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Wave packet dynamics in quantum mechanics and quantum cosmology

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Chapter 1

Introduction

This work consists of two parts that can be read independently and do not directly rely on each other. Yet they have have in common the aim to analyze and understand the transition between quantum and classical behaviour and the deviations of quantum dynamics from classical motion.

The first part deals with quantum mechanics. We focus on the semiclassical phase of time evolution before revivals occur but when quantum effects already come into play. Here we introduce the method of Laplace transformation that gives the solution of the time-dependent Schrödinger equation in terms of the initial wave function if the solution of the time-independent equation is known. Though the Laplace transformation has already been applied to several problems in quantum dynamics ([1], [2] ,[3] , [4] [5],[6];see also [7] for a more detailed discussion), the method has not been systematically used to solve the initial value problem of wave packet evolution. We obtain propagators of several systems that give a direct insight into the wave packet evolution and contain the quantum analogue of classical transmission and reflection processes. We are finally able to shed new light on the so-called Hartmann effect, predicting that for sufficiently thick barriers the tunneling time becomes independent of the thickness of the barrier.

The second part concerns quantum cosmology. In order to obtain an unambiguous time evolution we decided to choose unimodular gravity instead of general relativity in its common form as the starting point for the canonical quantization procedure. Unimodular gravity was already considered by Albert Einstein ([8]). It is obtained by constraining the space-time metric in the Einstein Hilbert action. This yields a theory that is practically indistinguishable from general relativity, with the only difference that the cosmological constant is a conserved quantity instead of a natural constant. Yet unimodular gravity has a different canonical structure and leads to a quantum theory that admits a time evolution. So the famous " problem of time " of canonical quantum gravity does not occur. We investigate unimodular quantum cosmology for a toy model. It is possible to construct solutions with a unitary time evolution. Unlike common quantum-mechanical systems (as the ones considered in the first part) the solutions become classical in a certain sense for the late phase of time evolution.

This thesis is structured as follows: After some considerations about the characterization of wave packets and their dynamics (chapter 2) we present the method of Laplace transformation in chapter 3. The following chapters contain the application of the method to: the infinite square well (chapter 4), the potential step (chapter 5), the asymmetric well (chapter 6) and the rectangular barrier (chapter 7). The contents of the chapters 3, 5, 6 and parts of chapter 4 have already been published in [7].

In chapter 8 we present unimodular gravity and discuss the steps of canonical quantization of general relativity versus the unimodular theory. Chapter 9 treats the symmetry reduced cosmological model of a scalar field in a spatially flat universe. We discuss the solutions in the even more special case of a massless scalar field, that can be related to a perfect fluid with a stiff matter equation of state. Chapter 10 finally contains the quantization of this model according to unimodular quantum gravity. Each chapter that contains new results closes with a short summary and a discussion of the literature.

Acknowledgments

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Part I

Quantum Mechanics

Chapter 2

The evolution of wave packets

In this chapter we discuss the equations which govern the time evolution of the characteristic variables of wave packets. Since the shape of the initial wave packet plays an important role, we introduce rather general initial functions for our analysis of quantum dynamics. We finally present the characteristic features of wave packet dynamics in at most quadratic potentials.

In classical mechanics, a dynamical system is said to be analyzed if the trajectories for all possible initial data can either be given analytically or at least be described in a satisfactory manner.

In quantum mechanics, dynamics is described by wave packets $\psi(x,t)$ which start at $t = 0$ and evolve according to the Schrödinger equation changing not only their position and momentum expectation values, but also their entire shape. Therefore, the description of the dynamics of a wave packet should not only contain the expectation values of the operators $\hat{x}$ and $\hat{p}$, but at least also the corresponding uncertainties of position and momentum.

Most investigations about quantum dynamics start with a family of wave packets (for instance Gauss functions), parameterized by the initial values of the expectation values of position and momentum x_0 and p_0 and the uncertainties Δx_0 and Δp_0. Of course the result for the time evolutions of expectation values and uncertainties will in general depend on the chosen family of initial wave packets. In fact, there are only few dynamical properties of quantum systems that have been properly analyzed and found out to be independent of the shape of the initial wave packet. (The most prominent example is undoubtedly the revival phenomenon which occurs in the long-term evolution of wave packets in many quantum systems [9].)

2.1 Equations of motion for the characteristic variables

The Schrödinger equation yields for the expectation values $\langle \hat{x} \rangle, \langle \hat{p} \rangle$ and the variances $(\Delta x)^2, (\Delta p)^2$ of a wave packet, which evolves subject to a Hamiltonian of the form

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) \,, \tag{2.1}$$

the equations of motion

$$\frac{d}{dt} \langle \hat{x} \rangle = \frac{\langle \hat{p} \rangle}{m} \qquad \frac{d}{dt} \langle \hat{p} \rangle = - \langle V'(\hat{x}) \rangle \tag{2.2a}$$

$$\frac{d}{dt}(\Delta x)^2 = \frac{1}{m} \langle \hat{x}\hat{p} + \hat{p}\,\hat{x} - 2 \langle \hat{x} \rangle \langle \hat{p} \rangle \rangle \tag{2.2b}$$

$$\frac{d}{dt}(\Delta p)^2 = - \langle (\hat{p} - \langle \hat{p} \rangle)\, V'(\hat{x}) \rangle - \langle V'(x)\, (\hat{p} - \langle \hat{p} \,\rangle) \rangle \tag{2.2c}$$

$$\frac{d^2}{dt^2}(\Delta x)^2 = \frac{2}{m^2}(\Delta p)^2 - \frac{2}{m} \langle (\hat{x} - \langle \hat{x} \rangle)\, V'(\hat{x}) \rangle \tag{2.2d}$$

$$\begin{aligned} \frac{d^2}{dt^2}(\Delta p)^2 = &-\frac{1}{2m} \left\langle \hat{p}^2 V''(x) + 2\hat{p}V''(\hat{x})\hat{p} + V''(\hat{x})\hat{p}^2 \right\rangle + \\ &\frac{1}{m} \langle \hat{p}V''(\hat{x}) + V''(\hat{x})\hat{p} \rangle \langle \hat{p} \rangle + 2 \left(\left\langle (V'(\hat{x}))^2 \right\rangle - \langle V'(\hat{x}) \rangle^2 \right) \quad . \end{aligned} \tag{2.2e}$$

The equations for the expectation values (2.2a) agree with Newton's equations of motion only if

$$\langle V'(\hat{x}) \rangle = V'(\langle \hat{x} \rangle) \quad . \tag{2.3}$$

All potentials of at most quadratic order in x fulfill this condition. For more general potentials the equations (2.2a) do not even constitute a closed system of first order differential equations. If we insert for example $V(x) = x^3/3$, we get

$$\frac{d}{dt} \langle \hat{x} \rangle = \frac{\langle \hat{p} \rangle}{m} \qquad \frac{d}{dt} \langle \hat{p} \rangle = \langle \hat{x} \rangle^2 - (\Delta x)^2 \quad .$$

This means that the equations for the expectation values become connected with the equations for the uncertainties. For potentials of even higher order in x more general so-called moments of the form $\langle x^n \rangle$ come into play. Moreover in general the equations (2.2) altogether do not constitute a closed system of differential equations. Only in the case of at most quadratic potentials the equations (2.2a) can be solved independently and the remaining equations represent also a closed system of differential equations, which governs the dynamics of the uncertainties (see section 2.3).

Equation (2.2b) still contains another interesting information. Since it does not depend on the potential, the derivative of the position variance at the starting time is only determined by the initial wave packet. We will call

$$\Delta_{xp} = \frac{1}{2}\left\langle \hat{x}\hat{p} + \hat{p}\,\hat{x} - 2\left\langle \hat{x}\right\rangle \left\langle \hat{p}\right\rangle \right\rangle \tag{2.4}$$

mixed uncertainty. The mixed uncertainty is always real, but not necessarily positive, which distinguishes it from the position and momentum uncertainty. According to (2.12a) the sign of the mixed uncertainty determines if the wave packet is going to spread or narrow at the beginning of the time evolution, regardless which potential is given. The mixed uncertainty is the counterpart of the covariance in classical statistical mechanics that indicates a correlation between position and momentum of classical phase-space densities [10].

Moreover $(\Delta x)^2, (\Delta p)^2$ and Δ_{xp} always satisfy the inequality

$$(\Delta x)^2(\Delta p)^2 - (\Delta_{xp})^2 \geq \frac{1}{4}\hbar^2 \quad , \tag{2.5}$$

which is stronger than Heisenberg's uncertainty inequality [11]. We will call it generalized uncertainty relation. As a consequence of the considerations in this section, we will include the mixed uncertainty in our investigations of wave packet dynamics. Moreover we will call wavepackets with $\Delta_{xp} \neq 0$ uncorrelated wave packets.

2.2 Papageno functions

For our analysis of quantum dynamics we will use initial wave packets of the form

$$\psi(x) \;=\; e^{i(\alpha\, x^2 + \beta\, x + \gamma)} F(x) \qquad \text{where} \qquad \alpha\,,\, \beta,\, \gamma \,\epsilon\, \mathbb{R} \quad . \tag{2.6}$$

The functions F(x) are twice differentiable real functions and should fulfill the condition

$$\int_{x_1}^{x_2} F(x)^2 dx = 1\,,$$

where $F(x) = 0$ outside (x_1, x_2). The values of x_1 and x_2 depend on the analyzed quantum system. If we want to define the wave function on the whole real line the boundaries have to be replaced by $-\infty$ and ∞. We will call all functions described by (2.6). Papageno functions. (We will explain the name below.) Of course not every initial wave packet can be represented by a Papageno function. But at least every initial probability density can be associated with a Papageno function. The Gauss functions are special cases of Papageno functions.

A Papageno function of the form $\psi(x) = F(x)$, where $F(x)$ fulfills the additional condition

$$\int_{x_1}^{x_2} F(x)^2 x\, dx = 0$$

describes an initial wave packet with the position and momentum expectation values

$$
\begin{aligned}
x_0 &= \langle \psi \, \hat{x} \, \psi \rangle = 0 \\
p_0 &= \langle \psi \, \hat{p} \ \ \psi \rangle = 0 \quad .
\end{aligned}
$$

For the variances of position and momentum we will write

$$
\begin{aligned}
(\Delta x_0)^2 &= \langle \psi \, \hat{x}^2 \, \psi \rangle = k \\
(\Delta p_0)^2 &= \langle \psi \, \hat{p}^2 \, \psi \rangle = l\hbar^2 \quad .
\end{aligned}
$$

.

For the mixed uncertainty we finally find

$$
\Delta^0_{xp} = \frac{1}{2} \langle \psi \, (\hat{x} \, \hat{p} + \hat{p} \, \hat{x}) \, \psi \rangle = 0 \quad .
$$

Then the family of functions

$$
\psi(A, B, a, b\,; x) = e^{\frac{iB(x-A)}{\hbar} + ia(x-A)^2} (\frac{1}{\sqrt{b}}) F(\frac{(x-A)}{b}) \tag{2.7}
$$

is a family of Papageno functions with the initial values

$$
\begin{aligned}
x_0 &= \langle \psi \, \hat{x} \, \psi \rangle = A \qquad & (\Delta x_0)^2 &= \langle \psi (\hat{x} - x_0)^2 \psi \rangle = kb^2 \\
p_0 &= \langle \psi \, \hat{p} \, \psi \rangle = B \qquad & (\Delta p_0)^2 &= \langle \psi (\hat{p} - p_0)^2 \psi \rangle = l \frac{\hbar^2}{b^2} + 4a^2 \hbar^2 b^2 k \\
& & &= \hbar^2 \frac{l\,k}{(\Delta x_0)^2} + 4a^2 \hbar^2 (\Delta x_0)^2 \quad .
\end{aligned} \tag{2.8}
$$

So b and $F(x)$ characterize the spatial width and the shape of the Papageno function, whereas B determines the momentum. The parameter a allows to choose Δx_0 and Δp_0 independently - except that they have to fulfill $(\Delta x_0)^2 (\Delta p_0)^2 \geq \hbar^2 \, k \, l$.

A closer look at the oscillating part of the Papageno function

$$
e^{\frac{ip_0(x-x_0)}{\hbar} + ia(x-x_0)^2} = e^{i\left(\frac{p_0}{\hbar} + a(x-x_0)\right)(x-x_0)}
$$

reveals that in the vicinity of $x = x_0$, more precisely if $|a(x-x_0)\hbar| \ll |p_0|$, the parameter a imposes an irregularity on the regularly oscillating factor $e^{\frac{ip_0(x-x_0)}{\hbar}}$. This looks like a signal with increasing (for $p_0 \cdot a > 0$) or decreasing (for $p_0 \cdot a < 0$) frequency (see figure 2.1). In the time domain such signals are commonly called chirps and we will use this name also for the parameter a as it was done in [12], where the chirp is defined with an additional factor $\hbar$. In order to emphasize that we treat functions with chirp (or functions with non-vanishing position-momentum correlation) we have named our initial wave packets Papageno functions.

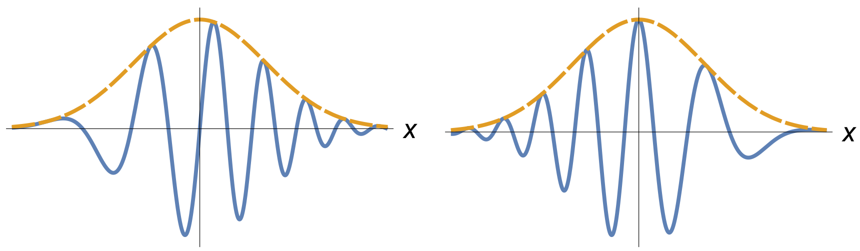


Figure 2.1: Papageno function $\mathrm{Re}\,[\psi(x)]$ with Gaussian $F(x)$ (dashed line) and $p_0 \cdot a > 0$ (left) respectively $p_0 \cdot a < 0$ (right)

The value of a determines the mixed uncertainty of the Papageno function. We find

$$\Delta^0_{xp} = 2a\hbar(\Delta x_0)^2 \quad . \tag{2.9}$$

The generalized uncertainty relation (2.5) for a family Papageno functions (2.7) reads

$$(\Delta x_0)^2(\Delta p_0)^2 - (\Delta^0_{xp})^2 = \hbar^2 lk \geq \frac{1}{4}\hbar^2 \quad . \tag{2.10}$$

If

$$F(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}$$

we will call the associated family of Papageno functions Gaussian wave packets. Since for those wave packets $k = l = 1/2$, Gaussian wave packets saturate the generalized uncertainty relation.

2.3 Potentials of at most quadratic order

If the potential has the form

$$V(x) = v_2\, x^2 + v_1\, x + v_0 \qquad \text{with} \qquad v_0\,,\, v_1,\, v_2 \,\epsilon\, \mathbb{R} \quad ,$$

the equations (2.2a) become

$$\frac{d}{dt}\,\langle \hat{x} \rangle = \frac{\langle \hat{p} \rangle}{m} \qquad \frac{d}{dt}\,\langle \hat{p} \rangle = -V'(\langle \hat{x} \rangle) \quad , \tag{2.11}$$

which ensures that the evolution of position and momentum expectation values agrees with the evolution of the classical observables.

The remaining equations (2.2b-2.2e) read

$$\frac{d}{dt}(\Delta x)^2 = \frac{2}{m}\Delta_{xp} \tag{2.12a}$$
$$\frac{d}{dt}(\Delta p)^2 = -4v_2\Delta_{xp} \tag{2.12b}$$
$$\frac{d^2}{dt^2}(\Delta x)^2 = \frac{2}{m^2}(\Delta p)^2 - \frac{4v_2}{m}(\Delta x)^2 \tag{2.12c}$$
$$\frac{d^2}{dt^2}(\Delta p)^2 = 8(v_2)^2(\Delta x)^2 - \frac{4v_2}{m}(\Delta p)^2 \,. \tag{2.12d}$$

The equations (2.12c) and (2.12d) represent a system of two linear second order differential equations which has a unique solution for fixed initial values of $(\Delta x)^2$, $(\Delta p)^2$, $\frac{d}{dt}(\Delta x)^2$ and $\frac{d}{dt}(\Delta p)^2$. In order to fulfill equation (2.12a) the initial value of $\frac{d}{dt}(\Delta x)^2$ has to be chosen in accordance with the initial mixed uncertainty. But if finally equation (2.12b) should also be satisfied, the relation

$$\frac{d}{dt}\left(2mv_2(\Delta x)^2 + (\Delta p)^2\right) = 0 \tag{2.13}$$

must hold for all times. Since a closer look at the system (2.12c,2.12d) reveals

$$\frac{d^2}{dt^2}\left(2mv_2(\Delta x)^2 + (\Delta p)^2\right) = 0 \tag{2.14}$$

we see that the constraint equation(2.13) is fulfilled during the time evolution of the system (2.12c,2.12d) if it is only satisfied at $t = 0$. So we get a unique solution for (2.12) if we solve (2.12c,2.12d) and choose the initial values according to (2.12a, 2.12b).

The system (2.12) has two constants of motions, namely

$$\mathcal{K} = (\Delta p)^2 + 2mv_2(\Delta x)^2 \quad \text{and} \quad U = (\Delta x)^2(\Delta p)^2 - (\Delta_{xp})^2 \quad . \tag{2.15}$$

The conservation of $\mathcal{K}$ is equivalent to the constraint equation (2.13). U is just the left hand side of the inequality (2.5). The conservation of U can be derived carrying out the time derivative of U and using (2.12a,2.12b,2.12c). If the mixed uncertainty takes the value zero, which is in particular the case when $(\Delta x)^2$ or $(\Delta p)^2$ have an extreme value (see (2.12a, 2.12b)), the uncertainty product P takes the value of its global minimum

$$P \equiv (\Delta x)^2(\Delta p)^2 = P_{min} = U\,. \tag{2.16}$$

So the system of equations (2.12)has a unique solution for fixed initial values of the three uncertainties $(\Delta x), (\Delta p), \Delta_{xp}$. It is important to notice that the initial data of momentum and position uncertainties are not enough to prescribe the time evolution of these two quantities. But together with the initial value of the mixed uncertainty the dynamics of all three quantities is determined.

Since U is the left hand side of the generalized uncertainty relation, a Gaussian wave packet continues to saturate the generalized uncertainty relation for all times. This is in accordance with the fact that a Gaussian wave packet evolves as a Gaussian, if the potential is at most quadratic:

The Gaussian wave packet

$$\psi(x,t) = \frac{1}{(\pi\alpha)^{1/4}} e^{-\frac{(x-A(t))^2}{2\alpha(t)} + \frac{iB(t)(x-x(t))}{\hbar} + ia(t)(x-A(t))^2 + i\frac{S(t)}{\hbar}} \tag{2.17}$$

$$\text{with} \quad \alpha(t) > 0 \quad \text{and} \quad A(t), B(t), a(t), S(t) \, \epsilon \, \mathbb{R}$$

has the properties

$$(\Delta x)^2(t) = \frac{\alpha(t)}{2}\,, \qquad \mu(t) \equiv \Delta_{xp}(t) = \alpha(t)\,a(t)\hbar\,, \tag{2.18}$$

$$\langle x\rangle(t) = A(t)\,, \qquad \langle\hat{p}\rangle(t) = B(t)\,. \tag{2.19}$$

If we insert this wave packet in the Schrödinger equation and expand the potential about $A(t)$ we can compare equal powers of $(x - A(t))$. So we find the following equations for the characteristic parameters of the wave packet

$$\dot{A} = \frac{B}{m} \qquad \dot{B} = -V'(A) \tag{2.20}$$

$$\dot{\alpha} = \frac{4\mu}{m} \qquad \dot{\mu} = \frac{\hbar^2}{2m\alpha}\left(1 + \frac{4\mu^2}{\hbar^2}\right) - V''\frac{\alpha}{2}$$

$$\dot{S} = \frac{B^2}{2m} - V(A) - \frac{\hbar^2}{2m\alpha}\,. \tag{2.21}$$

This system of equations can be solved for all appropriate initial conditions. So we see, that a Gaussian wave packet keeps its shape under the influence of at most quadratic potentials.

For an arbitrary family of Papageno functions the relation $U = \hbar^2 lk$ (see 2.10) must also hold for all times, where l, k are properties of the characteristic function $F(x)$. But in this only slightly more general case the Papageno functions will in general not keep their shape. We can show this, if we choose an arbitrary Papageno function as initial wave packet

$$\psi(x) = e^{\frac{iB_0(x-A_0)}{\hbar} + ia_0(x-A_0)^2} e^{i\frac{\phi_0}{\hbar}} \cdot F(x) \tag{2.22}$$

We assume that it has the properties

$$\langle x\rangle = A_0\,, \quad (\Delta x)^2 = \frac{\alpha}{2}\,,$$

$(\Delta p)^2$ is determined by $F(x)$. The remaining characteristic properties are given by

$$\langle\hat{p}\rangle = B_0\,, \quad \Delta_{xp}(t) = \alpha(t)\,a(t)\hbar\,.$$

We expand the non-oscillating part in terms of shifted harmonic oscillator eigenfunctions (see Appendix D.2):

$$F(x) = \sum_{n=0}^{\infty} c_n \varphi_n(x - A_0)$$

$$\text{with} \quad \varphi_n(x - A_0) = \frac{1}{(\pi\alpha_0)^{1/4}\sqrt{2^n n!}} H_n\left[\frac{x - A_0}{\sqrt{\alpha_0}}\right] e^{-\frac{(x-A_0)^2}{2\alpha_0}} \quad . \tag{2.23}$$

So the initial wave function reads

$$\psi(x) = \sum_{n=0}^{\infty} c_n \, \varphi_n(x - A_0) \, e^{\frac{iB_0(x-A_0)}{\hbar} + ia_0(x-A_0)^2} e^{i\frac{\phi_0}{\hbar}} \equiv \sum_{n=0}^{\infty} c_n u_n(x) \quad . \tag{2.24}$$

determine the time evolution for each term of the sum. Inserting the functions

$$\begin{aligned} u_n(x,t) = & \frac{1}{(\pi\alpha_n(t))^{1/4}\sqrt{2^n n!}} H_n\left[\frac{x - A_n(t)}{\sqrt{\alpha_n(t)}}\right] e^{-\frac{(x-A_n(t))^2}{2\alpha_n(t)}} \\ & \cdot e^{\frac{iB_n(t)(x-A_n(t))}{\hbar} + ia_n(t)(x-A_n(t))^2} e^{i\frac{S_n(t)}{\hbar}} \end{aligned} \tag{2.25}$$

in the Schrödinger equation yields with regard to (D.15) for all n the same equations of motion (2.20) for the variables $A_n(t), B_n(t), \alpha_n(t), \mu_n(t) = a_n(t), \alpha_n(t)$ which we have already found for the evolution of Gaussian wave packets ($n = 0$). For the variables $S_n(t)$ we find the equations

$$\dot{S}_n = \frac{B^2}{2m} - V(A) - \frac{\hbar^2}{m\alpha}\left(n + \frac{1}{2}\right) \quad . \tag{2.26}$$

So we get the time evolution

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n u_n(x,t) \quad , \tag{2.27a}$$

if we insert the solutions of (2.20,2.26)

$$A_n(t) = A(t), \quad B_n(t) = B(t), \quad \alpha_n(t) = \alpha(t), \quad a_n(t) = a(t), \quad S_n(t) \tag{2.27b}$$

with the initial conditions

$$A(0) = A_0, \quad B(0) = B_0, \quad a(0) = a_0, \quad \alpha(t) = \alpha_0, \quad S_n(0) = \phi_0 \tag{2.27c}$$

in the functions $u_n(x,t)$ (2.25).

Now we assume that the resulting function could be written as a Papageno function (2.6)for all times. Since the dynamics of the expectation values and uncertainties is determined by (2.11, 2.12) with the initial values of (2.22), the oscillating factor coincides with the corresponding expression for the functions $u_n(x,t)$ apart from a real function $\gamma(t)$. We get

$$\psi(x,t) \stackrel{!}{=} G(x,t)\, e^{\frac{iB(t)(x-A(t))}{\hbar}+ia(t)(x-A(t))^2} e^{i\gamma(t)} ,$$

where $G(x,t)$ is a real function. According to (2.27) this implies

$$\sum_{n=0}^{\infty} c_n \varphi_n(x-A(t)) \cdot e^{i\frac{S_n(t)}{\hbar}} \stackrel{!}{=} G(x,t)e^{i\gamma(t)}$$

$$\text{with} \quad \varphi_n(x-A(t)) = \frac{1}{(\pi\alpha(t))^{1/4}\sqrt{2^n n!}} H_n\left[\frac{x-A(t)}{\sqrt{\alpha(t)}}\right] e^{-\frac{(x-A(t))^2}{2\alpha(t)}} \quad .$$

The imaginary part of this equation yields

$$\sum_{n=0}^{\infty} c_n \varphi_n(x,t) sin\left[\frac{S_n(t)}{\hbar} - \gamma(t)\right] \stackrel{!}{=} Im\left[G(x,t)\right] = 0 \quad .$$

This condition can only be fulfilled if

$$c_n \cdot \sin\left[\frac{S_n(t)}{\hbar} - \gamma(t)\right] \stackrel{!}{=} 0 \quad \forall n \quad .$$

Since (2.26) leads to different phase factors $S_n(t)$, which can not be constant in t, we conclude that all expansion coefficients but one must be zero.

So the wave packet can only be written as a Papageno function throughout the time evolution if it has initially the shape of a shifted harmonic oscillator eigenfunction φ_n.

In the next two sections we will summarize the characteristic features of uncertainty dynamics for two potentials.

2.3.1 The free particle

If the potential $V(x)$ equals zero the constant of motion $\mathcal{K}$ turns out to be the variance of momentum :

$$\mathcal{K} = (\Delta p)^2 = (\Delta p_0)^2 \quad .$$

With the initial values $(\Delta x)^2_{t=0} = (\Delta x_0)^2$ and $(\Delta_{xp})_{t=0} = \Delta^0_{xp}$ the system of equations (2.12) yields

$$(\Delta x)^2 = (\Delta x_0)^2 + \frac{t^2}{m^2}(\Delta p_0)^2 + \frac{2t}{m}\Delta^0_{xp} \tag{2.28a}$$

$$\Delta_{xp} = \Delta^0_{xp} + \frac{t}{m}(\Delta p_0)^2 \tag{2.28b}$$

The mixed uncertainty is a monotonically increasing function. If $\Delta_{xp}^0 < 0$, the position uncertainty is decreasing until it reaches its minimum at

$$T = -\frac{m\Delta_{xp}^0}{(\Delta p_0)^2} \quad , \tag{2.29}$$

when the mixed uncertainty is zero. For $t > T$ the wave packet is going to spread which is the behavior commonly expected from a free particle wave function. A wave packet that starts with a negative mixed uncertainty reaches its original position uncertainty Δx_0 at $2T$ (see figure 2.2). If the initial wave function belongs to a family of Papageno functions (2.7) with the characteristic properties k, l and is further specified by the parameters b, $a > 0$, the time it takes the position uncertainty to reach its minimum reads

$$T = -\frac{2mak^2b^4}{\hbar(lk + 4a^2k^2b^4)} = -\frac{2ma(\Delta x_0)^4}{\hbar(lk + 4a^2(\Delta x_0)^4)} \quad . \tag{2.30}$$

If the initial wave packet has the shape of a shifted oscillator eigenfunction, we find for the time evolution with regard to the foregoing results for the time dependent parameters in $u_n(x,t)$ (2.25)

$$u_n(x,t) = \varphi_n(x - A(t)) \cdot e^{\frac{ip_0(x-A(t))}{\hbar} + ia(t)(x-A(t))^2} e^{i\frac{S_n(t)}{\hbar}} \tag{2.31a}$$

$$\text{with} \quad \varphi_n(x,t) = \frac{1}{(\pi\alpha(t))^{1/4}\sqrt{2^n n!}} H_n\left[\frac{x - A(t)}{\sqrt{\alpha(t)}}\right] \quad .$$

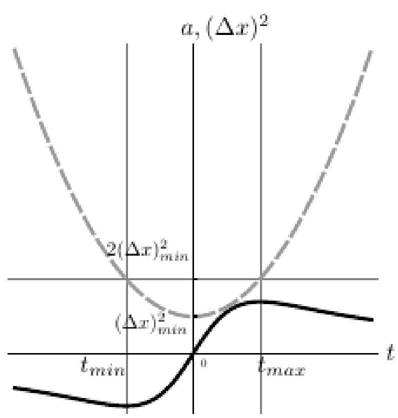


Figure 2.2: The evolution of the position variance for an arbitrary wave packet together with the chirp, in case the wave packet is a shifted harmonic oscillator eigenfunction. The chirp $a(t)$ has a maximum (minimum) at t_{max} (t_{min}) when $(\Delta x)^2$ (dashed line) reaches twice its minimum value $(\Delta x)^2_{min}$.

The parameters $A(t), a(t), \alpha(t)$ are given by

$$A(t) = x_0 + \frac{p_0}{m}\,t\,, \tag{2.31b}$$
$$\alpha(t) = \alpha_0\left\{1 + Q^2\left(1 + 4\alpha_0^2 a_0^2\right) + 4\,Q\,\alpha_0 a_0\right\}\,,$$
$$a(t) = \frac{2\,\alpha_0 a_0 + \,Q\,\left(1 + 4\alpha_0^2 a_0^2\right)}{2\,\alpha(t)}$$
$$\text{where} \quad Q = \frac{t\,\hbar}{m\alpha_0}\,.$$

The phase factor $S_n(t)$ is governed by the equation

$$\dot{S}_n = \frac{p_0^2}{2m} - \frac{\hbar^2}{m\alpha(t)}\left(n + \frac{1}{2}\right) \quad . \tag{2.31c}$$

2.3.2 The harmonic oscillator

The potential

$$V(x) = \frac{m\omega^2}{2}x^2$$

represents a harmonic oscillator with the particle mass m and the angular frequency ω. If we use the variables

$$\mathcal{K} = (\Delta p)^2 + m^2\omega^2(\Delta x)^2 \qquad Z = (\Delta p)^2 - m^2\omega^2(\Delta x)^2 \tag{2.32}$$

instead of $(\Delta x)^2$ and $(\Delta p)^2$ (2.12) yields

$$\mathcal{K} = const. \qquad Z = Z_0\cos(2\omega t) - \Delta_{xp}^0\,2m\omega\sin(2\omega t) \tag{2.33}$$
$$\Delta_{xp} = \Delta_{xp}^0\cos(2\omega t) + \frac{Z_0}{2m\omega}\sin(2\omega t)$$

with the initial values $Z_0 = Z_{t=0}$ and $\Delta_{xp}^0 = (\Delta_{xp})_{t=0}$. So we see that the variable Z and the mixed uncertainty Δ_{xp} oscillate twice as fast as the expectation values of the classical phase space variables and so will the uncertainties (Δx) and (Δp).

For the special initial conditions $Z_0 = \Delta_{xp}^0 = 0$, the mixed uncertainty and the variable Z remain zero for all times. In all other cases, Z has one maximum during the oscillation period $[0, \frac{\pi}{\omega}]$. We find for the maximal value of Z

$$Z_{max} = (Z_0^2 + 4m^2\omega^2(\Delta_{xp}^0)^2)^{1/2} = (\mathcal{K}^2 - 4m^2\omega^2 U)^{1/2} \tag{2.34}$$

where we have used the definitions of $\mathcal{K}, Z$ (2.32) and U (2.15) in the last step. At the time T when Z takes its maximum value, the mixed uncertainty reaches zero. We will now choose T as starting point and therefore make the replacement $\tau = t - T$. So we find for the time evolution of Z

$$Z = (\mathcal{K}^2 - 4m^2\omega^2 U)^{1/2} \cos(2\omega\tau)\,,$$

which yields for the time evolution of uncertainties

$$\begin{aligned} \Delta_{xp} &= \frac{(\mathcal{K}^2 - 4m^2\omega^2 U)^{1/2}}{2m\omega} \sin(2\omega\tau) \\ (\Delta x)^2 &= \frac{1}{2m^2\omega^2} \Big(\mathcal{K} - (\mathcal{K}^2 - 4m^2\omega^2 U)^{1/2} \cos(2\omega\tau) \Big) \\ (\Delta p)^2 &= \frac{1}{2} \Big(\mathcal{K} + (\mathcal{K}^2 - 4m^2\omega^2 U)^{1/2} \cos(2\omega\tau) \Big) \quad . \end{aligned} \tag{2.35}$$

The definitions of U and $\mathcal{K}$ imply

$$\mathcal{K}^2 - 4m^2\omega^2 U \, \geq \, 0 \qquad , \tag{2.36}$$

since

$$\begin{aligned} \mathcal{K}^2 - 4m^2\omega^2 U \; &= \; ((\Delta p)^2 + m^2\omega^2(\Delta x)^2)^2 - 4m^2\omega^2((\Delta p)^2(\Delta x)^2 - (\Delta_{xp})^2) \\ &\geq \; ((\Delta p)^2 + m^2\omega^2(\Delta x)^2)^2 - 4m^2\omega^2(\Delta p)^2(\Delta x)^2 \\ &= ((\Delta p)^2 - m^2\omega^2(\Delta x)^2)^2 \, \geq \, 0 \quad . \end{aligned} \tag{2.37}$$

In particular the initial condition

$$\mathcal{K}^2 - 4m^2\omega^2 U = 0\,, \tag{2.38}$$

is equivalent to

$$\Delta^0_{xp} = 0 \quad \text{and} \quad (\Delta p_0)^2 = m^2\omega^2(\Delta x_0)^2 \quad .$$

In this case the mixed uncertainty continues to be zero and the other two uncertainties remain constant. This corresponds to the special case of wavepackets evolving according to Newton's equations of motion with constant position and momentum uncertainties mentioned in textbooks and introductory quantum mechanics courses. Here we have shown that this special behaviour is not restricted to Gaussian wave packets, but a consequence of appropriate initial uncertainties. For all other initial conditions all three uncertainties will oscillate. When the mixed uncertainty is zero, the wave packet is going spread, if

$$(\Delta x_0)^2 m^2\omega^2/(\Delta p_0) < 1\,,$$

and going to narrow if

$$(\Delta x_0)^2 m^2\omega^2/(\Delta p_0) > 1 \quad ,$$

which can also be seen in figure (2.3) for the special case of a Gaussian wave packet.

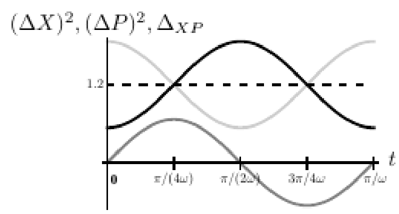


Figure 2.3: The oscillations of $(\Delta X)^2 \equiv (\Delta x)^2 \, \frac{2m\omega}{\hbar}$, $(\Delta P)^2 \equiv (\Delta p)^2 \frac{2}{m\omega\hbar}$ (light-gray) and $(\Delta_{XP}) \equiv (\Delta_{xp}) \frac{2}{\hbar}$ (gray) for a Gaussian wave packet with $\mathcal{K} = 1.2 \, m\omega\hbar$ during one full period.

Chapter 3

The method of Laplace Transforms

The Laplace transform is a useful tool to solve the time-dependent Schrödinger equation if the solution of the stationary equation is known.

The Laplace transformation (see Appendix C) of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\,\psi(x,t) = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \tag{3.1}$$

with respect to time yields

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x,s)}{\partial x^2} + V(x)\,\varphi(x,s) = i\hbar\,s\,\varphi(x,s) - i\hbar\,\psi(x,0) \tag{3.2}$$

where $\varphi(x,t)$ is the Laplace transform of the wavefunction $\psi(x,t)$:

$$\varphi(x,s) = \mathcal{L}(\psi(x,t)) = \int\limits_0^\infty \psi(x,t)e^{-st}dt \quad . \tag{3.3}$$

Here and from now on we always assume that the Laplace transform of the wave function exists which is ensured if the wavefunction does not grow faster than exponentially. Moreover we have used the differentiation rule (C.2) of the Laplace transformation to obtain (3.2).

Equation (3.2) is an inhomogeneous linear ordinary second order differential equation for the Laplace-transformed wavefunction $\varphi(x,s)$. When two linearly independent solutions of the homogeneous equation are known a particular solution of (3.2) can be obtained by the method of variation of constants. With the two homogeneous solutions $u_1(x,s)$ and $u_2(x,s)$ we get the particular solution

$$\varphi_p(x,s) = u_1(x,s) \int\limits_c^x \frac{2mi}{\hbar} \frac{u_2(y,s)}{W[u_1,u_2]} \psi(y,0)\, dy - u_2(x,s) \int\limits_c^x \frac{2mi}{\hbar} \frac{u_1(y,s)}{W[u_1,u_2]} \psi(y,0)\, dy \tag{3.4}$$

Here $W[u_1, u_2]$ is the Wronskian of the two homogeneous solutions:

$$W[u_1,u_2] = \frac{\partial u_1(y,s)}{\partial y} u_2(y,s) - \frac{\partial u_2(y,s)}{\partial y} u_1(y,s) \quad .$$

Therefore the general solution of (3.2) reads

$$\varphi_(x,s) = \varphi_p(x,s) + \alpha(s)\, u_1(x,s) + \beta(s)\, u_2(x,s) \tag{3.5}$$

The functions $\alpha(s)$ and $\beta(s)$ are determined by the boundary conditions on $\varphi(x,s)$, which stem from the physical boundary conditions on the wavefunction $\psi(x,t)$.

Since the homogeneous equation corresponding to (3.2) is just a stationary Schrödinger equation the Laplace transformed solution of the time-dependent Schrödinger equation is easily found when the solution of the stationary equation is known. It is not necessary to identify the eigenvalues. The only technical difficulty is to perform the inverse Laplace transform. In the next chapters we will apply the method to several piecewise constant potentials. We will find that we only need the inverse Laplace transform of very few functions that can be explicitly found in [25].

Chapter 4

The infinite square well

The application of the method of Laplace transforms to the infinite square well leads to the so-called mirror solution for the propagator. With the help of this propagator we will state two theorems which describe the transition from classical to quantum behaviour.

The infinite square well is a physical model system which can be interpreted as the one-dimensional description of a particle confined by infinitely rigid walls. The appropriate potential is $V(x) = 0$ for $0 < x < d$ and $V(x) = \infty$ at $x = 0$ and $x = d$. The dynamics of a wave packet $\psi(x, 0)$, starting at $t = 0$, is therefore determined by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{on} \qquad [0,d] \tag{4.1a}$$

with the boundary conditions

$$\psi(0,t) = \psi(d,t) = 0\,. \tag{4.1b}$$

The energy eigenvalues and the corresponding eigenfunctions read

$$E_n = \frac{\hbar^2\pi^2}{2md^2}\,n^2 \quad \phi_n(x) = \sqrt{\frac{2}{d}}\sin\left(\frac{n\pi x}{d}\right) \quad n = 1,2,3\ldots \quad .$$

Since the second derivative of the energy E_n with respect to n does not depend on n the system possesses a universal revival time (Appendix A,[9])

$$T_{rev} = 4\pi\hbar\left(\frac{d^2E_n}{dn^2}\right)^{-1} = \frac{4md^2}{\hbar\pi} \quad .$$

This means that any solution of the infinite square well fulfills

$$\psi(x,t) = \psi(x, t + T_{rev}) \quad .$$

4.1 The mirror solution

The Laplace transformation of the Schrödinger equation (4.1a) gives

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x,s)}{\partial x^2} = i\hbar\, s\,\varphi(x,s) - i\hbar\,\psi(x,0) \tag{4.2a}$$

with the boundary conditions for the Laplace transformed wave packet

$$\varphi(0,s) = \varphi(d,s) = 0 \quad . \tag{4.2b}$$

The general solution of the homogeneous equation corresponding to (4.2a) is a linear combination of the functions

$$u_1(x,s) = e^{i\sqrt{\frac{2msi}{\hbar}}x} \qquad u_2(x,s) = e^{-i\sqrt{\frac{2msi}{\hbar}}x} \quad .$$

With the Wronskian $W[u_1,u_2] = 2i\sqrt{\frac{2msi}{\hbar}}$ the general solution of (4.2a) reads

$$\varphi(x,s) = \sqrt{\frac{m}{2is\hbar}}\left\{u_1(x,s)\int_0^x u_2(y,s)\psi(y,0)dy \,-\, u_2(x,s)\int_0^x u_1(y,s)\psi(y,0)dy\right\}$$

$$+\,\alpha(s)u_1(x,s) \,+\, \beta(s)u_2(x,s)\ . \tag{4.3}$$

If we impose the boundary conditions (4.2b) we find for $\alpha(s)$ and $\beta(s)$

$$\begin{aligned}
\alpha(s) \;&= \sqrt{\frac{m}{2is\hbar}}\left\{\frac{u_1(d,s)}{u_2(d,s)-u_1(d,s)}\int_0^d u_2(y,s)\psi(y,0)dy\right.\\
&\qquad \left.-\,\frac{u_2(d,s)}{u_2(d,s)-u_1(d,s)}\int_0^d u_1(y,s)\psi(y,0)dy\right\} =\\
&-\sqrt{\frac{m}{2is\hbar}}\int_0^d u_1(y,s)\psi(y,0)dy+\\
&\sqrt{\frac{m}{2is\hbar}}\frac{u_1(d,s)}{u_2(d,s)-u_1(d,s)}\left\{\int_0^d u_2(y,s)\psi(y,0)dy - \int_0^d u_1(y,s)\psi(y,0)dy\right\}\ ,\\
\beta(s) \;&= -\alpha(s) \quad .
\end{aligned}$$

Inserting the result in (4.3) and rewriting the integrals so that each term goes to zero for $s\to\infty$ (which is a necessary condition for the existence of the inverse Laplace transform), we get

$$
\begin{aligned}
\varphi(x,s) = \frac{\kappa}{\sqrt{2is}}\{&\int_0^x e^{(i-1)\kappa\sqrt{s}(x-y)}\psi(y,0)dy \;+\; \int_x^d e^{(i-1)\kappa\sqrt{s}(y-x)}\psi(y,0)dy \\
&- \int_0^d e^{(i-1)\kappa\sqrt{s}(x+y)}\psi(y,0)dy\} + \frac{\kappa}{\sqrt{2i}}\, s\, w(s) \int_0^d \{e^{(i-1)\kappa\sqrt{s}(2d+x+y)} \\
- e^{(i-1)\kappa\sqrt{s}(2d+x-y)} \;+\; & e^{(i-1)\kappa\sqrt{s}(2d-x-y)} \;-\; e^{(i-1)\kappa\sqrt{s}(2d-x+y)}\}\psi(y,0)\, dy
\end{aligned}
\tag{4.4}
$$

where we have used the abbreviation

$$
\kappa = \sqrt{\frac{m}{\hbar}} \tag{4.5}
$$

and $w(s)$ stands for

$$
w(s) = \frac{1}{s^{\frac{3}{2}}(e^{2(i-1)\kappa d\sqrt{s}} - 1)} \qquad .
$$

The inverse Laplace transform of the first three terms in (4.4) can be determined with the formula (also given in Appendix C.3):

$$
\mathcal{L}^{-1}\{\frac{1}{\sqrt{s}}e^{-(1-i)\sqrt{as}}\} = \sqrt{\frac{1}{\pi}}(\frac{e^{\frac{ia}{2t}}}{t^{\frac{1}{2}}}) \qquad \text{where} \qquad a\,>\,0 \tag{4.6}
$$

If we write $w(s)$ as an infinite geometric series

$$
w(s) = \frac{1}{s^{\frac{3}{2}}(e^{2(i-1)\kappa d\sqrt{s}} - 1)} = -\frac{1}{s^{\frac{3}{2}}}\sum_{k=0}^{\infty} e^{2(i-1)d\kappa\sqrt{s}\,k} \tag{4.7}
$$

and insert this in $\varphi(x,s)$ (4.4) we get sums of the form

$$
\sum_{k=0}^{\infty}\varphi_{\alpha\beta}^{k}(x,s) \equiv \sum_{k=0}^{\infty}\sqrt{\frac{\kappa}{2is}}\int_0^d e^{-(1-i)\kappa\sqrt{s}(2d(k+1)+\alpha x+\beta y)}\psi(y)dy \tag{4.8}
$$

where α and β can take the values ±1. The inverse Laplace transform of the terms of (4.8) gives according to (4.6)

$$
\psi_{\alpha\beta}^{k}(x,t) = \frac{\kappa}{\sqrt{2\pi t\, i}}\int_0^d e^{\frac{i\kappa^2(2d(k+1)+\alpha x+\beta y)^2}{2t}}\psi(y)dy \tag{4.9}
$$

We can only be sure that the infinite sum of these terms gives the inverse Laplace transform of $\phi(x,s)$ if the requirements of Theorem C.3 are fulfilled. After a twofold partial integration and taking into account (D.8),(D.11) and the boundary conditions for $\psi(x,t)$ we get the estimation:

$$|\psi^k_{\alpha\beta}(x,t)| \le \frac{1}{a}\left| G^+\left(\frac{az}{2}\right)\psi'(y,0)\Big|_0^d - \int_0^d G^+\left(\frac{az}{2}\right)\psi''(y,0)dy\right|$$

$$\le \frac{C}{a}\sup_{y\in[0,d]}\left|G^+\left(\frac{az}{2}\right)\right| \le \frac{C}{\sqrt{2\pi}a^3(2dk+d+\alpha x)^2} \le \frac{C}{\sqrt{2\pi}}\cdot\frac{1}{(2dk)^2}\cdot\left(\frac{\sqrt{t}}{\kappa}\right)^3 \tag{4.10}$$

where $\quad a = \frac{\kappa}{\sqrt{t}} \qquad z = 2d(k+1)+\alpha x+\beta y$

and $\quad G^+(x) = x\mathrm{Erfc}\left((1-i)x\right) - \frac{e^{2ix^2}}{(1-i)\sqrt{\pi}x}$

Since C is independent of t and k we can conclude that the series of Laplace transforms of $|\hat{\varphi}^k_{\alpha\beta}(x,t)|$ is convergent.

So we can carry out the inverse Laplace transform before the summation of the terms in (4.8)and we finally get for the wave packet

$$\begin{aligned}\psi(x,t) = \frac{\kappa}{\sqrt{2\pi t\, i}}\Bigg(&\int_0^d \{e^{\frac{i(x-y)^2\kappa^2}{2t}} - e^{\frac{i(x+y)^2\kappa^2}{2t}}\}\psi(y,0)dy \\ &+\sum_{k=1}^{\infty}\int_0^d\{e^{\frac{i\kappa^2(2dk+x-y)^2}{2t}} - e^{\frac{i\kappa^2(2dk+x+y)^2}{2t}} \\ &+ e^{\frac{i\kappa^2(2dk-x+y)^2}{2t}} - e^{\frac{i\kappa^2(2dk-x-y)^2}{2t}}\}\psi(y,0)dy\Bigg)\end{aligned} \tag{4.11}$$

This expression is called the mirror solution for the infinite square well since it can also be derived in an argumentative way by the so-called ,method of images' technique, starting with the problem of one infinite wall which acts like a mirror on the wave function [13]. Here however we have derived the solution in a straightforward manner without considerations about the special symmetry of the problem.

4.2 Approximations for the early phase of time evolution

We will now investigate the quantum evolution of families of Papageno functions with certain boundary conditions. We start with wave packets of the form

$$\psi(x) = e^{i\frac{p_0(x-x_0)}{\hbar}}\; e^{ia_0(x-x_0)^2}\left(\frac{1}{\sqrt{b}}\right)F\left(\frac{(x-x_0)}{b}\right) \tag{4.12a}$$

We choose $F(x)$ and the parameters b, x_0 such that $\psi(x)=0$ outside an interval (x_1,x_2) that lies inside the well $(x_1,x_2)\subseteq(0,d)$. In order to fulfill the prerequisites of the following theorems $F(x)$ should be a twice differentiable function that satisfies

$$\int_{x_1}^{x_2} (F(x))^2 = 1\,, \qquad \int_{x_1}^{x_2} x\,(F(x))^2 = 0 \tag{4.12b}$$

The differentiability condition on $F(x)$ then implies also $\psi'(x) = 0$ outside (x_1, x_2).

The application of the mirror solution (4.11) to initial functions of the form (4.12) leads to infinite sums of integrals of the form

$$\begin{aligned}\psi^k_{\alpha\beta} &= \left(\frac{\kappa}{\sqrt{2\pi i t}}\right)\int_0^d (-\alpha\beta) e^{\frac{i\kappa^2(2dk+\alpha x+\beta y)^2}{2t}} e^{i\frac{p_0(y-x_0)}{\hbar}} e^{ia_0(y-x_0)^2}\mathcal{F}(y)dy \\ &= \left(-\frac{\alpha\,\kappa}{2\sqrt{2a_0t+\kappa^2}}\right)\int_0^d e^{\frac{-i(v_0(v_0t+2\beta(2dk+\alpha x+\beta x_0))\kappa^2+2a_0(2dk+\alpha x+\beta x_0)^2)\kappa^2}{2\kappa^2+4a_0t}} \\ &\mathrm{Erfc}\left(\frac{(1-i)((v_0t+\beta(2dk+\alpha x+\beta y))\kappa^2+2a_0t(y-x_0))}{2\beta\sqrt{t}\sqrt{2a_0t+\kappa^2}}\right)\mathcal{F}'(y)dy\,,\end{aligned} \tag{4.13a}$$

where we have used (D.8) and we have made the assumption $t \neq -\frac{\kappa^2}{2a_0}$. For $t = -\frac{\kappa^2}{2a_0}$ we get

$$\begin{aligned}\psi^k_{\alpha\beta} = \left(\frac{\alpha\beta}{i\kappa}\sqrt{\frac{t}{2\pi i}}\right)\int_0^d e^{\frac{i\kappa^2((2dk+\alpha x+\beta x_0)^2-2v_0tx_0-2x_0\beta(2dk+\alpha x+\beta x_0))}{2t}} \\ e^{\frac{i\kappa^2 y(v_0t+(2dk+\alpha x+\beta x_0)\beta)}{t}}\frac{\mathcal{F}'(y)}{(v_0t+(2dk+\alpha x+\beta x_0)\beta)}dy\,.\end{aligned} \tag{4.13b}$$

Here α and β can again take the values ± 1 and we have made the replacements

$$p_0 = mv_0 \qquad \text{and} \qquad \mathcal{F}(x) = \left(\frac{1}{\sqrt{b}}\right)F\left(\frac{(x-x_0)}{b}\right)$$

Further we have used the boundary conditions on $\psi(x)$. The time $t = -\frac{\kappa^2}{2a}$ will turn out to be related to the change from narrowing to spreading behaviour of the particular wavepackets (see the comment at the end of this section). The time evolution of the Papageno functions is then given by

$$\psi(x,t) = \sum_{k=0}^{\infty}\left(\psi^k_{1,-1}+\psi^k_{-1,-1}\right)+\sum_{k=1}^{\infty}\left(\psi^k_{-1,1}+\psi^k_{11}\right) \tag{4.14}$$

Looking at (4.13) we see that if the argument of the complementary error function (respectively the exponent) is large the contribution of the term to the wavefunction will be small. In order to express this more precisely we will state several theorems. We start with a theorem that is appropriate to Papageno functions without chirp.

Theorem 4.1. *Suppose $\psi(x) = e^{ip_0\frac{(x-x_0)}{\hbar}}\mathcal{F}(x)$ is a function with the following properties:*

- *$\psi(x) = 0$ outside the interval $(0, d)$*
- *$\psi(x)$ is twice differentiable*
- *x_0 and $p_0 = mv_0$ are real numbers*

We define $w_2 = \int_0^d |\mathcal{F}''(x)|dx$. Then the time evolution of $\psi(x)$ in an infinite square well of the width d satisfies:

- *For $\quad v_0 > 0 \quad$ and $\quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad$ where $l \,\epsilon\, \mathbb{N},\ 0 \le \epsilon < 2d$*

$$\psi(x,t) = \psi^{l}_{-1-1} + \psi^{l+1}_{-1-1} + \psi^{l+2}_{-1-1} + \psi^{l}_{1-1} + \psi^{l+1}_{1-1} + \delta\psi$$

- *For $\quad v_0 < 0 \quad$ and $\quad t = \frac{2dl}{|v_0|} + \frac{\epsilon}{|v_0|} \quad$ where $l \,\epsilon\, \mathbb{N},\ l > 1,\ 0 \le \epsilon < 2d$*

$$\psi(x,t) = \psi^{l-1}_{11} + \psi^{l}_{11} + \psi^{l+1}_{11} + \psi^{l}_{-11} + \psi^{l+1}_{-11} + \delta\psi$$

- *For $\quad v_0 < 0 \quad$ and $\quad t = \frac{2d}{|v_0|} + \frac{\epsilon}{|v_0|} \quad$ where $0 \le \epsilon < 2d$*

$$\psi(x,t) = \psi^{0}_{-1-1} + \psi^{1}_{-11} + \psi^{2}_{-11} + \psi^{1}_{11} + \psi^{0}_{11} + \delta\psi$$

- *For $\quad v_0 < 0 \quad$ and $\quad t = \frac{\epsilon}{|v_0|} \quad$ where $0 \le \epsilon < 2d$*

$$\psi(x,t) = \psi^{0}_{1-1} + \psi^{1}_{11} + \psi^{1}_{-11} + \psi^{1}_{-1-1} + \psi^{0}_{-1-1} + \delta\psi$$

- *For $\quad v_0 = 0$*

$$\psi(x,t) = \psi^{0}_{-1-1} + \psi^{0}_{1-1} + \psi^{1}_{-1-1} + \delta\psi$$

where

$$|\delta\psi| \le \frac{3\,d\,w_2}{2}\left(\frac{2\,t}{T_{rev}}\right)^{\frac{3}{2}}$$

and T_{rev} denotes the revival time of the infinite square well.

Proof. $v_0 > 0$: Using the abbreviation

$$g^k_{\alpha\beta} = (v_0 t + \beta(2dk + \alpha x + \beta y))\frac{1}{\beta} \tag{4.15}$$

the expressions 4.13a read

$$\psi^k_{\alpha\beta} = (-\frac{\alpha}{2})\int_0^d e^{\frac{-iv_0(v_0 t + 2\beta(2dk+\alpha x+\beta x_0)\kappa^2}{2}}\,\mathrm{Erfc}\left(\frac{(1-i)\kappa}{2\sqrt{t}}g^k_{\alpha\beta}\right)\mathcal{F}'(y)dy$$

We are now going to use the estimation for the complementary error functions for large argument (D.11) given in Appendix D.1. If $g^k_{\alpha\beta} > 0$ for all (x, y) in the interval [0,d] we can apply the formulas directly. But also for $g^k_{\alpha\beta} < 0$ in the whole interval $[0, d]$ we end up with a positive real part of the argument of the complementary error functions inserting $\mathrm{Erfc}(-z) = 2 - \mathrm{Erfc}(z)$ and taking into account the boundary conditions on $\mathcal{F}(x)$. So we have to make sure that we apply the estimation only to terms with positive or negative definite $g^k_{\alpha\beta}$.

At a certain time t, expressed as stated in the theorem, the following inequalities are valid for all (x, y) in the interval $[0, d]$:

$$
\begin{aligned}
g^k_{11} &= 2d(l+k) + \epsilon + x + y \;>\; 2d(l+k) \;>0 \text{ for } k \geq 1 \\
g^k_{-1,1} &= 2d(l+k) + \epsilon - x + y \;>\; d(2(l+k)-1) \;>0 \text{ for } k \geq 1 \\
g^k_{1,-1} &= -(2d(l-k) + \epsilon - x + y) \begin{cases} < \;\; -d(2(l-k)-1) \;<\; 0 & \text{for } k < l \\ > \;\; d(2(k-l)-3) \;>\; 0 & \text{for } k > l+1 \end{cases} \\
g^k_{-1,-1} &= -(2d(l-k) + \epsilon + x + y) \begin{cases} < \;\; -2d(l-k) \;<\; 0 & \text{for } k < l \\ > \;\; d(2(k-l)-4) \;>0 & \text{for } k > l+2\,. \end{cases}
\end{aligned}
\tag{4.16}
$$

We see that all terms $\psi^k_{\alpha\beta}$ which contribute to $\delta\psi$ contain a $g^k_{\alpha\beta}$ which is strictly positive or negative within the interval [0,d]. So we can apply (D.11, D.12) to these $\psi^k_{\alpha\beta}$ where a factor $\gamma = \pm 1$ will ensure that the real part of the argument is positive.

$$
\begin{aligned}
|\psi^k_{\alpha\beta}| &= \left| \frac{1}{2} \int_0^d \mathrm{Erfc}\left(\frac{(1-i)\kappa}{2\sqrt{t}} \gamma g^k_{\alpha\beta} \right) \mathcal{F}'(y) dy \right| = \frac{\sqrt{t}}{\kappa} \left| \int_0^d G^+ \left(\frac{\kappa}{2\sqrt{t}} \gamma g^k_{\alpha\beta} \right) \mathcal{F}''(y) dy \right| < \\
&\sup_{(x,y)\in[0,d]} \left(\frac{1}{|g^k_{\alpha\beta}|^2} \right) \cdot \frac{4t^{\frac{3}{2}}}{\kappa^3} \cdot \frac{1}{4\sqrt{2\pi}} \cdot \int_0^d |\mathcal{F}''(y)| dy \;=\; \sup_{(x,y)\in[0,d]} \left(\frac{1}{|g^k_{\alpha\beta}|^2} \right) \cdot \left(\frac{\sqrt{t}}{\kappa} \right)^3 \cdot \frac{w_2}{\sqrt{2\pi}}
\end{aligned}
\tag{4.17}
$$

Now we can apply this estimation to the sums in 4.14. With the help of 4.16 we get

$$
\begin{aligned}
&|g^k_{11}| \;>\; d\,(1 + 2(k-1)) \quad k : 1 \ldots \infty &&|g^k_{-1,1}| \;>\; d\,(1 + 2(k-1)) \quad k : 1 \ldots \infty \\
&|g^k_{1,-1}| > d\,(1 + 2(l-k-1)) \quad k : 0 \ldots l-1 &&|g^k_{1,-1}| > d\,(1 + 2(k-l-2)) \quad k : l+2 \ldots \infty \\
&|g^k_{-1,-1}| > d\,(1 + 2(l-k-1)) \quad k : 0 \ldots l-1 &&|g^k_{-1,-1}| > d\,(1 + 2(k-l-3)) \quad k : l+3 \ldots \infty
\end{aligned}
\tag{4.18}
$$

$\psi^k_{1,-1}$	describes the free time evolution of the initial wavefunction shifted by $2dk$ to the left.
$\psi^k_{-1,-1}$	describes the free time evolution of the initial wave function wavefunction, mirrored at the axis $x = 0$ and shifted by $2dk$ to the right.
$\psi^k_{-1,1}$	describes the free time evolution of the initial wavefunction shifted by $2dk$ to the right.
ψ^k_{11}	describes the free time evolution of the initial wavefunction, mirrored at the axis $x = 0$ and shifted by $2dk$ to the left.

Table 4.1: Meaning of the terms $\psi^k_{\alpha\beta}$

If we insert these estimations in (4.17) and carry out the summations we get for $\delta\psi$

$$\begin{aligned}
|\delta\psi| &\leq \sum_{k=1}^{\infty} |\psi^k_{11}| + \sum_{k=1}^{\infty} |\psi^k_{-11}| + \sum_{k=0}^{l-1} |\psi^k_{1-1}| + \sum_{k=l+2}^{\infty} |\psi^k_{1-1}| + \sum_{k=0}^{l-1} |\psi^k_{-1-1}| + \sum_{k=l+3}^{\infty} |\psi^k_{-1-1}| \\
&\leq \frac{d\,w_2}{\sqrt{2\pi}} \left(\frac{\sqrt{t}}{\kappa d}\right)^3 \cdot 6 \cdot \sum_{k=1}^{\infty} \frac{1}{(1+2(k-1))^2} = \frac{3\,d\,w_2}{2} \left(\frac{t\,\hbar\,\pi}{2md^2}\right)^{\frac{3}{2}} \\
&= \frac{3\,d\,w_2}{2} \left(\frac{2\,t}{T_{\text{rev}}}\right)^{\frac{3}{2}} \quad \text{with} \quad T_{\text{rev}} = \frac{4md^2}{\hbar\pi} \quad .
\end{aligned}$$

Since the proof of the cases where $v_0 \leq 0$ is analogous we will omit it.

□

In order to make the meaning of the theorem evident we will apply it to Papageno functions with $a = 0$, that fulfill the requirements of the theorem and have position and momentum expectation values x_0 and $p_0 = mv_0$. We start with the interpretation of the terms $\psi^k_{\alpha\beta}$(4.13). Since

$$\psi_{\text{free}}(x,t) = \left(\frac{\kappa}{\sqrt{2\pi i t}}\right) \int_0^d e^{\frac{i\kappa^2(x-y)^2}{2t}} \psi(y)dy$$

describes the free time evolution, these terms can be interpreted as the evolution of the shifted and/or mirrored initial wave function, as explained in table 4.1.

The mirrored wavefunctions have the opposite velocity of the original ones and therefore the corresponding terms clearly describe the wavefunction after an odd number of reflections. According to the shift property the terms with $\beta = -1$ show how the wavefunction with positive start velocity is reflected between the two walls (and vice versa for $\beta = 1$).

In the light of these considerations we will first have a closer look at the results of Theorem 4.1 for the case $v_0 = 0$. The three relevant terms are

$$\psi \sim \ \psi^0_{1,-1} + \psi^0_{-1,-1} + \psi^1_{-1,-1}$$

$\psi^0_{1,-1}$ describes the spreading of the initial wave packet and the terms $\psi^0_{-1,-1}$ and $\psi^1_{-1,-1}$ take into account the reflection at the left and the right wall. If the initial wavefunction is zero in the vicinity of the walls we can further improve the estimations of Theorem 4.1. The arguments of the complementary error functions that correspond to the reflection terms $\psi^0_{-1,-1}$ and $\psi^1_{-1,-1}$ fulfill the following inequalities if y lies in the interval $[x_1, x_2]$:

$$g^0_{-1,-1} = -x - y \geq -x_1 \qquad g^1_{-1,-1} = 2d - x - y \leq d - x_2 \qquad \forall x \in [0, d]$$

For a wavefunction which is zero outside the interval (x_1, x_2) we therefore get with the application of the estimation formula (4.17)

$$\begin{aligned} \left|\psi^0_{-1,-1}\right| &\leq \left(\frac{d}{x_1}\right)^2 \cdot \frac{w_2\, d}{\sqrt{2}\pi^2} \left(\frac{4\,t}{T_{\text{rev}}}\right)^{\frac{3}{2}} \\ \left|\psi^1_{-1,-1}\right| &\leq \left(\frac{d}{d - x_2}\right)^2 \cdot \frac{w_2\, d}{\sqrt{2}\pi^2} \left(\frac{4\,t}{T_{\text{rev}}}\right)^{\frac{3}{2}} . \end{aligned}$$

So we can say that as long as $\delta\psi$ is negligible in the sense of Theorem 4.1 the spreading wavefunction in the infinite square well does not 'feel' the walls if its distance was far enough at the beginning. In this case the dynamics is just the free time evolution described by a single term: $\psi \sim \psi^0_{1-1}$.

If $v_0 > 0$ the relevant terms during a full classical period of the infinite square well are

$$\begin{aligned} &\psi \sim \psi^l_{-1,-1} + \psi^l_{1,-1} + \psi^{l+1}_{-1,-1} + \psi^{l+1}_{1,-1} + \psi^{l+2}_{-1-1} \\ \text{for} \qquad &t \in \left[\frac{2dl}{v_0}, \frac{2d(l+1)}{v_0}\right) \qquad \text{where} \quad l = 0, 1, 2, \ldots \quad . \end{aligned}$$

We will now show that not all terms are relevant during the whole time interval. If we look again at the arguments of the corresponding complementary error functions (4.16), we find that at a time ϵ/v_0 after the beginning of the period at $T = 2d\,l/v_0$ the following inequalities are valid for all $(x, y)\,\epsilon\,[0, d] \times [0, d]$ and for any $\delta > 0$

$$\begin{aligned} &g^l_{-1,-1} < -\delta \quad \text{for} \quad \epsilon > \delta && g^{l+1}_{1,-1} > \delta \quad \text{for} \quad \epsilon < d - \delta \\ &g^l_{1,-1} < -\delta \quad \text{for} \quad \epsilon > d + \delta && g^{l+2}_{-1,-1} > \delta \quad \text{for} \quad \epsilon < 2d - \delta \\ &g^{l+1}_{1,-1} < -\delta \quad \text{for} \quad \epsilon > \delta && \end{aligned}$$

With $2\delta < d$ we get according to (4.17) the relevant terms of ψ during different parts of the whole time period, as given in table 4.2.

time interval	ψ^l_{-1-1}	ψ^l_{1-1}	ψ^{l+1}_{-1-1}	ψ^{l+1}_{1-1}	ψ^{l+2}_{-1-1}
$0 < \epsilon/v_0 < \delta/v_0$	$\surd$	$\surd$	$\surd$	$-$	$-$
$\delta/v_0 < \epsilon/v_0 < (d-\delta)/v_0$	$-$	$\surd$	$\surd$	$-$	$-$
$(d-\delta)/v_0 < \epsilon/v_0 < (d+\delta)/v_0$	$-$	$\surd$	$\surd$	$\surd$	$-$
$(d+\delta)/v_0 < \epsilon/v_0 < (2d-\delta)/v_0$	$-$	$-$	$\surd$	$\surd$	$-$
$(2d-\delta)/v_0 < \epsilon/v_0 < 2d/v_0$	$-$	$-$	$\surd$	$\surd$	$\surd$

Table 4.2: Relevant terms during a classical period

The contribution of each of the neglected terms to the wavefunction is restricted by

$$|\psi^k_{\alpha\beta}| \leq \left(\frac{d}{\delta}\right)^2 \cdot \frac{w_2\, d}{\sqrt{2}\pi^2} \left(\frac{4\,t}{T_{\text{rev}}}\right)^{\frac{3}{2}} \qquad .$$

We can try to describe this result as follows: At the beginning of a period the wavefunction consists of a part representing a particle moving from the left to the right which is the analog of the classical motion, and two additional terms which describe reflections on the walls and represent the previous and the next reflection from the classical point of view. When time proceeds the (previous) reflection on the left wall looses significance and for a certain time interval we end up with two relevant terms, describing wavefunctions before and after the reflection on the right wall. Finally the parts of the wavefunction which were reflected by the right wall already when the period began approach the left wall. So we have to take into account a further reflection on the left wall even before half of the period d/v_0 has passed (etc).

We can restrict the number of relevant terms even further if the distance of the initial wave packet from the walls is far enough. If the initial wavefunction is zero outside the interval (x_1, x_2) and if further $x_1 > \delta$ and $d - x_2 > \delta$, we get the following inequalities, valid for all $(x, y)\,\epsilon\,[0, d] \times [x_1, x_2]$,where ϵ/v_0 indicates again the time after the beginning of the period :

$$g^l_{-1,-1} < -\delta \quad \text{for} \quad \epsilon > 0$$
$$g^l_{1,-1} < -\delta \quad \text{for} \quad \epsilon > d - (x_1 - \delta)$$
$$g^{l+1}_{-1,-1} \begin{cases} > \delta & \text{for} \quad \epsilon < d - (x_2 + \delta) \\ < -\delta & \text{for} \quad \epsilon < 2d - (x_1 - \delta) \end{cases}$$
$$g^{l+1}_{1,-1} > \delta \quad \text{for} \quad \epsilon < 2d - (x_2 + \delta)$$
$$g^{l+2}_{-1,-1} > \delta \quad \text{for} \quad \epsilon < 2d$$

If we neglect all terms which are restricted by

$$|\psi^k_{\alpha\beta}| < \left(\frac{d}{\delta}\right)^2 \cdot \frac{w_2\, d}{\sqrt{2}\pi^2} \left(\frac{4\,t}{T_{\text{rev}}}\right)^{\frac{3}{2}} \qquad .$$

we see that we can omit further two terms during the whole interval according to 4.17. With the additional assumption $d - 2\delta - (x_2 - x_1) > 0$ we finally

time interval	ψ^l_{1-1}	ψ^{l+1}_{-1-1}	ψ^{l+1}_{1-1}
$0 < \epsilon/v_0 < (d-(x_2+\delta))/v_0$	$\surd$	$-$	$-$
$(d-x_2-\delta)/v_0 < \epsilon/v_0 < (d-(x_1-\delta))/v_0$	$\surd$	$\surd$	$-$
$(d-(x_1-\delta))/v_0 < \epsilon/v_0 < (2d-(x_2+\delta))/v_0$	$-$	$\surd$	$-$
$(2d-(x_2+\delta))/v_0 < \epsilon/v_0 < (2d-(x_1-\delta))/v_0$	$-$	$\surd$	$\surd$
$(2d-(x_1-\delta))/v_0 < \epsilon/v_0 < 2d/v_0$	$-$	$-$	$\surd$

Table 4.3: Further restriction of relevant terms

find that the following terms are relevant during different phases of one period (see table 4.3):

So the wavefunction consists of three terms which are the quantum mechanical analog of the three characteristic phases of the movement of a classical particle with positive velocity during a whole period. The particle starts somewhere inside the well and moves from the left to the right until it bumps into the right wall. After the reflection the particle covers the whole distance d until it reaches the left wall. After a second reflection the particle moves again from left to right and finally reaches the starting point with the initial velocity. The dynamics of the wavefunction can be interpreted in a similar way apart from the fact that shortly before and after the moment of classical reflection the terms describing the previous or next phase of movement become respectively stay relevant. The time intervals with two relevant terms both have the width

$$\Delta t = \frac{2\delta + x_2 - x_1}{v_0}\,.$$

Of course Theorem 4.1 can also be applied to Papageno functions with chirp when the chirp factor $e^{ia(x-x_0)^2}$ is included in $\mathcal{F}$. But according to (2.8) only a chirp of order $1/\delta x_0^2$ will produce a relevant contribution to Δp_0. This may cause a factor $w_2 d^{\frac{3}{2}} \gg 1$ which makes the estimation of Theorem 4.1 meaningless. So we will add a theorem which is more appropriate to Papageno functions with chirp.

Theorem 4.2. *Suppose* $\psi(x) = e^{ip_0\frac{(x-x_0)}{\hbar} + ia_0(x-x_0)^2}\mathcal{F}(x)$ *is a function with the following properties*

- $\psi(x) = 0$ *outside the interval* $(x_1, x_2) \subseteq (0, d)$ *with* $x_1 < x_0 < x_2$
- $\psi(x)$ *is twice differentiable*
- $p_0 = mv_0 \geq 0$
- $a_0 \neq 0$ *is real*

We define $w_2 = \int_0^d |\mathcal{F}''(x)|dx$. *Then the time evolution of* $\psi(x)$ *in an infinite square well of the width* d *satisfies:*

- *For* $v_0 > 0\,,\quad 0 < \frac{2a_0(x_0-x_1)}{\kappa^2 v_0} \leq 1$

$$and \quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad where \quad l\,\epsilon\,\mathbb{N}\ ,\ 0 \leq \epsilon < 2d$$

$$\psi(x,t) = \sum_{k=l-N^-_{1-1}}^{k=l+N^+_{1-1}} \psi^k_{1-1} + \sum_{k=l-N^-_{-1-1}}^{k=l+N^+_{-1-1}} \psi^k_{-1-1} + \delta\psi \qquad with$$

$$\begin{aligned}
N^+_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + \tfrac{3}{2} + \tfrac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)\right\}\\
N^+_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + 2 + \tfrac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)\right\}\\
N^-_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + 1 + \tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0}\, l\right\}\\
N^-_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + \tfrac{1}{2} + \tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0}\, l\right\}
\end{aligned}$$

- *For* $v_0 > 0\,,\quad 1 < \frac{2a_0(x_0-x_1)}{\kappa^2 v_0}$

$$and \quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad where \quad l\,\epsilon\,\mathbb{N}\ ,\ 0 \leq \epsilon < 2d$$

$$\psi(x,t) = \sum_{k=l-N^-_{1-1}}^{k=l+N^+_{1-1}} \psi^k_{1-1} + \sum_{k=l-N^-_{-1-1}}^{k=l+N^+_{-1-1}} \psi^k_{-1-1} + \sum_{k=1}^{k=N_{11}} \psi^k_{11} + \sum_{k=1}^{k=N_{-11}} \psi^k_{-11} + \delta\psi \qquad with$$

$$\begin{aligned}
N^+_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + \tfrac{3}{2} + \tfrac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)\right\}\\
N^+_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + 2 + \tfrac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)\right\}\\
N^-_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + \tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0}\,(1+l)\right\}\\
N^-_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} - \tfrac{1}{2} + \tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0}\,(1+l)\right\}\\
N_{11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + \tfrac{1}{2} + (\tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0} - 1)\,(1+l)\right\}\\
N_{-11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + 1 + (\tfrac{2a_0(x_0-x_1)}{\kappa^2 v_0} - 1)\,(1+l)\right\}
\end{aligned}$$

- *For* $v_0 > 0\,,\quad a_0 < 0\,,\quad t \leq \left|\frac{\kappa^2}{2a_0}\right|$

$$and \quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad where \quad l\,\epsilon\,\mathbb{N}\ ,\ 0 \leq \epsilon < 2d$$

$$\psi(x,t) = \psi^l_{-1-1} + \psi^{l+1}_{-1-1} + \psi^{l+2}_{-1-1} + \psi^l_{1-1} + \psi^{l+1}_{1-1} + \delta\psi$$

- *For* $\quad v_0 > 0\,, \quad -1 \leq \frac{2a_0(x_2-x_0)}{\kappa^2 v_0} < 0\,, \quad t > \left|\frac{\kappa^2}{2a_0}\right|$

$$and \quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad where \quad l\,\epsilon\,\mathbb{N}\ ,\ 0 \leq \epsilon < 2d$$

$$\psi(x,t) = \sum_{k=l-N^-_{1-1}}^{k=l+N^+_{1-1}} \psi^k_{1-1} + \sum_{k=l-N^-_{-1-1}}^{k=l+N^+_{-1-1}} \psi^k_{-1-1} + \delta\psi \qquad with$$

$$\begin{aligned}
N^+_{1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < \tfrac{x_1}{2d} + \tfrac{3}{2} + \tfrac{2|a_0|(x_0-x_1)}{\kappa^2 v_0}(l+1) \right\} \\
N^+_{-1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < \tfrac{x_1}{2d} + 2 + \tfrac{2|a_0|(x_0-x_1)}{\kappa^2 v_0}(l+1) \right\} \\
N^-_{1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} + 1 + \tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0}\, l \right\} \\
N^-_{-1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} + \tfrac{1}{2} + \tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0}\, l \right\}
\end{aligned}$$

- *For* $\quad v_0 > 0\,, \quad \frac{2a_0(x_2-x_0)}{\kappa^2 v_0} < -1\,, \quad t > \left|\frac{\kappa^2}{2a_0}\right|$

$$and \quad t = \frac{2dl}{v_0} + \frac{\epsilon}{v_0} \quad where \quad l\,\epsilon\,\mathbb{N}\ ,\ 0 \leq \epsilon < 2d$$

$$\psi(x,t) = \sum_{k=l-N^-_{1-1}}^{k=l+N^+_{1-1}} \psi^k_{1-1} + \sum_{k=l-N^-_{-1-1}}^{k=l+N^+_{-1-1}} \psi^k_{-1-1} + \sum_{k=1}^{k=N_{11}} \psi^k_{11} + \sum_{k=1}^{k=N_{-11}} \psi^k_{-11} + \delta\psi \qquad with$$

$$\begin{aligned}
N^+_{1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < \tfrac{x_1}{2d} + \tfrac{3}{2} + \tfrac{2|a_0|(x_0-x_1)}{\kappa^2 v_0}(l+1) \right\} \\
N^+_{-1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < \tfrac{x_1}{2d} + 2 + \tfrac{2|a_0|(x_0-x_1)}{\kappa^2 v_0}(l+1) \right\} \\
N^-_{1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} + \tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0}\,(1+l) \right\} \\
N^-_{-1-1} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} - \tfrac{1}{2} + \tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0}\,(1+l) \right\} \\
N_{11} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} + \tfrac{1}{2} + (\tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0} - 1)\,(1+l) \right\} \\
N_{-11} &= \sup_{n\in\mathbb{N}} \left\{ n < -\tfrac{x_2}{2d} + 1 + (\tfrac{2|a_0|(x_2-x_0)}{\kappa^2 v_0} - 1)\,(1+l) \right\}
\end{aligned}$$

- *For* $\quad v_0 = 0\,, \quad a_0 > 0$

$$\psi(x,t) = \sum_{k=0}^{k=N_{1-1}} \psi^k_{1-1} + \sum_{k=0}^{k=N_{-1-1}} \psi^k_{-1-1} + \sum_{k=1}^{k=N_{11}} \psi^k_{11} + \sum_{k=1}^{k=N_{-11}} \psi^k_{-11} + \delta\psi \qquad with$$

$$
\begin{aligned}
N_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + \tfrac{1}{2} + \tfrac{a_0 t(x_2-x_0)}{\kappa^2 d}\right\}\\
N_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_2}{2d} + 1 + \tfrac{a_0 t(x_2-x_0)}{\kappa^2 d}\right\}\\
N_{11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + \tfrac{1}{2} + \tfrac{a_0 t(x_0-x_1)}{\kappa^2 d}\right\}\\
N_{-11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_1}{2d} + 1 + \tfrac{a_0 t(x_0-x_1)}{\kappa^2 d}\right\}
\end{aligned}
$$

- *For* $v_0 = 0\,,\quad a_0 < 0\,,\quad t < \left|\frac{\kappa^2}{2a_0}\right|$

$$\psi(x,t) = \psi^0_{-1-1} + \psi^1_{-1-1} + \psi^0_{1-1} + \delta\psi$$

- *For* $v_0 = 0\,,\quad a_0 < 0\,,\quad t > \left|\frac{\kappa^2}{2a}\right|$

$$\psi(x,t) = \sum_{k=0}^{k=N_{1-1}} \psi^k_{1-1} + \sum_{k=0}^{k=N_{-1-1}} \psi^k_{-1-1} + \sum_{k=1}^{k=N_{11}} \psi^k_{11} + \sum_{k=1}^{k=N_{-11}} \psi^k_{-11} + \delta\psi \qquad \textit{with}$$

$$
\begin{aligned}
N_{1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_1}{2d} + \tfrac{1}{2} + \tfrac{|a_0| t(x_0-x_1)}{\kappa^2 d}\right\}\\
N_{-1-1} &= \sup_{n\in\mathbb{N}}\left\{n < \tfrac{x_1}{2d} + 1 + \tfrac{|a_0| t(x_0-x_1)}{\kappa^2 d}\right\}\\
N_{11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_2}{2d} + \tfrac{1}{2} + \tfrac{|a_0| t(x_2-x_0)}{\kappa^2 d}\right\}\\
N_{-11} &= \sup_{n\in\mathbb{N}}\left\{n < -\tfrac{x_2}{2d} + 1 + \tfrac{|a_0| t(x_2-x_0)}{\kappa^2 d}\right\}
\end{aligned}
$$

where

$$|\delta\psi| \leq \frac{3\,d\,w_2}{2}\left(\frac{2\,t}{T_{rev}}\right)^{\frac{3}{2}}$$

when T_{rev} denotes the revival time of the infinite square well.

Proof. We proceed similar as in the proof of Theorem 4.1 Using the abbreviations

$$
\begin{aligned}
g^k_{\alpha\beta} &= \left(\tfrac{2a_0 t(y-x_0)}{\kappa^2} + v_0 t + \beta(2dk + \alpha x + \beta y)\right)\tfrac{1}{\beta}\\
r &= \tfrac{\kappa^2}{2\sqrt{2a_0 t+\kappa^2}\sqrt{t}}
\end{aligned}
\tag{4.19}
$$

the expressions (4.13) read

$$\left|\psi^k_{\alpha\beta}\right| = \left|\frac{\kappa}{2\sqrt{2a_0 t+\kappa^2}}\int_{x_1}^{x_2} \mathrm{Erfc}\left((1-i)\,\gamma\,r\,g^k_{\alpha\beta}\right)\mathcal{F}'(y)dy\right| \quad \text{for} \quad t \neq -\frac{\kappa^2}{2a_0} \tag{4.20a}$$

and

$$\left|\psi^k_{\alpha\beta}\right| = \left|\left(\frac{\alpha\beta}{\kappa}\sqrt{\frac{t}{2\pi}}\right)\int_{x_1}^{x_2} e^{\left\{\frac{i\beta\kappa^2}{t}g^k_{\alpha\beta}y\right\}}\cdot\frac{\mathcal{F}'(y)}{g^k_{\alpha\beta}}dy\right| \quad \text{for} \quad t = -\frac{\kappa^2}{2a_0}\,. \tag{4.20b}$$

Since r can become imaginary for $a_0 < 0$, the argument of the error function will lie on one of the diagonals of the complex plane. For those $g^k_{\alpha\beta}$ that are positive or negative definite on the interval

$$I \equiv [0,d] \times [x_1, x_2]\,,$$

we will choose the factor $\gamma = \pm 1$ in order to ensure that the real part of the complementary error function is positive. Then we find according to the boundary conditions and with the help of (D.11, D.12) :

$$\begin{aligned}
&\left|\psi^k_{\alpha\beta}\right| = \left| \frac{\kappa}{2\sqrt{2a_0 t + \kappa^2}} \int_{x_1}^{x_2} \frac{G^{\pm}(|r\, g^k_{\alpha\beta}|)}{r} \left(\frac{\partial g^k_{\alpha\beta}}{\partial y} \right)^{-1} \mathcal{F}''(y) dy \right| \leq \\
&\sup_{(x,y)\in I} \left(\frac{1}{|g^k_{\alpha\beta}|^2} \right) \cdot w_2 \cdot \left| \frac{\kappa^3}{2(2a_0 t + \kappa^2)^{\frac{3}{2}}} \frac{1}{r^3} \right| \cdot \frac{1}{4\sqrt{2\pi}} = \\
&\sup_{(x,y)\in I} \left(\frac{1}{|g^k_{\alpha\beta}|^2} \right) \cdot \left(\frac{\sqrt{t}}{\kappa} \right)^3 \cdot \frac{w_2}{\sqrt{2\pi}} \quad \text{for} \quad t \neq -\frac{\kappa^2}{2a_0}\,, \quad \text{and} \qquad (4.21a) \\
&\left|\psi^k_{\alpha\beta}\right| \leq \sup_{(x,y)\in I} \left(\frac{1}{|g^k_{\alpha\beta}|^2} \right) \cdot \left(\frac{\sqrt{t}}{\kappa} \right)^3 \cdot \frac{w_2}{\sqrt{2\pi}} \quad \text{for} \quad t = -\frac{\kappa^2}{2a_0} \quad \text{respectively.} \qquad (4.21b)
\end{aligned}$$

In the case of (4.20b) $g^k_{\alpha\beta}$ does not depend on y and therefore plays just the role of a factor.

Now we have to make sure that the sum of the terms $\psi^k_{\alpha\beta}$ belonging to $\delta\psi$ fulfills the statement of the theorem.

- For $v_0 > 0$, $0 < \frac{2a_0(x_0 - x_1)}{\kappa^2 v_0} \leq 1$

  we find at a certain time t, expressed like stated in the theorem and for all $(x,y) \in [0,d] \times [x_1, x_2]$:

$$\begin{aligned}
g^k_{\pm 11} &\geq g^k_{\pm 11}(y = x_1, \epsilon = 0) \\
g^k_{\pm 1-1} &\geq g^k_{\pm 1-1}(y = x_2, \epsilon = 2d) \\
g^k_{\pm 1-1} &\leq g^k_{\pm 1-1}(y = x_1, \epsilon = 0)
\end{aligned}$$

This yields the following estimations for the terms contained in $\delta\psi$

$$\begin{array}{llll}
g^k_{11} & \geq & 2d\left(\left(1-\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}\right)l+k\right)+x_1 \geq 2dk & k:1....\infty \\
g^k_{-11} & \geq & 2d\left(\left(1-\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}\right)l+k-\frac{1}{2}\right)+x_1 \geq d(1+2(k-1)) & k:1....\infty \\
g^k_{1-1} & \geq & 2d\left\{k-l-\left(\frac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)+\frac{x_2}{2d}+1\right)\right\} & \\
 & \geq & d(1+2(k-l-N^+_{1-1}-1)) & k:l+N^+_{1-1}+1...\infty \\
g^k_{-1-1} & \geq & 2d\left\{k-l-\left(\frac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)+\frac{x_2}{2d}+\frac{3}{2}\right)\right\} & \\
 & \geq & d(1+2(k-l-N^+_{-1-1}-1)) & k:l+N^+_{-1-1}+1...\infty \\
g^k_{1-1} & \leq & -2d\left\{l-k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}l-\frac{x_1}{2d}+\frac{1}{2}\right)\right\} & \\
 & \leq & -d(1+2(l-k-N^-_{1-1}-1)) & k:0....l-N^-_{1-1}-1 \\
g^k_{-1-1} & \leq & -2d\left\{l-k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}l-\frac{x_1}{2d}\right)\right\} & \\
 & \leq & -d(1+2(l-k-N^-_{-1-1}-1)) & k:0....l-N^-_{-1-1}-1
\end{array}$$

where the expressions $N^+_{1-1}, N^+_{-1-1}, N^-_{1-1}, N^-_{-1-1}$ are defined like stated in the theorem.

- For $v_0 > 0$, $1 < \frac{2a_0(x_0-x_1)}{\kappa^2 v_0}$

  the corresponding inequalities read:

$$\begin{array}{rcl}
g^k_{\pm 11} & \geq & g^k_{\pm 11}(y=x_1, \epsilon=2d) \\
g^k_{\pm 1-1} & \geq & g^k_{\pm 1-1}(y=x_2, \epsilon=2d) \\
g^k_{\pm 1-1} & \leq & g^k_{\pm 1-1}(y=x_1, \epsilon=2d)
\end{array}$$

This yields the following estimations for the terms contained in $\delta\psi$

$$\begin{array}{llll}
g^k_{11} & \geq & 2d\left(k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}-1\right)(l+1)+\frac{x_1}{2d}\right) & \\
 & \geq & d(1+2(k-N_{11}-1)) & k:N_{11}+1...\infty \\
g^k_{-11} & \geq & 2d\left(k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}-1\right)(l+1)+\frac{x_1}{2d}-\frac{1}{2}\right) & \\
 & \geq & d(1+2(k-N_{-11}-1)) & k:N_{11}+1...\infty \\
g^k_{1-1} & \geq & 2d\left\{k-l-\left(\frac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)+\frac{x_2}{2d}+1\right)\right\} & \\
 & \geq & d(1+2(k-l-N^+_{1-1}-1)) & k:l+N^+_{1-1}+1...\infty \\
g^k_{-1-1} & \geq & 2d\left\{k-l-\left(\frac{2a_0(x_2-x_0)}{\kappa^2 v_0}(l+1)+\frac{x_2}{2d}+\frac{3}{2}\right)\right\} & \\
 & \geq & d(1+2(k-l-N^+_{-1-1}-1)) & k:l+N^+_{-1-1}+1...\infty \\
g^k_{1-1} & \leq & -2d\left\{l-k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}(l+1)-\frac{x_1}{2d}-\frac{1}{2}\right)\right\} & \\
 & \leq & -d(1+2(l-k-N^-_{1-1}-1)) & k:0....l-N^-_{1-1}-1 \\
g^k_{-1-1} & \leq & -2d\left\{l-k-\left(\frac{2a_0(x_0-x_1)}{\kappa^2 v_0}(l+1)-\frac{x_1}{2d}-1\right)\right\} & \\
 & \leq & -d(1+2(l-k-N^-_{-1-1}-1)) & k:0....l-N^-_{-1-1}-1
\end{array}$$

where the expressions $N^+_{1-1}, N^+_{-1-1}, N^-_{1-1}, N^-_{-1-1}, N_{11}, N_{-11}$ are defined like stated in the theorem.

- For $v_0 > 0$, $a_0 < 0, t < \left|\frac{2a}{\kappa^2}\right|$

  we find at a certain time t, expressed like stated in the theorem and for all $(x, y) \in [0, d] \times [x_1, x_2]$:

$$\begin{array}{lclcl} g^k_{\pm 11} & \geq & g^k_{\pm 11}(y = x_1) & \geq & g^k_{\pm 11}(y = x_1, a_0 = 0) \\ g^k_{\pm 1-1} & \geq & g^k_{\pm 1-1}(y = x_2) & \geq & g^k_{\pm 11}(y = x_2, a_0 = 0) \\ g^k_{\pm 1-1} & \leq & g^k_{\pm 1-1}(y = x_1) & \leq & g^k_{\pm 11}(y = x_1, a_0 = 0) \end{array}$$

  These inequalities lead to the same estimations for $g^k_{\alpha\beta}$ as stated in the proof of Theorem 4.1 (4.18).

Since the estimations for the remaining cases work analogous we will omit them. We finally get the result for $|\delta\psi|$ by summing up the relevant terms using (4.17) and inserting the estimations for $g^k_{\alpha\beta}$. We get for all cases

$$|\delta\psi| < \sum_{k=N_{11}+1}^{\infty} |\psi^k_{11}| + \sum_{k=N_{-11}+1}^{\infty} |\psi^k_{-11}| + \sum_{k=0}^{l-1-N^-_{1-1}} |\psi^k_{1-1}| +$$

$$\sum_{k=l+1+N^+_{1,-1}}^{\infty} |\psi^k_{1-1}| + \sum_{k=0}^{l-1-N^-_{-1-1}} |\psi^k_{-1-1}| + \sum_{k=l+1+N^+_{-1-1}}^{\infty} |\psi^k_{-1-1}|$$

$$\leq \frac{d\, w_2}{\sqrt{2\pi}} \left(\frac{\sqrt{t}}{\kappa d}\right)^3 \cdot 6 \cdot \sum_{k=1}^{\infty} \frac{1}{(1+2(k-1))^2} = \frac{3\, d\, w_2}{2} \left(\frac{t\, \hbar\, \pi}{2md^2}\right)^{\frac{3}{2}} = \frac{3\, d\, w_2}{2} \left(\frac{2\, t}{T_{rev}}\right)^{\frac{3}{2}}$$

$$\text{with} \quad T_{rev} = \frac{4md^2}{\hbar\pi}$$

where $N_{\pm 11} = 0$ for: $v_0 > 0, 0 < \frac{2a_0(x_0 - x_1)}{\kappa^2 v_0} \leq 1$ and $v_0 > 0, -1 \leq \frac{2a_0(x_2 - x_0)}{\kappa^2 v_0} < 0$.

$\square$

Note that for negative a_0 and $t \leq t_G = \frac{m}{2\hbar|a_0|}$, the relevant terms reduce to those already singled out for the case $a = 0$ by Theorem 4.1. This time is always larger than the time T (2.30) it takes the individual terms $\psi^k_{\alpha\beta}$, which evolve as free particle wave functions to change from narrowing to spreading behaviour:

$$T = \frac{2m|a_0|(\Delta x_0)^4}{\hbar(lk + 4a_0^2(\Delta x_0)^4)} < \frac{m}{2\hbar|a_0|} = t_G \quad . \tag{4.22}$$

4.3 Summary and discussion of the literature

We have derived the mirror solution of the infinite square well (4.11) in a straight forward way, using the method of Laplace transforms, without referring to the special symmetry of the infinite square well.

The theorems 4.1, 4.2 point out that at a certain stage of time evolution in the infinite square well, only a certain amount of terms of the mirror solution (4.11)is relevant. The discussion of theorem 4.1 shows that the reflection of a sufficiently peaked, uncorrelated Papageno function with nonzero start velocity at one of the walls is described by two terms (see table 4.3)that coincide with the exact solution for a wave packet reflected at a single infinite wall. This reflection was investigated for Gaussian wave packets in ([14],[15]). The wave packets are slowed down when they are approaching the wall. And even a wave packet that is initially at rest feels a repulsing force from a nearby wall (see [16]). This corresponds to the relevance of the terms $\psi^0_{1,-1}, \psi^1_{-1,-1}$ according to theorem 4.1 for Papageno functions with zero start velocity.

As time progresses the estimations of the two theorems loose significance. They become meaningless at the latest when the time comes close to the revival time, maybe already earlier depending on the magnitude of $w_2 = \int_0^d |\mathcal{F}''(x)| dx$. The decreasing relevance of the estimations is caused by the spreading of the particular wave packets. This is also an explanation for the higher number of terms in theorem 4.2, since a positive chirp implies a faster growing position uncertainty (2.28a). A numerical investigation of the dynamics of an uncorrelated wave packet in the infinite square well can be found in [17], which also shows that the wave packet is slowed down, when it approaches the wall. This is a further confirmation of the contents of the two theorems: In the semiclassical time range and for sufficiently peaked initial wave packets the dynamics of a wave packet within the infinite square well can be reduced to the much simpler problem of the dynamics near an infinite wall.

Chapter 5

The potential step

We solve the initial value problem of the potential step. We investigate the dynamics of wavepackets with energies beyond and beneath the energy of the step.

Our next model system is the potential step, described by the potential

$$\begin{array}{lll} V(x) = 0 & \text{for} & x < 0 \\ V(x) = V & \text{for} & x \geq 0 \quad . \end{array}$$

The evolution of the wave packet $\psi(x,0)$, is determined by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad x < 0 \tag{5.1}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad x \geq 0\,, \tag{5.2}$$

where $\psi(x,t)$ is supposed to be continuously differentiable. The solution will be square integrable for all times, if the initial function is chosen square integrable. We will from now on only consider initial wave packets that are located left of the potential step

$$\psi(x,0) = 0 \qquad \text{for} \qquad x \geq 0\,.$$

According to our method, we find for the Laplace transformed wave packet $\varphi(x,s)$

$$\varphi(x,s) = \sqrt{\frac{m}{2is\hbar}} \left\{ u_1(x,s) \int_{-\infty}^{x} u_2(y,s)\psi(y,0)dy - \quad u_2(x,s) \int_{-\infty}^{x} u_1(y,s)\psi(y,0)dy \right\}$$

$$+ \ \alpha(s)u_1(x,s) \ + \ \beta(s)u_2(x,s) \qquad \text{for} \quad x \ < \ 0 \tag{5.3a}$$

$$\varphi(x,s) = \gamma(s)u_3(x,s) \ + \ \delta(s)u_4(x,s) \qquad \text{for} \quad x \ > \ 0 \quad , \tag{5.3b}$$

where

$$u_1(x,s) = e^{i\sqrt{\frac{2msi}{\hbar}}x} \qquad u_3(x,s) = e^{i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x} \tag{5.4a}$$

$$u_2(x,s) = e^{-i\sqrt{\frac{2msi}{\hbar}}x} \qquad u_4(x,s) = e^{-i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x}\,. \tag{5.4b}$$

Since $\psi(x,t)$ must be square integrable, $\varphi(x,s)$ must vanish for $x \to \pm\infty$. We get

$$\alpha(s) = \delta(s) = 0\,.$$

Furthermore $\varphi(x,s)$ should be continuously differentiable at $x = 0$ which determines the functions $\beta(s)$ and $\gamma(s)$:

$$\gamma(s) = \sqrt{\frac{m}{2si\hbar}} \int_{-\infty}^{0} u_2(y,s)\psi(y,0)dy \cdot \frac{2}{1+\sqrt{1-\frac{V}{\hbar si}}} \tag{5.5a}$$

$$\beta(s) = \sqrt{\frac{m}{2si\hbar}} \int_{-\infty}^{0} u_2(y,s)\psi(y,0)dy \cdot \left(\frac{2}{1+\sqrt{1-\frac{V}{\hbar si}}} - 1 \right) + \sqrt{\frac{m}{2si\hbar}} \int_{-\infty}^{0} u_1(y,s)\psi(y,0)dy\,. \tag{5.5b}$$

This yields for the Laplace transformed wave packet $\varphi(x,s)$ (5.3)

$$\varphi(x,s) = \sqrt{\frac{m}{2si\hbar}} \left\{ \int_{-\infty}^{0} e^{i\sqrt{\frac{2msi}{\hbar}}|x-y|}\psi(y,0)dy + \int_{-\infty}^{0} e^{-i\sqrt{\frac{2msi}{\hbar}}(x+y)}\psi(y,0)dy \cdot \rho(s) \right\}$$

$$\text{for} \quad x \ < \ 0 \tag{5.6a}$$

$$\varphi(x,s) = \sqrt{\frac{m}{2si\hbar}} \int_{-\infty}^{0} e^{i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x} e^{-i\sqrt{\frac{2msi}{\hbar}}y}\psi(y,0)dy \cdot (\rho(s)+1)$$

$$\text{for} \quad x \ > \ 0\,, \tag{5.6b}$$

where

$$\rho(s) = \frac{2}{1+\sqrt{1-\frac{V}{\hbar si}}} - 1\,. \tag{5.7}$$

5.1 Solution for $x < 0$

The inverse Laplace transform of (5.7) (see Appendix C.3) is

$$\mathcal{L}^{-1}\{\rho(s)\} = r(t) = \frac{1}{ti} J_1\left[\frac{Vt}{2\hbar}\right] e^{\frac{-iVt}{2\hbar}}\,, \tag{5.8}$$

where $J_1(x)$ denotes the Bessel function. Applying the convolution theorem C.2 we find for the inverse Laplace transform of the wave packet (5.6a) in the region $x < 0$

$$\psi(x,t) = \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy + \int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\, i}} \int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2(t-\tau)}} \psi(y,0) r(\tau) dy\, d\tau\,, \tag{5.9}$$

where we have applied (4.6,4.5). The first term describes the free time evolution of the wave packet $\psi(x,0)$. The second term represents the reflected wave packet and has the form of a wavepacket reflected at an infinite wall, deformed by a convolution.

If we use the momentum representation

$$f(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,0) e^{\frac{-ipx}{\hbar}} dx\,, \tag{5.10}$$

we can rewrite the convolution integral in (5.9) as

$$\int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\, i}} \int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2(t-\tau)}} \psi(y,0)dy\, r(\tau)d\tau = \tag{5.11}$$

$$\int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\, i}} \int_{-\infty}^{\infty} e^{\frac{i(x+y)^2\kappa^2}{2(t-\tau)}} \psi(y,0)dy\, r(\tau)d\tau = \tag{5.12}$$

$$\int_0^t \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} f(p)dp\, r(\tau)d\tau = \tag{5.13}$$

$$\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} e^{-\frac{ip^2 t}{2m\hbar}} f(p)R(p,t)dp\,, \tag{5.14}$$

where

$$R(p,t) = \int_0^t e^{\frac{ip^2\tau}{2m\hbar} - \frac{iV\tau}{2\hbar}} J_1\left[\frac{V\tau}{2\hbar}\right] \frac{d\tau}{\tau i}\,.$$

We will approximate this function by

$$R(p,t) \approx R(p) \equiv \int_0^{\infty} e^{\frac{ip^2\tau}{2m\hbar} - \frac{iV\tau}{2\hbar}} J_1\left[\frac{V\tau}{2\hbar}\right] \frac{d\tau}{\tau i}\,. \tag{5.15}$$

Since the Bessel function fulfills

$$\left| J_1\left[\frac{Vt}{2\hbar}\right]\frac{1}{t}\right| \leq \frac{2\hbar}{V}\frac{1}{t^{3/2}}$$

the additional part of the integral

$$\left|\int_t^\infty e^{\frac{ip^2\tau}{2m\hbar}-\frac{iV\tau}{2\hbar}} J_1\left[\frac{Vt}{2\hbar}\right]\frac{d\tau}{\tau i}\right| \leq \int_t^\infty \sqrt{\frac{2\hbar}{V}}\frac{1}{\tau^{3/2}}d\tau = 2\sqrt{\frac{2\hbar}{Vt}}$$

does hardly contribute, if

$$t \gg \frac{\hbar}{V}\,,$$

and can therefore be neglected after a very short time. Moreover, if the initial function is reasonably peaked the second term of (5.9) does not become relevant until the wave packet approaches the barrier. So the approximation can always be used when

$$t_R \gg \frac{\hbar}{V}\,,$$

where t_R is the time, a classical particle corresponding to the wave packet would need to reach the barrier.

The solution for the region $x < 0$, then reads

$$\begin{aligned}\psi(x,t) \approx \frac{\kappa}{\sqrt{2\pi t\, i}}\int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}}\psi(y,0)dy + \\ \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} e^{-\frac{ip^2t}{2m\hbar}} f(p)R(p)dp\,.\end{aligned} \tag{5.16}$$

Since the integral (5.15) is itself a Laplace integral, we can apply (5.8) and find for $R(p)$

$$R(p) = \rho\left[-\frac{ip^2}{2m\hbar}\right] = -1 + 2k - 2\sqrt{k(k-1)} \quad \text{with} \quad k = \frac{p^2}{2mV}\,. \tag{5.17}$$

This function coincides with the reflection coefficient of the time independent solution (see for instance [18]).

5.2 Solution for $x > 0$

In order to determine the inverse Laplace transform of (5.6b) we use the momentum representation of $\psi(x,0)$. This yields for the integral

$$\sqrt{\frac{m}{2si\hbar}}\int_{-\infty}^{0} e^{i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x} e^{-i\sqrt{\frac{2msi}{\hbar}}y}\psi(y,0)dy = \tag{5.18}$$

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x}\sqrt{\frac{m}{2si\hbar}}\int_{-\infty}^{\infty} e^{\frac{ipy}{\hbar}} e^{i\sqrt{\frac{2msi}{\hbar}}|y|}dyf(p)dp = \tag{5.19}$$

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{i\sqrt{\frac{2msi}{\hbar}-\frac{2mV}{\hbar^2}}x}\frac{1}{s+\frac{ip^2}{2m\hbar}}\, f(p)dp\,. \tag{5.20}$$

Using the scaling property of the Laplace transform (see table C.1) and the formula given in Appendix C.3, we obtain

$$\mathcal{L}^{-1}\left\{2(s+b+c)^{-1}e^{-\sqrt{a(s+c)}}\right\} =$$
$$e^{-ct-bt}\left\{e^{-i\sqrt{ab}}\mathrm{Erfc}\left[\sqrt{\frac{a}{4t}}-i\sqrt{bt}\right]+e^{i\sqrt{ab}}\mathrm{Erfc}\left[\sqrt{\frac{a}{4t}}+i\sqrt{bt}\right]\right\}\,.$$

We find with

$$a=-\frac{2mi}{\hbar}x^2\,,\quad b=\frac{i}{2m\hbar}\left(p^2-2mV\right)\,,\quad c=\frac{iV}{\hbar}$$

for the inverse Laplace transform of the wave packet (5.6b) in the region $x > 0$

$$\psi(x,t)=\int_{-\infty}^{\infty}K\left(x,p,t\right)f(p)\,dp+\int_0^t\int_{-\infty}^{\infty}K\left(x,p,t-\tau\right)f(p)\,dp\,r(\tau)\,d\tau\,, \tag{5.21a}$$

with

$$K(x,p,t)=\frac{1}{2\sqrt{2\pi\hbar}}e^{\frac{-iVt}{\hbar}-\frac{itq^2}{2\hbar m}}\quad\cdot$$
$$\left\{e^{-\frac{ixq}{\hbar}}\,\mathrm{Erfc}\left[-i\sqrt{\frac{2mi}{\hbar t}}\frac{x}{2}-i\sqrt{\frac{i\,t}{2\hbar m}}q\right]+e^{\frac{ixq}{\hbar}}\,\mathrm{Erfc}\left[-i\sqrt{\frac{2mi}{\hbar t}}\frac{x}{2}+i\sqrt{\frac{i\,t}{2\hbar m}}q\right]\right\}\,, \tag{5.21b}$$

where we have again used the convolution theorem C.2 and we have introduced the abbreviation

$$q=\sqrt{p^2-2mV}\,.$$

A further interpretation of (5.21) is only possible if we distinguish between momentum distributions that are concentrated around $p_0 > \sqrt{2mV}$, where a classical transmission of the barrier would be possible and those which are concentrated around $p_0 < \sqrt{2mV}$, where the wave packet enters a classically forbidden region.

5.3 A wave packet climbing the potential step

We can write any initial wave packet $\psi(x,0)$ in momentum space (5.10)as

$$f(p) = e^{\frac{-ipx_0}{\hbar}} F\left(p - p_0\right) \quad , \tag{5.22a}$$

where $F(p)$ fulfills

$$\int_{-\infty}^{\infty} F^*(p)\, p\, F(p) dp = 0\,, \qquad \int_{-\infty}^{\infty} F^*(p) F'(p) dp = 0\,. \tag{5.22b}$$

The expectation values of $\psi(x,0)$ are then given by

$$\langle \hat{x} \rangle = x_0\,, \qquad \langle \hat{p} \rangle = p_0\,,$$

and the uncertainties will be denoted by Δx_0 and Δp_0.

We will now consider an initial function $f(p)$ (5.10) almost exclusively concentrated in a region $p > p_m > \sqrt{2mV}$, so that we can assume

$$f(p) \approx 0 \quad \text{for} \quad p < p_m, \tag{5.23}$$

Moreover we require the wave packet to be sufficiently peaked around the momentum expectation value p_0, so that

$$\frac{p_0}{mV} F(p - p_0)(p - p_0) \approx 0\,, \tag{5.24a}$$

$$e^{-\frac{i\sqrt{q^2+2mV}x_0}{\hbar}} F\left(\sqrt{q^2 + 2mV} - \sqrt{q_0^2 + 2mV}\right) \approx \tag{5.24b}$$

$$F\left(\lambda(q - q_0)\right) e^{-\frac{iq_0x_0}{\lambda\hbar} - \frac{ix_0\lambda}{\hbar}(q-q_0) - \frac{ix_0\lambda}{2\hbar q_0 k_0}(q-q_0)^2}\,,$$

where

$$p_0 = \sqrt{q_0^2 + 2mV}\,, \quad \lambda = \sqrt{1 - \frac{2mV}{p_0^2}}$$

Finally the difference $p_m - \sqrt{2mV}$ should be big enough to ensure

$$\frac{1}{\sqrt{\frac{p^2}{2mV} - 1}} = O(1) \quad \text{for} \quad p \geq p_m \tag{5.25}$$

which means that this factor does not have relevant influence on the approximations.

If we now insert the wave packet into the solution for $x < 0$ (5.16) we will use $R(p) \approx R(p_0)$ since according to (5.24a) and the mean value theorem

$$f(p)R(p) = f(p)R(p_0) + f(p)R'(p_1)(p - p_0) \approx f(p)R(p_0)\,,$$
$$\text{with} \quad p_1 \,\epsilon\, (p_0, p)$$

where (5.25) ensures that the derivative of $R(p)$ (5.17) will not spoil the approximation. We find for $x < 0$

$$\psi(x,t) \approx \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy \, + \frac{R(p_0)}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx}{\hbar}} e^{-\frac{ip^2 t}{2m\hbar}} f(p)dp \, =$$
$$\frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy \, + R(p_0) \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2t}} \psi(y,0)dy \, . \tag{5.26}$$

The solution consists of an incoming and a reflected wave packet. Within our approximation the reflected wave packet has the same shape as the wave packet reflected by an infinite barrier, but its probability density is reduced by a factor $R(p_0)^2$. This factor only depends on $k_0 = p_0^2/(2mV)$ and goes from 1 to zero when k_0 goes from 1 to infinity (5.17). If $p_0^2/2m$, which corresponds to the energy expectation value within our approximation, is much higher than the potential step, there is hardly any reflection at the step.

For the interpretation of the solution for $x > 0$ (5.21) we rewrite the error function according to D.2a

$$\mathrm{Erfc}\left[\frac{u}{2z}\right] = \frac{2z}{\sqrt{\pi}} e^{-\frac{u^2}{4z^2}} \int_0^{\infty} e^{-z^2 y^2 - uy} dy \, , \tag{5.27}$$

where we choose

$$z = \sqrt{\frac{-im}{2\hbar t}} \, , \quad u = -\frac{im}{\hbar t} x \mp \frac{i}{\hbar} q \, .$$

This yields

$$K(x,p,t) = e^{-\frac{iVt}{\hbar}} \left\{ \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} e^{\frac{i(x+y)^2\kappa^2}{2t}} e^{\frac{iqy}{\hbar}} dy \, + \, \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} e^{\frac{i(x+y)^2\kappa^2}{2t}} e^{\frac{-iqy}{\hbar}} dy \right\} \, .$$

We define

$$\widetilde{\psi}(y,0) := \frac{1}{\sqrt{2\pi\hbar}} \int_{\sqrt{2mV}}^{\infty} e^{\frac{iqy}{\hbar}} f(p)dp = \frac{1}{\sqrt{2\pi\hbar}} \int_{\sqrt{2mV}}^{\infty} e^{\frac{i\sqrt{p^2-2mV}y}{\hbar}} f(p)dp \, . \tag{5.28}$$

The substitution $q = \sqrt{p^2 - 2mV}$, $q_0 = \sqrt{p_0^2 - 2mV}$ yields

$$\frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} e^{\frac{iqy}{\hbar}} f(\sqrt{q^2+2mV}) \frac{q}{\sqrt{q^2+2mV}} dq =$$
$$\frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} e^{\frac{iqy}{\hbar}} e^{-\frac{i\sqrt{q^2+2mV}x_0}{\hbar}} F\left(\sqrt{q^2+2mV} - \sqrt{q_0^2+2mV}\right) \frac{q}{\sqrt{q^2+2mV}} dq \, .$$

Applying(5.24b)and expanding also $q/\sqrt{q_0^2+2mV}$ around q_0 and using (5.24a), we find

$$\widetilde{\psi}(y,0) \approx \frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} e^{\frac{iqy}{\hbar}} \lambda e^{-\frac{iq_0 x_0}{\lambda\hbar} - \frac{ix_0\lambda}{\hbar}(q-q_0) - \frac{ix_0\lambda}{2\hbar q_0 k_0}(q-q_0)^2} F\left(\lambda(q-q_0)\right) dq \, .$$

Because of (10.11) we can extend the integral

$$\widetilde{\psi}(y,0) \approx \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{iqy}{\hbar}} \lambda e^{-\frac{iq_0 x_0}{\lambda\hbar} - \frac{ix_0\lambda}{\hbar}(q-q_0) - \frac{ix_0\lambda}{2\hbar q_0 k_0}(q-q_0)^2} F\left(\lambda(q-q_0)\right) dq\,.$$

Note that in (5.24b)the argument of F is approximated by a Taylor expansion around q_0 up to first order, whereas the exponent is expanded to second order due to a factor $1/\hbar$

The function $\widetilde{\psi}(y,0)$ is a deformed version of the original wave packet $\psi(x,0)$, characterized by the following properties:

$$\left\langle \widetilde{\psi}|\widetilde{\psi} \right\rangle = \lambda\,, \quad \frac{1}{\lambda}\left\langle \widetilde{\psi}|\hat{p}|\widetilde{\psi} \right\rangle = q_0\,, \quad \frac{1}{\lambda}\left\langle \widetilde{\psi}|\hat{x}|\widetilde{\psi} \right\rangle = \lambda\, x_0\,,$$
$$\Delta x^2 = \lambda^2 \Delta x_0^2 + \frac{x_0^2}{q_0^2 k_0^2}\Delta p_0^2\,, \quad \Delta p^2 = \frac{1}{\lambda^2}\Delta p_0^2\,.$$

$\psi(x,0)$ was assumed to be zero for $x > 0$. If this function is sufficiently peaked around $x = x_0 < 0$ and p_0, then also Δx will be sufficiently small so that the deformed wave function will also vanish for $x > 0$, and

$$\int_{-\infty}^{\infty} dp \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} dy e^{\frac{i(x+y)^2\kappa^2}{2t}} e^{\frac{iqy}{\hbar}} f(p) = \tag{5.29a}$$
$$\frac{\kappa}{\sqrt{2\pi t\, i}} \int_0^{\infty} e^{\frac{i(x+y)^2\kappa^2}{2t}} \widetilde{\psi}(y,0) dy \approx 0\,. \tag{5.29b}$$

Therefore we find

$$\int_{-\infty}^{\infty} K(x,p,t) f(p) dp \approx \frac{\kappa}{\sqrt{2\pi t\, i}} e^{-\frac{iVt}{\hbar}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \widetilde{\psi}(y,0) dy\,.$$

Inserting this result in (5.21a),applying (5.15) for the convolution integral and proceeding further as for $x < 0$, we get for $x > 0$

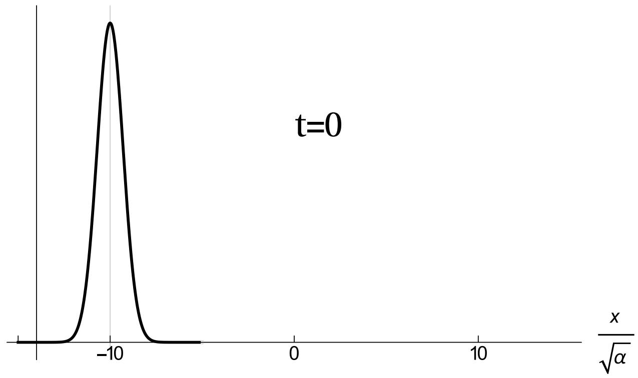
$$\psi(x,t) \approx (1 + R(p_0)) \frac{\kappa}{\sqrt{2\pi t\, i}} e^{-\frac{iVt}{\hbar}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \widetilde{\psi}(y,0) dy\,. \tag{5.30}$$

This means that the wave function is deformed after it has passed the potential step. It takes now the form of a free particle wave function that looked like $\widetilde{\psi}(x,0)$ at $t = 0$. Moreover it is slowed down, and has now the momentum expectation value $\sqrt{p_0^2 - 2mV}$ instead of p_0, which exactly coincides with the reduced momentum of a corresponding classical particle (see figure 5.1(c)).

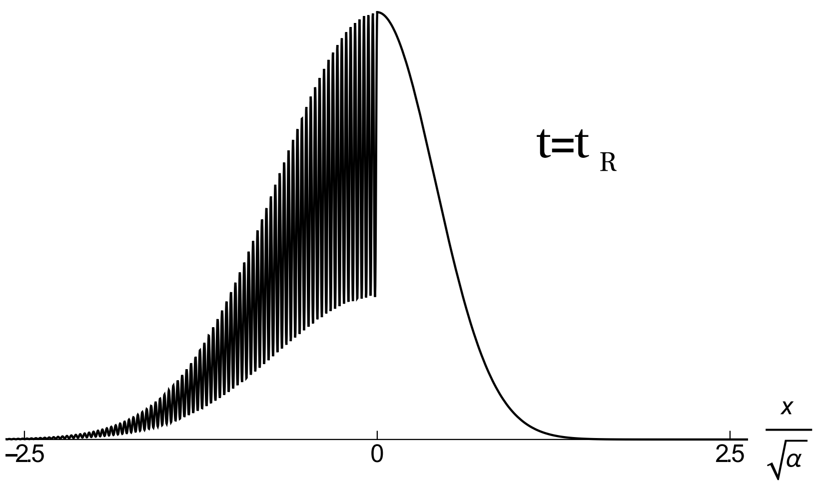
When the reflection/transmission process is finished

$$t \gg \frac{x_0 m}{p_0}\,,$$

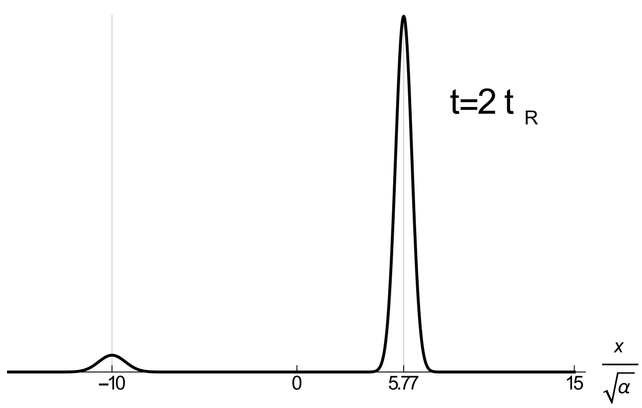
only the second term of (5.26), describing the reflected wave function is relevant and the solution consists of a reflected and a transmitted wave packet:



(a) The relative dimensionless probability density $|\psi|^2 \cdot (\pi\alpha)^{1/2}$ of the initial wave packet.



(b) The relative dimensionless probability density $|\Psi|^2 \cdot (\pi\alpha)^{1/2}$ at $t_R = |x_0|m/p_0$.



(c) The relative dimensionless probability density $|\Psi|^2 \cdot (\pi\alpha)^{1/2}$ at $t = 2t_R$. The momentum is reduced by a factor $\sqrt{\frac{k_0-1}{k_0}} = 0.577$.

Figure 5.1: As initial function we choose a Gaussian wave packet with the properties $\Delta x_0 = \sqrt{\alpha/2}$, $\Delta p_0 = \hbar/\sqrt{2\alpha}$, $x_0 = -10\sqrt{\alpha}$, $p_0 = 100\hbar/\sqrt{\alpha}$. The contributions of this Gaussian in the region $x \geq 0$ are so small that we can use (5.26,5.30) and we can extend the integrals to the whole real line. We show the wave packet before, during and after the reflection/transmission process that takes place around the classical reflection time t_R. We have chosen $k_0 = 1.5$.

$$\psi(x,t) \approx \psi_R(x,t) + \psi_T(x,t) = \tag{5.31}$$

$$R(p_0)\frac{\kappa}{\sqrt{2\pi t\, i}}\int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2t}}\psi(y,0)dy + (1+R(p_0))\frac{\kappa}{\sqrt{2\pi t\, i}}e^{-\frac{iVt}{\hbar}}\int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}}\widetilde{\psi}(y,0)dy\,. \tag{5.32}$$

Here we do not need to restrict ψ_R and ψ_T to the regions left and right of $x = 0$ anymore, since they will be concentrated in the respective regions anyway. The reflected and the transmitted part then fulfill

$$\langle\psi_R|\psi_R\rangle = (R(p_0))^2\,, \quad \langle\psi_T|\psi_T\rangle = (R(p_0)+1)^2\lambda = 1 - \langle\psi_R|\psi_R\rangle \tag{5.33}$$

So $|R(p_0)|^2$ denotes the reflection reflection probability for a sufficiently peaked wave packet.

5.4 A wave packet reflected by the potential step and swapping into the forbidden region

We now consider a wave packet represented by (5.22), and concentrated within a region $0 < p < p_m < \sqrt{2mV}$, so that we can assume

$$f(p) \approx 0 \quad \text{for} \quad p > p_m \quad \text{and} \quad p < 0\,, \tag{5.34}$$

and

$$\frac{1}{\sqrt{1-\frac{p^2}{2mV}}} = O(1) \quad \text{for} \quad 0 \leq p \leq p_m\,. \tag{5.35}$$

We also require (5.24a). Proceeding as in the case $p_0 > \sqrt{2mV}$, we get the same result (5.26) for $x < 0$

$$\psi(x,t) \approx \frac{\kappa}{\sqrt{2\pi t\, i}}\int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}}\psi(y,0)dy + R(p_0)\frac{\kappa}{\sqrt{2\pi t\, i}}\int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2t}}\psi(y,0)dy\,. \tag{5.36}$$

According to (5.17), $R(p_0)$ is a complex function with absolute value 1 for $k_0 = \frac{p_0^2}{2m} < 1$. For $k_0 \ll 1$, $R(p_0)$ is approximately -1 and $\psi(x,t)$ is completely reflected at the barrier.

Applying

$$\mathrm{Erfc}[x] = 2 - \mathrm{Erfc}[-x]$$

to the second term in (5.21b), and using (5.27) with

$$z = \sqrt{\frac{-im}{2ht}}\,, \quad u = \mp\frac{im}{\hbar t}x - \frac{i}{\hbar}q\,,$$

we get

$$K(x,p,t) = e^{-\frac{iVt}{\hbar}} \left\{ \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{itq^2}{2\hbar m}+\frac{ixq}{\hbar}} + \right.$$
$$\left. \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} \int_0^\infty e^{\frac{i(x+y)^2\kappa^2}{2t}} e^{\frac{iqy}{\hbar}} dy \,-\, \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} \int_0^\infty e^{\frac{i(x-y)^2\kappa^2}{2t}} e^{\frac{iqy}{\hbar}} dy \right\} . \tag{5.37}$$

With the help of the mean value theorem and (5.24a),(5.35) we determine

$$e^{\frac{iqy}{\hbar}} f(p) = e^{-\frac{\sqrt{2mV-p^2}y}{\hbar}} f(p) = e^{-\frac{\sqrt{2mV-p_0^2}y}{\hbar}} f(p) - e^{-\frac{\sqrt{2mV-p_1^2}y}{\hbar}} \frac{p_1 y}{\hbar\sqrt{2mV-p_1^2}}(p-p_0)f(p)$$
$$\approx e^{\frac{-\sqrt{2mV-p_0^2}y}{\hbar}} f(p) \,\text{with}\quad p_1 \,\epsilon\, (p_0,p).$$

Since according to (5.34)

$$\int_0^{\sqrt{2mV}} f(p)dp \approx \int_{-\infty}^{\infty} f(p)dp = \psi(0,0) = 0\,,$$

we conclude

$$\int_{-\infty}^{\infty} K(x,p,t)f(p)dp \approx e^{-\frac{\sqrt{2mV-p_0^2}x}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ip^2t}{2m\hbar}} f(p)dp\,.$$

Proceeding as for (5.30), we finally determine the solution for $x > 0$

$$\psi(x,t) \approx (1+R(p_0))e^{-\frac{\sqrt{2mV-p_0^2}x}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ip^2t}{2m\hbar}} f(p)dp\,. \tag{5.38}$$

We can again conclude that after the reflection process, when

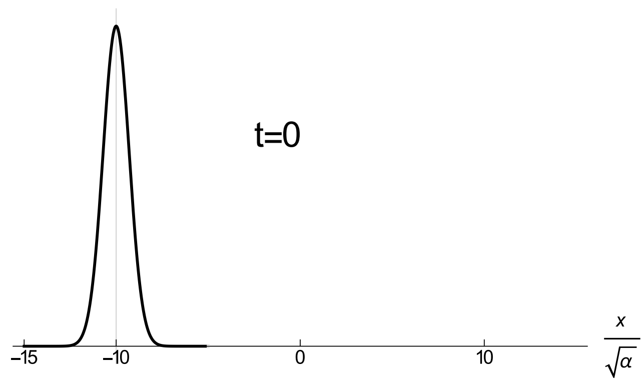
$$t \gg \frac{x_0 m}{p_0}\,,$$

the wavefunction only consists of a reflected and a transmitted part.

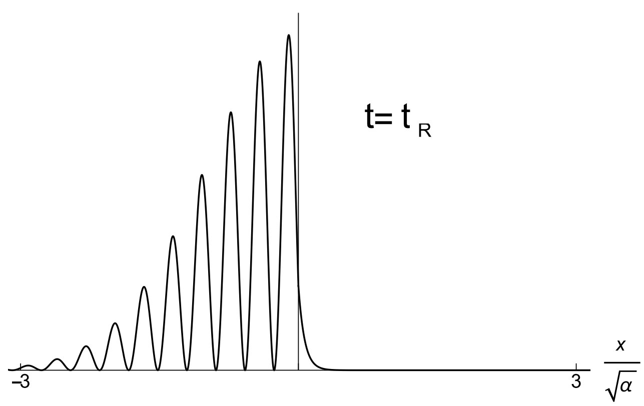
$$\psi(x,t) \approx \psi_R(x,t) + \psi_T(x,t) = \tag{5.39}$$
$$R(p_0)\frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2t}} \psi(y,0)dy + (1+R(p_0))e^{-\frac{\sqrt{2mV-p_0^2}x}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ip^2t}{\hbar}} f(p)dp\,. \tag{5.40}$$

But since $|R(p_0)| = 1$, we find

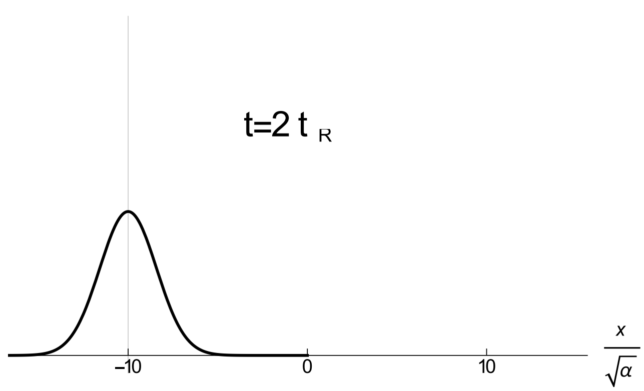
$$\langle\psi_R|\psi_R\rangle = \int_{-\infty}^{0} \psi^*(x,t)\psi(x,t)dx \approx \int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)dx = 1 \quad ,$$



(a) The relative dimensionless probability density $|\Psi|^2 \cdot (\pi\alpha)^{1/2}$ of the initial wave packet.



(b) The relative dimensionless density $|\Psi|^2 \cdot (\pi\alpha)^{1/2}$ at $t_R = |x_0|m/p_0$. Note that the exponential decay in the classically forbidden region is determined by the factor $e^{-\sqrt{1/k_0 - 1}p_0 x/\hbar}$



(c) The relative dimensionless probability density $|\Psi|^2 \cdot (\pi\alpha)^{1/2}$ at $t = 2t_R$. The whole wave function is reflected. There is no part of the probability density left in the classically forbidden region.

Figure 5.2: As initial function we choose a Gaussian wave packet with the properties $\Delta x_0 = \sqrt{\alpha/2}$, $\Delta p_0 = \hbar/\sqrt{\alpha 2}$, $x_0 = -10\sqrt{\alpha}$, $p_0 = 10\hbar/\sqrt{\alpha}$. The contributions of this function for $x \geq 0$ can again be neglected. We see that the wave packet swaps into the region $x > 0$ around the classical reflection time, but leaves it entirely when the reflection process is over. We have chosen $k_0 = 1/4$.

which means that when the reflected wave packet has left the neighborhood of the step the rest of the wave function also leaves the classically forbidden region (see figure 5.2(c))

$$\psi(x,t) \approx \psi_R(x,t) \quad \text{for} \quad t \gg \frac{x_0 m}{p_0} \, .$$

5.5 Summary and discussion of the literature

We derived an exact wave packet solution for the potential step. We could show that a wave packet with energy higher than the potential step will partly be reflected and partly transmitted and thereby slowed down (5.1(b)), as it would be expected from a classical particle that has passed the step. This effect was also obtained by [19] using the saddle point approximation. We found that the wave function with energy lower than the potential step will swap into the classically forbidden region only during the reflection process. Moreover we could show that for sufficiently peaked wave packets, the reflection probability can be denoted by the corresponding time-independent expression (5.33).

The derivation of the exact solution is significantly easier than the derivation of the propagator in [20],[21] where the PDX (path decomposition expansion) method for path integrals was applied. Apart from being of similar simplicity as the most explicit solutions available in the literature ([22],[21]) the obtained solutions admit a direct insight into the wave packet dynamics.

Chapter 6

The asymmetric square well

We solve the initial value problem of the asymmetric square well. The solution gives an intuitive picture of the wave packet dynamics reproducing all possible reflection processes. Under certain assumptions about the wave packet, we are able to determine the reflection and transmission probabilities.

We will consider a potential that is a combination of the infinite square well and the potential step, which can be described as a box with exit.

$$
\begin{array}{lll}
V(x) = \infty & \text{for} & x \le -d \\
V(x) = 0 & \text{for} & -d < x < 0 \\
V(x) = V & \text{for} & x \ge 0 \quad .
\end{array}
$$

The dynamics of the wave packet $\psi(x,0)$, is then governed by

$$
-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad -d \le x < 0 \tag{6.1}
$$

$$
-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t) = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad x \ge 0\,, \tag{6.2}
$$

where $\psi(x,t)$ is supposed to be continuously differentiable and square integrable and to fulfill the boundary condition

$$
\psi(-d,t) = 0\,. \tag{6.3}
$$

We will further assume that the initial wave packets are located within the box,

$$
\psi(x,0) = 0 \qquad \text{for} \qquad x \ge 0\,. \tag{6.4}
$$

We find for the Laplace-transformed wave packet $\varphi(x,s)$

$$\varphi(x,s) = \sqrt{\frac{m}{2is\hbar}} \left\{ u_1(x,s) \int_{-d}^{x} u_2(y,s)\psi(y,0)dy - \quad u_2(x,s) \int_{-d}^{x} u_1(y,s)\psi(y,0)dy \right\}$$

$$+ \ \alpha(s)u_1(x,s) \ + \ \beta(s)u_2(x,s) \qquad \text{for} \quad x < 0 \tag{6.5a}$$

$$\varphi(x,s) = \gamma(s)u_3(x,s) \ + \ \delta(s)u_4(x,s) \qquad \text{for} \quad x > 0 \quad , \tag{6.5b}$$

where the functions u_1, u_2, u_3, u_4 are defined as in the previous chapter (5.4). Since $\varphi(x,s)$ must vanish for $x \to \infty$, we find

$$\delta(s) = 0\,.$$

The boundary condition (6.3) implies

$$\alpha(s) = -\beta(s)e^{(i-1)2d\kappa\sqrt{s}}\,.$$

Since $\varphi(x,s)$ should be continuously differentiable at $x = 0$, we get

$$\gamma(s) = \frac{\kappa}{\sqrt{2\,s\,i}} \cdot \frac{2\,I_2 - 2\,I_1 e^{(i-1)2d\kappa\sqrt{s}}}{1 + \sqrt{1 - \frac{V}{si\hbar}} + e^{(i-1)2d\kappa\sqrt{s}}\left(1 - \sqrt{1 - \frac{V}{si\hbar}}\right)} \tag{6.6}$$

$$\beta(s) = \frac{\kappa}{\sqrt{2\,s\,i}} \cdot \frac{1}{1 - e^{(i-1)2d\kappa\sqrt{s}}} \left\{ I_1 - I_2 + \frac{2\,I_2 - 2\,I_1 e^{(i-1)2d\kappa\sqrt{s}}}{1 + \sqrt{1 - \frac{V}{si\hbar}} + e^{(i-1)2d\kappa\sqrt{s}}\left(1 - \sqrt{1 - \frac{V}{si\hbar}}\right)} \right\}, \tag{6.7}$$

where we have introduced

$$I_1 = \int_{-d}^{0} e^{(i-1)y\kappa\sqrt{s}}\psi(y,0)dy\,, \quad I_2 = \int_{-d}^{0} e^{-(i-1)y\kappa\sqrt{s}}\psi(y,0)dy\,.$$

Inserting these results in 6.5, using the abbreviations (5.7,4.5) and applying

$$\frac{1 - \sqrt{1 - \frac{V}{si\hbar}}}{1 + \sqrt{1 - \frac{V}{si\hbar}}} = \rho(s)$$

as well as the series expansion

$$\frac{1}{(1 + e^{(i-1)\kappa 2d\sqrt{s}}\rho(s))} = \sum_{k=0}^{\infty} (-1)^k \rho(s)^k \, e^{(i-1)2d\kappa\sqrt{s}\,k}\,, \tag{6.8}$$

we find for the Laplace transformed wave packet (6.5),

$$\varphi(x,s) = \left\{ \sum_{k=0}^{\infty} \frac{\kappa}{\sqrt{2si}} (\rho(s)+1)(-1)^k \rho(s)^k \int_{-d}^{0} e^{(i-1)(2dk-y)\kappa\sqrt{s}} \psi(y,0) dy \right.$$
$$\left. - \sum_{k=0}^{\infty} \frac{\kappa}{\sqrt{2si}} (\rho(s)+1)(-1)^k \rho(s)^k \int_{-d}^{0} e^{(i-1)(2d(k+1)+y)\kappa\sqrt{s}} \psi(y,0) dy \right\} e^{i\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}x}$$
$$\text{for} \quad x > 0 . \tag{6.9a}$$

Applying also

$$\frac{1}{1+e^{(i-1)2d\kappa\sqrt{s}}\rho(s)} \cdot \frac{1}{1-e^{(i-1)2d\kappa\sqrt{s}}} = \frac{e^{-(i-1)2d\kappa\sqrt{s}}}{1+\rho(s)} \left\{ \frac{1}{1-e^{(i-1)2d\kappa\sqrt{s}}} - \frac{1}{1+e^{(i-1)2d\kappa\sqrt{s}}\rho(s)} \right\}$$
$$= \frac{1}{1+\rho(s)} \sum_{k=0}^{\infty} (1-(-1)^k \rho(s)^k) e^{(i-1)2d(k-1)\kappa\sqrt{s}} ,$$

we conclude

$$\varphi(x,s) = -\sum_{k=0}^{\infty} \rho(s)^k (-1)^k \frac{\kappa}{\sqrt{2si}} \int_{-d}^{0} e^{(i-1)(2d(k+1)+x+y)\kappa\sqrt{s}} \psi(y,0) dy$$
$$+ \sum_{k=0}^{\infty} \rho(s)^{k+1} (-1)^{k+1} \frac{\kappa}{\sqrt{2si}} \int_{-d}^{0} e^{(i-1)(2d(k+1)+x-y)\kappa\sqrt{s}} \psi(y,0) dy$$
$$+ \frac{\kappa}{\sqrt{2si}} \int_{-d}^{0} e^{(i-1)|x-y|\kappa\sqrt{s}} \psi(y,0) dy$$
$$+ \sum_{k=0}^{\infty} \rho(s)^{k+1} (-1)^{k+1} \frac{\kappa}{\sqrt{2si}} \int_{-d}^{0} e^{(i-1)(2d(k+1)-x+y)\kappa\sqrt{s}} \psi(y,0) dy$$
$$- \sum_{k=0}^{\infty} \rho(s)^{k+2} (-1)^{k+2} \frac{\kappa}{\sqrt{2si}} \int_{-d}^{0} e^{(i-1)(2d(k+1)-x-y)\kappa\sqrt{s}} \psi(y,0) dy$$
$$+ \frac{\kappa}{\sqrt{2si}} \rho(s) \int_{-d}^{0} e^{(i-1)|x+y|\kappa\sqrt{s}} \psi(y,0) dy$$
$$\text{for} \quad x < 0 . \tag{6.9b}$$

Here we have again combined the integrals, so that each term goes to zero for $s \to \infty$. In order to determine the inverse Laplace transform of (6.9a), we will proceed similarly as in section (5.2). We will use the shifted momentum representation

$$f(K,p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x+K,0) e^{\frac{-ipx}{\hbar}} dx \; = \; e^{\frac{ipK}{\hbar}} f(p) \tag{6.10}$$

and we introduce

$$L(k,t) = \mathcal{L}^{-1} \left\{ (\rho(s)+1)\rho(s)^k \right\} , \tag{6.11}$$

which can be expressed as a sequence of convolutions of (5.8).

This yields for the wave function in the region $x > 0$

$$
\begin{aligned}
\psi(x,t) = & \int_{-\infty}^{\infty} K\left(x,p,t\right) f(0,p)\, dp + \int_{0}^{\infty}\int_{-\infty}^{\infty} K\left(x,p,t-\tau\right) f(0,p)\, dp\, r(\tau)\, d\tau + \\
& \sum_{k=1}^{\infty}(-1)^k \int_0^t \int_{-\infty}^{\infty} K\left(x,p,t-\tau\right) f(2dk,p)\, dp\, L(k,\tau) d\tau \\
& - \int_{-\infty}^{\infty} K\left(x,p,t\right) f(-2d,p)\, dp - \int_{0}^{\infty}\int_{-\infty}^{\infty} K\left(x,p,t-\tau\right) f(-2d,p)\, dp\, r(\tau)\, d\tau \\
& - (-1)^k \sum_{k=1}^{\infty} \int_0^t \int_{-\infty}^{\infty} K\left(x,p,t-\tau\right) f(-2dk,p)\, dp\, L(k,\tau) d\tau \,.
\end{aligned}
\tag{6.12a}
$$

Note that the first two terms are identical with the solution of the potential step (5.21). They describe the behavior of a wave packet that starts with positive momentum and undergoes its first transmission process. The following sum describes the transmitted parts of this wave packet after the kth reflection at the left wall $x = -d$. The remaining terms are relevant for the description of an initial wave packet with negative momentum.

The inverse Laplace transform of (6.9b) yields

$$
\begin{aligned}
\psi(x,t) = & -\sum_{k=0}^{\infty} \int_0^t \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i(t-\tau)}} e^{\frac{i\kappa^2(2d(k+1)+x+y)^2}{2(t-\tau)}} \psi(y,0) dy\, (-1)^k M(k,\tau) d\tau \\
& + \sum_{k=0}^{\infty} \int_0^t \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i(t-\tau)}} e^{\frac{i\kappa^2(2d(k+1)+x-y)^2}{2(t-\tau)}} \psi(y,0) dy\, (-1)^{k+1} M(k+1,\tau) d\tau \\
& + \sum_{k=0}^{\infty} \int_0^t \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i(t-\tau)}} e^{\frac{i\kappa^2(2d(k+1)-x+y)^2}{2(t-\tau)}} \psi(y,0) dy\, (-1)^{k+1} M(k+1,\tau) d\tau \\
& - \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \int_0^t \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i(t-\tau)}} e^{\frac{i\kappa^2(2d(k+1)-x-y)^2}{2(t-\tau)}} \psi(y,0) dy\, (-1)^{k+2} M(k+2,\tau) d\tau \\
& + \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i t}} e^{\frac{i\kappa^2(x-y)^2}{2t}} \psi(y,0) dy \; + \; \int_0^t \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i(t-\tau)}} e^{\frac{i\kappa^2(x+y)^2}{2(t-\tau)}} \psi(y,0) dy\, r(\tau) d\tau \\
& \text{for} \quad x < 0 \,,
\end{aligned}
\tag{6.13}
$$

where we have introduced

$$
M(k,t) \equiv \mathcal{L}^{-1}\left(\rho(s)^k\right) \,. \tag{6.14}
$$

The last two terms of (6.13)coincide with the solution of the potential step (5.9). If we compare (6.13) with the solution of the infinite square well (4.11), we find that (6.13) consists of the terms of (4.11) and their convolutions with $M(k,t)$.

According to Appendix C.3, we find

$$M(k,t) = \frac{k}{i^k t} J_k \left[\frac{Vt}{2\hbar}\right] e^{-\frac{iVt}{2\hbar}} \,. \tag{6.15}$$

The solution (6.13) consists of terms of the form

$$U(k,t) = \int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\,i}} \int_{-d}^{0} e^{\frac{i(Q\pm y)^2\kappa^2}{2(t-\tau)}} \psi(y,0)dy\, M(k,\tau)d\tau = \tag{6.16}$$

$$\int_0^t \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ipQ}{\hbar}} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} f(p)dpM(k,\tau)d\tau \quad \text{with} \quad Q = 2dk \pm x \tag{6.17}$$

If we approximate the τ-integral by an infinite Laplace integral as for (5.15), we obtain

$$\begin{aligned} U(k,t) \approx \int_0^\infty \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ipQ}{\hbar}} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} f(p)dpM(k,\tau)d\tau = \\ \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ipQ}{\hbar}} e^{-\frac{ip^2 t}{2m\hbar}} f(p) \left(\rho\left[\frac{-ip^2}{2m\hbar}\right]\right)^k dp = \\ \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ipQ}{\hbar}} \quad e^{-\frac{ip^2 t}{2m\hbar}} f(p)R(p)^k dp \,. \end{aligned} \tag{6.18}$$

For the neglected part of the integral

$$u(k,t) = \int_t^\infty e^{\frac{\mp ipQ}{\hbar}} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{-\frac{iV\tau}{2\hbar}} \frac{k}{i^k\,\tau} J_k\left[\frac{V\tau}{2\hbar}\right] d\tau \,, \tag{6.19}$$

we get the following estimate

$$\left|\int_t^\infty e^{\frac{ip^2\tau}{2m\hbar}-\frac{iV\tau}{2\hbar}} \frac{k}{\tau} J_k\left[\frac{Vt}{2\hbar}\right] d\tau\right| \le \int_{\frac{tV}{2\hbar}}^\infty \left|\frac{k\,J_k(y)}{y}\right| dy \le \tag{6.20a}$$

$$\left(\int_{\frac{tV}{2\hbar}}^\infty \frac{k}{y^{1+2\epsilon}} dy\right)^{\frac{1}{2}} \cdot \left(\int_0^\infty \frac{(J_k(y))^2}{y^{1-2\epsilon}}\right)^{\frac{1}{2}} = \tag{6.20b}$$

$$k\frac{1}{\sqrt{2\epsilon}} \left(\frac{2\hbar}{Vt}\right)^{\epsilon} \cdot \left(2^{2\epsilon}\frac{\Gamma[1-2\epsilon]\Gamma[k+\epsilon]}{2(\Gamma[1-\epsilon])^2\Gamma[1+k-\epsilon]}\right)^{\frac{1}{2}} \le \tag{6.20c}$$

$$k\frac{1}{\sqrt{2\epsilon}} \left(\frac{2\hbar}{Vt}\right)^{\epsilon} \cdot \left(2^{2\epsilon}\frac{\Gamma[1-2\epsilon]}{2(\Gamma[1-\epsilon])^2}\right)^{\frac{1}{2}} \quad \text{with} \quad 0 < \epsilon < \frac{1}{2} \,, \tag{6.20d}$$

where we have applied the Schwarz inequality and the integral formula ([26])

$$\int_0^\infty \frac{(J_k(y))^2}{y^{1-2\epsilon}} = 2^{2\epsilon} \frac{\Gamma[1-2\epsilon]\Gamma[k+\epsilon]}{2(\Gamma[1-\epsilon])^2\Gamma[1+k-\epsilon]} \,. \tag{6.21}$$

Therefore (6.18) will be a good approximation for $U(k,t)$ if $t \gg \frac{k^{\frac{1}{\epsilon}}\hbar}{V}$. Moreover, if the wave packet is sufficiently peaked around the momentum expectation value p_0, so that $R(p_0)^k$ can be put before the integral, we can write

$$U(k,t) \approx R(p_0)^k \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ipQ}{\hbar}} \quad e^{-\frac{ip^2 t}{2m\hbar}} f(p)dp =$$

$$R(p_0)^k \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-d}^{0} e^{\frac{i(Q\pm y)^2\kappa^2}{2t}} \psi(y,0)dy\,. \tag{6.22}$$

However, the estimation (6.20d) gets worse for increasing k and moreover the solution (6.13) consists of infinite sums of terms of the form $U(k,t)$ Therefore we can use the approximation only if the number of relevant terms is limited.

We will now show how the truncation of the series can be justified for an uncorrelated Papageno function (2.6)as initial wave packet

$$\psi(y,0) = e^{\frac{ip_0 y}{\hbar}} G(y)\,,$$

where $G(y)$ is a twice differentiable real function that is zero outside $[0,d]$ and $p_0 = mv_0$ denotes the momentum expectation value of $\psi(y,0)$. We will also assume that $G(y)$ is non-oscillatory so that a contribution

$$\int_{-d}^{0} |G''(y)|\; dy$$

will not spoil the estimations. Without loss of generality we will only discuss the sum

$$S_1 = \sum_{k=1}^{\infty} U_1(k,t)\,, \text{with} \tag{6.23a}$$

$$U_1(k,t) = \int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\, i}} \int_{-d}^{0} e^{\frac{i(2dk+x-y)^2\kappa^2}{2(t-\tau)}} \psi(y,0)dy\, M(k,\tau)d\tau\,. \tag{6.23b}$$

Considering only terms with

$$X = \kappa\frac{2dk - x + y - v_0(t-\tau)}{2\sqrt{t-\tau}} \;>\; 0$$

and applying D.7c

$$\left| -\mathrm{Erfc}[(1-i)X]X + \frac{e^{2iX^2}}{(1-i)\sqrt{\pi}} \right| \;\leq\; \frac{1}{4\sqrt{2\pi}X^2}$$

we find after a twofold partial integration for the spatial integral

$$\left|\int_{-d}^{0}\frac{\kappa}{\sqrt{2\pi(t-\tau)\,i}}e^{\frac{i(2dk+x-y)^2\kappa^2}{2(t-\tau)}}e^{\frac{ip_0 y}{\hbar}}G(y)dy\right| = \tag{6.24}$$

$$\left|\int_{-d}^{0}\frac{\sqrt{t-\tau)}}{\kappa}\left\{-\mathrm{Erfc}[(1-i)X]X+\frac{e^{2iX^2}}{(1-i)\sqrt{\pi}}\right\}G''(y)dy\right| \le \tag{6.25}$$

$$\left(\frac{\sqrt{t-\tau)}}{\kappa}\right)^3\frac{1}{\sqrt{2\pi}}\int_{-d}^{0}\frac{1}{(2dk-v_0\,(t-\tau)-x+y)^2}\left|G''(y)\right|dy \le \tag{6.26}$$

$$\left(\frac{\sqrt{t-\tau)}}{\kappa}\right)^3\frac{1}{\sqrt{2\pi}}\frac{1}{(2dk-v_0t-d)^2}\int_{-d}^{0}\left|G''(y)\right|dy\,. \tag{6.27}$$

Applying again the Schwarz inequality and (6.21) for $\epsilon=-1/2$,

$$\int_0^\infty\frac{(J_k(y))^2}{y^2}=2^{-1}\frac{\Gamma[2]\Gamma[k-\frac{1}{2}]}{2(\Gamma[\frac{3}{2}])^2\Gamma[k+\frac{3}{2}]}=\frac{1}{\pi\left(k^2-\frac{1}{4}\right)}\,,$$

we can write for the convolution integral

$$\left|\int_0^t\left(\frac{\sqrt{t-\tau}}{\kappa}\right)^3\frac{k}{i^k\tau}J_k\left(\frac{\tau V}{2\hbar}\right)d\tau\right| \le \tag{6.28}$$

$$\frac{1}{\kappa^3}\left\{\int_0^t(t-\tau)^3d\tau\right\}^{\frac{1}{2}}\cdot k\left\{\left(\frac{V}{2\hbar}\right)\int_0^\infty\frac{J_k^2(y)}{y^2}dy\right\}^{\frac{1}{2}} = \tag{6.29}$$

$$\frac{t^2\hbar}{2}\sqrt{\frac{V}{2m^3}}\cdot\frac{k}{\sqrt{\pi\left(k^2-\frac{1}{4}\right)}} \le t^2\hbar\sqrt{\frac{V}{6\pi m^3}}\,. \tag{6.30}$$

Then we find for the sum of all $U_1(k,t)$ (6.23b) with $k\ge l$, where l is the smallest positive integer with $l\,2d\ge v_0t+3d$,

$$\left|\sum_{k=l}^{\infty}U_1(k,t)\right| \le \sum_{k=l}^{\infty}\left|U_1(k,t)\right| \le \tag{6.31}$$

$$\frac{1}{\sqrt{2\pi}}\left(\sum_{n=1}^{\infty}\frac{1}{4d^2n^2}\right)t^2\hbar\sqrt{\frac{V}{6\pi m^3}}\int_{-d}^{0}\left|G''(y)\right|dy \le \frac{\pi t^2\hbar}{24d^2}\sqrt{\frac{V}{18\pi m^3}}\int_{-d}^{0}\left|G''(y)\right|dy\,, \tag{6.32}$$

which can be neglected if

$$\frac{t^2\hbar}{d^3}\sqrt{\frac{V}{m^3}} \ll 1\,. \tag{6.33}$$

So we can write for (6.23a)

$$S_1 \approx \sum_{k=1}^{l-1} U_1(k,t) = \sum_{k=1}^{l-1} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ip(2dk+x)}{\hbar}} \quad e^{-\frac{ip^2 t}{2m\hbar}} f(p) R(p)^k dp \tag{6.34}$$

$$- \sum_{k=1}^{l-1} \int_{-\infty}^{\infty} u_1(k,t) f(p) dp \,, \tag{6.35}$$

where $u_1(k,t)$ is defined as a special case of $u(k,t)$ (6.19),namely

$$u_1(k,t) = \int_t^{\infty} e^{\frac{ip(2dk+x)}{\hbar}} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{-\frac{iV\tau}{2\hbar}} \frac{k}{i^k\,\tau} J_k \left[\frac{V\tau}{2\hbar}\right] d\tau \,. \tag{6.36}$$

Applying (6.20d), we find

$$\left| \sum_{k=1}^{l-1} u_1(k,t) \right| \leq \sum_{k=1}^{l-1} |u_1(k,t)| \leq \tag{6.37}$$

$$\frac{1}{\sqrt{2\epsilon}} \left(\frac{2\hbar}{Vt}\right)^{\epsilon} \cdot \left(2^{2\epsilon} \frac{\Gamma[1-2\epsilon]}{2(\Gamma[1-\epsilon])^2}\right)^{\frac{1}{2}} \cdot \frac{l(l-1)}{2} \,. \tag{6.38}$$

So this sum can be neglected, if

$$\left(\frac{2\hbar}{Vt}\right)^{\epsilon} \cdot \frac{l(l-1)}{2} \ll 1 \,, \tag{6.39}$$

and we finally find

$$S_1 \approx \sum_{k=1}^{L_1} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{\mp ip(2dk+x)}{\hbar}} \quad e^{-\frac{ip^2 t}{2m\hbar}} f(p) R(p)^k dp \,, \tag{6.40}$$

if both conditions (6.33,6.39) are fulfilled. Here $L_1 = l - 1$. Similarly estimates for the other three types of sums in (6.13) can be found that will limit the number of relevant terms to L_2, L_3, L_4. So we find from (6.9b) for a sufficiently peaked uncorrelated Papageno function with momentum expectation value p_0

$$
\begin{aligned}
\psi(x,t) \approx & -\sum_{k=0}^{L_1}(-1)^k R(p_0)^k \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i t}} e^{\frac{i\kappa^2(2d(k+1)+x+y)^2}{2t}} \psi(y,0)dy \\
& + \sum_{k=0}^{L_2}(-1)^{k+1} R(p_0)^{k+1} \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i t}} e^{\frac{i\kappa^2(2d(k+1)-x+y)^2}{2t}} \psi(y,0)dy \\
& + \sum_{k=0}^{L_3}(-1)^{k+1} R(p_0)^{k+1} \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i t}} e^{\frac{i\kappa^2(2d(k+1)+x-y)^2}{2t}} \psi(y,0)dy \\
& - \sum_{k=0}^{L_4}(-1)^{k+2} R(p_0)^{k+2} \int_{-d}^{0} \frac{\kappa}{\sqrt{2\pi i t}} e^{\frac{i\kappa^2(2d(k+1)-x-y)^2}{2t}} \psi(y,0)dy \\
& + \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-d}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy \, + R(p_0) \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-d}^{0} e^{\frac{i(x+y)^2\kappa^2}{2t}} \psi(y,0)dy \\
& \text{for} \quad x \, < \, 0 \, . \qquad (6.41)
\end{aligned}
$$

This approximate solution of the asymmetric square well looks like the solution of the infinite well (4.11) supplemented by the appropriate reflection coefficients that make allowance for the fact that at each time the wave packet is reflected at $x = 0$, parts of the wave packet leave the box. If the wave packet is located between the walls (not too close to any of them) only one term of (6.41) is dominant at a certain time, as long as the wave packets do not spread too much (see also theorem 4.1). The probability of finding a corresponding particle within the well is then given by $|R(p_0)|^{2m}$, where m denotes the already undergone number of reflections at the right wall. The transmission probability is then given by $1 - |R(p_0)|^{2m}$.

6.1 Summary

We found that the exact solution of the asymmetric square well is an intuitive combination of the solution of the infinite square well and the potential step. Each term of the solution inside the well(6.13) describes the wave packet after a certain number of reflections. For uncorrelated Papageno functions as initial wave packets, we have shown how the convolution integrals can be approximated by powers of the reflection coefficient if the wave packet is sufficiently narrow (6.41) as long as the system still shows semiclassical behaviour. For this case we also determined the probability of finding a particle inside the box at a given time which yields the corresponding transmission probability. Note that this example illustrates the advantages of the method of Laplace transforms very well since from the point of view of the characterization in terms of eigenstates the box with exit differs fundamentally from the infinite square well since there are bound and unbound eigenstates. As far as we know the initial value problem of this model was not considered before.

Chapter 7

The barrier

We use the method of Laplace transform to determine the dynamics of a wave packet that passes a barrier by tunneling. We investigate the transmitted wave packet and find that it can be resolved into a sequence of subsequent wave packages. This result sheds new light on the Hartmann effect for the tunneling time.

We will finally apply the method of Laplace transform to the model system of a finite barrier, which is described by

$$\begin{array}{lll} V(x) = 0 & \text{for} & x \le 0 \\ V(x) = V & \text{for} & 0 < x < d \\ V(x) = 0 & \text{for} & x \ge d \quad . \end{array}$$

The dynamics of the wave packet $\psi(x,0)$, is then determined by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad x < 0 \tag{7.1}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t) = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad 0 < x < d \tag{7.2}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\,\frac{\partial\psi(x,t)}{\partial t} \qquad \text{for} \qquad x > d \tag{7.3}$$

where $\psi(x,t)$ is supposed to be continuously differentiable everywhere and square integrable .

We will further assume that the initial wave packets are located at the left side of the barrier

$$\psi(x,0) = 0 \qquad \text{for} \qquad x \ge 0\,. \tag{7.4}$$

We find for the Laplace transformed wave packet $\varphi(x,s)$:

$$\varphi(x,s) = \sqrt{\frac{m}{2is\hbar}} \left\{ u_1(x,s) \int_{-d}^{x} u_2(y,s)\psi(y,0)dy - \quad u_2(x,s) \int_{-d}^{x} u_1(y,s)\psi(y,0)dy \right\}$$

$$+ \; \alpha(s)u_1(x,s) \, + \, \beta(s)u_2(x,s) \qquad \text{for} \quad x < 0 \tag{7.5a}$$

$$\varphi(x,s) = \gamma(s)u_3(x,s) \, + \, \delta(s)u_4(x,s) \qquad \text{for} \quad 0 < x < d \tag{7.5b}$$

$$\varphi(x,s) = \mu(s)u_1(x,s) \, + \, \nu(s)u_2(x,s) \qquad \text{for} \quad x > d \quad , \tag{7.5c}$$

where the functions u_1, u_2, u_3, u_4 are defined as in the previous chapters (5.4).

Since $\varphi(x,s)$ must vanish for $x \to \infty$, we find

$$\alpha(s) = 0 \, , \quad \nu(s) = 0 \, .$$

If we evaluate $\varphi(x,s)$ and its first derivative at $x = 0$ and $x = d$, we obtain

$$\beta(s) = \sqrt{\frac{m}{2i\hbar s}}\,(I_1 - I_2) + \sqrt{\frac{m}{2i\hbar s}} \cdot \frac{2\,I_2}{1 + \sqrt{1 - \frac{V}{i\hbar s}}} \cdot \frac{\rho(s) - e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}}{\rho^2(s) - e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}} \tag{7.6}$$

$$\gamma(s) = -\sqrt{\frac{m}{2i\hbar s}} \cdot \frac{2\,I_2}{1 + \sqrt{1 - \frac{V}{i\hbar s}}} \cdot \frac{e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}}{\rho^2(s) - e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}} \tag{7.7}$$

$$\delta(s) = \sqrt{\frac{m}{2i\hbar s}} \cdot \frac{2\,I_2\,\rho(s)}{1 + \sqrt{1 - \frac{V}{i\hbar s}}} \cdot \frac{1}{\rho^2(s) - e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}} \, , \tag{7.8}$$

$$\mu(s) = \sqrt{\frac{m}{2i\hbar s}} \cdot \frac{2\,I_2}{1 + \sqrt{1 - \frac{V}{i\hbar s}}} e^{-id\sqrt{\frac{2msi}{\hbar}}} \cdot \frac{1 - \rho(s)}{\rho^2(s) - e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}} e^{-2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}} \tag{7.9}$$

where we have introduced the abbreviations

$$I_1 = \int_{-\infty}^{0} e^{i\sqrt{\frac{2msi}{\hbar}}y}\psi(y,0)dy \quad I_2 = \int_{-\infty}^{0} e^{-i\sqrt{\frac{2msi}{\hbar}}y}\psi(y,0)dy$$

and also used 5.7. Inserting this result into (7.5), applying a series expansion for

$$\frac{1}{1 - \rho^2(s)e^{2id\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}}}}$$

yields

$$\varphi(x,s) = \sqrt{\frac{m}{2si\hbar}} \left\{ \int_{-\infty}^{0} e^{i\sqrt{\frac{2msi}{\hbar}}|x-y|} \psi(y,0)dy + \int_{-\infty}^{0} e^{-i\sqrt{\frac{2msi}{\hbar}}(x+y)} \psi(y,0)dy \cdot \rho(s) \right\} +$$

$$\sqrt{\frac{m}{2si\hbar}} \sum_{l=0}^{\infty} \int_{-\infty}^{0} e^{2id(l+1)\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}} - i(x+y)\sqrt{\frac{2msi}{\hbar}}} \psi(y,0)dy \cdot (\rho^2(s) - 1)\rho^{2l+1}(s)$$

$$\text{for} \quad x < 0 \qquad (7.10a)$$

$$\varphi(x,s) = \sqrt{\frac{m}{2si\hbar}} \sum_{l=0}^{\infty} \int_{-\infty}^{0} e^{i(2dl+x)\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}} - iy\sqrt{\frac{2msi}{\hbar}}} \psi(y,0)dy \cdot (\rho(s) + 1)\rho^{2l}(s) -$$

$$\sqrt{\frac{m}{2si\hbar}} \sum_{l=0}^{\infty} \int_{-\infty}^{0} e^{i(2d(l+1)-x)\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}} - iy\sqrt{\frac{2msi}{\hbar}}} \psi(y,0)dy \cdot (\rho(s) + 1)\rho^{2l+1}(s)$$

$$\text{for} \quad 0 \le x \le d\,, \qquad (7.10b)$$

$$\varphi(x,s) = \sqrt{\frac{m}{2si\hbar}} \sum_{l=0}^{\infty} \int_{-\infty}^{0} e^{id(2l+1)\sqrt{\frac{2msi}{\hbar} - \frac{2mV}{\hbar^2}} + i(x-d-y)\sqrt{\frac{2msi}{\hbar}}} \psi(y,0)dy \cdot (-\rho^2(s) + 1)\rho^{2l}(s)$$

$$\text{for} \quad x > d\,. \qquad (7.10c)$$

Applying the shifted momentum representation (6.10)

$$f(K,p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x+K,0) e^{\frac{-ipx}{\hbar}} dx \; = \; e^{\frac{ipK}{\hbar}} f(p) \qquad (7.11)$$

and introducing

$$a_l(t) = \mathcal{L}^{-1}\left\{\rho^{2l+1}(s)(1-\rho^2(s))\right\}\,, \quad b_l(t) = \mathcal{L}^{-1}\left\{\rho^{2l}(s)(1+\rho(s))\right\}$$
$$c_l(t) = \mathcal{L}^{-1}\left\{\rho^{2l+1}(s)(1+\rho(s))\right\}\,, \quad g_l(t) = \mathcal{L}^{-1}\left\{\rho^{2l}(s)(1-\rho^2(s))\right\}\,,$$

we find proceeding as for the asymmetric square well, for the inverse Laplace transform of (7.10)

$$\psi(x,t) = \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0) dy + \int_0^t \frac{\kappa}{\sqrt{2\pi(t-\tau)\, i}} \int_{-\infty}^{0} e^{\frac{i(x+y)^2\kappa^2}{2(t-\tau)}} \psi(y,0) r(\tau) dy\, d\tau +$$
$$\sum_{l=0}^{\infty} \int_0^t \int_{-\infty}^{\infty} K\left(2d(l+1), p, t-\tau\right) f(-x,p) dp \cdot a_l(\tau) d\tau$$
$$\text{for} \quad x < 0 \,, \tag{7.12a}$$
$$\psi(x,t) = \sum_{l=0}^{\infty} \int_0^t \int_{-\infty}^{\infty} K\left(2dl + x), p, t-\tau\right) f(p) dp \cdot b_l(\tau) d\tau +$$
$$\sum_{l=0}^{\infty} \int_0^t \int_{-\infty}^{\infty} K\left(d(2l+1) - x), p, t-\tau\right) f(p) dp \cdot c_l(\tau) d\tau$$
$$\text{for} \quad 0 < x < d \,, \tag{7.12b}$$
$$\psi(x,t) = \sum_{l=0}^{l=\infty} \int_0^t \int_{-\infty}^{\infty} K\left(d(2l+1), p, t-\tau\right) f(x-d,p) dp \cdot g_l(\tau) d\tau$$
$$\text{for} \quad x > d \,, \tag{7.12c}$$

where $K(x,p,t)$ was already used for the potential step (5.21b) and we used again the abbreviation κ (4.5).

7.1 Tunneling of wave packets

In order to investigate the tunneling process,we consider a wave packet represented by (5.22), that is concentrated within a region $0 < p < p_m < \sqrt{2mV}$. Furthermore it should fulfill (5.345.35).

We start with the solution for $x > d$ (7.10c). If we rewrite $K(x,p,t)$ as in (5.37) for $q^2 = p^2 - 2mV < 0$ and use

$$X_l \equiv d(2l+1) \,,$$

we find proceeding as for (6.12a)

$$K(X_l,p,t) = U_0 + U_1 - U_2 \,, \quad \text{where} \tag{7.13}$$
$$U_0 = e^{-\frac{iVt}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{itq^2}{2\hbar m} + \frac{iX_l q}{\hbar}} = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ip^2 t}{2m\hbar} - \frac{X_l\sqrt{2mV-p^2}}{\hbar}} \,,$$
$$U_1 = \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{iVt}{\hbar}} \int_0^{\infty} e^{\frac{i(X_l+u)^2\kappa^2}{2t}} e^{\frac{i\sqrt{2mV-p^2}u}{\hbar}} du \,, \tag{7.14}$$
$$U_2 = \frac{\kappa}{\sqrt{2\pi t\, i}} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{iVt}{\hbar}} \int_0^{\infty} e^{\frac{i(X_l-u)^2\kappa^2}{2t}} e^{\frac{i\sqrt{2mV-p^2}u}{\hbar}} du \,.$$

Inserting

$$\frac{\kappa}{\sqrt{2\pi t\, i}} e^{\frac{i(X_l \pm u)^2\kappa^2}{2t}} = \int_{-\infty}^{\infty} \frac{1}{2\pi\hbar} e^{\frac{-iq^2 t}{2m\hbar} + \frac{iqX_l}{\hbar} \pm \frac{iqu}{\hbar}} dq\,,$$

we obtain

$$U_1 - U_2 = \frac{1}{(2\pi\hbar)^{3/2}} e^{-\frac{iVt}{\hbar}} \int_{-\infty}^{\infty} e^{\frac{-iq^2 t}{2m\hbar} + \frac{iqX_l}{\hbar}} \frac{2i\hbar q}{2mV - p^2 + q^2} dq\,. \tag{7.15}$$

If the initial wavefunction is sufficiently peaked (5.24a) to assume

$$F(p - p_0)(p - p_0) \approx 0\,,$$

the expansion of the non-oscillating part of U_0 around p_0 yields a contribution to $\psi(x,t)$ (7.10c) that is proportional to

$$e^{-\frac{X_l\sqrt{2mV - p0^2}}{\hbar}} \;\le\; e^{-\frac{d\sqrt{2mV - p_0^2}}{\hbar}}\,. \tag{7.16}$$

By contrast we find for $U_1 - U_2$, that contains no oscillatory part

$$\int_{-\infty}^{\infty} (U_1 - U_2) f(x - d, p) dp \approx 0\,, \tag{7.17}$$

since

$$\int_{-\infty}^{\infty} f(p) p^n e^{i\frac{p(x-d)}{\hbar}} dp = -i\hbar \frac{\partial^n}{\partial x^n}\psi(x - d, 0) = 0 \quad \text{for} \quad x > d\,,\; n = 0, 1, 2, \ldots N\,,$$

and so the contribution to (7.17) will be proportional to Δp^{N+1}, if $f(p)$ decays rapidly enough so that the integrals

$$\int_{-\infty}^{\infty} f(p) p^n dp$$

exist up to $n = N + 1$.

So we conclude that for sufficiently peaked wave packets, U_0 is the only relevant contribution.

We obtain for the wavefunction for $x > d$

$$\psi(x,t) \approx \sum_{l=0}^{\infty} \int_0^t \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{X_l\sqrt{2mV - p_0^2}}{\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p) dp \cdot g_l(\tau) d\tau\,. \tag{7.18}$$

This result contains the free time evolution of the initial wave packet that is shifted by d to the right. Proceeding as for the integral (6.16) we approximate the convolution integral by

$$\int_0^t \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp \cdot g_l(\tau)d\tau \approx$$
$$\int_0^{\infty} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp \cdot g_l(\tau)d\tau =$$
$$\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} R(p)^{2l}(1-R(p)^2) f(p)dp \tag{7.19}$$
$$\approx R(p_0)^{2l}(1-R(p_0)^2) \cdot \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp\,, \tag{7.20}$$

where $R(p)$ is given by (5.17). Here the assumptions about the concentration of the wave packet (5.24a, 5.35) justifies putting $R(p)$ before the integral. Evaluating the sum in (7.18), we obtain

$$\psi(x,t) \approx \sum_{l=0}^{\infty} \int_0^t \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{X_l\sqrt{2mV-p_0^2}}{\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp \cdot g_l(\tau)d\tau \approx$$
$$\frac{e^{\frac{-d\sqrt{2mV-p_0^2}}{\hbar}}}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}} R^2(p_0)} (1-R^2(p_0)) \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp\,. \tag{7.21}$$

For the neglected part of the time integral (7.20)

$$\Delta_l \equiv \int_t^{\infty} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2(t-\tau)}{2m\hbar}} e^{\frac{ip(x-d)}{\hbar}} f(p)dp \cdot g_l(\tau)d\tau\,, \tag{7.22}$$

we find using (6.21), setting $\epsilon = 1/4$ and performing the same steps as for the estimation of (6.19)

$$|\Delta_l| \sim O(l) \cdot O\left(\left[\frac{2\hbar}{Vt}\right]^{\frac{1}{4}} \right) \tag{7.23}$$

Since

$$\sum_{l=0}^{\infty} e^{-\frac{X_l\sqrt{2mV-p_0^2}}{\hbar}} \Delta_l \sim \frac{e^{\frac{d\sqrt{2mV-p_0^2}}{\hbar}}}{\left(-1+e^{\frac{2d\sqrt{2mV-p_0^2}}{\hbar}}\right)^2} \cdot O\left(\left[\frac{2\hbar}{Vt}\right]^{\frac{1}{4}} \right)$$

the approximation for $\psi(x,t)$ given by (7.21) can be used for $t \gg \frac{\hbar}{V}$. According to this result, the wave packet leaves the barrier without any time delay, it is instantaneously transmitted through the barrier attenuated by a factor of the magnitude

$$e^{\frac{-d\sqrt{2mV-p_0^2}}{\hbar}}\,.$$

If we investigate the wavefunction for $x < 0$ and $0 < x < d$ we see that the first two terms of 7.10a and the first term of 7.10a equal the solution for the potential step (5.6a, 5.6b). Performing the inverse Laplace transform and making the same approximations as in the previous case we find for the wavepacket to the left of and within the barrier:

$$
\begin{aligned}
&\psi(x,t) \approx \frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy + \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{-ipx}{\hbar}} R(p) f(p)dp + \\
&\sum_{l=0}^{\infty} e^{-\frac{2d(l+1)\sqrt{2mV-p_0^2}}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{-ipx}{\hbar}} R(p)^{2l+1}(R(p)^2-1) f(p)dp \approx \\
&\frac{\kappa}{\sqrt{2\pi t\, i}} \int_{-\infty}^{0} e^{\frac{i(x-y)^2\kappa^2}{2t}} \psi(y,0)dy + \\
&\left\{ 1 + \frac{e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}}}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}} R(p_0)^2} \cdot (R^2(p_0)-1) \right\} R(p_0) \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} e^{\frac{-ipx}{\hbar}} f(p)dp
\end{aligned}
$$

$$\text{for}\, x < 0\,, \tag{7.24}$$

$$
\begin{aligned}
&\psi(x,t) \approx \sum_{l=0}^{\infty} e^{-\frac{(2dl+x)\sqrt{2mV-p_0^2}}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} R(p)^{2l}(R(p)+1) f(p)dp \approx \\
&-\sum_{l=0}^{\infty} e^{-\frac{(2d(l+1)+x)\sqrt{2mV-p_0^2}}{\hbar}} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} R(p)^{2l+1}(R(p)+1) f(p)dp \approx \\
&\left\{ \frac{1}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}} R(p_0)^2} - \frac{e^{\frac{-2(d-x)\sqrt{2mV-p_0^2}}{\hbar}}}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}} R(p_0)^2} \cdot R(p_0) \right\} \\
&\cdot (R(p_0)+1) e^{\frac{-x\sqrt{2mV-p_0^2}}{\hbar}} \cdot \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip^2 t}{2m\hbar}} f(p)dp
\end{aligned}
$$

$$\text{for} \quad 0 < x < d\,. \tag{7.25}$$

The solution within the barrier differs from the solution of the potential step (5.38) only by a time-independent factor. So we see that the time it needs until the barrier is (approximately) empty again, is independent of the thickness of the barrier. The solution on the left side consists of the incoming and the reflected wave packet (7.24). In contrast to the potential step the reflected wavepacket experiences a permanent attenuation, since a part of the wavefunction has tunneled through the barrier. After the reflection process the wavefunction consists of a reflected and a transmitted wavepacket (7.21) only. An explicit calculation yields

$$\left|\left\{1+\frac{e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}}}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}}R(p_0)^2}\cdot(R^2(p_0)-1)\right\}R(p_0)\right|^2+ \tag{7.26}$$

$$\left|\frac{e^{\frac{-d\sqrt{2mV-p_0^2}}{\hbar}}}{1-e^{\frac{-2d\sqrt{2mV-p_0^2}}{\hbar}}R^2(p_0)}(1-R^2(p_0))\right|^2 \;=\; 1\,, \tag{7.27}$$

which confirms that the integral over the probability density is conserved and our approximations are consistent.

7.2 The tunneling time

Within our approximations we found the tunneling time to be zero, since our solution (7.21) indicates that the wavepacket leaves the tunnel, shifted by d to the right. Here we have assumed, that all functions of $R(p)$ can be pulled out of the integral (7.19), and therefore they do not influence the dynamics of the wave packet. If we take into account the first order contributions of $R(p)$, we find a small, but finite tunneling time. We will from now on assume that the initial wave function is an uncorrelated function of the form

$$f(p)=G(p)e^{\frac{-ipx_0}{\hbar}}\,,$$

where $G(p)$ is a real function that yields a momentum expectation value p_0. The position expectation value is then given by x_0.

An additional factor

$$Z(p)\equiv R(p)^{2l}(1-R(p)^2)$$

has an impact on the momentum as well as on the position expectation value of the initial wavepacket $f(p)$. We write

$$Z(p)f(p)=z(p)e^{i\mu(p)}f(p)\,,\text{where}\quad z(p)=|Z(p)|\,.$$

The probability density in momentum space is only affected by the absolute value $z(p)$. If we restrict ourselves to first order contributions in $p-p_0$,

$$z(p)\approx z(p_0)+z_1(p-p_0)$$

we find that we can neglect the momentum shift:

$$N^2\equiv\int_{-\infty}^{\infty}|f(p)|^2z(p)^2dp\approx z(p_0)^2\int_{-\infty}^{\infty}|f(p)|^2dp \;=z(p_0)^2 \tag{7.28}$$

$$\langle\hat{p}\rangle \;=\; N^{-2}\int_{-\infty}^{\infty}p|f(p)|^2z(p)^2dp \tag{7.29}$$

$$\approx p_0+2(z(p_0))^{-1}z_1\int_{-\infty}^{\infty}|f(p)|^2p(p-p_0)dp\approx p_0\,. \tag{7.30}$$

Using also a linear approximation for $\mu'(p)$

$$\mu'(p) \approx \mu_1 + \mu_2(p - p_0)$$

we find for the position expectation value

$$\langle x \rangle = N^{-2} \int_{-\infty}^{\infty} z(p) f^*(p) e^{-i\mu(p)} \left(i\hbar \frac{\partial}{\partial p} \right) z(p) f(p) e^{i\mu(p)} dp = \tag{7.31}$$

$$N^{-2} x_0 \int_{-\infty}^{\infty} G(p)^2 z(p)^2 dp - N^{-2} \hbar \int_{-\infty}^{\infty} G(p)^2 z(p)^2 \mu'(p) dp \tag{7.32}$$

$$\approx x_0 - \hbar \mu_1 \,. \tag{7.33}$$

Therefore the phase of the functions

$$R(p)^{2l}(1 - R(p)^2) \tag{7.34}$$

in (7.19) yields a a shift of the position of each particular wave packet of (7.21). We find

$$Arg\left[1 - R(p)^2\right] = Arctan\left[\frac{-1+2l}{2\sqrt{k-k^2}}\right] \approx Arctan\left[\frac{-1+2k_0}{2\sqrt{k_0-k_0^2}}\right] + \frac{2}{\sqrt{2mV - p_0^2}} \cdot (p - p_0) \tag{7.35}$$

$$Arg\left[R(p)\right] = -Arccos\left[1 - 2k\right] \approx -Arccos\left[1 - 2k_0\right] + \frac{2}{\sqrt{2mV - p_0^2}} \cdot (p - p_0)\,, \tag{7.36}$$

where we have used the definitions

$$k = \frac{p^2}{2mV}\,, \quad k_0 = \frac{p_0^2}{2mV}\,.$$

So we see that the lth term of (7.21) will experience a shift of

$$\frac{2(1+2l)}{\sqrt{2mV - p_0^2}}\,,$$

corresponding to a translation by

$$\frac{2(1+2l)\hbar}{\sqrt{2mV - p_0^2}}$$

to the left. So the delay time will be

$$T_l = \frac{2(1+2l)m\hbar}{p_0\sqrt{2mV - p_0^2}}$$

instead of zero. For thick barriers, if

$$d\frac{\sqrt{2mV - p_0^2}}{\hbar} \gg 1\,,$$

the first term will dominate the sum (7.21), and the tunneling time will be given by T_0. This is exact the time Hartmann ([34])found as upper limit for the tunneling time through thick barriers. If the barrier gets thinner the other wavepackets for $l > 0$ will also come into play. Each of them leaves the barrier at a different time T_l. But since they appear very shortly after each other they will look like one smeared out wavepacket with a delay time bigger than T_0. According to our calculations a contributions to the tunneling times that are proportional to the thickness of the barrier could only come from higher order contributions in $p - p_0$ that might yield a correction to smaller momenta.

7.3 Summary and discussion of the literature

There are several definitions of tunneling times and the discussion about their meaning is still ongoing ([30],[31],[29],[32]). Recently, experiments with atoms stimulated by ultrashort, infrared laser pulses, the so-called attoclock experiments, reinforced the interest in the prediction of tunneling times ([32]). Here we will only mention the so-called group delay or phase time τ_g. The solution of the time-dependent Schrödinger equation is represented as the integral over stationary solutions for different energies. Under the assumption that the energy distribution of the initial wave packet is sufficiently peaked the application of the stationary phase method yields a time for the arrival of the peak of the wavepacket at the end of the barrier that allows the determination of a traversal time through the barrier. One of the oldest results for tunneling times was obtained with this method. In 1932 Mac Coll ([33]) concluded that there was "no appreciable delay in the transmission of the packet through the barrier". These calculations were later refined by Hartmann ([34],[30]), who found a finite delay time. Moreover for thicker barriers this delay time becomes independent of the thickness of the barrier

$$\tau_{g\infty} = \frac{2m\hbar}{\sqrt{2mV - p_0^2}p_0} \ , \tag{7.37}$$

which is known as the Hartmann effect. We found that what hat comes out of the barrier is not a single wave packet, but infinitely many, one after the other. The time each of these wavepackets needs for the tunneling is completely independent of the thickness of the barrier. For thicker barriers, the later wavepackets are much more attenuated and there is only one relevant tunneling time which coincides with the delay time found by Hartmann.

Bernardini ([35]) got a similar result for the transmission of wave packets with energies higher than V. He finds that there is not only one reflected and one transmitted wave packet, but many of them that leave the barrier one after the other. This result was obtained by the decomposition of the transmission and reflection coefficients of the stationary solution in infinite series. Our result is the counterpart in the tunneling regime.

Part II

Quantum Cosmology

Chapter 8

Unimodular gravity and the Einstein equations

The variation of the action with respect to the metric $g_{\mu\nu}$ under the condition $\det g_{\mu\nu} = -1$ yields the Einstein equations with an unspecified cosmological constant. This theory is called unimodular gravity. Though it is physically indistinguishable from general relativity with a given cosmological constant the canonical formalism of this theory differs remarkably from canonical general relativity. Therefore unimodurar gravity also yields a fundamentally different quantum theory.

The Einstein-Hilbert action of general relativity is given by

$$S_{EH} = \frac{1}{2\kappa} \int_{\mathcal{M}} d^4x \sqrt{-g}\,(R - 2\Lambda) - \frac{1}{\kappa} \int_{\partial\mathcal{M}} d^3x \sqrt{h}\, K \,, \tag{8.1}$$

where

$$\kappa = \frac{8\pi G}{c^4}$$

contains the velocity of light c and the gravitational constant G. The second integral is defined on the spacelike boundary $\partial\mathcal{M}$ of the considered space-time region $\mathcal{M}$. The space-time metric $g_{\mu\nu}$ with $det\, g_{\mu\nu} \equiv g$ induces a three-dimensional metric h_{ab} with $det\, h_{ab} \equiv h$ on the boundary $\partial\mathcal{M}$. The corresponding second fundamental form is denoted by K_{ab} with the trace K. Since the cosmological constant Λ already appears in the action, it is also a constant of nature that has to be determined experimentally. In addition to the Einstein Hilbert action we have to take into account the matter action S_m that describes the fields. The variation of $S_{EH} + S_m$ with respect to the metric yields the Einstein equations

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = \kappa\, T_{\mu\nu} - \Lambda\, g_{\mu\nu}, \tag{8.2}$$

where the energy- momentum tensor is given by

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta S_m}{\delta g^{\mu\nu}}\,. \tag{8.3}$$

(We use the metric signature (-1,1,1,1) and the Riemann tensor is defined according to the convetion $R^{\alpha}_{\beta\gamma\delta} = \Gamma^{\alpha}_{\beta\gamma,\delta} - \dots ; thetimecoordinateisgivenbyx^0 = ct$).

The covariant divergence of the Einstein tensor $G_{\mu\nu}$ with respect to the metric is zero as a consequence of the Bianchi identity,

$$G_{\mu\nu}{}^{;\nu} = 0\,. \tag{8.4}$$

According to the Einstein equations this has also to be true for the energy momentum tensor,

$$T_{\mu\nu}^{;\nu} = 0\,. \tag{8.5}$$

Nevertheless (8.5) can be proven independently as a consequence of the invariance of the matter action integral with respect to coordinate transformations (see [36]).

We obtain unimodular gravity if we vary the action under the restriction $-g = 1$. This problem can be solved by introducing a Lagrangian multiplier $\Lambda(x)$ and varying the action functional ([37])

$$S_U \equiv S_{EH} + S_m + \int_{\mathcal{M}} d^4x\, 2\Lambda(x)\left(1 - \sqrt{-g}\right)$$

with respect to $g_{\mu\nu}(x)$ and $\Lambda(x)$. Applying

$$\delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta g^{\mu\nu}$$

we obtain the equations

$$G_{\mu\nu} = \kappa\, T_{\mu\nu} - \Lambda(x)\, g_{\mu\nu} \tag{8.6a}$$
$$\sqrt{-g} - 1 = 0\,. \tag{8.6b}$$

Since the covariant divergence of the Einstein tensor and the energy momentum tensor are both zero (8.4,8.5) the derivative of $\Lambda(x)$ has also to be zero and Λ is a constant:

$$\begin{aligned} 0 &= (\Lambda(x)g_{\mu\nu});^{\nu} = \Lambda(x),^{\nu} g_{\mu\nu} = \Lambda(x),_{\mu} \\ \Rightarrow &\quad \Lambda(x) \equiv \Lambda\,. \end{aligned}$$

Any solution of unimodular gravity (8.6) is also a solution of general relativity (8.2) for a specific cosmological constant and vice versa. The only difference between the two theories is, that Λ is a natural constant in general relativity while it is a conserved quantity in unimodular gravity. But since in both theories the cosmological constant can not vary over the whole universe, we would have to investigate different universes to determine if solutions with different Λ exist (unimodular theory) or if Λ is a "true" natural constant. So the two theories are practically indistinguishable.

8.1 Canonical general relativity

In this section we summarize the steps that lead to the canonical formulation of general relativity, we mainly follow the presentation in [38].

The implementation of the Hamiltonian formalism in general relativity requires the choice of a time function t and a timelike vector field t^μ such that the surfaces of constant time Σ_t are spacelike Cauchy hypersurfaces and such that $t,_\mu t^\mu = 1$ is fulfilled. The space-time metric $g_{\mu\nu}$ induces a metric $h_{\mu\nu}$ on Σ_t which is given by

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu \, ,$$

where n^μ denotes the unit normal to Σ_t. The decomposition of t^μ into its components normal and tangential to Σ_t

$$t^\mu = N n^\mu + N^\mu \, ,$$

yields the lapse function N and the shift vector N^μ. Both $h_{\mu\nu}$ and N^μ are three-dimensional objects and can be identified with their embeddings in Σ_t, h_{ab} and N^a. The decomposition of the space-time metric then reads

$$\begin{pmatrix} N_c N^c - N^2 & N_b \\ N_b & h_{ab} \end{pmatrix} . \tag{8.7}$$

The determinant of the metric is determined by $g = -N^2 \, h$. Applying this decomposition to the Einstein Hilbert action (8.1) gives the Langrangian density of the gravitational field

$$\mathcal{L}_G = \frac{1}{2\kappa} N\sqrt{h} \left(K_{ab}K^{ab} - K^2 + R_3 - 2\Lambda \right) \, , \tag{8.8}$$

where R_3 denotes the curvature scalar on Σ_t. K_{ab} is the extrinsic curvature of Σ_t with respect to $g_{\mu\nu}$ in the coordinates of the hypersurface

$$K_{ab} = \frac{1}{2N} \left(\dot{h}_{ab} - N_{a|b} - N_{b|a} \right) \, ,$$

where $|$ denotes the covariant derivative with respect to h_{ab}. The dot denotes the partial derivative with respect to the time coordinate determined by the vector field t^μ and the hypersurface foliation of the spacetime. The canonical variables of the theory are N, N^a, h_{ab} and the fields ϕ_A contained in the matter Lagrangian $\mathcal{L}_m(\phi_A, h_{\mu\nu})$. The Euler-Lagrange equations with respect to the Lagrange density $\mathcal{L} = \mathcal{L}_G + \mathcal{L}_m$ for these variables are equivalent to the Einstein equations. Since the Langrangian density does not depend on $\dot{N}, \dot{N}^a$, the Euler-Lagrange equations imply that the initial data of the canonical variables can not be chosen independently. Therefore the Hamiltonian equations of motion must be determined according to the so-called Dirac-Bergmann algorithm ([38],[39]).

The momenta are determined as usual

$$p_N \equiv \frac{\partial \mathcal{L}}{\partial \dot{N}} = 0 \, , \qquad p_a \equiv \frac{\partial \mathcal{L}}{\partial \dot{N}^a} = 0 \, , \tag{8.9}$$

$$p^{ab} \equiv \frac{\partial \mathcal{L}}{\partial \dot{h}_{ab}} = \frac{\sqrt{h}}{2\kappa} \left(K^{ab} - K h^{ab} \right) \, , \qquad p^A \equiv \frac{\partial \mathcal{L}_m}{\partial \dot{\phi}_A} \, . \tag{8.10}$$

The primary constraints of the theory are

$$p_N = 0 \,, \quad p_a = 0 \,.$$

The canonical Hamiltonian density of the theory reads

$$\mathcal{H}_c = \dot{h}_{ab} p^{ab} - \mathcal{L}_G + \mathcal{H}_m = N\,\mathcal{C} + N^a \mathcal{C}_a + \mathcal{H}_m \,, \tag{8.11}$$

where $\mathcal{H}_m$ denotes the canonical matter Hamiltonian density and $\mathcal{C}$ and $\mathcal{C}_a$ are given by

$$\mathcal{C} \equiv \frac{2\kappa}{\sqrt{h}} \left(p^{ab} p_{ab} - p^2 \right) - \frac{\sqrt{h}}{2\kappa} \left(R_3 - 2\Lambda \right) \,, \tag{8.12a}$$

$$\mathcal{C}_a \equiv -2 \left(p^{ab}{}_{|b} \right) \,. \tag{8.12b}$$

Moreover a total divergence was discarded from $\mathcal{H}_c$. This is justified, if Σ_t is assumed to be closed since the contribution to the total energy would be zero. In order to get the correct equations of the theory it is necessary to introduce the total Hamiltonian density

$$\mathcal{H}_T = \mathcal{H}_c + Z \cdot p_N + Z^a \cdot p_a \,,$$

where Z and Z^a are arbitrary functions of the canonical variables. The dynamics of the variables is then determined by the Hamiltonian equations with respect to $\mathcal{H}_T$ under the additional condition $p_N = p_a = 0$. Since the primary constraints have to be preserved in time the Poisson brackets yield further constraints for the canonical variables:

$$\{p_N, H_c\} = 0 \,, \{p_a, H_c\} = 0 \,. \tag{8.13}$$

For vacuum spacetimes ($\mathcal{H}_m = 0$) we find for the secondary constraints

$$\mathcal{C} = 0 \tag{8.14a}$$

$$\mathcal{C}_a = 0 \,. \tag{8.14b}$$

These equations are called the constraints of general relativity. The first one (2.1)is called Hamiltonian constraint, whereas (8.14b) are the diffeomorphism constraints. The secondary constraints are preserved automatically. The Poisson bracket with $\mathcal{H}_T$ does not yield further constraints, since the algebra of constraints is closed. Therefore there are no tertiary constraints.

The dynamics of N, N^a is determined by the arbitrary functions Z, Z^a. The remaining variables h_{ab}, p^{ab} evolve according to the Hamiltonian equations with respect to

$$\mathcal{H}_g \equiv N\,\mathcal{C} + N^a \mathcal{C}_a \,,$$

with the initial conditions $\mathcal{C} = \mathcal{C}_a = 0$.

If matter is involved the secondary constraints (8.14)contain additional terms and the dynamics is determined by the Hamiltonian density

$$\mathcal{H} = N(\mathcal{C} + \mathcal{C}^m) + N^a(\mathcal{C}_a + \mathcal{C}_a^m) \tag{8.15a}$$

and the initial conditions

$$\mathcal{C} + \mathcal{C}^m = 0\,, \tag{8.15b}$$
$$\mathcal{C}_a + \mathcal{C}_a^m = 0\,. \tag{8.15c}$$

8.2 Canonical unimodular gravity

In this section we review the canonical analysis of vacuum unimodular gravity that was performed in [37]. Since the 3 +1 decomposition of the metric (8.7) implies $\sqrt{-g} = N\sqrt{h}$, the restriction of unimodular theory $\sqrt{-g} = 1$ yields

$$N = h^{-\frac{1}{2}}\,. \tag{8.16}$$

We find then for the Lagrangian density of unimodular gravity

$$\mathcal{L}_G^{uni} = \frac{1}{2\kappa}\left(K_{ab}K^{ab} - K^2 + R_3\right)\,, \tag{8.17}$$

with

$$K_{ab} = \frac{\sqrt{h}}{2}\left(\dot{h}_{ab} - N_{a|b} - N_{b|a}\right)\,.$$

Since the lapse function is a fixed quantity the remaining canonical variables are N^a, h_{ab}, ϕ_A. The primary constraints of the theory are

$$p_a \equiv \frac{\partial \mathcal{L}}{\partial \dot{N}^a} = 0\,, \tag{8.18}$$

which yields the canonical Hamiltonian density

$$\mathcal{H}_c^{uni} = \dot{h}_{ab}p^{ab} - \mathcal{L}_G^{uni} = h^{-\frac{1}{2}}\,\mathcal{C} + N^a\mathcal{C}_a\,, \tag{8.19}$$

where $\mathcal{C}, \mathcal{C}_a$ are defined as in the previous section (8.12), with zero cosmological constant. This yields for the total Hamiltonian density

$$\mathcal{H}_T^{uni} = \mathcal{H}_c + Z^a \cdot p_a = \widetilde{\mathcal{H}}_0 + N^a\mathcal{C}_a + \mathcal{H}_m + Z^a \cdot p_a\,,$$

where we have introduced

$$\widetilde{\mathcal{H}}_0 \equiv h^{-\frac{1}{2}}\,\mathcal{C}\,,$$

and Z^a are arbitrary functions of the canonical variables.

For vacuum spacetimes the conservation of the primary constraints (8.18) yields the secondary constraints

$$\mathcal{C}_a = 0\,. \tag{8.20}$$

But in contrast to canonical general relativity, $\mathcal{C}$ does not represent a secondary constraint and therefore the Hamiltonian $\mathcal{H}_T^{uni}$ will not be zero on the constraint surface. Instead the conservation of the secondary constraints (8.20) yields according to the contraint algebra ([37])

$$\dot{\mathcal{C}}_a = \{\mathcal{C}_a, H_T\} = \left\{\mathcal{C}_a, \widetilde{\mathcal{H}}_0 + N^b\mathcal{C}_b\right\} = \mathcal{C}_{b,a}N^b + \mathcal{C}_b N^b_{\ ,a} + \widetilde{\mathcal{H}}_{0,a}\,.$$

This expression will vanish, if in the addition to the secondary contraints (8.20), also the tertiary constraints

$$\widetilde{\mathcal{H}}_{0,a} = 0$$

are fulfilled. This means that $\tilde{\mathcal{H}}_0$ has to remain constant which is equivalent to the constraint $\mathcal{C} = 0$ of general relativity with an arbitrary cosmological constant 8.14a. Because of the properties of the constraint algebra there are no quaternary constraints. The dynamics of h_{ab}, p^{ab} is therefore determined by

$$\mathcal{H}_g^{uni} = \widetilde{\mathcal{H}}_0 + \mathcal{C}_a N^a \tag{8.21}$$

and the initial conditions

$$C_a = 0, \quad \widetilde{\mathcal{H}}_{0,a} = 0\,. \tag{8.22}$$

Unimodular gravity is no longer time reparametrization invariant. Giving the theory again a reparametrization invariant form, Henneaux and Teitelboim have shown that the time difference in unimodular time between an initial and a final closed hypersurface equals the invariant four volume ([37]).

8.3 Unimodular quantum gravity and the problem of time

In canonical quantum gravity the operators that correspond to the canonical variables are implemented as functional operators, acting on the wavefunctional $\Psi[h_{ab}]$

$$\widehat{h}_{ab}\Psi[h_{ab}] = h_{ab}\Psi[h_{ab}]\,,$$
$$\widehat{p}^{ab}\Psi[h_{ab}] = -i\hbar\frac{\delta}{\delta h_{ab}}\Psi[h_{ab}]\,.$$

With the choice of an appropriate operator ordering, the constraints can then be expressed be as operators. The classical constraint equations (8.14) become according to the so-called Dirac quantization ([38])

$$\widehat{\mathcal{C}}\,\Psi = 0\,, \tag{8.23}$$

$$\widehat{\mathcal{C}_a}\,\Psi = 0\,. \tag{8.24}$$

It can be shown that the diffeomorphism constraint (8.24) ensures that the wave functional is invariant under three-dimensional coordinate transformations and therefore only depends on the three geometry. The Hamiltonian constraint equation is called the Wheeler-de Witt equation.

In the case of minisuperspace quantization where the three-geometry is determined by symmetry reduction (as for instance for a homogeneous and isotropic universe), it is the only remaining equation of canonical quantum gravity. If matter is added to the minisuperspace, the Wheeler-de Witt equation becomes a differential equation that only contains the scale factor of the universe and the matter variables. Because the Hamiltonian operator is just a sum of the constraints, the corresponding equation reads

$$\widehat{\mathcal{H}}\Psi = 0\,,$$

and according to most interpretations of quantum gravity ([38]), time has disappeared from the theory. This is not only hard to accept from a phenomenological point of view. The so-called frozen time formalism also implies difficulties when observables come into play, since in general, the observables will not commute with the Hamiltonian

$$\left[\widehat{O}, \widehat{\mathcal{H}}\right] \neq 0\,.$$

Even in the simplest case of a minisuperspace resulting from the quantization of a homogeneous universe and choosing the scale factor a as observable we find

$$\left[a, \widehat{H}_{mini}\right] \neq 0\,.$$

Some authors ([40]) try to use this relation to determine a time evolution from the Heisenberg equation

$$\left[\hat{a}(\tau), \widehat{H}_{mini}\right]\psi = \frac{i}{\hbar}\frac{\partial}{\partial\tau}\hat{a}(\tau)\,.$$

Another answer to this problem is to admit only observables that commute with the constraints, the so-called perennials which would exclude fundamental variables.

In contrary, the Hamiltonian of unimodular gravity does not equal zero. In addition to the quantum version of the secondary and tertiary constraint, unimodular quantum gravity contains a Schrödinger equation of the form [41]

$$i\hbar\frac{\partial}{\partial t}\Psi = \int \widehat{\widetilde{\mathcal{H}}}_0 dx^3 \Psi\,, \tag{8.25}$$

wher $\Psi\left[h_a, t\right]$ depends on the spatial geometry and on the time t. It must be admitted that this result also has its weak aspects. The time variable here is not on equal footing with the spatial geometry. There is no time expectation value, and time remains a classical variable. On the other hand it has lost its classical general relativistic meaning where time is always measured by an observer on a given worldline with respect to a certain geometry. This was especially pointed out by [42]. Nevertheless the interest in unimodular gravity has returned in the last years ([43], [44], [45]).

Moreover we think that apart from providing a time evolution there is another interesting aspect of unimodular quantum gravity: Instead of enforcing an operator version of a classical equation, it admits a superposition of eigensolutions with different cosmological constants

$$\Psi = \int e^{-i\Lambda t/\hbar} \Psi_\Lambda d\Lambda \,,$$
$$\text{with} \quad \Lambda \Psi_\Lambda = \int \widehat{\widetilde{\mathcal{H}}}_0 dx^3 \Psi_\Lambda \,.$$

With an appropriate scalar product equation (8.25) ensures that the expectation value of the Hamiltonian is conserved. This resembles much more the usual relation between quantum and classical mechanics where classical identities are transformed into relations between expectation values and not into operator identities. The counterpart of a classical solution $p = 0$ is not a constant function that would fulfill $\widehat{p}\,\psi = 0$, but a wavefunction with vanishing momentum expectation value $\langle \psi \,| \widehat{p} |\, \psi \rangle$=0.

Chapter 9

The flat Friedmann universe with a scalar field

Considering homogeneous and isotropic spacetimes we obtain the Euler-Lagrange equations for a flat Friedmann universe according to general relativity. We show that they are equivalent to the equations of unimodular theory for an appropriate choice of the lapse function. We assume that the matter is characterized by a scalar field. We determine the Hamiltonian for this model according to unimodular gravity and investigate the solutions of the field equations for the special case of a massless field.

The metric of a homogeneous and isotropic spacetime (Friedmann universe)

$$ds^2 = -N^2(t)c^2dt^2 + a^2(t)d\Omega_3^2 \tag{9.1}$$

is characterized by the lapse function and the scale factor $a(t)$. If the spatial curvature is zero, $d\Omega_3^2$ is the line element of three-dimensional flat space.

Inserting the metric into the Einstein-Hilbert action yields ([38])

$$S_{EH} = \frac{3}{\kappa}\int dt\, N\left(-\frac{\dot{a}^2 a}{c^2N^2} - \frac{\Lambda}{3}a^3\right) v_0\,,\,.$$

where v_0 is is the volume of the spacelike slices: $v_0 = \int d\Omega_3^2$.

The action of a scalar field in curved spacetime reads

$$S_m = \int_{\mathcal{M}} d^4x\,\sqrt{-g}\,\left(-\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - V(\phi)\right)\,. \tag{9.2}$$

If

$$V(\phi) = \left(\frac{m_0 c}{\hbar}\right)^2 \frac{\phi^2}{2}$$

the varation with respect to ϕ yields the Klein-Gordon equation for a particle with mass m_0

$$\nabla_\mu \nabla^\mu \phi = \left(\frac{m_0 c}{\hbar}\right)^2 \phi\,. \tag{9.3}$$

Since we consider a spatial homogeneous spacetime, the spatial derivatives of the field must be zero. Inserting (9.1), we find

$$S_m = \int dt\, N a^3 \left(\frac{\dot{\phi}^2}{2N^2c^2} - V(\phi)\right) v_0\,. \tag{9.4}$$

Therefore the Langrange function reads

$$L = v_0 \epsilon N \left(-\frac{\dot{a}^2 a}{c^2 N^2} - \Lambda \frac{a^3}{3}\right) + v_0 N a^3 \left(\frac{\dot{\phi}^2}{2N^2c^2} - V(\phi)\right)\,, \tag{9.5}$$

where we have introduced the abbreviation $\epsilon \equiv 3/(\kappa)$. If we incorporate v_0 into the variables a and N as well as $V(\phi)$, Λ by rescaling

$$a \to v_0^{\frac{1}{6}} a\,, \quad N \to v_0^{-\frac{1}{2}} N\,, \quad \Lambda \to v_0 \Lambda\,, \quad V(\phi) \to v_0 V(\phi)\,, \tag{9.6}$$

we find for the rescaled Lagrangian

$$L = \epsilon N \left(-\frac{\dot{a}^2 a}{c^2 N^2} - \Lambda \frac{a^3}{3}\right) + N a^3 \left(\frac{\dot{\phi}^2}{2N^2c^2} - V(\phi)\right)\,. \tag{9.7}$$

The variation with respect to N, a, ϕ yields the three equations:

$$\delta\phi: \quad G_1 \equiv \frac{\ddot{\phi}}{N^2c^2} + 3\frac{\dot{\phi}}{N^2c^2}\frac{\dot{a}}{a} - \frac{\dot{\phi}\dot{N}}{c^2N^3} + V'(\phi) = 0\,, \tag{9.8a}$$

$$\delta N: \quad G_2 \equiv -\left(\frac{\dot{a}}{aNc}\right)^2 + \frac{\Lambda}{3} + \frac{1}{\epsilon}\left(\frac{\dot{\phi}^2}{2N^2c^2} + V(\phi)\right) = 0\,, \tag{9.8b}$$

$$\delta a: \quad G_3 \equiv -\left(\frac{\dot{a}}{aNc}\right)^2 + \Lambda - \frac{3}{\epsilon}\left(\frac{\dot{\phi}^2}{2N^2c^2} - V(\phi)\right) - \frac{2}{c^2 N a}\frac{d}{dt}\left(\frac{\dot{a}}{N}\right) = 0\,. \tag{9.8c}$$

Since

$$(3\,G_2 - G_3)\frac{\dot{a}}{a} - \frac{d}{dt}G_2$$

is equivalent to G_2, the system of equations (9.8) can be reduced to two equations

$$G_1 = \frac{\ddot{\phi}}{N^2c^2} + 3\frac{\dot{\phi}}{N^2c^2}\frac{\dot{a}}{a} - \frac{\dot{\phi}\dot{N}}{c^2N^3} + V'(\phi) = 0\,, \tag{9.9a}$$

$$G_2 \equiv -\left(\frac{\dot{a}}{aNc}\right)^2 + \frac{\Lambda}{3} + \frac{1}{\epsilon}\left(\frac{\dot{\phi}}{2N^2c^2} + V(\phi)\right) = 0\ , \tag{9.9b}$$

where (9.9b) is the Hamiltonian constraint (8.15b) of our model.

In the unimodular theory he lapse function (8.16)is determined by $N = a^{-3}$ and the Friedmann metric (with unscaled quantities) has the form

$$ds^2 = -(c^2/a^6(t))dt^2 + a^2(t)d\Omega_3^2 \tag{9.10}$$

Note that the condition $Na^3 = 1$ is not influencde by the scaling (9.6). This yields for the Lagrange function (9.7)

$$L_{uni} = \epsilon(-\frac{\dot{a}^2a^4}{c^2}) + a^6\frac{\dot{\phi}^2}{2c^2} - V(\phi)\,. \tag{9.11}$$

We obtain by the variation with respect to a and ϕ

$$\delta\phi_{uni}: \qquad \frac{\ddot{\phi}a^6}{c^2} + 6\frac{\dot{\phi}a^5\dot{a}}{c^2} + V'(\phi) = 0 \tag{9.12a}$$

$$\delta a_{uni}: \qquad 4\dot{a}^2a^3 + 3\frac{1}{\epsilon}\dot{\phi}^2a^5 + 2\ddot{a}a^4 = 0 \tag{9.12b}$$

The system of equations (9.12) is equivalent (9.8) for certain choice of Λ and for the lapse function $N = 1/a^3$. In particular (9.8a) is equivalent to (9.12a). Inserting (9.12a) into (9.12b) yields

$$\frac{d}{dt}G_2 = 0\,.$$

This confirms the practical equivalence of general relativity and unimodular theory, as we discussed in the previous chapter in the general case. Whereas the Lagrange function of general relativity (9.7) yields the primary constraint

$$p_N \equiv \frac{\partial\mathcal{L}}{\partial\dot{N}} = 0$$

the Lagrange (9.11)function of the unimodular theory produces no constraints and the formulation of the Hamiltonian version of the theory can be performed as usual.

The momenta conjugate to the variables a and ϕ read

$$p_\phi = \frac{1}{c^2}\dot{\phi}a^6 \qquad p_a = -\frac{2\epsilon}{c^2}\dot{a}a^4\,. \tag{9.13}$$

We obtain for the Hamiltonian of the unimodular theory

$$H_{uni} = \frac{c^2}{2}\frac{p_\phi^2}{a^6} - \frac{c^2}{4\epsilon}\frac{p_a^2}{a^4} + V(\phi) \tag{9.14}$$

The Hamiltonian is a conserved quantity. If we write the Hamiltonian as a function of the configuration variables a, p_ϕ and their derivatives

$$H_{uni} == \frac{1}{2c^2}\dot{\phi}^2a^6 - \frac{\epsilon}{c^2}\dot{a}^2a^4 + V(\phi) \tag{9.15}$$

we find that

$$H_{uni} \equiv -\frac{\Lambda\epsilon}{3}$$

equals the Hamiltonian constraint of general relativity for $N = 1/a^3$. We see that this special labeling of the conserved quantity makes the solutions of unimodular gravity and general relativity coincide.

9.1 The flat Friedmann universe with a massless scalar field

The simplest case of a matter Lagrangian is $V = 0$, which would correspond to the field of a massless particle with spin zero (9.3). If instead a perfect fluid matter model is chosen, the solutions for a massless scalar field can be shown to be equivalent to the solutions for the special case of stiff matter (see Appendix B).

The Hamiltonian reads

$$H_{uni} = \frac{c^2}{2}\frac{p_\phi^2}{a^6} - \frac{c^2}{4\epsilon}\frac{p_a^2}{a^4}\,. \tag{9.16}$$

According to the equations of motion p_ϕ is a conserved quantity

$$\dot{p}_\phi = 0 \tag{9.17}$$

and the time-dependence of the field is given by

$$\dot{\phi} = \frac{p_\phi c^2}{a^6}\,. \tag{9.18}$$

If we assume $p_\phi = 0$, we obtain the de-Sitter solutions with $\Lambda > 0$, since a constant field

$$\dot{\phi} = 0 \tag{9.19}$$

is equivalent to zero matter density $\rho = 0$ in the perfect fluid model(see Appendix B). The conservation of the Hamiltonian

$$-\frac{c^2}{4\epsilon}\frac{p_a^2}{a^4} = H_{uni} = -\frac{\Lambda\epsilon}{3}$$

implies

$$\frac{\epsilon}{c^2}(\dot{a}a^2)^2 = \frac{\Lambda\epsilon}{3}\,.$$

We then find for the scale factor

$$a = (\sqrt{3\Lambda}ct)^{\frac{1}{3}} \tag{9.20}$$

This is the solution in unimodular theory which correspond to a solution in general relativity with $N = 1/a^3$.

If we express the solution in terms of the cosmological time Θ, that is defined by

$$d\theta = N\sqrt{v_0}dt\,,$$

we obtain

$$\theta = \int_{t_0}^{t} N\sqrt{v_0}dt = \frac{\sqrt{v_0}}{\sqrt{3\Lambda}c}\ln\frac{t}{t_0}\,,$$

which yields the de-Sitter solution in its usual form

$$a(\theta) = (\sqrt{3\Lambda}ct_0)^{\frac{1}{3}}e^{\theta c\sqrt{\frac{\Lambda}{3v_0}}}\,.$$

if $p_\phi \neq 0$,

$$-\frac{c^2}{4\epsilon}\frac{p_a^2}{a^4} + \frac{c^2p_\phi^2}{2a^6} = -\frac{\Lambda\epsilon}{3}$$

yields

$$\frac{\dot{a}^2a^{10}}{c^2} = \frac{\Lambda}{3}a^6 + \frac{1}{\epsilon}\frac{p_\phi^2c^2}{2}\,.$$

We obtain

$$a(t) = \left(6\sqrt{\frac{p_\phi^2}{2\epsilon}}ct + 3\Lambda\,c^2\,t^2\right)^{1/6} \tag{9.21a}$$

$$\phi(t) = \frac{1}{6}\sqrt{2\epsilon}Sign[p_\phi]\ln\left[\frac{t\,Z}{1+\frac{\Lambda}{2}\sqrt{\frac{2\,\epsilon}{p_\phi^2}}\,t}\right]\,, \tag{9.21b}$$

where Z is an integration constant that determines $\phi(0)$. For the scale factor we have assumed $a(0) = 0$.

Chapter 10

Quantization of a flat Friedmann universe with a massless scalar field

The canonical quantization of minisuperspaces according to unimodular gravity yields a Schrödinger equation for the wavefunction of the universe. For the case of a flat Friedmann universe with a massless scalar field, we obtain a class of wavepacket solutions that undergo a unitary time evolution. We investigate the expectation values of two characteristic variables and find that their longterm behaviour coincides with the classical time evolution.

The canonical quantization of the unimodular Hamiltonian of the model 9.16 yields

$$\hat{p}_a = -i\hbar \frac{\partial}{\partial a}\,, \quad \hat{p}_\phi = -i\hbar \frac{\partial}{\partial \phi}\,, \tag{10.1}$$

$$\widehat{H} = \frac{\hbar^2 c^2}{4\epsilon} \frac{1}{a^5} \frac{\partial}{\partial a} a \frac{\partial}{\partial a} - \frac{\hbar^2 c^2}{2} \frac{1}{a^6} \frac{\partial^2}{\partial \phi^2}\,.$$

Here we have chosen a factor ordering that gives the part of the Hamiltonian that is quadratic in the momenta the form of a Laplace Beltrami operator ([38])

$$G^{AB} p_A p_B \quad \Rightarrow \quad -\frac{\hbar^2}{\sqrt{-G}} \frac{\partial}{\partial x^A} G^{AB} \sqrt{-G} \frac{\partial}{\partial x^B}\,. \tag{10.2}$$

This operator is invariant with respect to a coordinate transformation if the metric G^{AB} tranforms as a covariant tensor.

This special form of operator ordering ensures that the quantization of the Hamiltonian commutes with a coordinate transformation if we understand classical coordinate tranformations as canonical point tranformations (see also [46],[47]). If we assume that the coordinate tranformation is given by

$$f^A{}_B = \frac{\partial \widetilde{x}^A}{\partial x^B},$$

the canonical momenta are transformed according to

$$p_A = f^B{}_A \widetilde{p}_B \,,$$

The canonical transformed Hamiltonian equals the original one and the part that is quadratic in the momenta therefore reads

$$G^{AB} p_A p_B = \widetilde{G}^{AB} \widetilde{p}_A \widetilde{p}_B \quad \text{where} \quad \widetilde{G}^{AB} = f^A{}_C f^B{}_D G^{CD} \,.$$

A quantization of this Hamiltonian with respect to the transformed momenta

$$\hat{p}_A = -i\hbar \frac{\partial}{\partial \widetilde{x}^A} \,, \quad \hat{p}_B = -i\hbar \frac{\partial}{\partial \widetilde{x}^B} \,, \tag{10.3}$$

and the operator ordering (10.2) yields the same result as a direct coordinate transformation of the Laplace Beltrami operator.

The evolution of the wavefunction $\psi(a, \phi, t)$ is determined by

$$\widehat{H}\psi = i\hbar \frac{\partial}{\partial t}\psi \,. \tag{10.4}$$

The Hamiltonian is symmetric with respect to the inner product defined by the measure $a^5 da d\phi$, where $a \in (0, \infty)$ and $\phi \in (-\infty, \infty)$.

With the transformation

$$A = a^3/3 \qquad B = \frac{3}{\sqrt{2\epsilon}}\phi \,, \tag{10.5}$$

and the volume element $3\sqrt{2\epsilon} A dA dB$, the Hamiltonian assumes the form

$$\widehat{H} = \frac{\hbar^2 c^2}{4\epsilon} \left\{ \frac{1}{A}\frac{\partial}{\partial A} A \frac{\partial}{\partial A} - \frac{1}{A^2}\frac{\partial^2}{\partial B^2} \right\} \,.$$

This expression has the appearance of the wave equation in polar coordinates, which shows that our minisuperspace is flat. The Hamilton operator equals the wave operator in Rindler spacetime. We bring the Hamiltonian into the simplest form using a transformation to light-cone coordinates:

$$u = Ae^{-B} \qquad v = Ae^{B} \,. \tag{10.6}$$

We obtain the Hamiltonian

$$\widehat{H} = \frac{\hbar^2 c^2}{\epsilon} \frac{\partial^2}{\partial u \partial v} \tag{10.7}$$

The volume element is given by $\frac{\sqrt{\epsilon}}{2} du dv$ and $u \in (0, \infty)$, $v \in (0, \infty)$. This is equivalent to a volume element $du\, dv$, if the wave functions are accordingly normalized.

10.1 The unitary time evolution

We will search for solutions of (10.4) that are square integrable. Moreover they should fulfill the condition for a unitary time evolution that is given by

$$\langle\psi(t_1)|\,\widehat{H}|\,\psi(t_2)\rangle \;=\; \langle\widehat{H}\,\psi(t_1)\,|\psi(t_2)\rangle \quad \forall\, t_1, t_2\,. \tag{10.8}$$

For $t_1 = t_2$ this condition ensures that the norm of the wavepackets is preserved:

$$\frac{d}{dt}\langle\Psi|\Psi\rangle = 0\,. \tag{10.9}$$

Differentiating (10.8) with respect to t_2 results in the conservation of the expectation value of the Hamiltonian

$$\frac{d}{dt}\langle\psi|\widehat{H}|\psi\rangle = 0\,.$$

Higher time derivatives yield

$$\frac{d}{dt}\langle\psi|\widehat{H}^n|\psi\rangle = 0 \quad \text{for} \quad n = 2, 3, \ldots\,.$$

For the Hamiltonian (10.7) the condition (10.8) is equivalent to

$$\int_0^\infty \psi^*(0,v,t_1)\frac{\partial}{\partial v}\psi(0,v,t_2)dv - \int_0^\infty \psi(u,0,t_2)\frac{\partial}{\partial u}\psi^*(u,0,t_1)du = 0\,. \tag{10.10}$$

If we choose two real functions $f_1(x), f_2(x)$ where $f_1(0) = \pm f_2(0)$ then any solution of (10.4) that obeys

$$\psi(0,v,t) = C(t)f_1(v) \qquad \psi(u,0,t) = C(t)f_2(u)\,, \tag{10.11}$$

fulfills (10.8). All solutions that evolve according to (10.11) with an arbitrary function $C(\tau)$ and are square integrable at $t = 0$ remain within the linear subspace of the space of square integrable function characterized by (10.11). Two elements of this subspace respectively meet the condition

$$\langle\varphi(t_1)|\,\widehat{H}|\,\psi(t_2)\rangle \;=\; \langle\widehat{H}\,\varphi(t_1)\,|\psi(t_2)\rangle \quad \forall\, t_1, t_2\,, \tag{10.12}$$

which implies

$$\frac{d}{dt}\langle\varphi|\widehat{H}^n|\psi\rangle = 0 \quad \text{for} \quad n = 0, 1, 2, \ldots\,.$$

10.2 Solutions with a negative expectation value of the Hamiltonian

Introducing

$$\tau = t\hbar c^2/\epsilon \tag{10.13}$$

we can write for the Schrödinger equation (10.4)

$$\frac{\partial^2}{\partial u \partial v}\psi = i\frac{\partial}{\partial \tau}\psi \tag{10.14}$$

This equation looks rather simple and there are many possibilities to solve it. The challenge here is to find solutions that ensure a unitary time evolution. We will obtain this goal by a superposition of eigensolutions. An eigenstate $\psi_\Lambda(u,v)$ with negative eigenvalue $h \equiv -\Lambda\,\epsilon/3 < 0$ fulfills the equation

$$\frac{\partial^2}{\partial u \partial v}\psi_\Lambda(u,v) = -\frac{\Lambda\epsilon}{3}\psi_\Lambda(u,v)\,, \tag{10.15}$$

which gives the time-dependent solution

$$\psi(u,v,\tau) = \psi_\Lambda(u,v)e^{\frac{i\Lambda\,\epsilon\tau}{3}} \tag{10.16}$$

The Laplace transformation (see Appendix C) of (10.15) with respect to v yields

$$s\frac{\partial L_\Lambda(u,s)}{\partial u} - \frac{\partial \psi_\Lambda(u,0)}{\partial u} = -\frac{\Lambda\epsilon}{3}L_\Lambda(u,0) \tag{10.17}$$

where $L_\Lambda(u,s)$ is given by

$$L_\Lambda(u,s) = \mathcal{L}(\psi_\Lambda(u,\cdot)) = \int_0^\infty \psi_\Lambda(u,0)e^{-sv}dv\,, \tag{10.18}$$

and we have used the differential rule of the Laplace transform given in table C.1. Solving (10.17), we obtain

$$L_\Lambda(u,s) = e^{-\frac{\Lambda\epsilon}{3s}u}\,L_\Lambda(0,s) + \int_0^u \frac{1}{s}e^{-\frac{\Lambda\epsilon}{3s}(u-x)}\,\frac{\partial\psi_\Lambda(u,0)}{\partial u}dx$$

Applying the formula for the inverse Laplace transform (see also C.3)

$$\mathcal{L}^{-1}\left\{\frac{1}{s}e^{-\frac{a}{s}}\right\} = J_0\left(2\sqrt{ax}\right)$$

and the convolution theorem (C.2) we find for the inverse Laplace transform

$$\begin{aligned}\psi_\Lambda(u,v) = &\int_0^v J_0\left[2\sqrt{\frac{\Lambda\,\epsilon u}{3}}\sqrt{v-x}\right]\,\frac{\partial f_1}{\partial x}dx\\ &+\int_0^u J_0\left[2\sqrt{\frac{\Lambda\,\epsilon v}{3}}\sqrt{u-x}\right]\,\frac{\partial f_2}{\partial x}dx\\ &+J_0\left[2\sqrt{\frac{\Lambda\,\epsilon}{3}vu}\right]\,f_1(0)\,,\\ &\text{where}\quad f_1(0) = f_2(0)\,.\end{aligned}$$

The functions $f_1(x), f_2(x)$ determine $\psi_\Lambda(u,v)$ at the edges

$$f_1(x) \equiv \psi_\Lambda(0,x) \qquad f_2(x) \equiv \psi_\Lambda(x,0).$$

The superposition of the corresponding eigensolutions (10.16) yields more general time-dependent wavepacket solutions of (10.14)

$$\psi(u,v,\tau) = \int_0^\infty e^{i\tau\,\epsilon\frac{\Lambda}{3}}\psi_\Lambda(u,v)F\,(\Lambda)\,d\Lambda\,. \tag{10.19}$$

The solution is then characterized by the functions $f_1(x), f_2(x), F(\Lambda)$. We assume that they can be chosen appropriately to ensure that $\psi(u,v,0)$ is square integrable. We obtain for the time evolution at the edges

$$\psi(0,v,\tau) = C(\tau)f_1(v) \qquad \psi(u,0,\tau) = C(\tau)f_2(u) \tag{10.20}$$
$$\text{where} \qquad C(\tau) = \int_0^\infty e^{i\epsilon\,\tau\frac{\Lambda}{3}}F(\Lambda)\,d\Lambda\,,$$

which means that (10.19) meets the condition (10.11) for a unitary time evolution if $f_1(x), f_2(x)$ are real functions. Moreover it follows from the Riemann-Lebesgue lemma (see for instance [24])for the Fourier transform that

$$\lim_{\tau\to\infty} C(\tau) = 0\,, \tag{10.21}$$

if $F(\Lambda)$ is an absolutely integrable function. This implies for the wavefunction at the edges

$$\lim_{\tau\to\infty}\psi(u,0,\tau) = \lim_{\tau\to\infty}\psi(0,v,\tau) = 0\,. \tag{10.22}$$

It will turn out to be more convenient to represent $F(\Lambda)$ as

$$F(\Lambda) = \int_0^\infty J_0\left[2\sqrt{\frac{\epsilon\,\Lambda r}{3}}\right]\frac{G(r)\,\epsilon}{3}\,dr\,. \tag{10.23}$$

The initial wavefunction then reads

$$\psi(u,v,0) = \int_0^v G\,[u(v-x)]\,\frac{\partial f_1}{\partial x}dx + \int_0^u G\,[v(u-x)]\,\frac{\partial f_2}{\partial x}dx + G\,[uv]\,\,f_1(0)\,. \tag{10.24}$$

This is a consequence of the selfreproducing property of the Hankel transformation ([24])

$$H(x) = \int_0^\infty \sqrt{xy}J_0(xy)\int_0^\infty \sqrt{yz}J_0(yz)H(z)dzdy\,, \tag{10.25}$$

which is equivalent to

$$G(\alpha) = \int_0^\infty J_0(2\sqrt{\alpha\beta})\int_0^\infty J_0(\sqrt{\beta\gamma})G(\gamma)d\gamma d\beta\,, \qquad \text{where} \quad G(\gamma) = H(\sqrt{2\gamma})/\gamma^{\frac{1}{4}}\,.$$

The relation (10.25) applies to any absolutely integrable function $H(z)$ on $\mathbb{R}_+$ of bounded variation. We also deduce from (10.23,10.25) that we can choose the function $G(z)$ in (10.24) arbitrarily under the restriction that $G(z^2/2)\sqrt{z}$ is an absolutely integrable function of bounded variation.

Inserting (10.23) into (10.19) yields for the time-evolution

$$
\begin{aligned}
&\psi(u,v,\tau) = \qquad\qquad (10.26)\\
&\frac{i}{\tau}\int_0^\infty\int_0^u e^{-\frac{iv(u-x)}{\tau}-\frac{ir}{\tau}} J_0\left[2\frac{\sqrt{v(u-x)r}}{\tau}\right]\frac{\partial f_1}{\partial x}dxG(r)dr\\
&\frac{i}{\tau}\int_0^\infty\int_0^v e^{-\frac{iu(v-x)}{\tau}-\frac{ir}{\tau}} J_0\left[2\frac{\sqrt{u(v-x)r}}{\tau}\right]\frac{\partial f_2}{\partial x}dxG(r)dr\\
&\frac{i}{\tau}\int_0^\infty e^{-\frac{iuv}{\tau}-\frac{ir}{\tau}} J_0\left[2\frac{\sqrt{u\,v\,r}}{\tau}\right] f_1(0)G(r)dr\,.
\end{aligned}
$$

We have obtained this result applying the formula for the Laplace transformation of a product of Bessel functions (C.3)

$$\int_0^\infty e^{-zs}J_0(2\sqrt{az})J_0(2\sqrt{bz})dz = \frac{1}{s}e^{-\frac{a+b}{s}}I_0\left(2\sqrt{ab}\right)$$

with the parameters

$$s=-i\,\tau\,,\quad z=\epsilon\Lambda/3\,,\quad a=r\,,\quad b=u(v-x)\quad \text{or } b=v(u-x)\quad \text{or } b=v\,u\;.$$

$I_0(x)$ is the modified Bessel function of the first kind (see for instance [26])and fulfills $I_0(ix)=J_0(x)$.

With the definition

$$G_\tau(z)\equiv\frac{i}{\tau}\int_0^\infty e^{-\frac{iz}{\tau}-\frac{ir}{\tau}}J_0\left[2\frac{\sqrt{u\,v\,r}}{\tau}\right]G(r)dr\,,$$

the solution (10.26) assumes the the form

$$\psi(u,v,\tau)=\int_0^v G_\tau\left[u(v-x)\right]\,\frac{\partial f_1}{\partial x}dx+\int_0^u G_\tau\left[v(u-x)\right]\,\frac{\partial f_2}{\partial x}dx+G_\tau\left[uv\right]\,f_1(0)\,. \tag{10.27}$$

So we see that the special form of the solution (10.24) is preserved during the time evolution.

10.3 General properties of the time evolution

As in ordinary quantum mechanics, the evolution of the expectation values of an observable $\widehat{O}$ with respect to a solution $\psi(u,v,t)$ of the Schrödinger equation (10.4) is given by

$$\frac{d}{dt}\langle\psi|\widehat{O}|\psi\rangle = -\frac{i}{\hbar}\left(\langle\psi|\widehat{O}\widehat{H}|\psi\rangle - \langle\widehat{H}\psi|\widehat{O}\psi\rangle\right) . \tag{10.28}$$

This implies the equation

$$\frac{d}{dt}\langle\psi|\widehat{O}|\psi\rangle = -\frac{i}{\hbar}\left\langle\psi\left[\widehat{O},\widehat{H}\right]\psi\right\rangle , \tag{10.29}$$

only if $\widehat{O}\psi$ obeys

$$\langle\widehat{H}\psi|\widehat{O}\psi\rangle \stackrel{!}{=} \langle\psi|\widehat{H}\widehat{O}|\psi\rangle . \tag{10.30}$$

In the case of our model (10.7), this condition reads

$$\int_0^\infty \psi^*(u,v,t)\frac{\partial}{\partial v}\widehat{O}\psi(u,v,t)dv\,\Big|_{u=0} - \int_0^\infty\left(\frac{\partial}{\partial u}\psi^*(u,v,t)\right)\widehat{O}\psi(u,v,t)du\,\Big|_{v=0} = 0 . \tag{10.31}$$

The observable (10.5,10.6)

$$A^2 = u\,v = \frac{a^6}{9}$$

fulfills this condition and we find for the first time derivative of the expectation value

$$\frac{d}{dt}\langle A^2\rangle = \langle\widehat{P}\rangle\,, \text{where}$$
$$\widehat{P} \equiv \frac{i\hbar c^2}{\epsilon}\left\langle\left\{v\frac{\partial}{\partial v} + u\frac{\partial}{\partial u} + 1\right\}\right\rangle .$$

But since $\widehat{P}$ does not meet the condition (10.31), the second derivative of $\langle A^2\rangle$ can not be determined by (10.29).

If we consider the solutions that we found in the previous section, and take into account the results for the time evolution at the edges (10.20,10.21),we obtain

$$\lim_{t\to\infty}\psi(0,v,t) = \lim_{t\to\infty}\left(\frac{\partial}{\partial u}(u,0,t)\right) = 0\,, \tag{10.32}$$

which means that (10.31) is fulfilled in the limit $t \to \infty$. This means that as far as (10.20,10.21) are fulfilled,the time evolution that we derive by the application of (10.29), gives the correct result for the limit $t \to \infty$, and is approximately valid in the late phase of time evolution.

We obtain for the second derivative of $\langle A^2\rangle$

$$\lim_{t\to\infty}\frac{d^2}{dt^2}\langle A^2\rangle = -\frac{i}{\hbar}\langle\left[\widehat{P},\widehat{H}\right]\rangle = -\frac{2c^2}{\epsilon}\langle\widehat{H}\rangle . \tag{10.33}$$

Setting for the expectation value of the Hamiltonian

$$\langle\widehat{H}\rangle = -\frac{\Lambda\epsilon}{3}\,,$$

yields

$$\frac{d^2}{dt^2}\langle A^2\rangle = \frac{2}{3}\,\Lambda\, c^2$$

which coincides with the classical result (9.21a).

The classical momentum p_ϕ (9.17) is a conserved quantity. The corresponding operator reads

$$\widehat{p}_\phi = -i\hbar\frac{\partial}{\partial\phi} = -i\hbar 3\sqrt{\frac{1}{2\epsilon}}\frac{\partial}{\partial B} = -i\hbar 3\sqrt{\frac{1}{2\epsilon}}\left(-u\frac{\partial}{\partial u} + v\frac{\partial}{\partial v}\right). \qquad (10.34)$$

Since

$$\left[\widehat{p}_\phi, \widehat{H}\right] = 0\,,$$

we conclude

$$\lim_{t\to\infty}\frac{d}{dt}\langle\widehat{p}_\phi\rangle = 0\,.$$

Note that the expectation value of $\hat{p}_\phi$ is in general not conserved, since without special assumptions the observable does not meet the condition (10.31). Instead it tends to a limit in the late phase of time evolution.

In order to investigate the late time behaviour of the uncertainty $\Delta(A^2)$, we determine

$$\lim_{t\to\infty}\frac{d^4}{dt^4}\langle A^2\rangle^2 = 6\left(\frac{d^2}{dt^2}\langle A^2\rangle\right)^2 = \frac{24c^2}{\epsilon^2}\langle\widehat{H}\rangle^2 \qquad (10.35)$$

$$\lim_{t\to\infty}\frac{d^4}{dt^4}\langle A^4\rangle = \frac{24c^2}{\epsilon^2}\langle\widehat{H}^2\rangle\,. \qquad (10.36)$$

We obtain

$$\lim_{t\to\infty}\frac{d^4}{dt^4}(\Delta(A^2))^2 = \frac{24c^2}{\epsilon^2}(\Delta H)^2\,,$$

which implies that the uncertainty $\Delta(A^2)$ is monotonically growing with t^2 in the late phase of time evolution.

Note that the results for the observables A and p_ϕ will apply to all wavefunctions with the properties (10.20,10.21). They will also apply to solutions that do not have the special initial form (10.24) or do not have a negative expectation value of the Hamiltonian.

Finally we discuss the special cases of solutions that are symmetric or antisymmetric in u and v. We will call them ψ_s or ψ_{as} respectively. The form of the Schrödinger equation (10.14) ensures, that the symmetry of the solution is conserved during the time evolution. Moreover we obtain for the expectation value of $\widehat{p}_\phi$ (10.34)

$$\langle\psi_s|\widehat{p}_\phi|\psi_s\rangle = \langle\psi_a|\widehat{p}_\phi|\psi_a\rangle = 0\,.$$

In these cases the expectation value of the field momentum operator is an exactly conserved quantity and has the value zero. The corresponding classical solutions with $p_\phi = 0$ are the de-Sitter solutions (9.19) with $\phi = const.$ Being (anti)symmetric in u and v means that the wavefunction is even (odd) in ϕ (10.5,10.6):

$$\begin{aligned} \psi(u,v) = \psi(v,u) \quad &\Leftrightarrow \quad \psi(a,\phi) = \psi(a,-\phi) \\ \psi(u,v) = -\psi(v,u) \quad &\Leftrightarrow \quad \psi(a,\phi) = -\psi(a,-\phi)\,. \end{aligned}$$

This implies for the expectation value of the field

$$\langle \psi_s | \widehat{\phi} | \psi_s \rangle = \langle \psi_{as} | \widehat{\phi} | \psi_{as} \rangle = 0\,,$$

which corresponds to a de Sitter solution with $\phi = 0$. Those solutions can be constructed according to (10.19), if the functions $f_1(x), f_2(x)$ fulfill

$$f_1(x) = f_2(x) \qquad \text{(symmetric case)}\,, \tag{10.37}$$

$$f_1(x) = -f_2(x) \quad \text{(antisymmetric case)}\,. \tag{10.38}$$

10.3.1 Remarks about the solution spaces

The solution spaces we found are characterized by the functions $f_1(x), f_2(x)$ and the specific shape given by (10.27). If we sum up two solutions belonging to two different spaces, the resulting solution of (10.7) will in general not fulfill the condition of unitary time evolution (10.10). Nevertheless we could not show that the solution spaces are maximal or if they are not, how their extensions would look like. It is conceivable that they can be completed to linear, dense spaces representing domains of selfadjointness of the oparator $\hat{H}$ in the Hilbert space $L^2(\mathbb{R}^2, a^5 da d\phi)$.

10.4 Example for a wavepacket evolution with a negative expectation value of the Hamiltonian

In section (10.2) we constructed solutions of (10.14) with a negative expectation value of the Hamiltonian and a unitary time evolution. We had to require that the functions $G(z), f_1(x), f_2(x)$ ensure that the initial wave function (10.24) is square integrable. Investigating an explicit example shows that an appropriate choice of these functions is possible. Moreover we are able to study the whole time evolution of the expectation values which is highly interesting since the general results we obtained in the last section apply only for the late phase of time evolution. The lengthy algebraic calculations of this section were performed with Wolfram Mathematica.

We define

$$G(z) = e^{-z}\left(z^3 - 6z^2 + 3z + 3\right) \tag{10.39}$$

$$f_1(x) = e^{-x}\left(-x^3 + 3x^2\right) \tag{10.40}$$

$$f_2(x) = 0 \tag{10.41}$$

With the additional real paramters λ and μ, we find for the initial function according to (10.24)

$$\psi(u,v,0) = \frac{1}{\sqrt{n_0}} \int_0^v G\left[\lambda u(v-x)\right] \frac{\partial f_1(\mu x)}{\partial x} dx \,, \tag{10.42}$$

where we have introduced a normalization factor that turns out to be

$$n_0 = \frac{135}{3\lambda} \,.$$

We obtain for the expectation value of the Hamiltonian

$$\langle \widehat{H} \rangle = -\frac{3\lambda}{2} \cdot \frac{\hbar^2 c^2}{\epsilon} \,. \tag{10.43}$$

The evaluation of $\langle A^2 \rangle$ according to (10.26) yields

$$\begin{aligned} \langle A^2 \rangle \; &= \frac{3}{40\lambda(1+\tau^2\lambda^2)^2} \\ &\cdot \left[30 + 71\tau^2\lambda^2 + 67\tau^4\lambda^4 + 20\tau^6\lambda^6 + 15\tau\lambda(1+\tau^2\lambda^2)^2 \arctan(\tau\lambda)\right] \,. \end{aligned} \tag{10.44}$$

We find for the late phase of the time evolution (where we have replaced τ by t (10.13)):

$$\lim_{t\to\infty} = \frac{d^2}{dt^2}\langle A^2 \rangle \; = \; \frac{3\lambda\left(\hbar c^2\right)^2}{\epsilon^2} \; = \; -\frac{2c^2}{\epsilon}\langle \widehat{H} \rangle \,,$$

which confirms the coincidence with the classical behaviour that we have already obtained as a general result (10.33). We also find that the expectation value of $\widehat{p}_\phi$ approaches a constant value

$$\lim_{t\to\infty} \langle \widehat{p}_\phi \rangle \; = \; \frac{9\pi}{16} \cdot \frac{3\hbar}{\sqrt{2\epsilon}} \,, \tag{10.45}$$

which reproduces the general result (10.33), see also figure 10.1.

Nevertheless at the beginning of the time evolution, the observable A^2 that is proportional to the sixth power of the scale factor assumes a constant value (10.2).

$$S = \frac{9}{4\lambda} \,.$$

In this explicit example we can also prove that the linear part of the classical time evolution of A^2 (9.21a)is reproduced by the late time behaviour of the expectation value. Inserting for (10.45), we find

$$\lim_{t\to\infty} \left(\frac{d}{dt}\langle A^2 \rangle - t \cdot \frac{d^2}{dt^2}\langle A^2 \rangle \right) = \frac{9\pi}{16} \cdot \frac{\hbar c^2}{\epsilon} = p_\phi \cdot \frac{\sqrt{2}}{\sqrt{\epsilon} 3\hbar} \,,$$

which shows that the time evolution of the expectation value approaches the classical evolution (see figure 10.2).

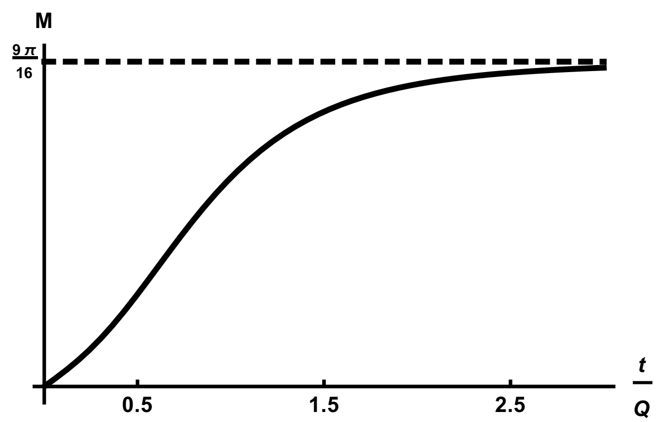


Figure 10.1: The quantity $M \equiv \langle p_\phi \rangle \left(\frac{3\hbar}{\sqrt{2\epsilon}}\right)^{-1}$ converges to $\frac{9\pi}{16}$. We have chosen $\lambda = 1 \cdot m^{-3}$, $\mu = 1 \cdot m^{-3/2}$ and time is scaled by $Q = \sqrt{\frac{2}{3}} \cdot \frac{\epsilon}{\hbar c^2 \lambda}$

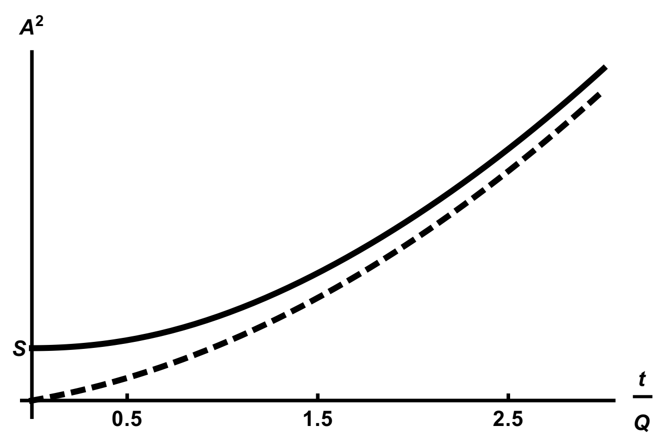


Figure 10.2: The time-evolution of the expectation value of A^2 according to the initial wave packet (10.42) ,compared to the classical evolution (dashed line). S is the minimal extension according to the quantum evolution. μ , λ and Q are defined as in figure 10.1.

10.5 Summary, conclusions and discussion of the literature

Investigations of unimodular quantum cosmology can be found in [41],[48] as well as more recently in [49] where unimodular quantum loop cosmology is discussed. In [48] a semiclassical wave function via path integral for an empty universe with positive curvature is constructed. The time evolution fails to be unitary. The model mentioned in [41] is the spatially flat universe with a massless scalar field. But the general solution is given only formally, and the properties of the wave packet evolution in particular the question of unitary time evolution are not discussed. The solutions in [49] apply for a flat universe filled with exotic matter with the equation of state $p = -2\rho c^2$. An approximate classical behaviour far away from the singularity is predicted. This is similar to our result for the massless scalar field.

We deem it remarkable to note that in the case of a singularity at the beginning of the time evolution, the system behaves more and more classically at late times. Since in common quantum mechanics, systems start with classical motion developping quantum properties appear in the late phase of time evolution (as the revival phenomena show impressively). However this classical behaviour for late times does not apply to all aspects of the time evolution because the uncertainty of the observable A^2, that is related to the scale factor increases with time. Maybe this would not happen with a more realistic matter model. The quantum analogue of the special case of de Sitter solutions could be constructed by assuming special symmetries for the wave function.

The construction of solutions according to (10.19) also works for negative times and so the solutions can be continued beyond the classical singularity at $t = 0$. In the special case we investigated (10.44) this would yield a contracting universe that passes a minimal extension before expanding again. The question of solutions with a positive expectation value of the Hamiltonian remains open.

Appendix A

Revivals

A revival is the occurrence of an exact or approximate periodicity in a quantum system that has no classical equivalence and can also not be reproduced by classical statistics. A revival can be predicted if some general conditions for the spectrum and the initial wave packet are fulfilled.

An initial wave packet that consists of $2\Delta n$ subsequent eigenfunctions that correspond to the eigenvalues $E(n)$ evolves according to

$$\psi(x,t) = \sum_{n=n_0-\Delta n}^{n=n_0+\Delta n} c_n \varphi_n(x) e^{\frac{-iE(n)t}{\hbar}} \,. \tag{A.1}$$

Extending the sequence $E(n)$ to a real analytic function, the mean value theorem yields

$$E(n) = E(n_0) + E'(n_0)\Delta n + \frac{1}{2}E''(n_0)(\Delta n)^2 + \frac{1}{3!}E'''(n_1(n))(\Delta n)^3 \,.$$

We introduce the classical period and the revival time by

$$T_{cl} = \frac{2\pi\hbar}{E'(n_0)} \,, \qquad T_{rev} = \frac{\pi\hbar}{E''(n_0)} \,. \tag{A.2}$$

The quantity T_{cl} corresponds to the classical period with the WKB approximation ([9]). We assume that

$$T_{cl} \ll T_{rev} \ll \frac{2\pi\hbar}{3!E'''(n_1(n))} \,, \quad t \ll \frac{2\pi\hbar}{3!E'''(n_1(n))}\Delta n^3 \qquad \forall\, n \,\epsilon\, [n_0 - \Delta n, n_0 + \Delta n] \,. \tag{A.3}$$

Then we can approximate (A.1) by

$$\psi(x,t) \approx e^{\frac{iE(n_0)t}{\hbar}} \sum_{n=n_0-\Delta n}^{n=n_0+\Delta n} c_n \varphi(x) e^{2\pi i \frac{t}{T_{cl}}\Delta n + 2\pi i \frac{t}{T_{rev}}\Delta n^2} \,. \tag{A.4}$$

When $t \ll T_{rev}\Delta n^2$ the wave function will oscillate with the classical period T_{cl}. With time the second term comes into play and the periodicity is no longer visible. When time comes close to T_{rev} within a few multiples of T_{cl}, the wave packet assumes its initial shape and oscillates again classically. Then a new revival cycle begins.

In the case of the harmonic oscillator T_{rev} is infinite ($E''(n) = 0$) and the wave packet undergoes exact oscillations with the classical frequency that is independent of the initial state. In the case of the infinite square well A.4 represents the exact solution ($E'''(n) = 0$), and the revival time denotes an exact and universal periodicity of the system. In general revivals are not exact and superrevivals may occur for

$$t \sim \frac{2\pi\hbar}{3!E'''(n_0)}\,.$$

Revivals were realized experimentally, for instance with Rydberg atoms (see [9] for a general overview).

Appendix B

The perfect fluid matter model compared to the scalar field

In the perfect fluid matter model the matter is characterized by its density ρ and pressure p which are connected by a barotropic equation of state $p = p(\rho)$. The energy-momentum tensor is given by

$$T^{PF}_{\mu\nu} = \rho c^2 u_\mu u_\nu + p(u_\mu u_\nu + g_{\mu\nu})\,,$$

where u^μ is the 4-velocity of the fluid.

In a reference frame that is at rest with respect to the fluid, the energy momentum tensor reads

$$\begin{pmatrix} \rho\, c^2 & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix}\,. \tag{B.1}$$

This is also the form, the energy-momentum tensor assumes if the perfect fluid is taken as matter source for the Friedmann universe in a coordinate system where the metric has the form (9.1) with $N = 1$. In this case ρ and p are spatially constant.

For the energy momentum tensor of the scalar field (9.2)we obtain according to (8.3)

$$T^S_{\mu\nu} = \phi,_\mu \phi,_\nu - g_{\mu\nu}\left(\frac{1}{2} g^{\alpha\beta}\phi,_\alpha \phi,_\beta + V(\phi)\right)$$

If we consider again the space-time to be the Friedmann universe the spatial derivatives have to be zero. Choosing the same coordinate system as before (9.1, N=1), we find for the energy momentum tensor

$$\begin{pmatrix} \frac{\dot\phi^2}{2c^2}+V(\phi) & 0 & 0 & 0 \\ 0 & \frac{\dot\phi^2}{2c^2}-V(\phi) & 0 & 0 \\ 0 & 0 & \frac{\dot\phi^2}{2c^2}-V(\phi) & 0 \\ 0 & 0 & 0 & \frac{\dot\phi^2}{2c^2}-V(\phi) \end{pmatrix} . \tag{B.2}$$

The two expressions (B.1,B.2) for the energy-momentum tensors coincide if

$$\rho\, c^2 = \left(\frac{\dot\phi^2}{2c^2}+V(\phi)\right) , \qquad p = \left(\frac{\dot\phi^2}{2c^2}-V(\phi)\right) . \tag{B.3}$$

In general, these relations are incompatible with a time-independent barotropic state equation. But in the special case $V(\phi)=0$ they imply $\rho c^2 = p$, which is the state equation of stiff matter.

Appendix C

Laplace transform

The Laplace transform of a function $f(t)$ on $\mathbb{R}_+$ is given by

$$\mathcal{L}(f(t)) = g(s) = \int_0^\infty f(t)\ e^{-st} dt \quad . \tag{C.1}$$

The Laplace transform is said to exist if the integral (C.1) converges for at least one value of s where s can be any complex number. If the Laplace transform of $|f(t)|$ also exists the Laplace transform of $f(t)$ is said to converge absolutely. Though the Laplace transform can in principle also be applied to more general functions most theorems and rules in the literature ([23],[24]) are stated for locally integrable functions $f(t)$. Therefore we will always assume (respectively make sure) that the Laplace transformed function is locally integrable on $[0, \infty)$.

C.1 The domain of convergence

If the Laplace transform exists for some complex number s_0 it will also converge in the region $\Re s > \Re s_0$. In more detail, the two important statements about the domain of convergence (respectively absolute convergence) are:

- The domain of convergence consists of a half-plane $\{\Re s > b\}$ and all, some or none of the points of the boundary line $\{\Re s = b\}$. The possible values for b are $-\infty \leq b \leq \infty$. The Laplace transform $g(s)$ is an analytic function in the half-plane $\{\Re s > b\}$ where it is also uniformly convergent.

- The domain of absolute convergence is either of the form $\Re s > a$ or $\Re s \geq a$ with $-\infty \leq a \leq \infty$.

C.2 The Rules of Laplace transformation

In this section we will list the rules and theorems applied in the text to derive the (inverse) Laplace transform of a function from the already known Laplace transforms of other functions.

For the Laplace transformation of derivatives we have the following theorem:

Theorem C.1. *Let $f(t)$ be a differentiable locally integrable function of exponential type with the additional assumption that $\lim_{t\to 0} f(t) = f(0)$ exists. If $\frac{d}{dt}f(t)$ is locally integrable then the Laplace transform of $\frac{d}{dt}f(t)$ exists and*

$$\mathcal{L}\left\{\frac{d}{dt}f(t)\right\} \;=\; sg(s) - f(0) \tag{C.2}$$

A function $f(t)$ is of exponential type if for some constants $M\,, t_0 \;>\; 0$ and some real γ, it satisfies

$$|f(t)| \leq Me^{\gamma t} \quad \text{for all} \quad t \;\geq\; t_0 \quad .$$

The Laplace transform of a convolution of two functions is the product of the Laplace transforms.

Theorem C.2. *Let $f_1(t)$ and $f_2(t)$ be locally integrable functions with the Laplace transforms $g_1(t)$ and $g_2(t)$. Assume that their Laplace integrals converge absolutely in some half-plane $\Re s \;>\; \alpha$. Then the convolution*

$$f(t) = \int_0^t f_1(t-\tau) f_2(\tau)\, d\tau$$

is a locally integrable function and has the Laplace transform

$$\mathcal{L}\{f(t)\} \;=\; g_1(s)g_2(s) \tag{C.3}$$

which is absolutely convergent for $\Re s \;>\; \alpha$.

Under certain conditions the infinite sum of Laplace transforms will be the Laplace transform of the sum of an infinite series.

Theorem C.3. *Let $g(s)$ be the sum of a series of absolutely convergent Laplace transforms $g_n(s)$ with a common half-plane of convergence $\Re s \;>\; s_0$:*

$$g(s) = \sum_0^\infty g_n(s) \qquad \textit{where} \qquad \mathcal{L}\{f_n(t)\} = g_n(s) \quad \textit{for} \quad \Re s \;>\; s_0$$

If the series

$$\sum_0^\infty \int_0^\infty e^{-s_0 t}\, |f_n(t)|\, dt$$

is convergent then

$$\sum_0^\infty f_n(t) = f(t) \quad \textit{converges absolutely and} \quad f(t) = \mathcal{L}^{-1}\{g(s)\} \qquad .$$

C.3 Special Laplace transforms

The Laplace transforms listed in the table below are taken from [25].

Table of general properties of Laplace transforms

$f(t)$	$g(s) = \int\limits_0^\infty f(t)\, e^{-st}\, dt$
$f(at) \quad a \,\epsilon\, \mathbb{R}$	$\frac{1}{a}\, g(s/a)$
$\frac{df(t)}{dt}$	$-f(0) \,+\, s\, g(s)$
$\int_0^t f_1(t-\tau) f_2(\tau) d\tau$	$g_1(s)\, g_2(s)$

Table C.1: Rules

Table of special Laplace Transforms

f(t)	$g(s) = \int\limits_0^\infty f(t)\, e^{-st}\, dt$
$\sqrt{\frac{1}{\pi t}}\, e^{\frac{ia}{2t}} \qquad a > 0$	$\frac{1}{\sqrt{s}} e^{-(1-i)\sqrt{as}}$
$\mathrm{Erfc}\left(\frac{(1-i)a}{2\sqrt{t}}\right) \qquad a > 0$	$\frac{1}{s} e^{-(1-i)a\sqrt{s}}$
$\frac{1}{i^k t} J_k\left(\frac{at}{2}\right) e^{-i\frac{at}{2}} \qquad \Re a > 0\,, \quad \Re k > 0$	$\left(2 \cdot \left(1 + \sqrt{1 - \frac{a}{is}}\right)^{-1} - 1\right)^k$
$e^{-bt}\left\{e^{-i\sqrt{ab}}\mathrm{Erfc}\left[\sqrt{\frac{a}{4t}} - i\sqrt{bt}\right] + e^{i\sqrt{ab}}\mathrm{Erfc}\left[\sqrt{\frac{a}{4t}} + i\sqrt{bt}\right]\right\}$ $\Re a \geq 0, \quad \Re b \geq 0$	$2(s+b)^{-1} e^{-\sqrt{as}}$
$J_0\left(2\sqrt{ax}\right)$	$\frac{1}{s} e^{-\frac{a}{s}}$
$e^{-zs} J_0(2\sqrt{az}) J_0(2\sqrt{bz})$	$\frac{1}{s} e^{-\frac{a+b}{s}} I_0\left(2\sqrt{ab}\right)$

Appendix D

Special functions

D.1 Error functions

In this section we will summarize some results concerning the error functions. All formulas that are not derived explicitly can be found in [26] or [27]. The error function $\mathrm{Erf}(x)$ and the complementary error function $\mathrm{Erfc}(x)$ are defined by

$$\mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du \tag{D.1a}$$

$$\mathrm{Erfc}(x) = 1 - \mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du \tag{D.1b}$$

The functions are entire functions of x. They satisfy the relations

$$\mathrm{Erf}(-x) = -\mathrm{Erf}(x) \qquad\qquad \mathrm{Erfc}(-x) = 2 - \mathrm{Erfc}(x)$$

The derivative and the integral of the complementary error function therefore read

$$\frac{d}{dx}\,\mathrm{Erfc}(x) = -\frac{2}{\sqrt{\pi}} e^{-x^2}$$

$$\int_x^\infty \mathrm{Erfc}(u)\,du = -\mathrm{Erfc}(x)\,x + \frac{1}{\sqrt{\pi}} e^{-x^2} \quad .$$

The complementary error function can also be represented by the integrals

$$\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} = \int_0^\infty e^{-\frac{u^2}{4} - ux} du \tag{D.2a}$$

and

$$x\,\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} = \int_0^\infty e^{-u} \left(1 + \frac{u}{x^2}\right)^{-\frac{1}{2}} du \qquad \text{for} \quad |\arg(x)| < \frac{\pi}{2} \quad . \tag{D.2b}$$

The asymptotic expansion of Erfc(x) for large arguments reads:

$$
\begin{aligned}
x\,\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} &= 1 + \sum_{m=1}^{N-1}(-1)^m \frac{1\cdot 3\cdot \ldots \cdot (2m-1)}{(2x^2)^m} + R_N \\
\text{where}\quad R_N &= (-1)^N \frac{1\cdot 3\cdot \ldots \cdot (2N-1)}{(2x^2)^N}\,\Theta_N(x) \\
\text{with}\quad \Theta_N(x) &= \int_0^\infty e^{-u}(1+\frac{u}{x^2})^{-N-\frac{1}{2}}\,du \quad \text{for} \quad |\arg(x)| < \frac{\pi}{2} \\
\text{and} \quad |\Theta_N(x)| &< 1 \quad \text{for} \quad |\arg(x)| \le \frac{\pi}{4} \quad . \qquad \text{(D.3)}
\end{aligned}
$$

In accordance with (D.2a, D.2b, D.3) the following estimations are valid:

$$
\begin{aligned}
&|\mathrm{Erfc}\,(x)\,| = \left|\frac{e^{-x^2}}{\sqrt{\pi}}\int_0^\infty e^{-\frac{u^2}{4}-u\,x}du\right| && \text{(D.4a)} \\
&\le \frac{1}{\sqrt{\pi}}\int_0^\infty e^{-\frac{u^2}{4}}du \;=\; 1 \qquad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{2}\,, \\
&|\,\mathrm{Erfc}\,(x)\,e^{x^2}\sqrt{\pi}| \;\le\; \frac{1}{|x|}\int_0^\infty e^{-u}\left|1+\frac{u}{x^2}\right|^{-\frac{1}{2}}du && \text{(D.4b)} \\
&\le \frac{1}{|x|} \qquad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{4}\,, \\
&\left|\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} - \frac{1}{x}\right| = \left|\frac{R_1}{x}\right| && \text{(D.4c)} \\
&\le \frac{1}{|2\,x^3|} \qquad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{4}\,, \\
&\left|\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} - \frac{1}{x} + \frac{1}{2x^3}\right| = \left|\frac{R_2}{x}\right| && \text{(D.4d)} \\
&\le \frac{3}{|4\,x^5|} \qquad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{4}\,, \\
&\left|\mathrm{Erfc}(x)\,e^{x^2}\sqrt{\pi} - \frac{1}{x} + \frac{1}{2x^3} - \frac{3}{4\,x^5}\right| = \left|\frac{R_3}{x}\right| && \text{(D.4e)} \\
&\le \frac{15}{|8\,x^7|} \qquad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{4}\,.
\end{aligned}
$$

If we integrate (D.2a) by parts, we find estimations that are valid for a wider range of arguments:

$$
\mathrm{Erfc}\,(x)\,e^{x^2}\sqrt{\pi} = \int_0^\infty e^{-\frac{u^2}{4}-u\,x}\,du = -\frac{1}{x}\cdot e^{-\frac{u^2}{4}-u\,x}\Big|_0^\infty + \frac{1}{x}\cdot\int_0^\infty e^{-\frac{u^2}{4}-u\,x}\left(-\frac{u}{2}\right)du =
$$

$$
\frac{1}{x}\cdot\left\{1-\int_0^\infty e^{-\frac{u^2}{4}-u\,x}\left(\frac{u}{2}\right)du\right\} = \frac{1}{x}\cdot\left\{\int_0^\infty e^{-\frac{u^2}{4}}\left(\frac{u}{2}\right)\left(1-e^{-u\,x}\right)du\right\}.
$$

This yields

$$\left|\mathrm{Erfc}\,(x)\,e^{x^2}\,\sqrt{\pi}\right| \;\le\; \left|\frac{1}{x}\right|\cdot\left\{\int_0^\infty e^{-\frac{u^2}{4}}\,u\,du\right\} = \left|\frac{2}{x}\right| \quad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{2}\,. \tag{D.5}$$

If we integrate (D.2a) three times by part , we get

$$\mathrm{Erfc}\,(x)\,e^{x^2}\,\sqrt{\pi} - \frac{1}{x} = -\frac{1}{x^3}\cdot\left\{\frac{1}{2} + \int_0^\infty \frac{u\,(u^2-6)}{8}e^{-\frac{u^2}{4}-u\,x}\,du\right\}.$$

The estimation of the integral yields

$$\left|\int_0^\infty \frac{u\,(u^2-6)}{8}e^{-\frac{u^2}{4}-u\,x}\,du\right| \le \int_0^\infty \frac{u\,|u^2-6|}{8}e^{-\frac{u^2}{4}}\,du$$
$$= \frac{1}{2} + 2e^{-3/2} \;<\; 1 \quad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{2}\,.$$

So we find the estimation

$$\left|\mathrm{Erfc}\,(x)\,e^{x^2}\,\sqrt{\pi} - \frac{1}{x}\right| \;\le\; \left|\frac{3}{2\,x^3}\right| \quad \text{for} \quad |\arg(x)| \;\le\; \frac{\pi}{2}\,. \tag{D.6}$$

We will now derive several formulas for error functions with arguments that lie on one of the diagonals of the complex plane:

$$\arg(x) = \pm\frac{\pi}{4} \quad \text{or} \quad x = (1\pm i)\,y \quad \text{with} \quad y \;>\; 0.$$

The estimations (D.4) then read, if the particular arguments have positive real part ($y > 0$).

$$|\mathrm{Erfc}\,((1\pm i)\,y)\,| \;\le\; 1\,, \tag{D.7a}$$

$$|\,\mathrm{Erfc}\,((1\pm i)\,y)\;\sqrt{\pi}| \;\le\; \frac{1}{\sqrt{2}\,y}\,, \tag{D.7b}$$

$$\left|\mathrm{Erfc}\,((1\pm i)\,y)\,e^{\pm 2iy^2}\,\sqrt{\pi} - \frac{1}{(1\pm i)\,y}\right| \;\le\; \frac{1}{4\sqrt{2}\,y^3}\,, \tag{D.7c}$$

$$\left|\mathrm{Erfc}\,((1\pm i)\,y)\,e^{\pm 2iy^2}\,\sqrt{\pi} - \frac{1}{(1\pm i)\,y} + \frac{1}{2(1\pm i)^3\,y^3}\right| \;\le\; \frac{3}{16\sqrt{2}\,y^5}\,, \tag{D.7d}$$

$$\left|\mathrm{Erfc}\,((1\pm i)\,y)\,e^{\pm 2iy^2}\,\sqrt{\pi} - \frac{1}{(1\pm i)\,y} + \frac{1}{2(1\pm i)^3\,y^3} - \frac{3}{4(1\pm i)^5\,y^5}\right| \;\le\; \frac{15}{64\sqrt{2}\,y^7}\,. \tag{D.7e}$$

If we carry out the complex integration in (D.1a) along the diagonals, we find

$$\mathrm{Erf}\left((1-i)\,x\right) = \frac{4}{\sqrt{2\pi i}} \int_0^x e^{2iu^2}\, du\,,$$
$$\mathrm{Erf}\left((1+i)\,x\right) = \frac{4}{\sqrt{2\pi(-i)}} \int_0^x e^{-2iu^2}\, du\,,$$

which implies

$$\frac{1}{2}\mathrm{Erf}\left(\frac{(1-i)a\,x}{2}\right) = \frac{a}{\sqrt{2\pi i}} \int_0^x e^{\frac{ia^2u^2}{2}}\, du\,, \tag{D.8}$$
$$\frac{1}{2}\mathrm{Erf}\left(\frac{(1+i)a\,x}{2}\right) = \frac{a}{\sqrt{2\pi(-i)}} \int_0^x e^{\frac{-ia^2u^2}{2}}\, du\,.$$

We find for the integral of the complementary error function

$$G^+(x) \equiv -\int_x^\infty \mathrm{Erfc}\left((1-i)u\right)\, du = x\,\mathrm{Erfc}\left((1-i)\,x\right) - \frac{e^{2i\,x^2}}{\sqrt{\pi}(1-i)}\quad, \tag{D.9}$$
$$G^-(x) \equiv -\int_x^\infty \mathrm{Erfc}\left((1+i)u\right)\, du = x\,\mathrm{Erfc}\left((1+i)\,x\right) - \frac{e^{-2i\,x^2}}{\sqrt{\pi}(1+i)}\quad.$$

With the help of the representation (D.2b) we find

$$\begin{aligned}
\left|G^\pm(x)\right| &= \left|\frac{e^{\pm 2ix^2}}{\sqrt{\pi}(1\mp i)}\left(\int_0^\infty e^{-u}\cdot\frac{du}{\sqrt{1\pm\frac{iu}{2x^2}}} - 1\right)\right| \\
&= \frac{1}{\sqrt{2\pi}}\left|\left(\int_0^\infty e^{-u}\cdot\frac{du}{\sqrt{1\pm\frac{iu}{2x^2}}} - \int_0^\infty e^{-u}du\right)\right| \\
&\le \frac{1}{\sqrt{2\pi}}\sup_{u\in[0,\infty]}\left|1-\frac{1}{\sqrt{1\pm\frac{iu}{2x^2}}}\right| \\
&\le \frac{1}{\sqrt{2\pi}}\quad \text{for}\quad x\,\ge\,0\,.
\end{aligned} \tag{D.10}$$

The application of (D.7c) to (D.9) yields the estimation

$$\left|G^+(x)\right|\,\le\,\frac{1}{4\sqrt{2\pi}x^2}\,,\quad \left|G^-(x)\right|\,\le\,\frac{1}{4\sqrt{2\pi}x^2}\qquad \text{for}\quad x\,>\,0\,. \tag{D.11}$$

So we find for an appropriate function $f(x)$

$$\int_{x_1}^{x} \mathrm{Erfc}\left((1 \mp i)ay\right) f(y)dy = \frac{G^{\pm}(ay)}{a} f(y) \Bigg|_{x_1}^{x} - \int_{x_1}^{x} \frac{G^{\pm}(ay)}{a} f'(y)dy$$

$$\text{with} \qquad \left|\frac{G^{\pm}(ay)}{a}\right| \leq \frac{1}{4\sqrt{2\pi}y^2a^3} \quad \text{for} \quad a > 0,\, x > x_1 \geq 0. \tag{D.12}$$

D.2 Hermite polynomials and harmonic oscillator eigenfunctions

The functions

$$\varphi_n(x) = \frac{1}{(\pi\alpha)^{1/4}\sqrt{2^n n!}} H_n\left(\frac{x}{\sqrt{\alpha}}\right) e^{-\frac{x^2}{2\alpha}} \quad \text{with} \quad \alpha = \frac{\hbar}{m\omega} \tag{D.13}$$

are eigenfunctions of the harmonic oscillator with the potential

$$V = \frac{1}{2}m\omega^2x^2$$

for the eigenvalues

$$E_n = \left(n + \frac{1}{2}\right) \cdot \hbar\omega\,.$$

The Hermite polynomials $H_n(\xi)$ are polynomials of order n (see for instance [12] for the definition), and fulfill the relationships

$$H_n'\left(\xi\right) = 2n\, H_{n-1}\left(\xi\right) \tag{D.14a}$$

$$H_{n+1}\left(\xi\right) - 2\xi\, H_n\left(\xi\right) + 2n\, H_n\left(\xi\right) = 0\,. \tag{D.14b}$$

According to (D.14 we obtain for the harmonic oscillator eigenfunctions

$$\frac{m\omega}{\hbar}\, x\varphi_n(x) = \sqrt{\frac{n+1}{2}}\varphi_{n+1}(x) \;+\; \sqrt{\frac{n}{2}}\varphi_{n-1}(x) \tag{D.15}$$

$$\frac{\hbar}{m\omega}\varphi_n'(x) = \sqrt{\frac{n+1}{2}}\varphi_{n+1}(x) \;+\; \sqrt{\frac{n}{2}}\varphi_{n-1}(x) \quad .$$

Abstract

This work consists of two parts, one concerning quantum mechanics, the other quantum cosmology. They have in common the aim to analyze and understand the transition between quantum and classical behaviour and the deviations of quantum dynamics from classical motion.

In the first part we focus on the semiclassical phase of time evolution before revivals occur but when quantum effects already come into play. Here we introduce the method of Laplace transformation that gives the solution of the time-dependent Schrödinger equation in terms of the initial wave function if the solution of the time-independent equation is known. The solution is obtained without summing up eigenstates, nor do we need the path integral. We derive the propagators for the infinite square well, the potential step, the asymmetric square well (box with exit) and the finite barrier. The solutions give a direct insight into the wave packet evolution and contain the quantum analogue of classical transmission and reflection processes.

In the case of the infinite square well we reproduce the mirror solution in a straightforward way without referring to the special symmetry of the system. We state two theorems that point out that at a certain stage of time evolution only a certain number of terms of the mirror solution is relevant. We find that a wave function with energy lower than the potential step will swap into the classically forbidden region only during the reflection process. Moreover we show that for sufficiently peaked wave packets the reflection probability can be expressed in terms of the corresponding time-independent expression. The exact solution of the asymmetric square well turns out to be an intuitive combination of the solutions of the infinite square well and the potential step. This is remarkable since from the point of view of the characterization in terms of energy eigenstates the box with exit differs fundamentally from the infinite square well because there are bound and unbound eigenstates. As far as we know the initial value problem of this model was not considered before. In the case of the finite barrier we shed new light on the so-called Hartmann effect, predicting that for sufficiently thick barriers the tunneling time becomes independent of the thickness of the barrier. Remarkably, what comes out of the barrier is not a single wave packet, but infinitely many, one after the other. The time each of these wavepackets needs for the tunneling is completely independent of the thickness of the barrier. But for thicker barriers, the later wavepackets are much more attenuated.

In order to obtain an unambiguous time evolution in quantum cosmology, we decided to choose unimodular gravity instead of general relativity in its common form as the starting point for the canonical quantization procedure. This theory is practically indistinguishable from general relativity, with the only difference that the cosmological constant is a conserved quantity instead of a constant of nature. But since the theory has a different canonical structure it leads to a quantum theory that admits a time evolution. We investigate the toy model of a massless scalar field in a spatially flat universe and construct solutions with a unitary time evolution. Unlike common quantum-mechanical systems (as the ones considered in the first part) the solutions become classical in a certain sense in the late phase of time evolution. The quantum analogue of the special case of de Sitter solutions is obtained by assuming special symmetries of the wave function. The solutions provided in an explicit example can be continued beyond the singularity at $t = 0$, passing a finite minimal extension of the universe.

Zusammenfassung

Diese Arbeit besteht aus zwei Teilen, der erste betrifft die Quantenmechanik, im zweiten geht es um Quantenkosmologie. Beiden liegt das Bestreben zu Grunde, den Übergang von klassischer Dynamik zu quantenmechanischem Verhalten zu verstehen, und die auftretenden Abweichungen zu analysieren.

Im ersten Teil liegt das Interesse bei der semiklassischen Phase der Zeitentwicklung, in der zwar noch keine Revivalphänomene, auftreten, aber dennoch bereits Quanteneffekte zum tragen kommen. Es wird die Methode der Laplacetransformation eingefhrt, mit deren Hilfe man die Lösung der zeitabhängigen Schrödingergleichung angeben kann, wenn die Lösung der zeitunabhängigen Gleichung bekannt ist. Dabei ist es nicht nötig, Eigenzustände zu summieren oder das Pfadintegral zu Hilfe zu nehmen. Es werden die Propagatoren für das Kastenpotential, die Potentialstufe, das asymmetrische Kastenpotential (Kasten mit Ausgang) und die endliche Barriere hergeleitet. Die Lösungen geben anschaulich die Dynamik der Wellenpakete wieder und beinhalten das quantenmechanische Analogon zum klassischen Reflexionsprozess.

Im Fall des Kastenpotentials gelingt es, die Spiegellösung herzuleiten, ohne dabei die Symmetrie des Potentials zu Hilfe zu nehmen. Es werden zwei Theoreme präsentiert, die zeigen, dass in einer bestimmten Phase der Zeitentwicklung nur bestimmte Terme der Spiegiellösung zum tragen kommen. Bei der Potentialsufe wird gezeigt, dass Wellenpakete, die eine niedrigere Enegrie als die der Stufe haben, nur während des Reflexionsprozesses in den verbotenen Bereich jenseits der Stufe hineinfließen. Der Reflexionkoeffizient für genügend konzentrierte Wellenpakete enspricht dem bekannten Wert für das zeitunabhängige Problem. Die Propagator für das asymmetrische Kastenpotential stellt sich als intuitive Kombination der Lösungen für das das gewöhnliche Kastenpotential und die Potentialstufe heraus. Dieses Ergebnis unterscheidet sich grundsätzlich von dem, was unter dem Gesichtspunkt der Darstellung als einer Kombination von Eigenzuständen erwartbar ist, da der Kasten mit Ausgang zum Unterschied vom unendlich hohen Potentialtopf sowohl gebundene als auch ungebunde Eigenzustände besitzt. Soweit bekannt ist, ist das Anfangswertproblem für das asymetrische Kastenpotential noch nicht betrachtet worden. Bei der Untersuchung der endlichen Barriere ist es gelungen, den Hartmann Effekt in einem neuen Licht erscheinen zu lassen. Dieser besagt, dass für genügend dicke Barrieren die Tunnelzeit nicht von der Barrierendicke abhängt. Interessanter Weise ist es jedoch nicht ein Wellenpacket, das die Barriere verlässt, sondern es sind unendlich viele, die eines nach dem anderen hindurchtunneln. Die Zeit, die jedes davon für das Durchtunneln der Barriere benötigt hängt nicht von der Dicke der Barriere ab. Aber je dicker die Barriere ist, desto stärker werden die späteren Wellenpackete abgeschwächt.

Um eine eindeutige Zeitentwicklung in der Quantenkosmologie zu erhalten, wurde die unimodulare Theorie anstatt der allgemeinen Relativitättheorie als Ausgangpunkt für die kanonische Quantisierung verwendet. Diese Theorie ist praktisch ununterscheidbar von der allgemeinen Relativitätstheorie. Der einzige Unterschied besteht darin, dass die kosmologische Konstante eine Erhaltungsgrö ße und nicht eine Naurkonstante ist. Da die unimodulare Theorie jedoch eine andere kanonische Struktur hat, führt sie auf eine Quantentheorie, die eine Zeitentwicklung zulässt. Im Rahmen des untersuchten Modells eines räumlich flachen Universums mit einem masselosen skalaren Feld werden Lösungen mit einer unitären Zeitentwicklung konstruiert. Im Gegensatz zu den geläufigen quantenmechanischen Modellen (wie den im ersten Teil untersuchten), bekommen die Lösungen in diesem Modell mit der Zeit in einem gewissen Sinn immer mehr klassischen Charakter. Außerdem ist es gelungen das Analogon zu den de Sitter Lösungen zu finden, indem bestimmte Symmetriebedingungen an die Lösungen gestellt werden. In einem expliziten Beispiel werden Lösungen präsentiert, die über die Singularität bei $t = 0$ hinaus fortgesetzt werden können, wobei die minimale Ausdehnung das Universums endlich bleibt.

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