  

(1.12)
After eliminating $dx$ and integrating both hand sides we obtain

$$S_1(x) = \frac{i}{2} \log(C_1 p). \quad (1.13)$$

Note that we have constants similar to $C_1$ in the formulae for $S_0$ and $S_2$ as well, but we have hidden them into the integrals. Eventually, we get rid of all these constants by absorbing them into the preexponential factor.

The third equation (1.10) gives us

$$S_2(x) = \int \frac{1}{\frac{dx}{d\gamma}} \left( \frac{d^2 S_1}{dx^2} - \left( \frac{dS_1}{dx} \right)^2 \right) dx =$$

$$= \pm \int \frac{1}{p} \left( -\frac{1}{2} \left( \frac{p'}{p} \right)' + \frac{1}{4} \left( \frac{p'}{p} \right)^2 \right) dx =$$

$$= \mp \frac{1}{4} \int \left( \frac{2p''}{p^2} - \frac{3p'^2}{p^3} \right) dx =$$

$$= \mp \left( \frac{p'}{2p^2} + \frac{1}{4} \int \frac{p'^2}{p^3} dx \right) =$$

$$= \pm \left( \frac{mV'}{2p^3} - \frac{m^2}{4} \int \frac{V'^2}{p^5} dx \right)$$

where we denoted $d/dx$ by a prime and used integration by parts as well as the fact that $p = \sqrt{2m(E - V(x))}$. Putting all together we have

$$S(x) = \pm \int p dx + \frac{i\hbar}{2} \log(C_1 p) \pm \frac{\hbar^2}{2} \left( \frac{mV'}{2p^3} - \frac{m^2}{4} \int \frac{V'^2}{p^5} dx \right) + \ldots \quad (1.15)$$

Considering the condition (1.4) we now see that the term proportional to $\hbar^2$ can be neglected. So can the higher terms, which is a fact that we will not prove here (it seems rather intuitive, though).

Finally we have obtained the expression

$$\Psi(x) \approx \frac{A}{k^{3/2}} \exp \left( i \int k dx \right) + \frac{B}{k^{3/2}} \exp \left( -i \int k dx \right), \quad (1.16)$$

where we used $k = p/\hbar$.

At this point a discussion is needed. In (1.3) we can see that near the turning point (i.e. point, where $E = V(x)$, see figure 1.1) our approximation is no longer valid. It means that we can use the formula (1.16) only in the regions far from these points (in our case far left and far right of the point $b$, respectively). A question arises concerning the nature of the solutions in the regions excluded or at least about the relation of the coefficients in the respective domains (we mean preexponential coefficients in (1.16)). Let us now briefly describe how to (partially but rather satisfactorily) resolve these issues.


1.2 Matching the solutions

A “standard” approach [10, p. 236] is to linearise the potential in the region near the turning point and presume that the domain of validity of this approximation overlaps with the domains where we have used the WKB approximation. By solving the Schrödinger equation in the linearised case we obtain Airy functions, which we then use to relate the WKB coefficients from the “left” and from the “right”. There is, however, another method, described in [9, p. 164], which uses analytic continuation of the solution to bypass in the complex plane the “dangerous” turning point. Of course, both ways we come to the same result. However, the latter method is rather elegant and we can easily generalise it to our case of tunnelling in 2D. We therefore turn our attention to it.

Consider a potential similar to that depicted in figure 1.1. To avoid confusion when using square roots we define the function

$$w(x) = \frac{2m}{\hbar^2} (E - V(x)).$$

In terms of $w$ the solution in the left region is

$$\Psi_L = \frac{C_1}{w^{1/4}} \exp \left( i \int_b^x \sqrt{w} dx \right) + \frac{C_2}{w^{1/4}} \exp \left( -i \int_b^x \sqrt{w} dx \right).$$

For the wavefunction on the right we have

$$\Psi_R = \frac{C}{2(-w)^{1/4}} \exp \left( - \int_b^x \sqrt{-w} dx \right).$$

(in the latter formula we have omitted the solution increasing to infinity when $x \to \infty$).
We now claim that it is possible to solve the time independent Schrödinger
equation in the complex plane and that the left and right solutions will be smoothly
connected by a (smooth) solution in the complex region between the two segments
of the real axis to which the solutions refer (see figure 1.2; the grey colour marks
the region where we are not allowed to use the WKB approximation - we have to
“go” around). Thus, both $\Psi_L$ and $\Psi_R$ being parts of the same solution, we can easily
unveil the relation between the coefficients appearing in them.

![Figure 1.2: Region where the WKB approximation is not valid](image)

From now on, we set the cut of the (complex) square root function on the
negative real axis. In other words, we have

$$\sqrt{e^{i\varphi}} = e^{\frac{i}{2}\varphi} \quad \text{for } \varphi \in (-\pi, \pi).$$  \hspace{1cm} (1.20)

We start from the solution on the right and analytically continue it first to the upper
complex half plane and then to the lower complex half plane. We must also analyt-
ically continue the potential $V(x)$. For this purpose, we get along with the linear
approximation like in the method of Airy functions.

The expression (1.19) is valid not only on the real axis for $x \gg b$, but in the
whole upper region far from $B$ up to the real axis on “the other side” (i.e. for $x \ll b$).\(^1\)
After we choose small $\epsilon$, set $x = b + re^{i(\pi - \epsilon)}$ (figure 1.3, in this case $\varphi = \pi - \epsilon$), and
denote $\alpha = V'(b)$, we have

$$\sqrt{-w(x)} \approx \sqrt{\frac{2m}{\hbar^2} \alpha r e^{i(\pi - \epsilon)}} \approx i \sqrt{\frac{2m}{\hbar^2} \alpha r} \approx i \sqrt{w(x)},$$  \hspace{1cm} (1.21)

\(^1\)On the axis itself (left to $b$) the square root in solution (1.19) has a cut, which is why we must
stop our analytic continuation before reaching the axis. However, this is not a problem, because
without any further trouble we can continue (1.18) so that it meets the solution just next to the real
axis.

\(^2\)When we consider only the beginning and the end, the complexity of the expression may look a
and the solution carried over from the right has the form
\[
\frac{C}{2\sqrt{i(w)^{1/4}}} \exp \left( -i \int_b^x \sqrt{w} dx \right) = \frac{C e^{-i\pi/4}}{2w^{1/4}} \exp \left( -i \int_b^x \sqrt{w} dx \right),
\]
which is exactly the second term in (1.18). We would be perfectly satisfied were it not the fact that we reconstructed only half of the solution. What is the reason?

One good idea is to look at the behaviour of the terms in (1.18) when analytically continuing \( \Psi_L \). When continuing the left solution towards the right region in the upper plane, the first term becomes negligible compared to the second. To see this, consider an upper semicircle around \( b \) with the radius \( R \). For \( x = b + R e^{i\varphi} \), \( \tilde{x} = b + r e^{i\varphi} \), \( \varphi \in (0, \pi] \), we have
\[
\int_b^x \sqrt{w} d\tilde{x} = \alpha \sqrt{\frac{2m}{\hbar^2}} \int_0^R \sqrt{-r e^{i\varphi} e^{i\varphi} dr} = \alpha \sqrt{\frac{2m}{\hbar^2}} \int_0^R \sqrt{r e^{i(\varphi - \pi)} e^{i\varphi}} dr = \frac{2}{3} \alpha \sqrt{\frac{2m}{\hbar^2}} R^{3/2} e^{i\varphi/2},
\]
where we integrated along the path of constant \( \varphi \). Notice that we have used \(-1 = e^{-i\pi}\)

\[
\left| \exp \left( i \int_b^x \sqrt{w} dx \right) \right| = \exp \left[ \frac{2}{3} \alpha \sqrt{\frac{2m}{\hbar^2}} R^{3/2} \cos \left( \frac{3}{2} \varphi \right) \right]
\]

Figure 1.3: Coordinates description

instead of (perhaps more popular) \(-1 = e^{i\pi}\). This is in order to satisfy the condition that the phase of the exponential lies in the interval \((-\pi, \pi)\) so that we can use (1.20). Now we can see that the module

\[
\text{bit absurd at first sight. But it is actually very important to distinguish whether we obtain } \sqrt{-w} = i\sqrt{w} \text{ or } \sqrt{-w} = -i\sqrt{w}, \text{ which we achieve by realising that } \pi - \epsilon < \pi \text{ implies } e^{i(\pi - \epsilon)} \approx e^{i\pi/2} = i \text{ due to (1.20).}
\]
decreases exponentially when $\varphi$ decreases from $\pi$, while the module of the second term in (1.18) increases exponentially. The implication is that we cannot expect the first term in (1.18) to appear in the analytic continuation of $\Psi_R$, because it could have been produced only by a term too small to survive the WKB approximation\(^3\).

Let us return to our result. We obtained the relation

$$C_2 = \frac{C}{2} e^{-i\frac{\pi}{4}}.$$  

(1.25)

When considering analytic continuation to the lower half plane and performing a similar analysis (the crucial formula now being $\sqrt{-\bar{w}} = -i\sqrt{w}$), we arrive at the condition

$$C_1 = \frac{C}{2} e^{i\frac{\pi}{4}}.$$  

(1.26)

As a result, we can write

$$\Psi_L = \frac{C}{w^{1/4}} \cos \left( \int_b^x \sqrt{w} dx + \frac{\pi}{4} \right).$$  

(1.27)

Putting all together we have

$$\Psi_L = \frac{C}{\sqrt{k}} \cos \left( \int_b^x k dx + \frac{\pi}{4} \right), \quad \Psi_R = \frac{C}{2 \sqrt{|k|}} \exp \left( - \int_b^x |k| dx \right).$$  

(1.28)

We now derive a rather famous consequence of these formulae (see [9, p. 170]). Imagine a situation similar to the one depicted on 1.4. The matching formulae for the turning point $b$ are given by (1.28), so for the internal solution we have

$$\Psi_{\text{inside}} = \frac{C}{\sqrt{k}} \cos \left( \int_b^x k dx + \frac{\pi}{4} \right).$$  

(1.29)

After performing another analysis, this time of the left turning point (the solution to the far left of $a$ is $C'/\sqrt{|k|} \exp \left( \int_a^x |k| dx \right)$), we arrive at

$$\Psi_{\text{inside}} = \frac{C'}{\sqrt{k}} \cos \left( \int_b^x k dx - \frac{\pi}{4} \right).$$  

(1.30)

We require this to be equal to (1.29), and as a result, we arrive at the condition

$$\int_a^b k dx - \frac{\pi}{2} = n\pi,$$

(1.31)

\(^3\)In other words, in our approximation, the function that gives birth only to the second term in (1.18) is in the region (relatively) far above the real axis indistinguishable from the function that produces both terms. Because of this, we can say that the continued $\Psi_R$ function smoothly becomes the second term in (1.18) modulo any function with the behaviour of the first term from (1.18).

\(^4\)In this context from now on we will use the following (perhaps barbaric) notation: by $|p|$ we will mean $\sqrt{|w|}$. (The barbarism is in the fact that if $V > E$, then $p$ lies precisely on the cut of the square root function.)
which is better known in its equivalent form
\[ \frac{1}{2\pi} \oint kdx = n + \frac{1}{2} \]
(1.32)
as the Bohr-Sommerfeld quantisation rule (by \( \oint \) we now mean simply going from \( a \) to \( b \) and back again).

This condition answers a natural question concerning the nature of the relation between the WKB formula (1.16) and the time-independent Schrödinger equation: The Schrödinger equation gives us stationary states as well as values of energy belonging to them. Energy spectrum is simply the spectrum of the Hamiltonian operator present in the equation. On the other hand, the formula (1.16) allows us to compute (approximately) the wavefunctions of the stationary states, but does not itself describe which energies actually belong to the spectrum. It is the Bohr-Sommerfeld rule (or possibly anything else describing the relations between the solutions from different regions) which gives us the answer to the possible energy values and thus tells us which energies we are allowed to use (through \( k \)) when working with (1.16).

### 1.3 2D tunnelling outwards

We now describe the technique developed by Banks, Bender and Wu [4] (for a detailed description see also [5]) for treating multidimensional QM tunnelling out of a non-rotationally symmetric potential well. We focus on the case of two dimensions and the potential of the form
\[ V(x, y) = \frac{1}{4}(x^2 + y^2) - \frac{1}{4}\epsilon(x^4 + y^4 + 2cx^2y^2), \]
(1.33)
where $0 < \epsilon \ll 1$ and $|c| < 1$ (for a typical visage of the potential, see figure 1.5). We are interested in the situation when a particle in the ground state is put inside the well and then tunnels out of it. We may visualise this for example by considering a 2D quadratic potential with a particle in the ground state and then quickly changing the potential to the one in (1.33), which causes the particle to slowly escape from the well.

The most penetrable parts of the barrier are the domains close to the $x$ and $y$ axes. These are called MPEP - the most probable escape paths. We will focus on the domain near the positive $x$ axis. It is useful in this case to set a condition that the wavefunction behaves like an outgoing wave when $x \to \infty$. This boundary condition causes the hamiltonian to be non-hermitian. As a consequence, the eigenstates, which we call quasistationary states, have an imaginary part in their energy. The claim is that we can describe the situation of the particle tunnelling out by a quasistationary state with energy close to the one of the ground state in the quadratic potential.

Near the $x$-axis the potential can be also expressed in a rather simple form

$$V(x, y) = V_0(x) + \frac{1}{4} k(x)y^2, \quad k = 1 - 2\epsilon cx^2, \quad V_0 = \frac{1}{4} x^2(1 - \epsilon x^2), \quad (1.34)$$

where we have neglected the $y^4$ term.

In our case with $\epsilon \ll 1$ we are allowed to use the WKB approximation. The reason is that as a characteristic length of our potential we may choose the distance

\footnote{When “shifting” the hamiltonian operator in $\int (H\Psi)^* \Phi dV$ from $\Psi$ to $\Phi$ by means of integration by parts, the boundary term does not vanish.}

\footnote{Among other things this causes $\frac{d}{dt} \int |\Psi(t)|^2 dV \neq 0$, where we have integrated over some compact region centered around the well. This is very convenient for our purpose.}
of the maximum of the potential (on the $x$-axis) from the centre, which is $1/\sqrt{2\epsilon}$ and this is much larger than the mean squared displacement of the particle in the ground state of the one-dimensional quadratic potential, $(\Delta x)^2 = 1$, which is a quantity we can in our case take instead of the de Broglie wavelength.

Now we set $\hbar = 1$ to simplify the expressions. We will investigate the Schrödinger equation for a particle of mass $m = 1/2$

$$[-\partial_x^2 - \partial_y^2 + \frac{1}{4}(x^2 + y^2) - \frac{1}{4}\epsilon(x^4 + y^4 + 2cx^2y^2) - E]\Psi(x, y) = 0. \quad (1.35)$$

We begin the calculations with an observation that the ground state of the parabolic approximation of our potential (the ground state of a 2D QM oscillator; it has energy $E = 1$) is equivalent to two 1D QM oscillators. Thus, we can, when constructing our solution, assign energy $1/2$ to the $x$ and $y$ directions respectively. Using this fact along with the WKB approximation we write the wavefunction in the following form:

$$\Psi(x, y) = A(x, y)p^{-\frac{1}{2}}\exp\left(-\int pdx - \frac{1}{4}f(x)y^2\right), \quad (1.36)$$

where

$$p = \sqrt{V_0 - E} = \sqrt{\frac{1}{4}x^2(1 - \epsilon x^2) - \frac{1}{2}}. \quad (1.37)$$

We have introduced two new functions $f(x)$ and $A(x, y)$. Our plan is to put this expression into (1.35), use again the WKB approximation to neglect some terms and choose $f(x)$ so that it eliminates another group of “unpleasant” terms.

After inserting the expression into the Schrödinger equation, neglecting the $y^4$ term and imposing a condition that the terms proportional to $y^2$ vanish$^8$, we obtain equations

$$-f^2A + 2f_Ax - f_xAp^{-1}p_x - 2f_xAp + f_xxA + kA = 0 \quad (1.38)$$

and

$$-A_{yy} + f_yA_y + \frac{1}{2}fA - A_{xx} + A_xp^{-1}p_x + 2A_xp - \frac{3}{4}Ap^{-2}p_x^2 +$$

$$+ \frac{1}{2}yp^{-1}p_{xx} - Ap^2 + \frac{1}{4}x^2(1 - \epsilon x^2)A - A = 0, \quad (1.39)$$

where we have used subscripts to denote the derivatives with respect to $x$ and $y$.

$^7$We factored out of the function $\Psi(x, y)$ a 1D WKB function. Obviously, this function must correspond to the energy $1/2$ in order that it matches properly with the ball-shaped function describing the motion of the particle in the $x$-direction inside the well.

$^8$This gives us the condition for $f$. 

20
Thanks to our approximation, we can neglect \( A_x, p_x, f_x, A_{xx}, p_{xx} \) and \( f_{xx} \) compared to \( Ap, p^2, fp, A_xp, p_xp \) and \( f_xp \), respectively. The reason is that we can assert for example \( A_x \sim A/l \ll A/\lambda \sim Ap \), where \( l \) is the “radius” of the potential. Due to (1.37) we also have

\[
-Ap^2 + \frac{1}{4}x^2(1 - \epsilon x^2)A - A = -\frac{1}{2}A. \tag{1.40}
\]

Now we introduce new variables: \( x \rightarrow \epsilon^{-1/2}x \), \( p \rightarrow \epsilon^{-1/2}p \), which we are going to use from now on (we have for example \( k = 1 - 2cx^2 \)). We can also write

\[
p = \sqrt{\frac{1}{4}x^2(1 - x^2) - \frac{\epsilon}{2}x(1 - x^2)^{\frac{1}{2}}}. \tag{1.41}
\]

Putting all together, we obtain

\[
-2pf_x = f^2 - k \tag{1.42}
\]

\[
-A_{yy} + f_yA_y + \frac{1}{2}fA + 2Axp - \frac{1}{2}A = 0. \tag{1.43}
\]

Let us now define \( w = \sqrt{1 - x^2} \). We have \(-w \partial_x = x \partial_w \) and therefore

\[
2p \partial_x = xw \partial_x = -x^2 \partial_w, \tag{1.44}
\]

so we can write equations (1.42) and (1.43) in the form

\[
x^2f_w = f^2 - k \tag{1.45}
\]

\[
-A_{yy} + f_yA_y + \frac{1}{2}fA - x^2Aw - \frac{1}{2}A = 0. \tag{1.46}
\]

The equation (1.45) is known as the Riccati equation. The standard substitution for its linearisation is

\[
f = -x^2\frac{u_w}{u}, \tag{1.47}
\]

where we have introduced a new function \( u(w) \). Inserting the substitution into (1.45) we get the well known associated Legendre equation (see Appendix A)

\[
(1 - w^2)u'' - 2wu' + \left(2c - \frac{1}{1 - w^2}\right)u = 0 \tag{1.48}
\]

(in this case we have denoted the derivative with respect to \( w \) with prime to make the equation look more familiar). The solutions are the associated Legendre functions \( P^\mu_\nu \) and \( Q^\mu_\nu \) with their indices given by

\[
\nu(\nu + 1) = 2c, \quad \mu^2 = 1. \tag{1.49}
\]
It can be shown that
\[ P^1_{\nu} \propto P^{-1}_{\nu}, \quad Q^1_{\nu} \propto Q^{-1}_{\nu}, \tag{1.50} \]
and in our calculations we are also free to choose and fix one of the two roots of \( \nu(\nu + 1) = 2c \). We therefore take
\[ u(w) = a_1 P^{-1}_{\nu}(w) + a_2 Q^1_{\nu}(w) \tag{1.51} \]
with \( \nu \) being the larger root of \( \nu(\nu + 1) = 2c \) and \( a_1, a_2 \) being some fixed coefficients.

We now return to the equation (1.46). Instead of variables \( w \) and \( y \) we take \( w \) and \( s = \frac{y}{u(w)} \). The equation will then have the form
\[ A_{ss} = -u^2(1 - w^2)A_w + \frac{1}{2} u^2 A(f - 1). \tag{1.52} \]
Using the method of separation we set \( A(w, s) = W(w)S(s) \) and obtain the equations
\[ S_{ss} = CS, \tag{1.53} \]
\[ u^2(1 - w^2)W_w = \left( \frac{1}{2} u^2(f - 1) - C \right) W. \tag{1.54} \]
The solutions for \( S \) are
\[ S \propto \begin{cases} \cos(\sqrt{-C}s) & \text{for } C \leq 0 \\ \cosh(\sqrt{C}s) & \text{for } C > 0 \end{cases} \tag{1.55} \]
and for \( W \) we have
\[ \int \frac{dW}{W} = \int \left[ \frac{f - 1}{2(1 - w^2)} - \frac{C}{u^2(1 - w^2)} \right] dw, \tag{1.56} \]
\[ \log |W| = - \int \frac{C}{u^2(1 - w^2)} dw - \int \frac{u_w dw}{2u} - \int \frac{dw}{2(1 - w^2)} = \]
\[ = - \int \frac{C}{u^2(1 - w^2)} dw - \frac{1}{2} \log |u| + \frac{1}{4} \log \left| \frac{1 - w}{1 + w} \right|, \tag{1.57} \]
and finally
\[ W \propto |u|^{-\frac{1}{2}} \left( \frac{1 - w}{1 + w} \right)^{\frac{1}{4}} \exp \left[ -C \int_{w_0}^w \frac{dw}{u^2(1 - w^2)} \right]. \tag{1.58} \]

The purpose of \( f \) from (1.36) is to make our calculations easier. Thus, once we have learned that it should be of the form (1.51), we are free to choose the coefficients \( a_1 \) and \( a_2 \). Either way it eliminates the unpleasant terms. However, not all choices lead to “nice” formulas, as we will now show.
Let us start with considering the asymptotic behaviour of the functions $P^{-1}_\nu$ and $Q^1_\nu$ for small $x$:

$$P^{-1}_\nu \sim \frac{x}{2}, \quad Q^1_\nu \sim -\frac{1}{x},$$

(1.59)

In (1.58) we choose the lower bound of integration $w_0$ to lie in the region where this approximation is valid.

Now we examine the situation when $u$ is chosen so that it contains $Q^1_\nu$, i.e.

$$u(w) = \eta P^{-1}_\nu + Q^1_\nu,$$

(1.60)

$\eta$ being some coefficient. For the $f$ function we have $f \approx -1$ for small $x$, the factor $(1 - w_0 + w)^{1/4}$ from (1.58) equals approximately $\sqrt{x/2}$ in the same limit and for the integral in (1.58) we obtain

$$\int_{w_0}^w \frac{dw}{u^2(1 - w^2)} = \int_x^{x_0} \frac{dx}{x\sqrt{1 - x^2}u^2} = \int_x^{x_0} xdx = K - \frac{x^2}{2},$$

(1.61)

where $K$ is a constant. Imagine now a linear superposition of functions belonging to different separation constants. We will inspect whether it is possible to obtain a plausible solution by means of such a superposition. More specifically, we will try to construct a function with the asymptotic form proportional (up to some function of $x$) to $e^{-y^2/4}$ for very small $x$.

In other words we search for $C(\alpha)$, $D(\alpha)$ such that

$$\int_0^\infty d\alpha |u|^{-\frac{1}{2}} p^{-\frac{1}{2}} \left( \frac{1 - w}{1 + w} \right)^{\frac{1}{4}} \exp \left( -\frac{1}{\epsilon} \int pdx - \frac{1}{4} \frac{f}{y^2} \right) \cdot \left\{ C(\alpha) \cosh \left( \frac{\alpha y}{u} \right) \exp \left[ -\alpha^2 \int_{w_0}^w \frac{dw}{u^2(1 - w^2)} \right] \right\} +$$

$$+ D(\alpha) \cos \left( \frac{\alpha y}{u} \right) \exp \left[ \alpha^2 \int_{w_0}^w \frac{dw}{u^2(1 - w^2)} \right] \sim e^{-\frac{x^2}{4}},$$

(1.62)

where by $\sim$ we mean that the two expressions match asymptotically up to some function of $x$ multiplying one or another hand side.

Changing our integration path from the real axis to the imaginary one (by means of the standard method of analytic continuation and using $\oint \Phi(z)dz = 0$ for...

---

9As can be seen from the equations, the result does not depend on the “global” constant in $u(w)$ (both $u(w)$ and $au(w)$ produce the same outcome). This is why we set the constant in front of $Q^1_\nu$ to 1.

10This is the behaviour we require in order to match our solution with the internal bell-shaped function correctly. (We presume that there is a region, where both the tunelling and the internal solution are valid simultaneously.)

11The factor $\epsilon^{-1}$ in the first exponent is due to the rescaling of variables.
analytic Φ) for the integral containing the hyperbolic cosine we obtain precisely the form of the other term containing the (ordinary) cosine, because

\[
\cosh \left( \frac{i\alpha y}{u} \right) \exp \left[ -\left( i\alpha \right)^2 \int_{w_0}^{w} \frac{dw}{u^2(1 - w^2)} \right] = \\
= \cos \left( \frac{\alpha y}{u} \right) \exp \left[ \alpha^2 \int_{w_0}^{w} \frac{dw}{u^2(1 - w^2)} \right].
\] (1.63)

Thus, we can consider only one function \( F \) instead of \( C, D \) and the expression simplifies to

\[
\int_{0}^{\infty} d\alpha |u|^{-\frac{1}{2}} p^{\frac{1}{2}} \left( \frac{1}{1 + w} \right)^{\frac{1}{4}} \exp \left( -\frac{1}{\epsilon} \int pdx - \frac{1}{4} f_y^2 \right) \cdot F(\alpha) \cos \left( \frac{\alpha y}{u} \right) \exp \left[ \alpha^2 \int_{w_0}^{w} \frac{dw}{u^2(1 - w^2)} \right] \sim e^{-\frac{y^2}{4}}
\] (1.64)

or

\[
e^{\frac{y^2}{4}} \int_{0}^{\infty} d\alpha F(\alpha) \cos(\alpha xy) e^{\alpha^2(K - x^2/2)} \sim e^{-\frac{y^2}{4}},
\] (1.65)

when the asymptotic behaviour is taken into account. The function

\[
\cos(\alpha xy) \exp \left( \alpha^2(K - x^2/2) \right)
\] (1.66)

is even in \( \alpha \), which leads us to define

\[
F(-\alpha) = F(\alpha) \quad \text{for } \alpha > 0
\] (1.67)

and write the equation (1.65) as

\[
\int_{-\infty}^{\infty} d\alpha F(\alpha) e^{i\alpha xy} e^{\alpha^2(K - x^2/2)} \sim e^{-\frac{y^2}{4}}.
\] (1.68)

Multiplying both hand sides by \( \exp(-i\beta xy) \), integrating with respect to \( y \), and using

\[
\int_{-\infty}^{\infty} e^{i(\alpha - \beta)xy} dy = 2\pi \delta(x(\alpha - \beta)),
\] (1.69)

\[
\int_{-\infty}^{\infty} e^{-y^2/2 - i\beta xy} dy = \sqrt{2\pi} e^{-\beta^2 x^2/2},
\] (1.70)

\[
\delta(x(\alpha - \beta)) = x^{-1} \delta(\alpha - \beta) \quad \text{(when computing } \int d\alpha)\]
(1.71)

we obtain approximately

\[
F(\beta) \propto e^{-K\beta^2}.
\] (1.72)

According to this result we are allowed to set

\[
u(w) = \eta P_{\nu}^{-1} + Q_{\nu},
\] (1.73)
but then we have to use the whole superposition of solutions with the weight $F(\beta) \propto e^{-K\beta^2}$.\footnote{Here it is appropriate to note that we have actually proven the other options (other weights) to be “bad behaved”. We have not rigorously proven, nor we ever will in this text, that the option $F(\beta) \propto e^{-K\beta^2}$ is correct in all conceivable aspects. For example it is possible that the respective wavefunction will be unacceptable due to its behaviour in some region where our approximation is no longer valid. It is therefore impossible to prove any further results in this direction without exceeding completely the (WKB) framework of this thesis.} This seems rather inconvenient for any further calculations. Fortunately, the case $u = P_{\nu}^{-1}$ will provide us with a (much) more suitable alternative. Let us therefore turn our attention to this option.

For $u = P_{\nu}^{-1}$ we have (for small $x$) $u \approx x/2$, $f \approx 1$, and for the integral in (1.58) we write

$$\int_{w_0}^{w} \frac{dw}{u^2(1 - w^2)} = \int_{x}^{x_0} \frac{dx}{x\sqrt{1 - x^2}u^2} \approx \int_{x}^{x_0} \frac{4dx}{x^3} \approx \frac{2}{x^2}. \quad (1.74)$$

In the latter we have used the fact that we are interested in $x$ which is much closer to 0 than $x_0$. Putting all together and requiring the plausible solution (i.e. solution with the same correct asymptotic behaviour as we tried to construct in the previous case) we arrive at the condition (compare with (1.65))

$$e^{-\frac{x^2}{4}} \int_{0}^{\infty} d\alpha F(\alpha) \cos(2\alpha y/x)e^{2\alpha^2/x^2} \sim e^{-\frac{x^2}{4}}. \quad (1.75)$$

Performing the next step as in the previous case we obtain the form

$$\int_{-\infty}^{\infty} d\alpha F(\alpha)e^{2i\alpha y/x}e^{2\alpha^2/x^2} \sim \text{constant in } y. \quad (1.76)$$

After multiplying both hand sides by $\exp(-2i\beta y/x)$ and integrating with respect to $y$ we have approximately

$$F(\beta) e^{\frac{2\beta^2}{x^2}} \propto \delta(\beta) \quad (1.77)$$

or equivalently

$$F(\beta) \propto \delta(\beta), \quad (1.78)$$

which is really good news for us, because it means that we have to set the separation constant from (1.53) and (1.54) to zero. Thanks to this, we (gladly) take $u = P_{\nu}^{-1}$.\footnote{One might argue that this analysis was perhaps unnecessarily long and complicated. Some would probably have said from the beginning that from the two functions $P_{\nu}^{-1}$ and $Q_{1\nu}$ the first is much more convenient (because of its nice behaviour) than the latter. This might indeed be true. Nevertheless, our analysis will be important for us in the next section, when it will turn out that the situation (i.e. the correct asymptotic behaviour) requires the presence of the $Q_{1\nu}$ function.}

The solution is

$$\Psi(x, y) \approx A|u|^{-1/2} \left(\frac{1 - w}{1 + w}\right)^{1/4} p^{-1/2} \exp \left(-\frac{1}{\epsilon} \int pdx + \frac{x^2}{4} \frac{u_w}{u} y^2\right), \quad (1.79)$$
A being a constant, \( w = \sqrt{1 - x^2} \), and \( u = P^{-1}_\nu \). We can also take \( |u| = u \) due to the fact that \( P^{-1}_\nu(w) \) is positive on \( w \in (0, 1) \), \( \nu \in \left( -\frac{1}{2}, 1 \right) \) (\( c \in \left( -\frac{1}{8}, 1 \right) \)), as can be seen from numerical computations.

Finally, we show that our solution matches the internal solution not only in the \( y \), but also in the \( x \) direction. The internal solution, when written in our rescaled variables, is

\[
\Psi_{\text{internal}} \propto \exp \left[-\frac{1}{4} \left(\frac{x^2 + y^2}{\epsilon}\right)\right]. \tag{1.80}
\]

In (1.79) we now consider \( x \) to be much smaller than 1 (so that it refers to positions near the centre), but sufficiently far (to the right) from the inner turning point (so that the WKB approximation is still valid). We have

\[
|u|^{-1/2} \approx \sqrt{\frac{2}{x}}, \quad \left(\frac{1 - w}{1 + w}\right)^{1/4} \approx \sqrt{\frac{x}{2}}, \quad p^{-1/2} \approx \sqrt{\frac{2}{x}}, \quad f \approx 1. \tag{1.81}
\]

For the integral in the exponent we need also the next-to-leading order,

\[
\int_{\sqrt{2x}}^{x} p dx = \int_{\sqrt{2x}}^{x} \frac{1}{2} \sqrt{x^2 - 2\epsilon} dx = \frac{x^2}{4} - \frac{\epsilon}{2} \log \left(\frac{2x}{\epsilon}\right) - \frac{\epsilon}{4} + O \left(\frac{1}{x^2}\right) \tag{1.82}
\]

where we have used (1.41) and integrated (approximately) from the inner turning point\(^{14}\). Putting all together we obtain

\[
\Psi \approx \text{constant} \cdot \exp \left[-\frac{1}{4} \left(\frac{x^2}{\epsilon} + y^2\right)\right], \tag{1.83}
\]

which exactly matches (1.80).

\(^{14}\)One might argue that we have another term in the exponential, \( \frac{1}{4} fy^2 \), and this we should also expand up to the next-to-leading order. However, we would obtain an expression proportional to \( x^2 y^2 \) without any \( \frac{1}{\epsilon} \) factor and this can be neglected compared to the term \( \frac{1}{4} y^2 \) (because the rescaled \( x \) variable is very small in this sector).
Chapter 2

Modification of the problem

2.1 2D tunnelling inwards

Now we turn our attention to the inverse problem (see [3]). Imagine a beam of particles with \( E = 1 \) coming from both the plus and minus infinity in the \( x \) direction and heading towards the central potential well\(^2\). The wavefunction will have the following form: In the region outside the barrier it will be a superposition of the incoming and outcoming wave (due to reflection) while in the barrier its module will decrease in the \( x \) direction towards the centre. Our task is to determine the form of the wavefunction in this region.

Near the centre itself we assume that we have \( \Psi \sim e^{-y^2/4} \), where by \( \sim \) we again mean that the two functions match assymptotically each other, up to some function of \( x \). This can happen in at least two different cases:

- The incoming wave is strongly focused around the \( x \) axis so that the module of the function near the upper or lower “pass” is smaller than the module inside the well. As a consequence, it is reasonable to assume \( \Psi_{\text{inside}} \rightarrow 0 \) for large \( y \).

- The potential has some form that is more complicated than \( V(x, y) = \frac{1}{2}(x^2 + y^2) - \frac{1}{4}\epsilon(x^4 + y^4 + 2cx^2y^2) \), and the form which we use is only approximate near the \( x \) axis. If the complete potential does not contain any other “passes”, we deduce again \( \Psi_{\text{inside}} \rightarrow 0 \) for large \( y \).

\(^1\)In the paper [3] the author deals with both problems simultaneously.

\(^2\)Note that this problem allows us to choose the value of energy from a continuous spectrum as opposed to the previous case, where the wavefunction originated from a state with energy from the discrete spectrum of parabolic potential. We have chosen the value 1 just to demonstrate clearly the correspondence with the previous case.
When solving the Schrödinger equation in the well (after neglecting the terms of higher order in $x$ and $y$) we can use the method of separation of variables and for $\Psi_{\text{internal}}(x,y) = X(x)Y(y)$ we arrive at two equations for a quantum harmonic oscillator. Both options mentioned imply that $E_y = 1/2 + n$ for some $n \in \mathbb{N}$. The choice $E_y = 1/2$ (and thus $\Psi \sim e^{-y^2/4}$) corresponds to the previous problem and therefore we choose to study this case.

From $E_y = 1/2$ we immediately have $E_x = 1/2$. For the $X$ function we then obtain

$$-X_{xx}(x) + \left(\frac{1}{4}x^2 - \frac{1}{2}\right)X(x) = 0, \tag{2.1}$$

$$X(x) \propto e^{-x^2/4} \left(1 + a \int_0^x e^{x^2/2} dx\right), \tag{2.2}$$

$a$ being an integration constant. The value of $\int_0^x e^{x^2/2} dx$ is for large $x$ approximately $\frac{1}{x} e^{x^2/2}$. Putting all together, we write (for large $x$)

$$\Psi_{\text{internal}} \approx \text{constant} \cdot e^{-x^2/4} \frac{1}{x} e^{x^2/2} = \text{constant} \cdot e^{\frac{1}{4}(x^2-y^2)}. \tag{2.3}$$

This result will be needed later (during the matching process).

Returning to our search for the tunnelling solution, we now write the wavefunction as

$$\Psi(x,y) = A(x,y)p^{\frac{1}{2}} \exp \left(\int p dx - \frac{1}{4} f(x)y^2\right), \tag{2.4}$$

where

$$p = \sqrt{V_0 - \frac{E}{2}} = \sqrt{\frac{1}{4}x^2(1 - e^2x^2) - \frac{1}{2}}. \tag{2.5}$$

Note that the only difference between these formulae and (1.36), (1.37) is the opposite sign in front of $\int p dx$. After inserting the expression into the Schrödinger equation, neglecting the same terms as in the previous case and rescaling $x$ and $p$, we obtain\(^3\)

$$2pf_x = f^2 - k \tag{2.6}$$

$$-A_{yy} + f_y A_y + \frac{1}{2} f A + 2 A_x p - \frac{1}{2} A = 0. \tag{2.7}$$

This time we choose our substitution with the sign plus

$$f = x^2 \frac{u_w}{u} \tag{2.8}$$

to arrive again at the associated Legendre equation

$$(1 - w^2)u'' - 2wu' + \left(2c - \frac{1}{1 - w^2}\right)u = 0. \tag{2.9}$$

\(^3\)It may be useful to compare the following expressions to their counterparts in section 1.3.
We choose the same form of the solution as before,
\[ u(w) = a_1 P_{\nu}^{-1}(w) + a_2 Q_{\nu}^{1}(w), \]  
(2.10)
\( \nu \) being the larger root of \( \nu(\nu + 1) = 2c \) and \( a_1, a_2 \) being some fixed coefficients.

After changing the variables in (2.10) from \( w, y \) to \( w, s = \frac{y}{u(w)} \) and using the method of separation of variables, we have
\[ S_{ss} = CS, \]  
(2.11)
\[ -u^2(1 - w^2)W_w = \left[ \frac{1}{2} u^2 (f - 1) - C \right] W. \]  
(2.12)
This time the solutions are
\[ S \propto \begin{cases} \cos(\sqrt{-C}s) & \text{for } C \leq 0 \\ \cosh(\sqrt{C}s) & \text{for } C > 0 \end{cases} \]  
(2.13)
and
\[ W \propto |u|^{-\frac{1}{2}} \left( \frac{1 - w}{1 + w} \right)^{-\frac{1}{4}} \exp \left[ C \int_{w_0}^{w} \frac{dw}{u^2(1 - w^2)} \right]. \]  
(2.14)
To simplify the analysis, we again choose \( w_0 \) to lie in the region where the leading term approximation to \( P_{\nu}^{-1} \) and \( Q_{\nu}^{1} \) is valid.

Let us now consider different linear combinations of \( P_{\nu}^{-1} \) and \( Q_{\nu}^{1} \) and perform a similar analysis as in the previous case. We start with
\[ u(w) = P_{\nu}^{-1}. \]  
(2.15)
For small \( x \) we have \( u \approx x/2, f \approx -1 \), and the integral in (2.14) equals approximately \( 2/x^2 \) (see (1.74)). We again want to find out whether it is possible to form a linear combination of solutions with different separation constants \( C \) such that the result has the correct asymptotic behaviour (for small \( x \)) \(^4\). After repeating the steps in the section 1.3 we arrive at
\[ \int_{-\infty}^{\infty} d\alpha F(\alpha)e^{2i\alpha y/x}e^{-2\alpha^2/x^2} \sim e^{-y^2/4}, \]  
(2.16)
and after multiplying by \( \exp(-2i\beta y/x) \), integrating with respect to \( y \), and using
\[ \int_{-\infty}^{\infty} e^{-y^2-2i\beta y/x} dy = \sqrt{2\pi} e^{-2\beta^2/x^2}, \]  
(2.17)
we have approximately
\[ F(\beta)e^{-2\beta^2/x^2} \propto e^{-\frac{2\beta^2}{x^2}} \]  
(2.18)
\(^4\)i.e. we can possibly match it with the internal solution (we again presume that there is a region where both the internal and tunnelling solution are valid simultaneously)
or equivalently

\[ F(\beta) = \text{constant}. \]  \hspace{1cm} (2.19)

The result is that \( u = P_{\nu}^{-1} \) can be used, but in order to satisfy the conditions of good asymptotic behaviour, we have to use solutions with all \( C' \)s in the superposition. However, we still have the option \( u = \eta P_{\nu}^{-1} + Q_{\nu}^1 \). This, as we will now show, leads to much more elegant formulae.

In this case we have \( u \approx -1/x \), \( f \approx 1 \) and the integral in (2.14) equals approximately \( K - x^2/2 \) (see (1.61)). We repeat the same steps and obtain

\[
\int_{-\infty}^{\infty} d\alpha F(\alpha)e^{i\alpha xy}e^{-\alpha^2(K-x^2/2)} \sim \text{constant},
\]  \hspace{1cm} (2.20)

from which we deduce (after multiplying by \( e^{i\beta xy} \) and integrating with respect to \( y \))

\[
F(\beta)e^{-\beta^2(K-x^2/2)} \sim \delta(\beta)
\]  \hspace{1cm} (2.21)

or equivalently

\[
F(\beta) \propto \delta(\beta).
\]  \hspace{1cm} (2.22)

We therefore choose and will examine the case of

\[
u = \eta P_{\nu}^{-1} + Q_{\nu}^1,
\]  \hspace{1cm} (2.23)

when we have

\[
\Psi(x,y) \approx A|u|^{-1/2} \left( \frac{1-w}{1+w} \right)^{-1/4} p^{-1/2} \exp \left( \frac{1}{\epsilon} \int pdx - \frac{x^2}{4} \frac{uw}{u} y^2 \right). \]  \hspace{1cm} (2.24)

It is easy to show that for all values of \( \eta \) function (2.24) matches (2.3).

Using

\[
|u|^{-1/2} \approx \sqrt{x}, \quad \left( \frac{1-w}{1+w} \right)^{-1/4} \approx \frac{2}{x}, \quad p^{-1/2} \approx \frac{2}{x}, \quad f \approx 1
\]  \hspace{1cm} (2.25)

and (1.82) for the integral in the exponent, we have (in the same limit as in the previous case)

\[
\Psi \approx \text{constant} \cdot \frac{1}{x} \exp \left[ \frac{1}{4} \left( \frac{1}{\epsilon} x^2 - y^2 \right) \right],
\]  \hspace{1cm} (2.26)

which corresponds to (2.3).

Now we must emphasise that the setting with a particle (or a beam of particles) tunnelling inwards is in some sense much more complicated than the case of tunnelling outwards. The complication arises from the fact that it was natural to expect that the problem of particle escaping from the well has a unique solution. This readily follows from the formulation of the problem: One has a particle in a well in the
ground state and the particle slowly escapes; what will be the probability amplitude? In the case of a beam of incoming particles we can no longer expect that the solution will be unique, because we have substantial freedom in choosing the exact form of the incoming wave. This is reflected in different wavefunctions in the tunnelling region. As a consequence, it is plausible that different values of the \( \eta \) coefficient in (2.23) will result in different \( \Psi \)'s. This is indeed the case. Before demonstrating all this, we now show how to relate the wavefunction in the tunnelling region to the wavefunction outside the barrier.

### 2.2 Outside the barrier

We use the technique described in 1.2. Again it is reasonable to expect that the WKB approximation is valid not only on the real axis, but also throughout the complex plane, as long as we stay far away from the turning point. Thus, we can construct the analytic continuation of our solution, bypass the turning point by going in the upper half-plane, arrive again at the real axis on the other side of “the dangerous region” and proclaim that the solution obtained is “half” of the correct solution. The other “half” we get when we bypass the turning point in the opposite half-plane.

We now presume that the function \( u \) does not change the sign for \( x \in (0, 1) \), from which it immediately follows that \( |u| = -u \) due to (1.59). This is a reasonable assumption, as we will show later\(^5\).

The formula

\[
\Psi(x, y) \approx A u^{-1/2} \left( \frac{1 - w}{1 + w} \right)^{-1/4} p^{-1/2} \exp \left( \frac{1}{\epsilon} \int p dx - \frac{x^2}{4} u w y^2 \right) \tag{2.27}
\]

is valid in the complex plane up to the real axis on the opposite side of the point \( P \) (see figure 2.1). In the regions \( A \) and \( B \) (both of them being very close to the real axis), the functions \( w, p \) and \( \sqrt{p} \) in (2.24) have the form

\[
\begin{align*}
A \ (\text{up}) & \\
\frac{1}{w_u(x)} &= -i \sqrt{x^2 - 1} \\
\frac{1}{p_u(x)} &= -i/2 \sqrt{x^2 - 1} \\
\sqrt{p_u(x)} &= e^{-i \pi/4} \sqrt{1/2x \sqrt{x^2 - 1}} \\
B \ (\text{down}) & \\
\frac{1}{w_d(x)} &= i \sqrt{x^2 - 1} \\
\frac{1}{p_d(x)} &= i/2 \sqrt{x^2 - 1} \\
\sqrt{p_d(x)} &= e^{i \pi/4} \sqrt{1/2x \sqrt{x^2 - 1}},
\end{align*}
\]

\(^5\)The basic idea will be that when \( u \) passes 0, the wavefunction behaves non-physically (see \( u \) in the denominator of (2.24)).
where we have chosen the indices \( u \) and \( d \) so that it is obvious to which region do the functions refer. Contrary to this, let us write \( u \) without indices, i.e. \( u(w) = \eta P_u^{-1}(w) + Q_u^1(w) \) and again use the subscript to denote the derivative with respect to \( x \). Then we can write for \( x > 1 \)

\[
\Psi \approx C \left[ p_u^{-1/2}(u(w_u))^{-1/2} \left( \frac{1 + w_u}{1 - w_u} \right)^{1/4} \exp \left( \frac{1}{\epsilon} \int p_u dx + \frac{xw_u u_x(w_u)}{4 u(w_u)^2} \right) + \right.
\]

\[
+ p_d^{-1/2}(u(w_d))^{-1/2} \left( \frac{1 + w_d}{1 - w_d} \right)^{1/4} \exp \left( \frac{1}{\epsilon} \int p_d dx + \frac{xw_d u_x(w_d)}{4 u(w_d)^2} \right) \right].
\]

(2.31)

In Appendix A ((A.12), (A.13)) we prove the following equalities for \( \eta \in \mathbb{R} \):

\[
u(\overline{w}) = \overline{u(w)}, \quad u'(\overline{w}) = \overline{u'(w)},
\]

(2.32)

where \( \overline{z} \) denotes the complex conjugate of \( z \) and the prime denotes derivative with respect to the argument. As a consequence, we have

\[
u(w_u) = \overline{u(w_d)}
\]

(2.33)

and

\[
u_x(w_u) = u_x(-i\sqrt{x^2 - 1}) = -iu'(w_u)(\sqrt{x^2 - 1})_x =
\]

\[
- iu'(w_d)(\sqrt{x^2 - 1})_x = iu'(w_d)(\sqrt{x^2 - 1})_x =
\]

\[
u_x(i\sqrt{x^2 - 1}) = \overline{u_x(w_d)}.
\]

(2.34)

Putting all together, it can easily be seen that the second term in (2.31) is
a complex conjugate of the first term. Thus, we finally have

\[ \Psi \approx 2C \Re \left\{ p_d^{-1/2}(u(w_d))^{-1/2} \left( \frac{1 + w_d}{1 - w_d} \right)^{1/4} \cdot \exp \left( \frac{1}{\epsilon} \int p_d dx + \frac{x w_d u_d(w_d)}{4 \cdot u(w_d) y^2} \right) \right\}, \tag{2.35} \]

where \( \Re z \) is the real part of \( z \in \mathbb{C} \).

### 2.3 Some pictures

Now we show how the results for the case of tunnelling inwards look like, both inside and outside the barrier. Figures 2.2 to 2.8 show \(|\Psi|^2\) in the region \( x \in (0,1) \) near the \( x\)-axis (small \( y \)). The parameters have values \( \epsilon = 0.1, \nu = 0.5, \eta \in \{-4, -2, -1, 0, 1, 2, 4\} \).

As can be seen from the graphs, the function \( \Psi \) behaves unacceptable for large \( \eta \), because the module goes to infinity for some \( x \) smaller than 1. We must therefore abandon such solutions\(^6\). Similarly, for \( \eta \) much smaller than 0 the wavefunction starts to increase in the transversal direction for some fixed \( x < 1 \), which is unacceptable for the particle in the barrier. These solutions are therefore “bad”, too.

The first problem (singularity in \( \Psi \)) is caused by the fact that \( u(x) \) crosses 0 for some \( x \in (0,1)\).\(^7\) A generic example of such bad-behaved function \( u(x) \) is depicted on 2.9. From the asymptotic form we also know that for every \( \eta \neq 0 \) the function \( u \) is negative near \( x = 0 \). It is therefore tempting to try to find out for which \( \eta \) and \( \nu \) has the function negative value also in \( x = 1 \). Clearly the answer gives us a necessary condition for determining whether the solution is well-behaved.

From (A.7), (A.15), (A.16), and

\[ \Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin(\pi x)} \tag{2.36} \]

we have

\[
u(x = 1) = \eta P_{\nu}^{-1}(w = 0) + Q_{\nu}^{1}(w = 0) =
\]

\[ = -\frac{\eta}{\nu(\nu + 1)} P_{\nu}^{1}(w = 0) + Q_{\nu}^{1}(w = 0) =
\]

\[ = -\frac{\sqrt{\pi}}{\Gamma \left( -\frac{\nu}{2} \right) \Gamma \left( \frac{1}{2} + \frac{\nu}{2} \right)} \left[ \frac{2\eta}{\nu(1+\nu)} + \pi \tan \frac{\pi(\nu + 1)}{2} \right] =
\]

\(^6\)This is not something new, we have already abandoned solutions with other separations con-
stants/weight functions due to their wrong (assymptotical) behaviour.

\(^7\)Another implication is divergence of \( f \).
Figure 2.2: $\nu = 0.5$, $\eta = -4$

Figure 2.3: $\nu = 0.5$, $\eta = -2$

Figure 2.4: $\nu = 0.5$, $\eta = -1$

Figure 2.5: $\nu = 0.5$, $\eta = 0$

\[
= \frac{\sqrt{\pi}}{\sin \frac{\pi \nu}{2}} \frac{\Gamma \left(1 + \frac{\nu}{2}\right)}{\Gamma \left(\frac{1}{2} + \frac{\nu}{2}\right)} \left[ \frac{2\eta}{\nu(1+\nu)} - \pi \cot \frac{\pi \nu}{2} \right].
\]  

(2.37)

Recall that we chose $\nu$ to be the larger root of $\nu(\nu + 1) = 2c$. Thus

\[
\nu = -1 + \sqrt{1 + 8c}.
\]

(2.38)

If we restrict ourselves to $c \in \left(-\frac{1}{8}, 1\right)$ so that both roots are real, we have

\[
\nu \in \left(-\frac{1}{2}, 1\right).
\]

(2.39)

Moreover, for real positive arguments we have $\Gamma(x) > 0$. Putting all together we see that $u(x = 1) > 0$ is equivalent to

\[
\frac{1}{\sin \frac{\pi \nu}{2}} \left[ \frac{2\eta}{\nu(\nu + 1)} - \pi \cot \frac{\pi \nu}{2} \right] < 0,
\]

(2.40)
which can be simplified to

\[ \eta < \eta_{\text{crit}}, \quad \eta_{\text{crit}} = \frac{\pi}{2} \nu(\nu + 1) \cot \frac{\pi \nu}{2}. \]  

(2.41)

This is the neccessary condition for the solution to be well-behaved.

The second problem (the increase in transversal direction) is caused by negative \( f(x) \). Again, from the assymptotic form we have that for small \( x \) the \( f \) function is positive,

\[ f(x) = x^2 \frac{u_x}{u} = -xw \frac{u_x}{u} \approx -x \frac{1}{1-x} = 1. \]  

(2.42)

One more time, we can formulate the neccessary condition for the function to be "acceptable":

\[ f(x = 1) > 0. \]  

(2.43)
We first find for which $\eta$ we have $u_w < 0$. With the help of (A.7), (A.15), (A.16), (A.17), (A.18), and $x \Gamma(x) = \Gamma(x + 1)$ (2.44)

we have

$$u_w(x = 1) = \left(\frac{1}{w^2 - 1} \left\{ \eta \left[ w\nu P^{-1}_\nu - (-1 + \nu) P^{-1}_\nu \right] + \right. \right.$$ 

$$+ \left. \left[ w\nu Q^1_\nu - (1 + \nu) Q^1_\nu \right] \right\} \right|_{x=1} =$$

$$= \eta(\nu - 1)P^{-1}_{\nu-1}(w = 0) + (\nu + 1)Q^1_{\nu-1}(w = 0) =$$

$$= -\frac{\eta}{\nu}P^1_{\nu-1}(0) + (\nu + 1)Q^1_{\nu-1}(0) =$$

$$= \frac{\sqrt{\pi}}{\Gamma\left(\frac{\nu}{2}\right)\Gamma\left(\frac{1}{2} - \frac{\nu}{2}\right)} \left[ -\frac{2\eta}{\nu} - \pi(\nu + 1) \tan \frac{\pi \nu}{2} \right] =$$

$$= -\frac{\sqrt{\pi}}{2\Gamma\left(1 + \frac{\nu}{2}\right)\Gamma\left(\frac{1}{2} - \frac{\nu}{2}\right)} \left[ 2\eta + \pi\nu(\nu + 1) \tan \frac{\pi \nu}{2} \right]$$

(2.45)

As a result, when using $\nu \in (-\frac{1}{2}, 1)$, the inequality $u_w(x = 1) < 0$ is equivalent to

$$2\eta + \pi\nu(\nu + 1) \tan \frac{\pi \nu}{2} > 0,$$

(2.46)

which gives us

$$\eta > \eta_{\text{crit}}', \quad \eta_{\text{crit}}' = -\frac{\pi}{2} \nu(\nu + 1) \tan \frac{\pi \nu}{2}. (2.47)$$

Consequently, for $\eta < \eta_{\text{crit}}'$ (the first condition) the value $f(x = 1)$ is negative if and only if (2.47) is satisfied. We thus have another necessary condition.

Putting all together, we have

$$-\frac{\pi}{2} \nu(\nu + 1) \tan \frac{\pi \nu}{2} < \eta < \frac{\pi}{2} \nu(\nu + 1) \cot \frac{\pi \nu}{2},$$

(2.48)

which defines a region in the $\eta, \nu$ plane (see (2.10)). Although we have only proven that the conditions are necessary, numeric computation suggests that they might be also sufficient (or perhaps sufficient everywhere except for some small regions). However, a rigorous proof (if the reversed implication indeed holds) would probably be much more complicated than the one we gave in this text.

Finally, in figures 2.11 to 2.24 we provide graphs of the $|\Psi|^2$ function behind the barrier, i.e. for $x > 1$ (again we focus only on the case of tunnelling inwards). The parameters have values $\epsilon = 0.1, \nu \in \{0.5, 0.9\}, \eta \in \{-2, -1, -0.5, 0, 0.5, 1, 2\}$

8We included also several graphs corresponding to values of $\nu$ and $\eta$ lying outside the grey area in figure 2.10. We can see that the incoming waves constructed in the same way as for the well-behaved solutions have qualitatively the same form.
We can now confirm that various $\eta$ values indeed correspond to different incoming waves.

As a curiosity, observe that while for $x < 1$ was the behaviour of $|\Psi|^2$ for fixed $x$ always of the form $e^{-\frac{1}{4}f(x)y^2}$ (see (1.79)), behind the barrier it is no longer so. The reason is that we have used only the real part of the function (see (2.35)).
Figure 2.13: $\nu = 0.5$, $\eta = -0.5$

Figure 2.14: $\nu = 0.5$, $\eta = 0$

Figure 2.15: $\nu = 0.5$, $\eta = 0.5$

Figure 2.16: $\nu = 0.5$, $\eta = 1$

Figure 2.17: $\nu = 0.5$, $\eta = 2$

Figure 2.18: $\nu = 0.9$, $\eta = -2$
Figure 2.19: $\nu = 0.9$, $\eta = -1$

Figure 2.20: $\nu = 0.9$, $\eta = -0.5$

Figure 2.21: $\nu = 0.9$, $\eta = 0$

Figure 2.22: $\nu = 0.9$, $\eta = 0.5$

Figure 2.23: $\nu = 0.9$, $\eta = 1$

Figure 2.24: $\nu = 0.9$, $\eta = 2$
Chapter 3

In polar coordinates

This short chapter deals with the same problem, but shows how to obtain solutions when working in polar coordinates (again see [3]). It will be useful in the quantum-cosmological problem, because, as we will show in the next chapter, the Wheeler-DeWitt equation has (in our case) a form very similar to Schrödinger equation in polar coordinates. However, as it is unnecessary to provide all details of the calculation (the ideas are practically the same as in the sections 1.3 and 2.1), we will focus only on differences from the previous calculations and main results. We again consider the case $E = 1$ (although the wave can have any energy from a continuous spectrum) and this time we compute the wavefunctions for tunnelling inwards and outwards simultaneously.

Let us begin with writing equation (1.35) in the $r, \varphi$ variables:

\[
-\frac{1}{r} \partial_r r \partial_r - \frac{1}{r^2} \partial_\varphi^2 + \frac{1}{4} r^2 - \frac{1}{4} \epsilon r^4 \left( \cos^4 \varphi + \sin^4 \varphi + 2c \cos^2 \varphi \sin^2 \varphi \right) - 1 \right] \Psi(r, \varphi) = 0.
\] (3.1)

After restricting ourselves to $\varphi \ll 1$ and defining $\hat{\Psi} = \sqrt{r} \Psi$, for which

\[
\frac{1}{r} \partial_r r \partial_r \Psi = \frac{1}{\sqrt{r}} \left( \partial_\varphi^2 \hat{\Psi} + \frac{1}{4r^2} \hat{\Psi} \right) \approx \frac{1}{\sqrt{r}} \partial_\varphi^2 \hat{\Psi},
\] (3.2)

we arrive at

\[
\left[ -\partial_\varphi^2 - \frac{1}{r^2} \partial_\varphi^2 + \frac{1}{4} r^2 (1 - \epsilon r^2 + 2c r^2 \varphi^2) - 1 \right] \hat{\Psi}(r, \varphi) = 0,
\] (3.3)

where $\gamma = 1 - c$.

\[1\] The last is due to the WKB approximation and the fact that we are interested in large values of $r$. 

40
We look for the solution in the form
\[ \Psi(r, \varphi) = B(r, \varphi) q^{-\frac{1}{2}} \exp \left( \mp \int q dr - \frac{1}{4} g(r) \varphi^2 \right), \]  \hspace{1cm} (3.4)\]
where
\[ q = \sqrt{\frac{1}{4} r^2(1 - \epsilon r^2) - E} = \sqrt{\frac{1}{4} r^2(1 - \epsilon r^2) - 1} \]  \hspace{1cm} (3.5)\]
and the \(-\) and \(+\) signs refer to tunnelling outwards and inwards, respectively. We introduced two new functions, \( B(r, \varphi) \) and \( g(r) \). Again, the purpose of the latter is to eliminate a group of unpleasant terms (this time the terms with the common factor \( \varphi^2 \)). After inserting (3.4) into (3.3), using the WKB approximation to neglect some terms, redefining the variables and functions according to
\[ r \rightarrow \epsilon^{-1/2} r, \hspace{0.5cm} \varphi \rightarrow \epsilon^{1/2} \varphi, \hspace{0.5cm} q \rightarrow \epsilon^{-1/2} q, \hspace{0.5cm} g \rightarrow \epsilon^{-1} g, \]  \hspace{1cm} (3.6)\]
and defining
\[ \kappa = 2 \gamma r^4, \hspace{0.5cm} \xi = \sqrt{1 - r^2}, \]  \hspace{1cm} (3.7)\]
we obtain
\[ \pm r^2 g_\xi = \frac{1}{r^2} g^2 - \kappa, \]  \hspace{1cm} (3.8)\]
\[ \pm 2 r^3 \xi q B_\xi + B_\varphi \varphi - \frac{1}{2} g B - g \varphi B_\varphi = 0, \]  \hspace{1cm} (3.9)\]
\[ q \approx \frac{1}{2} r \sqrt{1 - r^2}, \]  \hspace{1cm} (3.10)\]
where we have again denoted the respective derivatives with subscript.

To solve (3.8) we make a substitution (as proposed by Genzor in [5])
\[ g = \mp r^4 \frac{v_\xi}{v} \]  \hspace{1cm} (3.11)\]
and obtain the Gegenbauer equation (see (A.31))
\[ (1 - \xi^2) v'' - 4 \xi v' - 2 \gamma v = 0, \]  \hspace{1cm} (3.12)\]
where we have again used \( v_\xi = v' \). According to (A.34) the solution is
\[ v(\xi) = \frac{1}{r} \left[ a_1 P_{\nu}^{-1}(\xi) + a_2 Q_{\nu}^1(\xi) \right], \]  \hspace{1cm} (3.13)\]
where again \( \nu \) is the larger root of \( \nu(\nu + 1) = 2c \) and \( a_1, a_2 \) are arbitrary constants.

In (3.9) we change the variables \( \xi \) and \( \varphi \) to \( \xi \) and \( \psi = \frac{\varphi}{v(\xi)} \). Now the equation assumes the form
\[ \mp r^4 \left( v^2 B_\xi + \frac{1}{2} v v_\xi B \right) = B_\psi \psi, \]  \hspace{1cm} (3.14)\]
We again use the method of separation of variables, and after setting
\[ B(\xi, \psi) = \Xi(\xi) \tilde{\Psi}(\psi)^2 \]  
we obtain
\[ \mp r^4 (v^2 \Xi + \frac{1}{2} v \nu \Xi) = C \Xi, \]  
\[ \tilde{\Psi}_{\psi \psi} = C \tilde{\Psi}. \]

The solutions for \( \tilde{\Psi} \) are
\[ \tilde{\Psi} \propto \begin{cases} \cos(\sqrt{-C} \psi) & \text{for } C \leq 0 \\ \cosh(\sqrt{C} \psi) & \text{for } C > 0 \end{cases} \]  
and from (3.16) we have
\[ \int \frac{d\Xi}{\Xi} = -\frac{1}{2} \int \frac{dv}{v} \mp C \int \frac{d\xi}{r^4 v^2}, \]  
\[ \Xi \propto |v|^{-1/2} \exp \left[ \mp C \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^2 v^2} \right]. \]

Once again, we choose \( \xi_0 \) to lie in the region where our approximation of associated Legendre functions is valid.

We now try to construct a superposition of solutions with different separation constants \( C \) so that it has the correct asymptotic behaviour. First we deal with the particle tunnelling outwards. We expect that near the centre, the wavefunction will not depend on \( \varphi \). In other words, we would like to find a function \( G(\alpha) \) such that
\[ \int_{-\infty}^{\infty} d\alpha |v|^{-1/2} q^{-1/2} \exp \left( -\frac{1}{\epsilon} \int qr - \frac{1}{4} g \varphi^2 \right) \cdot G(\alpha) \exp \left( i \frac{\alpha \varphi}{\nu} \right) \exp \left[ \alpha^2 \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^2 v^2} \right] \sim \text{constant in } \varphi, \]  
where by \( \sim \) we mean that the two expressions asymptotically match (for small \( r \)) up to some function of \( r \).

Consider the case \( v = \frac{1}{r} P_{\nu}^{-1}(\xi) \). Then, for small \( r \), we have \( v \approx 1/2, g \approx 2r^4 v''(r = 0), \) and the integral in the third exponential in (3.21) can be written as
\[ \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^2 v^2} = \int_{r}^{r_0} \frac{dr}{r^3 \sqrt{1 - r^2 v^2}} \approx 4 \int_{r}^{r_0} \frac{dr}{r^3} \approx \frac{2}{r^2}. \]  

\footnote{We denote the function of \( \psi \) by tilde to avoid confusion with the wavefunction.}
\footnote{We skip the steps which are similar to those in the previous chapters.}
\footnote{The second derivative is due to absence of a linear term in \( v \) (see (A.19)).}
From (3.21) we have
\[ \int_{-\infty}^{\infty} d\alpha G(\alpha) e^{2i\alpha \varphi} e^{\frac{2\alpha^2}{r^2}} \sim \text{constant in } \varphi \] (3.23)
and finally
\[ G(\beta) e^{\frac{2\beta^2}{r^2}} \propto \delta(\beta), \] (3.24)
\[ G(\beta) \propto \delta(\beta). \] (3.25)

In the case \( v = \frac{1}{r}(\eta P_{\nu} - Q_{\nu}) \) we have \( v \approx -1/r^2 \), \( g \approx -2r^2 \) and the integral is
\[ \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^{v/2}} = \int_{r}^{r_0} \frac{dr}{r^3 \sqrt{1 - r^2 v^2}} \approx \int_{r}^{r_0} rdr = K - \frac{r^2}{2}. \] (3.26)
Condition (3.21) is equivalent to
\[ \int_{-\infty}^{\infty} d\alpha G(\alpha) e^{-i\alpha r^2 \varphi} e^{\alpha^2 (K - \frac{r^2}{2})} \sim e^{-\frac{1}{2}r^2 \varphi^2}, \] (3.27)
\[ G(\beta) e^{\frac{\beta^2}{r^2} (K - \frac{r^2}{2})} \propto e^{-\frac{1}{2}r^2 \beta^2}, \] (3.28)
\[ G(\beta) \propto e^{-K\beta^2}. \] (3.29)

As a result, we choose the first option \( v = \frac{1}{r} P^{-1}_{\nu} \), because the expressions will be much simpler. The wavefunction then has the form
\[ \Psi(r, \varphi) \approx B |v|^{-1/2} q^{-1/2} r^{-1/2} \exp \left( -\frac{1}{\epsilon} \int qdr + \frac{r^4 v\xi}{4v^2} \right), \] (3.30)
\( B \) being a constant.

For tunnelling inwards the task is again more complicated. We cannot expect that the wavefunction in the centre will be independent of \( \varphi \). However, the precise dependence on \( \varphi \) can be easily determined when we (once again) presume that the wavefunction in the centre is suppressed in the \( y \) direction in the same manner as before. From (2.3) we then have (in the rescaled variables and again restricting ourselves to \( \varphi \ll 1 \))
\[ \Psi_{\text{internal}} \approx \text{constant} \cdot \frac{1}{r \cos(\sqrt{\epsilon} \varphi)} \exp \left( -\frac{r^2}{4\epsilon} \right) \exp \left[ \frac{r^2}{2\epsilon} \cos^2 \left( \sqrt{\epsilon} \varphi \right) \right] \approx \] (3.31)
\[ \approx \text{constant} \cdot \frac{1}{r} \exp \left( -\frac{r^2}{4\epsilon} \right) \exp \left[ \frac{r^2}{2\epsilon} \left( 1 - \epsilon \varphi^2 \right) \right] \approx \] (3.32)
\[ \approx \text{constant} \cdot \frac{1}{r} \exp \left( \frac{r^2}{4\epsilon} \right) \exp \left( -\frac{1}{2} r^2 \varphi^2 \right). \] (3.33)
We therefore want the tunnelling solution to satisfy $\Psi \sim e^{-\frac{1}{2} r^2 \varphi^2}$ instead of $\Psi \sim \text{constant}$. Next, we search for a correct weight function $G(\alpha)$.

For $v = \frac{1}{r} P_{\nu}^{-1}$ we arrive at

$$\int_{-\infty}^{\infty} G(\alpha) e^{2i\alpha \varphi} e^{-\frac{2\alpha^2}{r^2}} d\alpha \sim e^{-\frac{1}{2} r^2 \varphi^2},$$

(3.34)

from which we deduce

$$G(\beta) = \text{constant}. \quad (3.35)$$

For $v = \frac{1}{r} (\eta P_{\nu}^{-1} + Q_{\nu}^1)$ we have

$$e^{-\frac{1}{2} r^2 \varphi^2} \int_{-\infty}^{\infty} G(\alpha) e^{-i\alpha r \varphi} e^{-\alpha^2 \left( \frac{K-r^2}{2} \right)} d\alpha \sim e^{-\frac{1}{2} r^2 \varphi^2},$$

(3.36)

which implies

$$G(\beta) \propto \delta(\beta). \quad (3.37)$$

Consequently, we choose $v = \frac{1}{r} (\eta P_{\nu}^{-1} + Q_{\nu}^1)$. Again, we obtained a one-parametric class of solutions. The wavefunction has the same form as in (3.30), difference being only in the choice of $v$.

Finally, we check that the results indeed match the respective internal solutions correctly even in the $r$ direction. For tunnelling outwards we have

$$|v|^{-1/2} \approx \sqrt{2}, \quad q^{-1/2} \approx \sqrt{\frac{2}{r}}, \quad g \approx 2r^4 v''(r = 0), \quad (3.38)$$

$$\int_{\sqrt{4\epsilon}}^{r} q dr = \int_{\sqrt{4\epsilon}}^{r} \frac{1}{2} \sqrt{r^2 - 4\epsilon} dr = \frac{r^2}{4} - \epsilon \log \left( \frac{r}{\epsilon} \right) - \frac{\epsilon}{2} + O \left( \frac{1}{r^2} \right), \quad (3.39)$$

$$\Psi \approx \text{constant} \cdot \exp \left( -\frac{r^2}{4\epsilon} \right), \quad (3.40)$$

which corresponds to the ground state of the parabolic potential.

The case of tunnelling inwards differs in

$$|v|^{-1/2} \approx r, \quad g \approx 2r^2, \quad (3.41)$$

which produces

$$\Psi \approx \text{constant} \cdot \frac{1}{r} \exp \left( \frac{r^2}{4\epsilon} \right) \exp \left( -\frac{1}{2} r^2 \varphi^2 \right), \quad (3.42)$$

This is in accordance with (3.33).
Chapter 4

Tunnelling in cosmology

In this chapter we consider the quantum cosmological problem of closed, homogeneous and isotropic universe with spatially homogeneous scalar field $\Phi$ with potential $V(\Phi)$. At the beginning we describe the equation that governs quantum cosmology, both in its most general form and in its form restricted to our case.

4.1 Wheeler–DeWitt equation

The Wheeler–DeWitt equation arises in the “canonical” approach to quantisation of the general theory of relativity. Let us briefly describe its derivation. The procedure of rewriting the general theory of relativity into Hamiltonian formalism is due to Arnowitt, Deser and Misner (see [11]). The quantisation process is done according to [7]. We use the metric tensor of signature $(-, +, +, +)$.

In the general case, we define functions $N$ and $N_i$ (lapse and shift functions) which describe some particular choice of coordinates. We also need the metric $h_{ij}$ inducted on the hypersurfaces of constant time,

$$h_{ij} = g_{ij}, \quad i, j = 1, 2, 3.$$  \hfill (4.1)

Using these functions we rewrite the Lagrangian density

$$\mathcal{L} = -\frac{1}{2\kappa_E}(R + 2\Lambda)\sqrt{-g},$$ \hfill (4.2)

$R$ being the scalar curvature, $\Lambda$ the cosmological constant, $\kappa_E$ the Einstein constant ($\kappa_E = 8\pi G$) and $g$ the determinant of $g_{\mu\nu}$ (this is the $\mathcal{L}$, from which we can derive the left hand side of Einstein equations by means of the principle of least action). We then construct the Hamiltonian density $\mathcal{H}_0$, which turns out to have an elegant form

$$\mathcal{H}_0 = N_i\mathcal{H}^i + N\mathcal{H},$$ \hfill (4.3)
where \( \mathcal{H} \) and \( \mathcal{H}^i \) are functions of \( h_{ij} \)'s and their conjugate momenta \( \pi_{ij} \)'s only. Finally, using the procedure of canonical quantisation, we define \( \Psi \) to be a functional from the space of all \( h_{ij} \)'s to \( \mathbb{C} \). The only restriction imposed on this functional is that it is annihilated by \( \mathcal{H} \) and \( \mathcal{H}^i \), i.e. by the operators formed by the standard procedure

\[
\pi_{ij} \to -i \frac{\delta}{\delta h_{ij}}. \tag{4.4}
\]

It is easy to show that the equations \( \mathcal{H}^i \Psi = 0 \) are equivalent to the statement that the \( \Psi \) functional in fact depends only on the three-geometries \( ^3\mathcal{G} \), i.e. 3D manifolds equipped with a metric tensor. In other words, \( \Psi \) is the same for different coordinate representations of the same geometry. As a result, we are left with only one condition

\[
\mathcal{H} \Psi = 0, \tag{4.5}
\]

which is called the Wheeler–DeWitt equation. We refer to the space of all three-geometries as superspace and to the functional \( \Psi[^3\mathcal{G}] \) as the wavefunction (wavefunctional) of the universe.

In our case we are interested in a closed FLRW (Friedmann–Lemaître–Robertson–Walker) universe, i.e. a universe with the metric of the form

\[
d s^2 = -N^2 d t^2 + a^2(t)(d\chi^2 + \sin^2 \chi d\Omega^2), \tag{4.6}
\]

where \( d\Omega^2 = d\theta^2 + \sin^2 \theta d\phi^2 \). In this universe there “resides” a spatially homogeneous scalar field \( \Phi \) with potential \( V(\Phi) \). Its Lagrangian density is

\[
\mathcal{L}_\Phi = \left[ -\frac{1}{2} (\partial \Phi)^2 - V(\Phi) \right] \sqrt{-g}. \tag{4.7}
\]

For every fixed moment \( t \) we therefore have a universe fully characterised by two numbers: \( a, \Phi \). In quantum cosmology, the wavefunction \( \Psi \) is a function of these two variables. We now construct the corresponding Wheeler–DeWitt equation.

Due to the fact that we restricted ourselves to three-geometries of a special form, the only freedom left is reparametrisation of the \( t \) variable. We therefore choose

\[
d s^2 = -N^2 d t^2 + a^2(t)(d\chi^2 + \sin^2 \chi d\Omega^2) \tag{4.8}
\]
as our starting point. It contains all possible spacetime metrics of the required form and their parametrisations (when we glue together the three-spheres in the natural way). The scalar curvature corresponding to (4.8) is

\[
R = -6a^{-2} [aN^{-1}(N^{-1}\dot{a}) - N^{-2}\dot{a}^2 + 1]. \tag{4.9}
\]

\(^1\)A quick derivation consists in the substitution \( dt \to N dt \) in the scalar curvature for the closed FLRW universe.
Similarly, the scalar field Lagrangian density has the form
\[ L_\Phi = \left( \frac{1}{2} N^{-2} \dot{\Phi}^2 - V(\Phi) \right) \sqrt{-g}. \] (4.10)

Putting all together, we obtain action
\[ S = \int L_{\text{grav}} d^4x + \int L_\Phi d^4x = \] (4.11)
\[ = \int \left\{ \frac{3}{\kappa E} \left[ N^{-1} a(N^{-1} \dot{a}) + N^{-2} \dot{a}^2 + 1 \right] a^{-2} - \right. \] (4.12)
\[ - \left. \frac{1}{\kappa E} \Lambda + \left( \frac{1}{2} N^{-2} \dot{\Phi}^2 - V(\Phi) \right) \right\} N a^3 2 \pi^2 dt \] (4.13)

Now we set \( \frac{12 \pi^2}{\kappa E} \) to 1, define \( \lambda = \frac{A}{\Lambda} \), rescale the scalar field, \( \Phi \rightarrow \frac{1}{\sqrt{2\pi}} \Phi \), and skip the total derivatives. As a result, for the Lagrangian (i.e. the integrand when integrating with respect to \( t \)) we have
\[ L = \frac{1}{2} (-N^{-1} a \ddot{a}^2 + Na - N\lambda a^3 + N^{-1} a^3 \dot{\Phi}^2 - 2N V(\Phi) a^3). \] (4.14)

Using the canonical momenta corresponding to \( a \) and \( \Phi \),
\[ \pi_a = -N^{-1} a \dot{a}, \quad \pi_\Phi = N^{-1} a^3 \Phi, \] (4.15)
we construct the Hamiltonian,
\[ H = \pi_a a + \pi_\Phi \Phi - L = \] (4.16)
\[ = -\frac{N}{2a} \left[ \pi_a^2 - a^{-2} \pi_\Phi^2 + a^2 (1 - \lambda a^2 - 2a^2 V(\Phi)) \right]. \] (4.17)

In the quantum theory, we define the wavefunction of the universe \( \Psi(a, \Phi) \). As was mentioned earlier, this is a function on the space of \( a \)'s and \( \Phi \)'s\(^3\). \( \Psi \) must satisfy the Wheeler–DeWitt equation
\[ \left[ -a^{-p} \partial_a a^p \partial_a + a^{-2} \partial_\Phi^2 + a^2 (1 - \lambda a^2 - 2a^2 V(\Phi)) \right] \Psi(a, \Phi) = 0, \] (4.18)
where \( p \) is a constant. The complicated form of the first term arises due to the operator ordering problem – in the Hamiltonian we have a product of two operators \( a^{-1} \) and \( \pi_a \), which do not commute in the quantum theory. In general, it should be of the form \( a^\alpha \partial_a a^\beta \partial_a a^\gamma \), \( \alpha + \beta + \gamma = 0 \). However, similarly as in [14], we restrict ourselves to the case \( \gamma = 0 \). (The only difference between the form in (4.18) and the one containing \( \alpha, \beta, \gamma \), is in some multiplicative factor \( a^\beta \) in the solution.)

\(^2\)This is due to \( (\partial \Phi)^2 = \Phi_{\mu \nu} \Phi^{\mu \nu} = g^{\mu \nu} \Phi_{\mu \nu} = g^{\mu \nu} \Phi_{\mu \nu} \Phi_{\nu} = g^{\mu \nu} \Phi^2 = -\frac{1}{N^2} \Phi^2 \).

\(^3\)We call it the minisuperspace.
4.2 Vilenkin’s solution

In the paper [14] the author investigated equation (4.18) for the case of a universe “created from nothing” and found a tunnelling solution. Let us now describe his approach. We consider a scalar field with a potential that is bounded from above. We presume it to be of the form

$$V(\Phi) = \rho_v - \frac{1}{2} \mu^2 \Phi^2$$  \hspace{1cm} (4.19)

near the global maximum at $\Phi = 0$.\(^4\) Moreover, we set $\rho_v = 0$, because the term is exactly the same as the one containing $\lambda$.\(^5\) Such a potential corresponds to a scalar field with imaginary mass $m = i\mu$. We also define $U(a, \Phi) = a^2(1 - \lambda a^2 - 2a^2V(\Phi))$ and $\eta = \mu^2/\lambda$. The equation can be written as

$$[-a^{-p}\partial_a a^p \partial_a + a^{-2} \partial_\Phi^2 + U(a, \Phi)] \Psi(a, \Phi) = 0, \hspace{1cm} (4.20)$$

with

$$U(a, \Phi) = a^2 \left[1 - \lambda a^2 (1 - \eta \Phi^2)\right]. \hspace{1cm} (4.21)$$

Vilenkin divides the half-plane $a \in [0, \infty), \Phi \in (-\infty, \infty)$ into two domains: so called Euclidean region, where $U > 0$, and Lorentzian region, where $U < 0$. These roughly correspond to classically forbidden and allowed region, respectively. In general, the border between the two domains is defined by

$$a^2 = \frac{1}{\lambda + 2V(\Phi)}. \hspace{1cm} (4.22)$$

We search for a solution that decreases exponentially for increasing $a$. Condition (4.22) together with (4.19) implies that the highest tunnelling probability will be along the $a$-axis, i.e. for small $\Phi$, as the barrier is most penetrable at this point.

In the computations, we restrict ourselves to the case $\eta \ll 1, \lambda \ll 1$. According to Vilenkin, the first is required when we want to study a cosmologically interesting inflationary scenario\(^6\) and the second must be satisfied if we want to use the WKB approximation\(^7\). Vilenkin also keeps the value of $p$ unspecified (his computation is therefore valid for all $p$’s).

\(^4\)In most cases we can find a global maximum and expand the potential near it to obtain a parabolic approximation. All we have to do is to shift the scalar field and we arrive at the potential of the form (4.19).

\(^5\)We can redefine $\lambda \rightarrow \lambda + 2\rho_v$.

\(^6\)We want the lifetime of the false vacuum, i.e. of the state $\Phi = 0$, to be much greater than the expansion rate of a de Sitter space (which is a classical analogy of our problem).

\(^7\)The condition is equivalent to the statement that the energy is much smaller than the Planck energy.
For small $a$ we can simplify the form of the Wheeler–DeWitt equation (4.20) as
\[
(-a^{-p}\partial_a a^p \partial_a + a^{-2}\partial^2_{\Phi} + a^2) \Psi(a, \Phi) = 0, \tag{4.23}
\]
or equivalently
\[
\left(\partial^2_a + \frac{p}{a} \partial_a - a^{-2}\partial^2_{\Phi} - a^2\right) \Psi(a, \Phi) = 0. \tag{4.24}
\]
Vilenkin then searches for a solution that does not depend on $\Phi$ in this region. This is an important presumption, which distinguishes his solution from the solution that we will obtain in section 4.3. In his case the equation takes the form
\[
\left(\partial^2_a + \frac{p}{a} \partial_a - a^{-2}\partial^2_{\Phi} - a^2\right) \Psi(a) = 0. \tag{4.25}
\]
Changing the independent variable from $a$ to $b = a^2/2$ and the function from $\Psi$ to $\Omega = b^{1-p}\Psi$, we can rewrite (4.25) as
\[
b^2\Omega'' + b\Omega' - \left[\left(\frac{1-p}{4}\right)^2 + b^2\right] \Omega = 0, \tag{4.27}
\]
where we have denoted the derivative with respect to $b$ by a prime. This is the modified Bessel differential equation, which has the general solution
\[
\Omega(b) = a_1 I_{\frac{1-p}{2}}(b) + a_2 K_{\frac{1-p}{2}}(b), \tag{4.28}
\]
$a_1$, $a_2$ being some coefficients and $I$, $K$ being the modified Bessel functions of the first and second kind, respectively. Due to the fact that we describe tunnelling “outwards”, we want the modulus of the solution to decrease for $a \to \infty$. We therefore take $\Omega = K_{\frac{1-p}{2}}$. Returning to $a$ and $\Phi$ we have
\[
\Psi(a) \propto a^{\frac{1-p}{2}} K_{\frac{1-p}{2}} \left(\frac{a^2}{2}\right). \tag{4.29}
\]
For large $a$ we obtain
\[
\Psi(a) \approx \text{constant} \cdot a^{-\frac{p+1}{2}} e^{-\frac{a^2}{2}}. \tag{4.30}
\]
We now return to the “full” Wheeler–DeWitt equation and construct a tunnelling solution that matches (4.30). From (4.22) we see that the tunnelling region

---

8Note that we do not need to consider only small values of $\Phi$. However, $\Phi$ must not leave the domain of validity of our parabolic approximation of the potential.
ends at \( a = \lambda^{-1/2} \). This motivates the change of variable \( a \to \lambda^{-1/2}a \). We first rewrite (4.30) and obtain (for \( a \ll 1 \))

\[
\Psi(a) \approx \text{constant} \cdot a^{-\frac{p+1}{2}} e^{-\frac{a^2}{2}}. \tag{4.31}
\]

The Wheeler–DeWitt equation has the form

\[
\left\{ -a^p \partial_a a^p \partial_a + a^2 \partial_\Phi^2 + \frac{a^2}{\lambda^2} \left[ 1 - a^2(1 - \eta \Phi^2) \right] \right\} \Psi(a, \Phi) = 0, \tag{4.32}
\]

Vilenkin then proposes an approach to WKB approximation which uses an expansion in \( \lambda \), i.e.

\[
\Psi(a, \Phi) = e^{\pm S(a, \Phi)}, \quad S = S_0 + \lambda S_1 + \lambda^2 S_2 + \ldots \tag{4.33}
\]

Inserting this expression into (4.32), collecting the terms with the same order of \( \lambda \) and defining \( v(a, \Phi) = 1 - a^2 + \eta a^2 \Phi^2 \), we arrive at

\[
\left( \frac{\partial S_0}{\partial a} \right)^2 - \frac{1}{a^2} \left( \frac{\partial S_0}{\partial \Phi} \right)^2 + a^2 v(a, \Phi) = 0, \tag{4.34}
\]

\[
-2 \frac{\partial S_0}{\partial a} \frac{\partial S_1}{\partial a} + 2 \frac{\partial S_0}{\partial \Phi} \frac{\partial S_1}{\partial \Phi} + i \frac{\partial^2 S_0}{\partial a^2} + i \frac{p}{a} \frac{\partial S_0}{\partial a} - i \frac{\partial^2 S_0}{\partial \Phi^2} = 0. \tag{4.35}
\]

Since the wavefunction does not depend on \( \Phi \) for small \( a \) (we have chosen it so) and \( \Phi \) is in \( U \) accompanied by the small parameter \( \eta \), Vilenkin concludes that the terms having derivatives with respect to \( \Phi \) can be neglected. As a result, we have

\[
\left( \frac{\partial S_0}{\partial a} \right)^2 + a^2 v(a, \Phi) = 0, \tag{4.36}
\]

\[
2 \frac{\partial S_0}{\partial a} \frac{\partial S_1}{\partial a} - i \frac{\partial^2 S_0}{\partial a^2} - \frac{ip}{a} \frac{\partial S_0}{\partial a} = 0. \tag{4.37}
\]

The first equation implies

\[
S_0 = \pm ia \int \sqrt{1 - a^2(1 - \eta \Phi^2)} da = \frac{i}{3(1 - \eta \Phi^2)} \left[ (1 - a^2(1 - \eta \Phi^2))^{3/2} + H_0(\Phi) \right], \tag{4.38}
\]

where \( H_0 \) is some function of \( \Phi \). We want the solution to decrease as \( a \to \infty \), which means that we use the upper sign. The function \( H_0 \) can be determined using the requirement that the exponential factor in (4.31) matches correctly with that appearing in the function (4.33). In other words, we want to satisfy

\[
\frac{ia^2}{2\lambda} = -\frac{i}{3\lambda(1 - \eta \Phi^2)} \left[ 1 - \frac{3}{2} a^2(1 - \eta \Phi^2) + H_0 \right]. \tag{4.39}
\]

9The leading term contains \( \lambda^{-1} \) so that we can reproduce (4.31) in the limit \( a \to 0 \).
which implies $H_0 = -1$.

From equation (4.37) we have

$$\frac{\partial S_1}{\partial a} = i\frac{\partial^2 S_0}{\partial a^2} + \frac{i p}{2a}, \quad (4.40)$$

$$S_1 = i\frac{1}{2} \log \frac{\partial S_0}{\partial a} + \frac{i p}{2} \log a + \tilde{H}_1(\Phi), \quad (4.41)$$

$$S_1 = i\frac{1}{2} \log \left( a^{p+1} \sqrt[3]{v(a, \Phi)} H_1(\Phi) \right), \quad (4.42)$$

where $\tilde{H}_1$ and $H_1$ are some functions of $\Phi$. Requiring that the expression asymptotically corresponds to the preexponential factor in (4.31), we arrive at

$$H_1 = \text{constant}.$$ \hfill (4.43)

Putting all together, we obtain

$$\Psi \approx \text{constant} \cdot a^{\frac{-p+1}{2}} v^{-1/4} \exp \left[ -\frac{1 - v^{3/2}}{3\lambda(1 - \eta\Phi^2)} \right]. \quad (4.44)$$

In [14] Vilenkin also mentions the resemblance between his solution and the wavefunctions of Banks, Bender and Wu [4]. However, Vilenkin’s approach seems to be less precise due to the larger number of neglected terms during the computation. It is therefore interesting to obtain the Vilenkin-type wavefunction using the methods of Banks, Bender and Wu, and compare the two. This will be done as a byproduct in the following section.

### 4.3 Alternative solutions

We now show how to obtain another set of solutions using the techniques developed in previous chapters. The difference from the Vilenkin’s solution lies in a requirement that our function matches a different internal solution, this time dependent on $\Phi$. However, we restrict ourselves to $p = 1$. This is a choice motivated by Hawking and Page [8] (mentioned also in [14]), who proposed that the differential operator in the Wheeler–DeWitt equation should be the Laplace operator in the canonical metric of the superspace. We also choose to study the case $\mu \ll 1$, $\lambda \ll 1$, the potential is assumed to be of the same form as in the previous case and we use the notation $\eta = \mu^2/\lambda$.

We again presume that the most probable escape path leads through the region close to the $a$-(half-)axis, i.e. where $\Phi$ is small, and we will investigate this
domain. After introducing new variables
\[ X = a \cosh \Phi, \quad (4.45) \]
\[ Y = a \sinh \Phi, \quad (4.46) \]
we use them to rewrite the differential operator as
\[ a^{-1} \partial_a a \partial_a - a^{-2} \partial^2_\Phi = \partial^2_X - \partial^2_Y. \quad (4.47) \]
For small \( a \) we therefore have the following equivalent form of equation (4.18):
\[ (-\partial^2_X + X^2) \Psi(X, Y) = (-\partial^2_Y + Y^2) \Psi(X, Y). \quad (4.48) \]
We have used \( a^2[1 - \lambda a^2(1-\eta \Phi^2)] \approx a^2 = X^2 - Y^2 \). Motivated by a similar condition in the chapter 3, we now require that the wavefunction is suppressed in the \( Y \) direction and from all possible options we choose the one corresponding to the lowest energy. In other words, we want that after the separation of variables, \( \Psi(X, Y) = \Psi^K(X)\Psi^Y(Y) \), the function \( \Psi^Y(Y) \) satisfies
\[ (-\partial^2_Y + Y^2) \Psi^Y(Y) = 1 \cdot \Psi^Y(Y) \quad (4.49) \]
and thus
\[ \Psi^Y(Y) \propto e^{-Y^2/2}. \quad (4.50) \]
As a consequence, we have
\[ \Psi^K(X) \propto e^{-X^2/2} \quad (4.51) \]
and for the internal wavefunction we obtain
\[ \Psi(X, Y) \propto e^{-\frac{1}{2}(X^2+Y^2)}. \quad (4.52) \]
This solution has the asymptotic form (for large \( a \) and small \( \Phi \), similarly as in previous chapters)
\[ \Psi(a, \Phi) \propto e^{-\frac{a^2}{2}(\cosh^2 \Phi + \sinh^2 \Phi)} = e^{-\frac{a^2}{2}(1+2\sinh^2 \Phi)} \approx e^{-a^2/2} e^{-a^2\Phi^2}. \quad (4.53) \]
Now we compute the wavefunction in the tunnelling region and match it with (4.53).

In the WKB region it is convenient to use \( \hat{\Psi} = \sqrt{a}\Psi \), because we have
\[ \frac{1}{a} \partial_a a \partial_a \frac{1}{\sqrt{a}} \hat{\Psi} = \frac{1}{\sqrt{a}} \left( \partial^2_a \hat{\Psi} + \frac{1}{4a^2} \hat{\Psi} \right) \approx \frac{1}{\sqrt{a}} \partial^2_a \hat{\Psi}, \quad (4.54) \]
\[ \text{At this point we use the "original"/non-rescaled } a \text{ variable.} \]
\[ \text{This can be quickly derived from the well-known formula for the Laplace operator in polar coordinates, } \partial^2_\rho + \rho^2 \partial^2_\phi = -r^{-1}\partial_r r \partial_r + r^{-2} \partial^2_\phi, \text{ after setting } X = x, \ Y = iy, \ a = r, \ \Phi = -i\phi. \]
\[ \text{This is the ground state of the harmonic oscillator in 1 dimension.} \]
52
where the second term vanished due to the WKB approximation. The equation (4.18) then has the form

$$\begin{align*}
\{-\partial_a^2 + a^{-2}\partial_\Phi^2 + a^2 \left[ 1 - \lambda a^2 (1 - \eta \Phi^2) \right] \} \tilde{\Psi}(a, \Phi) &= 0. \\
\end{align*}$$

(4.55)

We again search for the solution

$$\tilde{\Psi}(a, \Phi) = B(a, \Phi) q^{-\frac{3}{2}} \exp \left( -\int q da - \frac{1}{4} g(a) \Phi^2 \right),$$

(4.56)

where

$$q = \sqrt{a^2(1 - \lambda a^2)}. \quad \text{(4.57)}$$

After inserting these expressions into (4.55), repeating the procedure from previous chapters, redefining

$$a \rightarrow \lambda^{-1/2} a, \quad \Phi \rightarrow \lambda^{1/2} \Phi, \quad q \rightarrow \lambda^{-1/2} q, \quad g \rightarrow \lambda^{-1} g,$$

(4.58)

and using $\xi = \sqrt{1 - a^2}$, we arrive at

$$-2a^2 g_\xi = 4\eta a^4 + a^{-2} g^2,$$

(4.59)

$$-2a^3 \xi q B_\xi + B_{\Phi\Phi} - \frac{1}{2} g B - g B_{\Phi} = 0,$$

(4.60)

$$q = a\sqrt{1 - a^2}. \quad \text{(4.61)}$$

These equations are very similar to their analogues in section 3, (3.8) – (3.10), when the signs for tunnelling outwards are chosen in them. In fact, the only difference between (3.9) and (4.60) is the opposite sign of the first term.

To linearise equation (4.59) we define

$$g = \frac{2a^4}{v} v_\xi \quad \text{(4.62)}$$

and obtain the Gegenbauer differential equation

$$(1 - \xi^2) v'' - 4\xi v' + \eta v = 0. \quad \text{(4.63)}$$

The general solution can be written in the form

$$v = \frac{1}{a} \left( a_1 P_{\nu}^{-1}(\xi) + a_2 Q_{\nu}^1(\xi) \right) \quad \text{(4.64)}$$

with the coefficient $\nu$ given by

$$\nu(\nu + 1) = 2 + \eta. \quad \text{(4.65)}$$
In the second equation, (4.60), we change the variables from $\xi, \Phi$ to $\xi, \psi = \frac{\Phi}{v}$ and arrive at

$$B \psi \psi = a^4 v^2 \left( 2B \xi + \frac{\psi}{v} B \right).$$

(4.66)

This equation is almost identical to (3.14) as is the process of its solution. The result (for $B(\xi, \psi) = \Xi(\xi) \tilde{\Psi}(\psi)$) is

$$\tilde{\Psi} \propto \begin{cases} \cos(\sqrt{-C} \psi) & \text{for } C \leq 0 \\ \cosh(\sqrt{C} \psi) & \text{for } C > 0 \end{cases}$$

(4.67)

$$\Xi(\xi) \propto |v|^{-1/2} \exp \left( \frac{C}{2} \int_{\xi_0}^{\xi} \frac{d\xi}{a^4 v^2} \right).$$

(4.68)

Before continuing in our task, we examine the Vilenkin’s condition, i.e. that the dependence on $\Phi$ vanishes for small $a$. We are searching for a weight function $G(\alpha)$ such that

$$\int_{-\infty}^{\infty} d\alpha |v|^{\frac{1}{2} q - \frac{1}{2}} a^{-\frac{1}{2}} \exp \left( -\frac{1}{\lambda} \int q \, da - \frac{1}{4} q \Phi^2 \right) \cdot G(\alpha) \exp \left( i \frac{\alpha}{v} \Phi \right) \exp \left[ \frac{-\alpha^2}{2} \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^2 v^2} \right] \sim \text{constant in } \Phi.$$  

(4.69)

For $v = \frac{1}{a} P_{\nu}^{-1}$, we quickly obtain (as in chapter 3)

$$F(\alpha) \propto \delta(\alpha),$$

(4.70)

while for $v = \frac{1}{a} (\eta P_{\nu}^{-1} + Q_{\nu}^1)$ we arrive at

$$F(\alpha) \propto e^{\frac{K}{2} a^2}.13$$

(4.71)

The conclusion is that we have obtained a solution (considering the one with $v = \frac{1}{a} P_{\nu}^{-1}$; the final form of wavefunction is the same as in (4.75)) of Vilenkin’s type that seems to be more accurate than that of Vilenkin in [14].14 The reason, as was mentioned before, is that using the methods of Banks, Bender and Wu [4], we have neglected fewer terms in the equation than Vilenkin.

13In the latter case we must overcome a small obstacle during the computation. This arises due to the fact that we have an opposite sign in the exponent of the right hand side of the equation analogous to (3.27) (instead of $r$ we now have $a$). However, we can define $a = ib$ and after presuming $b \in \mathbb{R}$ perform the integration. After the analytic continuation we then obtain the answer for $a \in \mathbb{R}$. Note that despite the fact that the weight function increases exponentially, this does not cause any divergence in the integral, because the term is cancelled by a corresponding factor with opposite sign, present in the other exponential.

14In Vilenkin’s solution there are only elementary functions as opposed to the wavefunction we obtained.
Let us turn to our case, i.e. searching for a solution with the asymptotic (4.53). Hence, we need to examine
\[ \int_{-\infty}^{\infty} d\alpha |v|^{-\frac{1}{2}} q^{-\frac{1}{2}} a^{-\frac{1}{2}} \exp \left( -\frac{1}{\lambda} \int q da - \frac{1}{4} g \Phi^2 \right) \cdot G(\alpha) \exp \left( i \frac{\alpha \Phi}{v} \right) \exp \left[ -\frac{\alpha^2}{2} \int_{\xi_0}^{\xi} \frac{d\xi}{(1 - \xi^2)^2 v^2} \right] \sim e^{-a^2 \Phi^2}. \] (4.72)

For \( v = \frac{1}{a} P_{\nu}^{-1} \) we have
\[ G(\alpha) = \text{constant in } \alpha \] (4.73)
and for \( v = \frac{1}{a} (\eta P_{\nu}^{-1} + Q_{\nu}^1) \)
\[ G(\alpha) \propto \delta(\alpha). \] (4.74)

We are interested in the latter case, because it contains a whole new class of solutions that differ in their very nature (i.e. in their asymptotic behaviour) from the Vilenkin’s one. The wavefunction is
\[ \Psi(a, \Phi) \approx B |v|^{-1/2} q^{-1/2} a^{-1/2} \exp \left( -\frac{1}{\lambda} \int q da - \frac{a^4 v''(a = 0)}{2 v} \Phi^2 \right). \] (4.75)

We now show that the results match correctly the internal solutions in both directions (\( a \) and \( \Phi \)). For the case \( v = \frac{1}{a} P_{\nu}^{-1} \), \( G(\alpha) \propto \delta(\alpha) \), which satisfies the Vilenkin’s condition of independence on \( \Phi \) for small \( a \), we have
\[ |v|^{-1/2} \approx \sqrt{2}, \quad q^{-1/2} \approx a^{-1/2}, \quad g \approx -4a^4 v''(a = 0), \] (4.76)
\[ \int_0^a q da \approx \frac{a^2}{2}, \] (4.77)
\[ \Psi \approx \text{constant} \cdot \frac{1}{a} \exp \left( \frac{a^2}{2\lambda} \right), \] (4.78)
which corresponds to (4.31).

In the case of the one-parametric class of solutions \( v = \frac{1}{a} (\eta P_{\nu}^{-1} + Q_{\nu}^1) \), \( G(\alpha) \propto \delta(\alpha) \), the only difference is
\[ |v|^{-1/2} \approx a, \quad g \approx 4a^2, \] (4.79)
which gives us
\[ \Psi \approx \text{constant} \cdot \exp \left( -\frac{a^2}{2\lambda} - a^2 \Phi^2 \right) \] (4.80)
in accordance with (4.53).

Although all values of \( \eta \) correspond to the same leading term in \( g(a) \) (and thus to the same leading behaviour in transversal direction), the difference between
various \( \eta \) can be seen clearly in the next-to-leading term. This follows from (A.19) and (A.29):

\[
v = \frac{1}{a} \left[ \eta P_{\nu}^{-1} \left( \sqrt{1 - a^2} \right) + Q_{\nu}^{1} \left( \sqrt{1 - a^2} \right) \right]
\]

\[
= -\frac{1}{a^3} + \frac{\eta}{2} + \frac{\nu(\nu + 1)}{2} \left[ \log \frac{a}{2} + \Psi(\nu + 1) + \gamma - \frac{1}{2} \right] + o(1), \quad (4.81)
\]

\[
v_a = \frac{2}{a^3} + \frac{\nu(\nu + 1)}{2a} + o\left(\frac{1}{a}\right), \quad (4.82)
\]

\[
g = 4a^4 \left[ 1 + \omega(a) \right] + o(a^4), \quad (4.83)
\]

where

\[
\omega(a) = \frac{\nu(\nu + 1)}{2} \log \frac{a}{2} + \frac{\eta}{2} + \frac{\nu(\nu + 1)}{4} + \Psi(\nu + 1) + \gamma - 1. \quad (4.84)
\]

The result is in agreement with [3].
Conclusion

In the thesis we focused on the topic of quantum cosmology. More specifically, we studied the solutions of the Wheeler–DeWitt equation for the case of a closed FLRW universe with spatially homogeneous scalar field with quadratic potential. Firstly, we described the procedure, developed by Banks, Bender and Wu [4], for finding a tunnelling solution in two-dimensional quantum mechanics. We than showed how to alter the technique (according to [3]) so that it covers the case of an incoming beam of particles, which tunnel through the barrier to the inside of the well.

We contributed to the calculations with our own arguments, for example when dealing with the separation constant (analysis around formula (1.62) and similar ones in the following chapters). Using the technique of analytic continuation [9, p. 164], we also constructed the form of the incoming beam of particles corresponding to the tunnelling solutions. We demonstrated that some solutions are not physically acceptable and we found a necessary condition for a solution to be well-behaved.

In the last chapter we studied the case of a “universe created from nothing”. We first described the approach of Vilenkin [14], in which he used the condition that the dependence of the wavefunction on the values of the scalar field vanishes as the radius of the universe approaches zero. Motivated by [8], we then chose a special value of the ordering parameter, $p = 1$. In this case, we proposed an alternative boundary condition. Finally, employing the techniques from the previous chapters we constructed a new one-parametric class of solutions.

Using the method of analytic continuation it should be again possible to find the forms of the respective solutions in the Lorentzian domain (i.e. region of large radii). As we are working in the WKB approximation, it is plausible that a classical trajectory can emerge by interference of waves [6] and finding it we would obtain the information about the very early evolution of the universe with scalar field. This may be useful when investigating possible inflationary scenarios.
Appendix A

Associated Legendre functions

In this appendix we use formulae from [1], [2] and [5, Appendix].

Consider the differential equation

\[
(1 - w^2) u''(w) - 2wu'(w) + \left[ \nu(\nu + 1) - \frac{\mu^2}{1 - w^2} \right] u(w) = 0, \tag{A.1}
\]

which is called the associated Legendre equation. The solutions can be written in the form

\[
u(w) = a_1 P^\mu_\nu(w) + a_2 Q^\mu_\nu(w), \tag{A.2}
\]

where \(a_1\) and \(a_2\) are some coefficients and \(P^\mu_\nu\), \(Q^\mu_\nu\) are the associated Legendre functions of the first and second kind, respectively.

The following identities hold for the functions \(P^\mu_\nu\) and \(Q^\mu_\nu\):

\[
P^\mu_\nu(w) = \frac{1}{\Gamma(1 - \mu)} \left( \frac{1 + w}{1 - w} \right)^{\mu/2} 2F_1 \left( -\nu, \nu + 1; 1 - \mu; \frac{1 - w}{2} \right), \tag{A.4}
\]

\[
Q^\mu_\nu(w) = \frac{\pi}{2 \sin(\pi \mu)} \left( \cos(\pi \mu) P^\mu_\nu(w) - \frac{\Gamma(\mu + \nu + 1)}{\Gamma(-\mu + \nu + 1)} P^{-\mu}_\nu(w) \right), \tag{A.5}
\]

where \(2F_1\) is the hypergeometric function defined by the series

\[
2F_1(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} \sum_{n=0}^{\infty} \frac{\Gamma(n + \alpha)\Gamma(n + \beta)}{n!\Gamma(n + \gamma)} z^n \tag{A.6}
\]

and in (A.4), (A.5) we have to take the respective limits in \(\mu\) when we are interested in the case \(\mu \in \{-1, 1\}\).
Observe also the following useful identities:

\[
P_1^\nu = -\nu(\nu + 1)P_{-1}^{-\nu}(w), \quad (A.7)
\]

\[
Q_1^\nu = -\nu(\nu + 1)Q_{-1}^{-\nu}(w), \quad (A.8)
\]

\[
P_{-\nu-1}^\mu = P_{-\nu}^\mu(w), \quad (A.9)
\]

\[
Q_{-\nu-1}^\mu = Q_{-\nu}^\mu(w) + \cos(\pi\nu)\Gamma(\mu - \nu)\Gamma(\mu + \nu + 1)P_{-\mu}^{-\nu}(w). \quad (A.10)
\]

These imply that it is possible to choose and fix some \(\nu\) and some \(\mu\) (for either of the functions \(P_{-1}^{-\nu}\) and \(Q_1^\nu\) we have two options for each index).

We will now prove the equalities used in section 2.2. We presume that \(P_\nu^\mu(w)\) and \(Q_\nu^\mu(w)\) are analytic (in the region we are interested in)\(^1\). Let us consider a solution \(u(w) = \alpha P_\nu^\mu + \beta Q_\nu^\mu, \alpha, \beta \in \mathbb{R}\). The key point is to realise that the function \(v(w) = \overline{u(w)}\) is then equal to \(u(w)\) for all \(w \in (0, 1)\) and also in some region above and under the real axis. The reason is that one can expand \(u(w)\) into Taylor series around any point \(x_0 \in (0, 1)\) and in this expansion all coefficients are real (because all the derivatives of \(u(w)\) are real on \((0, 1))\). The claim then follows from

\[
\sum_{n=0}^{\infty} a_n z^n = \sum_{n=0}^{\infty} a_n \overline{z^n}, \quad \text{when} \quad a_n \in \mathbb{R} \quad \forall n. \quad (A.11)
\]

Finally, due to the uniqueness of analytic continuation, we have that there holds

\[
\overline{u(w)} = u(\overline{w}) \quad (A.12)
\]

in the entire region.

The other equality we used in (2.2),

\[
\overline{u'(w)} = u'(\overline{w}), \quad (A.13)
\]

follows readily from

\[
u'(\overline{w}) = \lim_{\epsilon \to 0} \frac{u(\overline{w} + \epsilon) - u(\overline{w})}{\epsilon} = \lim_{\epsilon \to 0} \frac{u(\overline{w} - \epsilon) - u(\overline{w})}{\epsilon} = \lim_{\epsilon \to 0} \frac{u(w + \epsilon) - u(w)}{\epsilon} = u'(w). \quad (A.14)
\]

\(^1\)This is of course true, but we will not prove it in this text.
In section 2.3 the following formulae were needed:

\[ P_{\nu}^{\mu}(w = 0) = \frac{2^\mu \sqrt{\pi}}{\Gamma \left( \frac{1-\mu-\nu}{2} \right) \Gamma \left( 1 - \frac{\mu-\nu}{2} \right)} \]  \hspace{1cm} (A.15)

\[ Q_{\nu}^{\mu}(w = 0) = -\frac{2^{\mu-1} \pi^{3/2}}{\Gamma \left( \frac{1-\mu-\nu}{2} \right) \Gamma \left( 1 - \frac{\mu-\nu}{2} \right)} \tan \left( \frac{\pi (\mu + \nu)}{2} \right) \]  \hspace{1cm} (A.16)

\[ \frac{\partial P_{\nu}^{\mu}(w)}{\partial w} = \frac{1}{w^2 - 1} \left[ w \nu P_{\nu}^{\mu}(w) - (\mu + \nu) P_{\nu-1}^{\mu}(w) \right] \]  \hspace{1cm} (A.17)

\[ \frac{\partial Q_{\nu}^{\mu}(w)}{\partial w} = \frac{1}{w^2 - 1} \left[ w \nu Q_{\nu}^{\mu}(w) - (\mu + \nu) Q_{\nu-1}^{\mu}(w) \right]. \]  \hspace{1cm} (A.18)

The asymptotic formula for \( P_{\nu}^{-1}(\sqrt{1-x^2}) \), \( x \to 0 \) can be derived quickly from (A.4) and (A.6):

\[ P_{\nu}^{-1}(\sqrt{1-x^2}) = \frac{x}{2} + \frac{1}{16} \left[ 2 - \nu(\nu + 1) \right] x^3 + o(x^3). \]  \hspace{1cm} (A.19)

To obtain the asymptotic formula for \( Q_{\nu}^{1}(w) \), \( x \to 0 \) we have to perform the limit \( \mu \to 1 \). For the sake of completeness, we first construct the whole series expansion. In other words, we compute

\[ \lim_{\epsilon \to 0} \frac{\pi}{2 \sin(\pi \epsilon)} \left( \cos(\pi(1 + \epsilon)) P_{\nu}^{1+\epsilon}(w) - \frac{\Gamma(\nu + 2 + \epsilon)}{\Gamma(\nu - \epsilon)} P_{\nu}^{-1-\epsilon}(w) \right) = \]  \hspace{1cm} (A.20)

\[ = \lim_{\epsilon \to 0} \frac{\pi}{2 \sin(\pi \epsilon)} \left( \cos(\pi \epsilon) P_{\nu}^{1+\epsilon}(w) + \frac{\Gamma(\nu + 2 + \epsilon)}{\Gamma(\nu - \epsilon)} P_{\nu}^{-1-\epsilon}(w) \right). \]

The factor in large brackets equals zero for \( \epsilon = 0 \) because of (A.7). As a result

\[ Q_{\nu}^{1}(w) = \frac{1}{2} \left. \frac{\partial}{\partial \epsilon} \right|_{\epsilon=0} \left( \cos(\pi \epsilon) P_{\nu}^{1+\epsilon}(w) + \frac{\Gamma(\nu + 2 + \epsilon)}{\Gamma(\nu - \epsilon)} P_{\nu}^{-1-\epsilon}(w) \right) = \]  \hspace{1cm} (A.21)

\[ \frac{1}{2} \left. \frac{\partial}{\partial \epsilon} \right|_{\epsilon=0} \left( P_{\nu}^{1+\epsilon}(w) + \frac{\Gamma(\nu + 2 + \epsilon)}{\Gamma(\nu - \epsilon)} P_{\nu}^{-1-\epsilon}(w) \right). \]

We introduce the digamma function

\[ \Psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} \]  \hspace{1cm} (A.22)

and using

\[ z \Gamma(z) = \Gamma(z + 1), \]  \hspace{1cm} (A.23)

\[ \Gamma(\epsilon) = \frac{1}{\epsilon} \Gamma(1 + \epsilon) = \frac{1}{\epsilon} + o \left( \frac{1}{\epsilon} \right) \]  \hspace{1cm} (A.24)
we write
\[ \frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} P^{1+\epsilon}_\nu(w) = \frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} \left[ \left( \frac{1+w}{1-w} \right)^{1/2} \frac{1}{\Gamma(-\nu)\Gamma(\nu+1)} \right]. \]

\[ \cdot \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n)} \left( \frac{1-w}{2} \right)^n = \left( \frac{1+w}{1-w} \right)^{1/2} \frac{1}{\Gamma(-\nu)\Gamma(\nu+1)}. \]

\[ \cdot \left[ \frac{1}{2} \log \frac{1+w}{1-w} \sum_{n=1}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \left( \frac{1-w}{2} \right)^n \right] + \]

\[ + \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \Psi(n+2) \left( \frac{1-w}{2} \right)^n \]. \tag{A.25}

\[ \frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} \frac{\Gamma(\nu+2+\epsilon)}{\Gamma(\nu)} = \frac{\Gamma(\nu+2)}{\Gamma(\nu)} \left[ \Psi(\nu+2) + \Psi(\nu) \right], \tag{A.26} \]

\[ \frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} P^{-1-\epsilon}_\nu(w) = \frac{\partial}{\partial \epsilon} \bigg|_{\epsilon=0} \left[ \left( \frac{1+w}{1-w} \right)^{1/2} \frac{1}{\Gamma(-\nu)\Gamma(\nu+1)} \right]. \]

\[ \cdot \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2+\epsilon)} \left( \frac{1-w}{2} \right)^n = \left( \frac{1+w}{1-w} \right)^{-1/2} \frac{1}{\Gamma(-\nu)\Gamma(\nu+1)}. \]

\[ \cdot \left[ \frac{1}{2} \log \frac{1+w}{1-w} \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \left( \frac{1-w}{2} \right)^n \right] + \]

\[ + \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \Psi(n+2) \left( \frac{1-w}{2} \right)^n \]. \tag{A.27}

The result is
\[ Q^1_\nu(w) = \frac{1}{2\Gamma(-\nu)\Gamma(\nu+1)} \left\{ \sqrt{1+w} \int \frac{1}{1-w} \frac{1}{2} \log \frac{1+w}{1-w} \right. \]

\[ \cdot \sum_{n=1}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n)} \left( \frac{1-w}{2} \right)^n - \]

\[ - \Gamma(-\nu)\Gamma(\nu+1) + \sum_{n=1}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n)} \Psi(n) \left( \frac{1-w}{2} \right)^n \right\} + \]

\[ + \nu(\nu+1) \sqrt{1+w} \left[ \left( \Psi(\nu+2) + \Psi(\nu) - \frac{1}{2} \log \frac{1+w}{1-w} \right) \right. \]

\[ \cdot \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \left( \frac{1-w}{2} \right)^n - \]

\[ - \sum_{n=0}^{\infty} \frac{\Gamma(n-\nu)\Gamma(n+\nu+1)}{n!\Gamma(n+2)} \Psi(n+2) \left( \frac{1-w}{2} \right)^n \right\}. \tag{A.28} \]
Now we can deduce
\[ Q_1^1(\sqrt{1 - x^2}) = -\frac{1}{x} + \frac{1}{2} \nu(\nu + 1) \left[ \log \frac{x}{2} + \Psi(\nu + 1) + \gamma - \frac{1}{2} \right] x + o(x), \tag{A.29} \]
where we have used \( \Gamma'(1) = -\gamma \) (\( \gamma \) being the Euler–Mascheroni constant) and the formula
\[
\Psi(z + 1) = \frac{1}{\Gamma(z + 1)} \lim_{\epsilon \to 0} \frac{\Gamma(z + 1 + \epsilon) - \Gamma(z + 1)}{\epsilon} = \frac{1}{z} \lim_{\epsilon \to 0} \frac{(z + \epsilon)\Gamma(z + \epsilon) - z\Gamma(z)}{\epsilon} = \Psi(z) + \frac{1}{z}. \tag{A.30}
\]

Another equation, which is closely related to associated Legendre equation, is the Gegenbauer differential equation,
\[ (1 - w^2)u''(w) - 2(\mu + 1)wu'(w) + (\nu - \mu)(\nu + \mu + 1)u(w) = 0. \tag{A.31} \]
This equation arises for example when one deals with the Sturm-Liouville problem for the Laplace operator on a \((n\text{-dimensional})\) sphere considering functions dependent on only one spherical angle \([5]\). Making a substitution
\[ u(w) = (1 - w^2)^{-\mu/2}v(w), \tag{A.32} \]
computing the respective derivatives (for simplicity we deal only with cases \( \mu \neq 0, -2 \))
\[
\begin{align*}
    u' &= (1 - w^2)^{-\mu/2} \left[ \mu w(1 - w^2)^{-1}v + v' \right], \\
    u'' &= (1 - w^2)^{-\mu/2} \left[ \mu(1 - w^2)^{-1}v + \mu(\mu + 2)w^2(1 - w^2)^{-2}v + 2\mu w(1 - w^2)^{-1}v' + v'' \right],
\end{align*}
\tag{A.33}
\]
and inserting the expressions into (A.31), we arrive at the associated Legendre equation (A.1). The solution to (A.31) is therefore
\[ u(w) = (1 - w^2)^{-\mu/2} (a_1 P_\mu^\nu(w) + a_2 Q_\mu^\nu(w)). \tag{A.34} \]
Bibliography


