Subdiffusive reaction-diffusion equations

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1 Introduction

Diffusion is a widely investigated and common phenomenon. Already the preparation of a cup of tea possibly yields the question why the colour of the tea spreads throughout the whole cup without stirring a single time. The first scientist who occupied himself with this problem, and hence with the question why two substances, when brought together, tend to mix, was Adolf Fick. In 1855 he formulated the principles of diffusion on an empirical basis and elaborated the diffusion equation [13]. Mathematically, the equation was not new. It was just a new application of the already known heat equation, which Fourier had stated in 1822 [17]. A more general derivation of the diffusion equation is based on a work by Einstein [7]. He was motivated by investigations of Brown, who had described a random movement of suspended particles in a fluid. Later on it was referred to as Brownian motion. Within a simple model, the so-called random walk model, he deduced the diffusion equation which describes the evolution of the probability density function of these suspended particles. He could show that this motion and also the process of mixing of different substances, the diffusion, is driven by the kinetic energy each particle of a substance has according to its temperature.

Considering diffusion in a fluid, the obvious feature, which can be observed, is the spreading of a number of particles in a given space throughout time. The conclusion of the diffusion equation is that the dependence of a particle density on time is linear. Mathematically this means $\langle x^2 \rangle \sim t$, the mean squared displacement of a Brownian particle is proportional to time. It is a consequence of the underlying Gaussian statistics each Brownian particle can be described with according to the diffusion equation. The physical equivalence of Brownian motion and diffusion is therefore easily deduced in terms of the central limit theorem. There are also processes where the typical spreading behaviour is observed but the dependence on time is not linear. Hence, the term "diffusion" is generalised and in all these cases where this linearity is not observable one speaks of anomalous diffusion, with $\langle x^2 \rangle \sim t^\alpha$, where α is larger than zero but not unity. In case of a sublinear dependence, where $0 < \alpha < 1$, the according process is called subdiffusion. Whenever the linear spreading relation is violated the diffusion equation fails to describe the process. Thus, the question is how to deal with such a process adequatly.

Within this thesis there are two different approaches to that issue. The first one, which I called the method of subordination, deals with the diffusion equation directly. It yields a description of the process in an alternative variable of time, the system time. Therefore, the process is described in this new time scale via the diffusion equation, which was stated by Fick. That entails the problem of finding the distribution this system time and the physical time have and finally leads to a certain class of so-called Lévy distributions. Another and more general way, which is also capable of describing processes where the mentioned time dependence is superlinear, is the so-called continuous time random walk. This model was derived in 1965 by Montroll and Weiss [29]. It leads to the same description of subdiffusion as the method of subordination but

the starting point is analogous to the one Einstein chose. This model for a random movement on the level of particles leads to the so-called fractional diffusion equation. The most important feature of this equation is its nonlocality in time. The Fickian diffusion equation includes a spatial and a temporal derivative of a density function, whereas the spatial derivative is bound to a temporal integration, in case of the fractional diffusion equation. Nowadays many phenomenons showing anomalous diffusion are well-known. Subdiffusion for example is found in charge carrier transport in amorphous semi-conducters [36], the transport of contaminants through soil [5] and in the spread of tumors [10], to name just a few.

An important class of systems, which are able to model a wide range of different phenomenons, are the reaction-diffusion systems. The application to chemistry is apparent, considering two substances that are brought together and mix and that are additionally capable of reacting with each other. Nevertheless, the most famous examples of employing reaction-diffusion equations as model equations come from other fields of science.

In 1952 Alan Turing published the article "The chemical Basis of Morphogenesis" [38] where he explained the evolution of spatial patterns as a result of a reaction-diffusion system containing two different reactants, which yields a possible explanation for the structured colouring of animal fur, for example. Another famous application was to model the spread of advantageous genes in a population by a single nonlinear reaction diffusion equation as it was done by Fisher in 1937 [15]. In the same year also Andrey Kolmogorov worked on this equation [25], which is today referred to as the Fisher-Kolmogorov-Petrovskii-Piskounov equation, consequently. It will be a main object of investigation concerning this thesis. This equation with different extensions has been widely investigated and employed as a model equation for different phenomena in ecology and also epidemiology [30]. An important feature in most of the applications is the convergence of the different solutions for large values of time to a uniform front. One aim of this thesis is to study a generalisation of this equation that also accounts for subdiffusion with different values of the characteristic exponent, see [8]. Another feature of the normal diffusive Fisher-Kolmogorov-Petrovskii-Piskounov equation is that it does not only converge to a front with a uniform speed but also that this speed can be evaluated in terms of a simplified linearised equation. So the two questions this thesis deals with, concerning this equation, can be formulated as follows: Does the solution of the subdiffusive Fisher-Kolmogorov-Petrovskii-Piskounov equation also converge to a uniform front? And is there furthermore a simple method available to predict its asymptotic velocity?

The mentioned front behaviour is not only characteristic for the Fisher-Kolmogorov-Petrovskii-Piskounov equation. Many nonlinear reaction-diffusion equations exhibit these propagating fronts. Nevertheless, depending on the symmetry of the reaction term, they can also be stationary. In this case they are often referred to as domain walls. The Zeldovich equation, the second object of investigation in this thesis, or better to say the specific form of Zeldovich equation that I was working on, exhibits the evolution of such domain walls. Reaction-diffusion equations providing this feature can therefore be used to model phenomenons, where such domain walls arise. The Newell-Whitehead-Segel equation for example, which is similar to the Zeldovich equation I dealt with, is used to model Rayleigh-Benard convection [31]. The method of deriving a subdiffusive reaction-diffusion equation, which was developed by Eule, Friedrich, Jenko,

and Sokolov [8], also in this case serves as a basis to reach a formulation of the Zeldovich equation that also accounts fore subdiffusion. The question the thesis deals with, concerning the subdiffusive Zeldovich equation, was quite similar to the ones regarded for the Fisher-Kolmogorov-Petrovskii-Piskounov equation: Does a domain wall arise? And how is the dependence of the evolution of such a domain wall on the exponent α to be characterised?

The structure of this diploma thesis is similar to the structure of the introduction. The second chapter characterises the mathematical description of diffusion in general and how further generalisations are made to meet with subdiffusion. In the third chapter reaction-diffusion equations with a normal diffusivity are discussed. The two mentioned equations are introduced as examples and discussed in terms of linear stability analysis. An option to reach approximate solutions, which also accounts for the nonlinearities, the singular perturbation approximation, is presented and applied to both of the equations. The fourth chapter finally deals with the according subdiffusive equations. The way to derive subdiffusive reaction-diffusion equations generally and the two equations particularly is explained. Afterwards, once again, a linear stability analysis for both of them is performed. In the last parts of this chapter the singular perturbation approximation is applied to the subdiffusive equations and their behaviour is discussed taking into account the mentioned questions.

2 From Brownian motion to anomalous diffusion

In the following chapter the Brownian motion and diffusion will be introduced and the expansion to anomalous diffusion will be carried out. Consequently, in the first section Brownian motion, its first investigation and the postulates which are necessary to deal with it will be described. In the second section stochastic processes and a way to handle them will be explained. The so-called Markov property and its importance concerning these processes will be announced and the master equation will be derived in an elementary way, which was taken from [21]. The random walk model, which is a model for the Brownian particles and which is able to predict charateristic features of Brownian motion and diffusion, will be introduced in section 2.3 – similar explanations of this model can be found in [9, 21, 24]. Characteristic features of diffusion will be explained in section 2.4, the extension to anomalous diffusion and especially subdiffusion will be motivated and described – this is also found in [9]. In section 2.5 the method of subordination will be derived. It is a method that leads to a description of subdiffusion starting from the diffusion equation. This section is mainly based on a talk Prof. Dr. Friedrich held in a seminary. Basic features of my description like the process $s(t)$ and the distribution $p(s,t)$ are also introduced in [16]. The section 2.6 is going to deal with a mathematical technique, which is used to handle probability density functions – the so-called characteristic functions will be introduced. With the help of these functions the central limit theorem, which enables the calculation of probability density functions concerning sums of stochastic variables, will be derived, taking account of Gaussian distributions. A further generalisation of this theorem will be announced in section 2.7 – both of these sections are similar to explanations in [9, 24]. Section 2.8 is going to start with the introduction of an integral transform, the Laplace transform, which is common, concerning the treatment of time dependent functions and distributions. Hence, some important features will be outlined and in the following an application of this transform concerning stochastic processes depending on time, the renewal theory, will be described. Basic descriptions of the Laplace transform can also be found in [6,33], whereas an introduction of the renewal theory is also contained in [9]. Section 2.9 will provide the derivation of an equation, the fractional diffusion equation, to describe subdiffusion. This equation will also be solved and a number of graphic examples will be given. The treatment of the problem of subordination, which I used to derive this equation, is also found in [9] and the solutions were taken from [28]. In section 2.10 the so-called continuous time random walk, a generalisation of the random walk, will be introduced and another derivation of the fractional diffusion equation will be shortly outlined. The explanations of the continuous time random walk were also taken from [9]. The last section of this chapter is going to demonstrate the possibility of taking account of certain initial conditions that are different from the ones implemented in the solution of the fractional diffusion equation given by [28].

2.1 Brownian motion

In the year 1826 the Scottish botanist Robert Brown discovered a new and exciting physical phenomenon. Looking through a microscop at plant pollen suspended in water, he found the microscopic seeds in a state of restless and undirected movement. In this time there were no theories that could explain why they did not rest and where they got their energy from. In 1828 Brown wrote "While examining these particles immersed in water, I observed many of them very evidently in motion[...] These motions were such as to satisfy me, after frequently repeated observation, that they arose neither from currents in the Fluid, nor from its gradual evaporation, but belonged to the particle itself." [27]. Although Maxwell and Boltzmann discovered their famous probability distribution 32 years later, which related the particle velocity in an ideal gas to its temperature, it still took 45 years more until this phenomenon was explained. In 1905 Albert Einstein first published his theory about the observations made by Brown, from there on referred to as Brownian motion. In [7] he could show that this motion is enforced by the motion of the microscopic fluid molecules and thus an essential implication of the statistic movement described by statistical thermodynamics and governed by the Maxwell-Boltzmann-distribution.

To reach a macroscopic description of the Brownian motion – from the point of the fluid molecules, immersed particles such as pollen can be regarded as macroscopic – he claimed the Brownian particles to

1. be independent of each other
2. possess a time scale τ, such that the movement of one particle only depends on its past within such an interval but not on the τ-intervals before
3. choose their direction at the beginning of each interval from a probability density function, that means by chance
4. posses a mean squared displacement and therefore a finite standard deviation for each τ-interval

2.2 Markov processes and the master equation

Trying to find a probability density function (pdf) for one Brownian particle to be at a given time t at some position x, some simplifications shall be employed. Let us first concentrate on a one dimensional discrete space and discrete time durations. In order to make a statistical investigation about where the particle will be after n time steps, one measures its position after each step. A large number of iterations yields a joint probability, $P_n(x_n, t_n;\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1)$, which describes the probabilities for all of the possible positions after all different steps in time. To reduce the number of arguments which are contained by the probability, one has to sum over all the possibilities for the arguments which are not of interest

$$P_n(x_n, t_n;\, x_{n-2}, t_{n-2}; ...;\, x_1, t_1) = \sum_{x_{n-1}} P_n(x_n, t_n;\, x_{n-1}, t_{n-1};\, x_{n-2}, t_{n-2}; ...;\, x_1, t_1)\,. \tag{2.1}$$

One can also consider the probability for the Brownian particle to be at x_n at the given time t_n under the condition that it was for sure at the sites x_{n-1}, x_{n-2} and so on at the corresponding times. This is called a conditional probability which in this case is expressed as $P(x_n, t_n|\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1)$. Then the following expression is valid

$$P_n(x_n, t_n;\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1) = P(x_n, t_n|\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1) \times P_{n-1}(x_{n-1}, t_{n-1}; ...;\, x_1, t_1)\,, \quad (2.2)$$

so that the conditional probability is calculated as

$$P(x_n, t_n|\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1) = \frac{P_n(x_n, t_n;\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1)}{P_{n-1}(x_{n-1}, t_{n-1}; ...;\, x_1, t_1)}\,. \quad (2.3)$$

Remembering the characteristics of the Brownian particles that were postulated by Einstein (sec. 2.1), it is now convenient to take the duration times between each measurement of the position to be at least as large as τ. According to the second postulate the expression reduces to

$$P(x_n, t_n|\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1) \overset{t_n - t_{n-1} \geq \tau}{=} P(x_n\,, t_n|\, x_{n-1}, t_{n-1})\,. \quad (2.4)$$

The probability of a Brownian particle is only related to its past within an interval of duration τ. More generally one says that in a scale of time steps which are at least as large as τ the process has Markovian character or that it is a Markov process. Simplifying the notation, I will go on writing

$$P(x_n, t_n|\, x_{n-1}, t_{n-1}) = p_{t_n,\, t_{n-1}}(x_n, x_{n-1})\,. \quad (2.5)$$

According to the Markov property, it is possible to factorise the joint probability

$$P_n(x_n, t_n;\, x_{n-1}, t_{n-1}; ...;\, x_1, t_1) = p_{t_n,\, t_{n-1}}(x_n, x_{n-1}) \times p_{t_{n-1},\, t_{n-2}}(x_{n-1}, x_{n-2}) \cdot ... \cdot P_1(x_1, t_1)\,. \quad (2.6)$$

Let us now consider three different times t_1, t_2, t_3 with $t_1 < t_2 < t_3$, the difference of two of them being an integer multiple of τ. As described before the following equation holds

$$P_2(x_3, t_3;\, x_1, t_1) = \sum_{x_2} P_3(x_3, t_3;\, x_2, t_2;\, x_1, t_1)\,. \quad (2.7)$$

This can again be factorised

$$p_{t_3,\, t_1}(x_3, x_1) = \sum_{x_2} p_{t_2,\, t_1}(x_1, x_2) p_{t_3,\, t_1}(x_3, x_1)\,. \quad (2.8)$$

This is the Chapman-Kolmogorov equation, which can easily be applied to a higher dimensional or continuos space by replacing the sum by an integral. Multiplying again by $P_1(x_1, t_1)$ entails another form of the equation

$$p_{t_3,\, t_1}(x_3, x_1) P_1(x_1, t_1) = P_2(x_3, t_3;\, x_1, t_1)\,, \quad (2.9)$$

which is similar to equation (2.2). Hence, it follows that

$$P_1(x_3,t_3) = \sum_{x_1} p_{t_3,\,t_1}(x_3,x_1)P_1(x_1,t_1)\,. \tag{2.10}$$

To put the whole thing in a more general framework I will now omit the index 1 of the probabilities and take account of the difference between the t's and x's by just stressing them

$$P(x,t) = \sum_{x'} p_{t,\,t'}(x,x')P(x',t')\,. \tag{2.11}$$

For the following it will be necessary to evaluate the time evolution of the probabilities. Hence, a limiting process concerning the time instant τ will be essential. To perform this limiting process the next step has to be made

$$\frac{1}{\tau}\left(P(x,t-\tau) - P(x,t)\right) = \frac{1}{\tau}\sum_{x'}\left(p_{t+\tau,\,t}(x,x')P(x',t) - p_{t,\,t-\tau}(x,x')P(x',t-\tau)\right)\,, \tag{2.12}$$

The probability that was stated in equation (2.11) is considered at two different times, at τ and at $t-\tau$. Moreover, their difference was multiplied by $\frac{1}{\tau}$. With the substitution $t-\tau \to t'$ the limit $\tau \to 0$ leads to

$$\dot{P}(x,t) = \sum_{x'} \dot{p}_t(x,x')P(x',t)\,. \tag{2.13}$$

The dot denotes the derivative with respect to t. $\dot{p}_t(x,x')$ can be interpreted as the transition rate per time for $x \neq x$' and will be expressed as $w(x|x')$ in the following. The case $x = x'$ is more difficult. Due to conservation of probability, the probability of not having a transition in the intervall τ is given as

$$p_\tau(x,x) = \left(1 - \sum_{x'\neq x} p_\tau(x',x)\right)\,. \tag{2.14}$$

Performing the same procedure as before to (beginning with expr. (2.12)), leads to

$$w(x|\,x) = \sum_{x'\neq x} w(x'|\,x) \tag{2.15}$$

Applying this to expression (2.12), yields the master equation

$$\dot{P}(x,t) = \sum_{x'\neq x}\left(w(x|\,x')P(x',t) - w(x'|\,x)P(x,t)\right)\,. \tag{2.16}$$

Again higher dimensional or continuos cases can also be handled, treating the spatial variables as vectors and replacing the sum by an integral. The master equation has a simple interpretation. The time derivative of a probability at a certain position x equals the sum over all transition rates into that position times the probabilities of finding it at the according sites before, minus the sum over all transition rates out of this position x times the probability of already being there at position x. The master equation with its

simple interpretation provides a good framework to model different types of stochastic and essentially Markovian processes.

2.3 The random walk

To develop an appropriate model to describe Brownian motion it is necessary to make some further approximations. I already considered the system to be one dimensional and discrete. The further approximation will be that all steps are of unit size Δx. The Brownian particle at site x is only able to perform steps to the neighbouring sites $x \pm \Delta x$. The time span between two successive steps is again considerered to be always the same, it will be called τ as before. Furtermore, the steps will be regarded as statistically independent of each other. The master equation then reads

$$\dot{P}(x,t) = w(x|\, x+\Delta x)P(x+\Delta x,t) + w(x|\, x-\Delta x)P(x-\Delta x,t) \\ - \left(w(x+\Delta x|\, x) + w(x-\Delta x|\, x)\right) P(x,t)\,. \quad (2.17)$$

Let the particle start at position $x = 0$. After the time span τ it will perform a step to the right or to the left with equal probabilties (each with probability $\frac{1}{2}$). This is why the model is referred to as random walk (RW), and why it is often explained as to have a proband walking on a line and deciding after each time span via coin flipping about what direction to take next. The most probable position after any number of steps seems to be the starting position again, which is almost right. An urgent consequence of the discretised space is that the particles position after an odd number of steps is $k \cdot \Delta x$ with k being odd as well. For an even number of steps k has also to be even so that it is impossible to find the particle at the starting position after an odd number of steps. The distance travelled by the particle has to be equal to the number of steps times the unit step size Δx. But what about the probabilities of the particle concerning different sites? There is a number of possible ways to get there. One is to solve the master equation, which would lead, with the help of Taylor expansion, to the diffusion equation, and consequently to a Gaussian distribution. Another one would be finding the discretised version of the pdf with the help of the joint probability, which asymptotically, so for large values of n, is a Gaussian, as well. The way I will present is a bit like a mixture of both. Due to the Markovian property of Brownian motion the pdf can be expressed via a recursion formula

$$P(x,t+\tau) = \frac{1}{2}P(x-\Delta x,t) + \frac{1}{2}P(x+\Delta x,t)\,, \quad (2.18)$$

with $x = k\Delta x$ and $t = n\tau$, where n denotes the total number of steps. Taylor expansion of the left hand side (lhs) with regard to small deviations τ leads to

$$P(x,t+\tau) \approx P(x,t) + \frac{\partial}{\partial t}P(x,t)\tau\,. \quad (2.19)$$

A similar expansion of the right hand side (rhs), considering small values of Δx entails

$$\begin{aligned} P(x \pm \Delta x, t) \approx & P(x,t) + \frac{\partial}{\partial x} P(x,t)(\pm \Delta x) \\ & + \frac{1}{2} \frac{\partial^2}{\partial x^2} P(x,t)(\pm \Delta x)^2 \,. \end{aligned} \tag{2.20}$$

Applying this to the recursion formula, one ends up with

$$\frac{\partial}{\partial t} P(x,t) = \frac{(\Delta x)^2}{2\Delta t} \frac{\partial^2}{\partial x^2} P(x,t) \,. \tag{2.21}$$

To get a continuous description of Brownian motion, one has to deal with the unit step size and time span. This is provided by a special kind of limiting process, the so-called diffusion limit. That means

$$\lim_{\substack{\Delta x \to 0 \\ \tau \to 0}} \frac{(\Delta x)^2}{2\tau} = konst. = D \,, \tag{2.22}$$

where D is named the diffusion constant. The derived equation

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial^2}{\partial x^2} P(x,t) \tag{2.23}$$

is called the diffusion equation. Also here the changeover to a higher dimensional space is easy to perform, turning the spatial derivative into a Laplace operator. The solution of the diffusion equation then appears to be the Gaussian distribution

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} \tag{2.24}$$

for the initial condition

$$P(x, t=0) = \delta(x) \,. \tag{2.25}$$

The statistically important values that were discussed shortly in the beginning of this section are now to be defined mathematically because now they can be calculated with the analytical expression that was evaluated for the pdf. The expectancy value for any function $Y(X)$ of a stochastic variable X which is distributed according to a certain pdf $P_X(x)$ is defined as

$$\langle Y(X) \rangle_P = \int_\Omega \mathrm{d}x y(x) P_X(x) \,, \tag{2.26}$$

where Ω is the set of possible values x, see e.g. [21]. The mean value for the position of the Brownian particle, in that case one also speaks of the first moment of the pdf, consequently reads

$$\langle X \rangle_P = \int_{-\infty}^{\infty} \mathrm{d}x x \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} = 0 \,, \tag{2.27}$$

which is due to the symmetry of the Gaussian. Generally any pdf is related to the stochastic variable it stands for with an index. It will be omitted throughout this thesis, if this relation is clear. The standard deviation for any stochastic variable is in

general defined as

$$\sigma_Y = \sqrt{\langle Y(X)^2 - [\langle Y(X)\rangle_P]^2\rangle_P}\,. \tag{2.28}$$

In the given case it reduces to the square root of the mean squared displacement, which is also called the second moment of the pdf and reads

$$\langle X^2\rangle_P = \int_{-\infty}^{\infty} \mathrm{d}x x^2 \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} = Dt\,. \tag{2.29}$$

This result is the most important characteristic of Brownian motion and diffusion. As the pdf, which was obtained via the RW, is the solution of the diffusion equation, diffusion and Brownian motion is mathematically the same thing, even though the physical phenomenons, which belong to both of the terms are not entirely the same. In the sense of Brownian motion the Gaussian embodies a distribution function for the probabilities a single particle has, to be at a certain position x concerning a given time t. In the sense of the physical phenomenon of diffusion the Gaussian assigns each position x with a particle density according to a given time t. Nevertheless, interpreting this density as the one concerning a number of Brownian particles also leads to the conclusion that the density function has to be a Gaussian.

2.4 Diffusion

The first scientist who reached a mathematical description of diffusion was Adolf Fick in 1855. Although the equation he derived empirically, the diffusion equation, was already known concerning the transport of heat, it was him who understood it applied for processes of mixing and random transport in general, as well. Thus, the diffusion equation is also called the second Fickian law. The most important characteristic of diffusion is the proportionality of the mean squared displacement to time

$$\left\langle x^2\right\rangle_P \sim t\,. \tag{2.30}$$

It was calculated in (2.29), where the relation reads $\left\langle x^2\right\rangle_P = Dt$. The diffusion constant was later on directly related to the temperature and friction of the fluid [7]. Albert Einstein derived the relation

$$D = \frac{k_B T}{m\gamma}\,, \tag{2.31}$$

where γ is the coefficient of friction, k_B Boltzmann‘s constant and m the particle mass [35]. It is also referred to as the fluctuation-dissipation relation. The characteristic proportionality has its importance in the fact that it is something experimentally observable. But also other processes of random transport are observed in which this proportionality and as a matter of fact the second Fickian law is violated. Nevertheless, they are still named diffusion. Diffusive behaviour as a technical term is therefore extended to all processes exhibiting

$$\left\langle x^2\right\rangle_P \sim t^\alpha\,, \tag{2.32}$$

where $\alpha > 0$. α is the so-called characteristic exponent. In the cases discussed above it was always equal to one. This kind of diffusion will be termed normal diffusion in the following. Cases where the mean squared displacement is subproportional to time, which means $0 < \alpha < 1$, are denoted as subdiffusive, cases where the mean squared displacement is superproportional to time ($\alpha > 1$), are classified as superdiffusive. In general diffusion with $\alpha \neq 1$ is called anomalous. There are various cases in many physical disciplines as well as in other sciences where anomalous diffusion is observed, as mentioned in the introduction. In the preceeding discussions the normal diffusive behaviour proved to be a consequence of the RW model and is, therefore, due to the Markovian character of Brownian motion. As this model is evidently not able to describe sub- or supersiffusion, the question arises how to model such systems and if they are still to be seen as Markovian systems. As this thesis is concerned with subdiffusive equations I will concentrate on subdiffusion in the following.

2.5 The method of subordination

Imagine two different types of particles, A an B, immersed in a fluid. Let both of them undergo a normal diffusion. Particles A shall be considered as very small in comparison to particles B, which results in different diffusion constants. Considering the fluctuation-dissipation relation and taking into account that the friction of a particle depends on its volume, it is clear that $D_A > D_B$. The ratio of both of them can also be regarded as a parameter varying the time scale on which one of the particle types diffuses

$$\begin{aligned} \frac{\partial}{\partial t}A(\mathbf{x},t) &= D_A \Delta_{\mathbf{x}} A(\mathbf{x},t) \\ &= \tau D_B \Delta_{\mathbf{x}} A(\mathbf{x},t)\,, \\ \frac{1}{\tau}\frac{\partial}{\partial t}A(\mathbf{x},t) &= \frac{\partial}{\partial t'}A(\mathbf{x},\frac{t'}{\tau}) \\ \overset{t'\to t}{\Longleftrightarrow} \frac{\partial}{\partial t}A(\mathbf{x},\frac{t}{\tau}) &= D_B \Delta_{\mathbf{x}} A(\mathbf{x},\frac{t}{\tau})\,. \end{aligned} \tag{2.33}$$

Thus, both types of particles diffuse in the same manner but, as $\tau > 1$, the time is running faster for particles A. Now let us furthermore assume that particles A and B are able to interact. Particles A can bind to the B ones and stay fixed to them for a random time span, which is still small in comparison to the time scale in which the particles B move. Only considering the random movement of particles A one says that they undergo a normal diffusion which is interrupted by waiting times when they are bound to the particles of type B. These waiting times make it difficult to define a certain time scale in which the described process is still Markovian. It can and will be shown that for a certain class of waiting time distributions the process is subdiffusive but there are also waiting time distributions for which the Markovian property is conserved.

The distributions that can be chosen as the underlying ones, concerning these waiting times, will be discussed in section 2.8. In the concept of subordination the pdf of the particles of type A is assigned with a random time scale, in which the particles still behave in a Markovian manner and undergo normal diffusion. This time scale is the so-called system time s. This system time is regarded as a time dependent stochastical process, see [16]. Consequently, there has to be a distribution function for

the probabilities of different values of s for a given physcal time t. In the described example this distribution function, which will from now be referred to as $p(s,t)$, is obviously related to the waiting times. Due to the importance for the whole issue of subdiffusion section 2.8 will concentrate on the analytic structure of the waiting time distribution, which will be termed $\Psi(\tau)$, and the relationship to the distribution $p(s,t)$. The advantage of these distributions is that the pdf of the A particles, knowing the analytic form of $p(s,t)$, can be related to the solution of the Markovian problem in system time

$$A(\mathbf{x},t) = \int_0^\infty \mathrm{d}s p(s,t) A_0(\mathbf{x},s)\,. \tag{2.34}$$

2.6 Characteristic functions and the central limit theorem

An important tool concerning the analysis of stochastic systems is the so-called central limit theorem (CLT). It deals with sums of stochastic variables and provides a powerful tool to investigate the corresponding underlying pdf's. An elementary derivation of the CLT can be carried out with the help of the so-called characteristic functions, which shall be introduced in the following. Each stochastic variable can be related to such a function taking account of its pdf by means of integral transformation. The normal way to calculate the characteristic function is provided by evaluating the Fourier transform of the pdf with respect to the variable under consideration. The Fourier transform of a function is generally defined as

$$\mathrm{FT}\left[f(x)\right] = \hat{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x f(x) \mathrm{e}^{\mathrm{i}kx}\,, \tag{2.35}$$

with the inversion formula

$$\mathrm{FT}^{-1}\left[\hat{f}(k)\right] = f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \hat{f}(k) \mathrm{e}^{-\mathrm{i}kx}\,. \tag{2.36}$$

The characteristic function then reads

$$\hat{P}_Y(k) = \int_\Omega \mathrm{d}x P_Y(x) \mathrm{e}^{\mathrm{i}ky(x)} = \left\langle \mathrm{e}^{\mathrm{i}kY(x)} \right\rangle_P\,. \tag{2.37}$$

It has a certain advantage considering the expectancy values of the variable in different powers under the given pdf. They can be calculated via derivation with respect to the variable k.

$$\begin{aligned}(-\mathrm{i})^n \left[\frac{\mathrm{d}^n}{\mathrm{d}k^n}\hat{P}_Y(k)\right]_{k=0} &= \left[\frac{\mathrm{d}^n}{\mathrm{d}k^n}\int_\Omega \mathrm{d}x P_Y(x)\mathrm{e}^{\mathrm{i}ky(x)}\right]_{k=0} \\ &= \int_\Omega \mathrm{d}x \left(y(x)\right)^n P(x) \\ &= \langle Y^n \rangle_P\,. \end{aligned} \tag{2.38}$$

The derivative for $k = 0$ gives the expectancy value. The characteristic function at $k = 0$ is always equal to one, which is due to the standardisation of pdf's. Therefore, it is easy to approximate the characteristic function, by means of Taylor expansion

$$\hat{P}_Y(k) = \sum_{n=0}^{\infty} \left[\frac{\mathrm{d}^n}{\mathrm{d}k^n} \hat{P}_Y(k) \right]_{k=0} \frac{(k)^n}{n!} \,. \tag{2.39}$$

The different orders of approximation are proportional to the corresponding expectancy values.

Let us now apply this techique to a number n of Brownian particles that are independently and identically distributed. They accordingly all possess the same mean value and standard deviation, for the sake of simplicity they will be 0 and σ throughout this example. One is now able to define a new stochastic variable as the sum over all particle positions

$$Y = X_1 + X_2 + ... + X_n \,. \tag{2.40}$$

The characteristic function of this new variable consequently simplifies

$$\begin{aligned} \hat{P}_Y(k) &= \left\langle \mathrm{e}^{\mathrm{i}kY} \right\rangle_P = \left\langle \mathrm{e}^{\mathrm{i}k \sum_{q=1}^{n} X_q} \right\rangle_P \\ &= \prod_{q=1}^{n} \left\langle \mathrm{e}^{\mathrm{i}kX_q} \right\rangle_P = \left(\left\langle \mathrm{e}^{\mathrm{i}kX} \right\rangle_P \right)^n \\ &= \left(\hat{P}_X(k) \right)^n \,. \end{aligned} \tag{2.41}$$

In the concrete case the pdf is a simple Gaussian. Its characteristic function reads

$$\hat{P}(k) = \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{\sigma\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2} = \mathrm{e}^{-\frac{\sigma^2 k^2}{2}} \,, \tag{2.42}$$

and consequently

$$\hat{P}_Y(k) = \mathrm{e}^{-n\frac{\sigma^2 k^2}{2}} \,. \tag{2.43}$$

If one then defines the scaled sum as to be

$$Z = \frac{1}{\sqrt{n}} \sum_{q=0}^{n} X_q \,. \tag{2.44}$$

Calculating the characteristic function leads to the same distribution, which underlies the positions of the single particles. This is one of the main statements of the CLT. But it can be generalised a bit more. Considering a large number of particles, identically and independently distributed, it is sufficient to assume that their mean value and standard deviation are known. Claiming that all of them have a mean value of zero and a standard deviation of σ, Taylor expansion provides the approximate characteristic function for each particle position X_q

$$\hat{P}_{X_q}(k) \approx 1 + \frac{\sigma^2 k^2}{2} \tag{2.45}$$

(see expr. (2.38) and expr. (2.38)). Hence, the characteristic function of the scaled sum (expr. (2.44)) reads

$$\hat{P}_Z(k) = \left(1 + \frac{\sigma^2 k^2}{2n}\right)^n . \tag{2.46}$$

For a sufficiently large number of particles this expression is approximatly equal to its limit $n \to \infty$, which entails

$$\hat{P}_Z(k) \approx \mathrm{e}^{-\frac{\sigma^2 k^2}{2}} . \tag{2.47}$$

So also in this case the large number of particles is distributed according to a Gaussian.

2.7 Generalisation of the central limit theorem and stable distributions

The CLT that was shown to be valid for the sum of identically and independently distributed stochastic variables, having a finite mean value and standard deviation, can be expanded to stochastic variables that lack these characteristics. This will become more important in the course of this thesis. The central feature of the generalised CLT can be expressed as follows

$$\sum_i (a_i X_i + b_i) \stackrel{d}{=} aX + b . \tag{2.48}$$

For arbitrary constants b_i and a_i, with the constraint $a_i \neq 0$, the parameters a and b exist, so that the expressions on both sides have the same underlying pdf (see [24]). This is ment by the "$\stackrel{d}{=}$", it represents the distributional equality. There is a broad class of distribution functions that provide this feature, subsumed under the term stable or Lévy distributions. A general formula for these distributions is only given in terms of their characteristic functions

$$\hat{L}_{\alpha,\beta}(k) = \exp\left(\mathrm{i}k\gamma - C\,|k|^\alpha \left[1 + \mathrm{i}\beta\frac{k}{|k|}\delta(k,\alpha)\right]\right), \tag{2.49}$$

(cf. [9, 24, 28]) with

$$\delta(\omega,\alpha) = \begin{cases} \tan(\frac{\pi}{2}\alpha) & ,\text{for } \alpha \neq 1, \\ \frac{2}{\pi}\ln(k) & ,\text{for } \alpha = 1 . \end{cases} \tag{2.50}$$

There are several other definitions with different parameters of these stable distributions. A rigorous derivation of the generalised CLT can be found in [19]. In the definition (2.49) there is first of all the real valued constant γ denoting a stiff displacement of the pdf. α is named characteristic exponent, with $0 < \alpha \leq 2$. Moreover, there is β, with $-1 \leq \beta \leq 1$, parameterising the asymmetry of the distribution. For $\beta = 1$ and $\alpha \neq 2$ the pdf is completely one sided and has nonzero values only for positive values of the stochastic variable. At last there is the scaling parameter C, which is always positive. An expression for the pdf in physical values is provided by the inverse transform. But not for any choice of parameters it can be evaluated. In the case $\alpha = 2$, the inverse transform is a Gaussian. For all values with $\alpha < 2$ the standard deviation does not exist and for $\alpha < 1$ also the mean value vanishes. In the following sections the choice

$\beta = 1, \alpha < 1, \gamma = 0$ will be of great interest. A possible way to express the corresponding Lévy distributions in physical values is given by the so-called Fox functions [28], which will be discussed a bit more in the course of this thesis. The reason why these one-sided

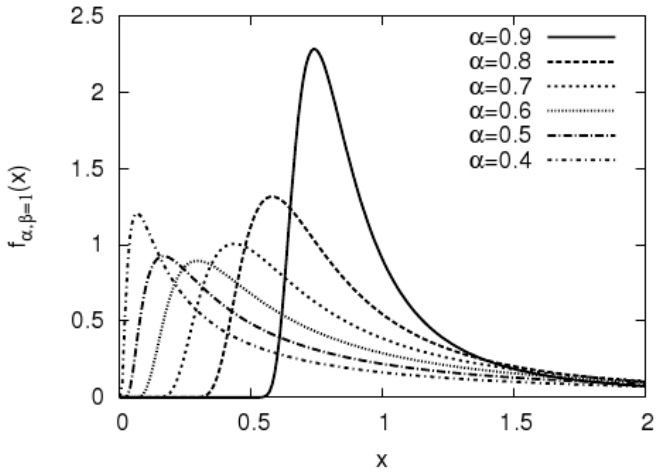

Figure 2.1: The Lévy distribution for $\beta = 1$ and for different values of $0 < \alpha < 1$, taken from [24]

Lévy distributions with $0 < \alpha < 1$ are so important concerning this thesis will become clear in the ongoing thesis. To prepare this let me perform a procedure that leads to these distribution, which is similar to the one performed in the last section and lead to the CLT. For this special form of Lévy distribution the following proportionality holds

$$\hat{L}_{\alpha,1}(\omega) \sim \mathrm{e}^{-C|\omega|} \,. \tag{2.51}$$

Let us now take a number n of indepentently identically distributed stochastic variables X_q into account. The asymptotic behaviour of the underlying pdf shall be described by the proportionality

$$\psi_{X_q}(x) \sim C\frac{1}{x^\alpha} \,. \tag{2.52}$$

Pdf's that show this behaviour are referred to as to posses a power-law tails or as power-law distributions [9]. They will play a key role in the following sections. For the characteristic function the corresponding proportionality reads

$$\hat{\psi}_{X_q}(\omega) \sim 1 - \hat{C}\,|\omega|^\alpha \,, \tag{2.53}$$

which is due to the so-called Tauberian theorems [12], where the asymptotic behaviour for large values of x corresponds to the behaviour for small values of ω concerning the characteristic function. In this case th scaled sum shall be defined as

$$Z = \sum_q \frac{X_q}{n^{\frac{1}{\beta}}} \tag{2.54}$$

We are now looking for the underlying pdf of the scaled sum. Steps similar to the ones performed in section 2.6 lead to the pdf

$$\hat{\psi}_Z(\omega) = \left(1 - \hat{C}\,|\omega|^\alpha\right)^n \tag{2.55}$$

In the limit $n \to \infty$, so for a large number of stochastic variables, the mentioned proportionality of the one-sided Lévy distribution (expr. 2.51) is obtained

$$\hat{\psi}_Z(\omega) = \mathrm{e}^{\hat{C}|\omega|^\alpha} \tag{2.56}$$

Speaking in terms of equation (2.48), the conclusion is that one-sided Lévy distributions posses a power-law tail, which is also demonstrated by figure 2.1.

2.8 Laplace transformation and the renewal theory

The following essential problem is finding the analytic relation between the two mentioned distributions $\psi(\tau)$ and $p(s,t)$ and the concrete structure of both of them. The theory which is concerned with distributions in time is named renewal theory. Before I introduce into that theory let me present another kind of integral transform, which is not as common in physics as the Fourier transform. The Laplace transform is applied in connection with variables that are defined on $\mathbb{R}_+$ exclusively. It is defined as

$$\mathrm{LT}\left[f(t)\right] = \tilde{f}(\lambda) = \int_0^\infty \mathrm{d}t f(t)\mathrm{e}^{-\lambda t}\,. \tag{2.57}$$

The advantages of dealing with a function in the Laplace domain instead of treating the corresponding function depending on physical values are similar to the advantages of the Fourier transform. The most important ones are

$$\mathrm{LT}\left[f(at)\right] = \frac{1}{|a|}\tilde{f}(\frac{\lambda}{a})\,, \tag{2.58}$$

$$\mathrm{LT}\left[\frac{\mathrm{d}}{\mathrm{d}t}f(t)\right] = \lambda\tilde{f}(\lambda) - f(t=0)\,, \tag{2.59}$$

$$\mathrm{LT}\left[\int_o^t \mathrm{d}\tau f(\tau)\right] = \frac{1}{\lambda}\tilde{f}(\lambda)\,, \tag{2.60}$$

$$\mathrm{LT}\left[f(t)\mathrm{e}^{at}\right] = \tilde{f}(\lambda - a)\,, \tag{2.61}$$

$$\mathrm{LT}\left[\int_0^t \mathrm{d}\tau f(t-\tau)v(\tau)\right] = \tilde{f}(\lambda)\tilde{v}(\lambda)\,, \tag{2.62}$$

see [6]. A disadvantage of the Laplace transform in comparison to the Fourier transform is the difficult inverse transformation

$$\mathrm{LT}^{-1}\left[\tilde{f}(\lambda)\right] := f(t) = \frac{1}{2\pi \mathrm{i}} \int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \mathrm{d}\lambda \tilde{f}(\lambda) \mathrm{e}^{\lambda t}\,, \tag{2.63}$$

where γ is a parameter that cares for a path of integration lying inside the region of convergence. In most practicle cases one compares a given transform with tabulated ones in order to find the function in time domain (for example [6]). It is also a good tool for calculating the characteristic functions of distributions in time, what makes the Laplace transform an indispensable technique for this thesis and especially for the following discussion.

The so-called renewal theory deals with random processes in time. Many processes in physics consisting of a number of single events distributed in time can be regarded as dots on a time axis. One can think of a Geiger-Müller counter that records the radioactive decay of a given substance. Each time a single event of decay is detected it clicks. The time durations elapsed between two succesive events of decay, or clicks respectively, can then be regarded as random variables, which are independently identically distributed. These time durations will be denoted as the waiting times, τ, in the following, with the underlying distribution, $\Psi(\tau)$, the waiting time distribution. With the first event a duration or waiting time τ_1 is drawn from the waiting time distribution, so that the first point in the scale t, is determined with $t_1 = \tau_1$. For the second event the point in time t is again defined by drawing a waiting time from $\Psi(\tau)$ with $t_2 = t_1 + \tau_2$. Each drawing of a waiting time is referred to as one process of renewal. The process is renewed until a number n is reached, with $t_{n+1} > t$. t denotes the boundary of an arbitrary time interval, $[0, t]$), in which a random number, n, of renewals can be observed. The pdf of this random number will be denoted as $p_n(t)$

The connection to section 2.5 is at hand. The waiting time distribution discussed above is the same that was introduced into the method of subordination. Moreover, the number of renewals within a given time interval is a discrete version of the distribution function $p(s, t)$. One can then define an auxiliary function $\phi_n(t)$ denoting the probability that the nth event lies in the interval $[t, t + \mathrm{d}t]$, for which the following recursion formula holds

$$\phi_n(t) = \int_0^t \mathrm{d}\tau \phi_{n-1}(t-\tau)\Psi(\tau)\,. \tag{2.64}$$

This relation simplifies in Laplace space to

$$\tilde{\phi}_n(\lambda) = \tilde{\phi}_{n-1}(\lambda)\tilde{\Psi}(\lambda)\,. \tag{2.65}$$

The characteristic function was this time calculated as the Laplace transform of the given pdf, which is the conventional way to deal with distributions depending on time. With the help of this relation the expression $\tilde{\phi}_n(\lambda)$ factorises

$$\tilde{\phi}_n(\lambda) = \left(\tilde{\Psi}(\lambda)\right)^n\,, \tag{2.66}$$

with $\phi_1(t) = \Psi(t)$. One is also able to express the distribution $p_n(t)$ in terms of the auxiliary distribution. As a result of the conservation of probability the distribution concerning the case of not having a process of renewal in a given time interval reads

$$w(t) = 1 - \int_0^t \mathrm{d}\tau \Psi(\tau)\,, \tag{2.67}$$

which results in

$$p_n(t) = 1 - \int_0^t \mathrm{d}\tau \phi_n(t-\tau) w(\tau)\,. \tag{2.68}$$

The Laplace transform then gives the searched for expression for p_n in terms of the waiting times

$$\begin{aligned} \tilde{p}_n(\lambda) &= \left(\tilde{\Psi}(\lambda)\right)^n \tilde{w}(\lambda) \\ &= \left(\tilde{\Psi}(\lambda)\right)^n \frac{1-\tilde{\Psi}(\lambda)}{\lambda}\,. \end{aligned} \tag{2.69}$$

So the problem of subdiffusion reduces to the problem of choosing a distribution function for $\Psi(\tau)$ or $\tilde{\Psi}(\lambda)$. To model subdiffusion not all kinds of distribution functions can be chosen as waiting time distributions. Distributions with a finite mean value lead to normal diffusion. In the following I will use a form of distribution that was introduced in section 2.7, a distribution exhibiting a power-law tail

$$\Psi(\tau) \sim C \frac{1}{\tau^\alpha}\,. \tag{2.70}$$

The asymptotic behaviour in Laplace space reads (see eq. (2.53))

$$\tilde{\Psi}(\lambda) \sim 1 - \tilde{C}\lambda^\alpha\,. \tag{2.71}$$

The application of expression (2.71) to equation (2.69) leads to

$$\tilde{p}_n(\lambda) \sim \tilde{C}\lambda^{\alpha-1}\left(1-\tilde{C}\lambda^\alpha\right)^n = \tilde{C}\lambda^{\alpha-1}\mathrm{e}^{n\ln(1-\tilde{C}\lambda^\alpha)}\,. \tag{2.72}$$

As the behaviour of the pdf concerning small values of λ was evaluated, it is in this case reasonable to assume

$$\ln(1-\tilde{C}\lambda^\alpha) \approx -\tilde{C}\lambda^\alpha\,. \tag{2.73}$$

Including the constant $\tilde{C}$ into the variable λ, one finally obtains

$$\tilde{p}_n(\lambda) \approx \lambda^{\alpha-1}\mathrm{e}^{-n\lambda^\alpha} \tag{2.74}$$

as an approximation for small values of λ. In this formulation the transmission to continuous values of n is easy to perform. A simple substitution $n \to s$ yields

$$\tilde{p}(s,\lambda) \approx \lambda^{\alpha-1}\mathrm{e}^{-s\lambda^\alpha} = -\frac{\partial}{\partial s}\left(\frac{1}{\lambda}\mathrm{e}^{-s\lambda^\alpha}\right)\,. \tag{2.75}$$

With the help of this function I shall meet with the principle of subordination once again. The form of this function is proportional to the Laplace transform of a one-sided Lévy distribution (see fig. 2.1), with $\beta = 1$ and $0 < \alpha < 1$ (see expr. (2.51)). It is also referred to as inverse Lévy distribution. Inverse Laplace transformation leads to the distribution $p(s,t)$, which governs the mapping of the systemtime s to the physical time t, see [9].

2.9 Subordination in Laplace space and fractional calculus

With the help of the derived expression (2.75) for the characteristic function $\tilde{p}(s,\lambda)$ the equation that was derived in section 2.5 can be used as the starting point to reach a description of subdiffusion. The equation reads

$$f(\mathbf{x},t) = \int_0^\infty \mathrm{d}s p(s,t) f_0(\mathbf{x},s)\,, \tag{2.76}$$

which is equal to (2.34). The solution $f(\mathbf{x},t)$ is within this framework related to the function $f_0(\mathbf{x},s)$, which is the solution of the normal diffusion equation. A possible way to solve it is caused by a different interpretation of the equation in Laplace space, which shall be introduced in the following. The Laplace transform of equation (2.76) takes the form

$$\tilde{f}(\mathbf{x},\lambda) = \int_0^\infty \mathrm{d}s \tilde{p}(s,\lambda) f_0(\mathbf{x},s)\,. \tag{2.77}$$

Inserting the given distribution

$$\tilde{p}(s,\lambda) = \lambda^{\alpha-1}\mathrm{e}^{-s\lambda^\alpha} \tag{2.78}$$

leaves us with

$$\tilde{f}(\mathbf{x},\lambda) = \int_0^\infty \mathrm{d}s A\lambda^{\alpha-1}\mathrm{e}^{-As\lambda^\alpha} f_0(\mathbf{x},s)\,. \tag{2.79}$$

The integral can be interpreted as another Laplace transform with respect to λ^α. This leads to a simple relation

$$\tilde{f}(\mathbf{x},\lambda) = \lambda^{\alpha-1}\tilde{f}_0(\mathbf{x},\lambda^\alpha)\,, \tag{2.80}$$

or

$$\tilde{f}_0(\mathbf{x},\lambda^\alpha) = \lambda^{1-\alpha}\tilde{f}(\mathbf{x},\lambda)\,. \tag{2.81}$$

The normal diffusion equation transforms as follows

$$\begin{aligned} &\mathrm{LT}\left[\frac{\partial}{\partial t}P(\mathbf{x},t) = D\Delta_{\mathbf{x}}P(\mathbf{x},t)\right] \\ &\Leftrightarrow u\tilde{P}(\mathbf{x},u) - P(x,t=0) = D\Delta_{\mathbf{x}}\tilde{P}(\mathbf{x},u)\,, \end{aligned} \tag{2.82}$$

with u being the Laplace variable (see sec. 2.8). Now the substitutions $u \to \lambda^\alpha$ and $\tilde{P}(\mathbf{x}, u) \to \tilde{f}_0(\mathbf{x}, \lambda^\alpha)$ yield

$$\lambda^\alpha \tilde{f}_0(\mathbf{x}, \lambda^\alpha) - f_0(x, s = 0) = D\Delta_\mathbf{x} \tilde{f}_0(\mathbf{x}, \lambda^\alpha)\,. \tag{2.83}$$

The relation (2.81) can be applied

$$\lambda \tilde{f}(\mathbf{x}, \lambda) - f(\mathbf{x}, t = 0) = \lambda^{1-\alpha} D\Delta_\mathbf{x} \tilde{f}(\mathbf{x}\,\lambda)\,, \tag{2.84}$$

where $f_0(\mathbf{x}, t = 0) = f_0(\mathbf{x}, s = 0)$ was assumed. The inverse transformation of equation (2.84) leads to an equation describing subdiffusion. As already indicated, the multiplication of a Laplace transform with the Laplace variable to any integer power, abandoning the needed initial conditions, always leads to a differentiation or integration of the same order (see relations (2.59) and (2.60)) in time domain. So the question arises, what is about to happen to the function in time domain if the power of the Laplace variable is not an integer. Is there a fractional generalisation of infinitesimal calculus? Yes, there is. A number of different definitions for fractional integrals and derivatives is given in literature (for an exhaustive treatment see [23, 33]). The most frequently used one is probably the Riemann-Liouville fractional calculus, which is defined as

$${}_0\mathrm{D}_t^\gamma g(t) = \frac{1}{\Gamma(\gamma)} \int_0^t \mathrm{d}\tau (t - \tau)^{\gamma-1} g(\tau)\,, \tag{2.85}$$

with the explicit form of the Γ-function being

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

${}_a\mathrm{D}_t^\gamma$ is the operator of fractional integration and differentiation, which depends on the sign of γ. If γ is positive the operator the corresponding mathematical operation is regarded as fractional derivation. The Laplace transform of expression (2.85) reads

$$\mathrm{LT}\left[{}_a\mathrm{D}_t^\gamma g(t)\right] = \lambda^\gamma \tilde{g}(\lambda)\,. \tag{2.86}$$

It is a linear operator. Hence, the differetial equation concerning subdiffusion is constituted as the inverse transform of equation (2.84)

$$\frac{\partial}{\partial t} f(\mathbf{x}, t) = D\,{}_0\mathrm{D}_t^{1-\alpha} \Delta_\mathbf{x} f(\mathbf{x}, t)\,. \tag{2.87}$$

Due to the time derivative of fractional order – it will be demonsrated later on that $\alpha < 1$ – it is also named fractional diffusion equation (FDE). In this partial differential equation (PDE) the pdf is related to its past, which is completely incompatible with a Markovian process. The memory effect is also often met by writing this equation in another way

$$\frac{\partial}{\partial t} f(\mathbf{x}, t) = D\Delta_\mathbf{x} \int_0^t \mathrm{d}\tau Q(t - \tau) f(\mathbf{x}, \tau)\,, \tag{2.88}$$

where $Q(t)$ is called the time or memory kernel. In that way it is possible to generalise this subdiffusive nature also on reaction diffusion equations, which will become more important in the course of this thesis. An analytical expression for the time kernel is only given in Laplace [8]. It can be derived from the following differential equation

$$\frac{\partial}{\partial t}p(s,t) = -\int_0^t \mathrm{d}t' Q(t-t')\frac{\partial}{\partial s}p(s,t')\,. \tag{2.89}$$

The Laplace transform reads

$$\lambda\tilde{p}(s,\lambda) - p_0 = -\frac{\partial}{\partial s}(\tilde{Q}(\lambda)\tilde{p}(s,\lambda))\,, \tag{2.90}$$

with the condition $p_0 = 0$. The derived solution for $\tilde{p}(s,\lambda)$ (expr. 2.75) yields an analytical expression for the time kernel in the Laplace domain

$$\tilde{Q}(\lambda) = \lambda^{1-\alpha}\,. \tag{2.91}$$

The solution of the FDE, concerning the initial condition $f(\mathbf{x}, t=0) = \delta(\mathbf{x})$, is given in terms of a so-called Fox function. Functions of that type often appear in connection with inverse integral transformations and fractional order infinitesimal calculus. In general they are defined as follows

$$\begin{aligned}\mathrm{H}_{p,\,q}^{m,\,n}\left[z\middle|\begin{matrix}(a_1,A_1),...,(a_p,A_p)\\(b_1,B_1),...,(b_q,B_q)\end{matrix}\right]&\\ = \frac{1}{2\pi\mathrm{i}}\int_{\mathfrak{L}}\mathrm{d}s\frac{\prod_{i=1}^{m}\Gamma\left(b_i+B_is\right)\prod_{i=1}^{n}\Gamma\left(1-a_i-A_is\right)}{\prod_{i=n+1}^{p}\Gamma\left(a_i+A_is\right)\prod_{i=m+1}^{q}\Gamma\left(1-b_i-B_is\right)}z^{-s}&\end{aligned} \tag{2.92}$$

(see [23]). $\mathfrak{L}$ denotes the contour of integration which goes from $\omega - \mathrm{i}s$ to $\omega + \mathrm{i}s$. The solution of the FDE reads

$$f(\mathbf{x},t) = \frac{1}{\sqrt{4Dt^\alpha}}\mathrm{H}_{1,\,1}^{1,\,0}\left[\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}}\middle|\begin{matrix}\left(1-\frac{\alpha}{2},\frac{\alpha}{2}\right)\\(0,1)\end{matrix}\right] \tag{2.93}$$

(see [28]). In the case of $\alpha = \frac{1}{2}$ it reduces to a so-called Meijer-G function, which belongs to the implemented functions of the computer program Mathematica. The deviation from Gaussian statistics is quite apparent (fig 2.2). The slope on the flanks of the distribution is steeper than the slope of a Gaussian distribution. It has the same symmetry as the Gaussian, which is in this case due to dependence of the solution on the norm of $\mathbf{x}$. This is also the explanation of the sharp peak at position $\mathbf{x} = 0$. The generalisation of expression (2.93) to other values of α is possible via a series expansion

$$f(\mathbf{x},t) = \frac{1}{\sqrt{4Dt^\alpha}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma\left(1-\frac{\alpha}{2}(k+1)\right)}\left(\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}}\right)^k \tag{2.94}$$

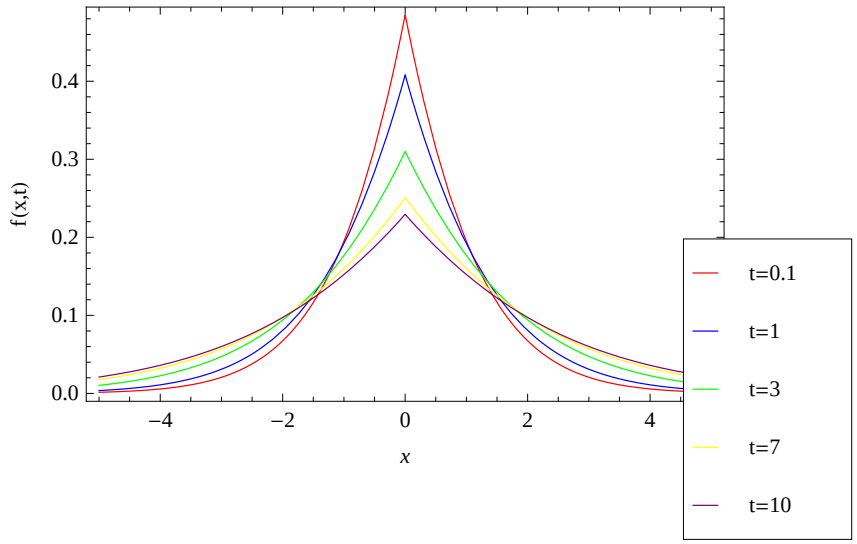

Figure 2.2: The solution (2.93) of the FDE (2.87) in one spatial dimension for $\alpha = 0.5$ and for different values of t.

(see [23, 28]). Comparing the case of $\alpha = \frac{1}{2}$ to the resulting series, shows that it is sufficient to abort the series at $k = 100$. On the considered spatial interval the plot does not change taking more terms of the sum into account. The plot for $\alpha = \frac{2}{3}$ (fig. 2.3) shows that the steepness of the flanks is decreased with increasing α.

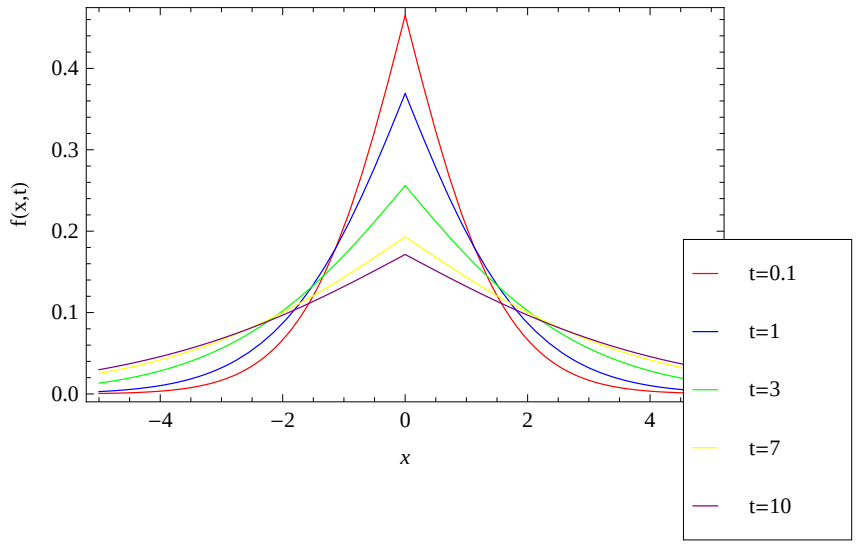

Figure 2.3: The solution (2.94)of the FDE (2.87) in one spatial dimension for $\alpha = \frac{2}{3}$ and for different values of t.

Analytically it can be shown that the series expansion reduces to a Gaussian in the limit $\alpha \to 1$, which can also be clarified graphically (see fig. 2.4).

To calculate the mean squared displacement terminally one takes the FDE in the

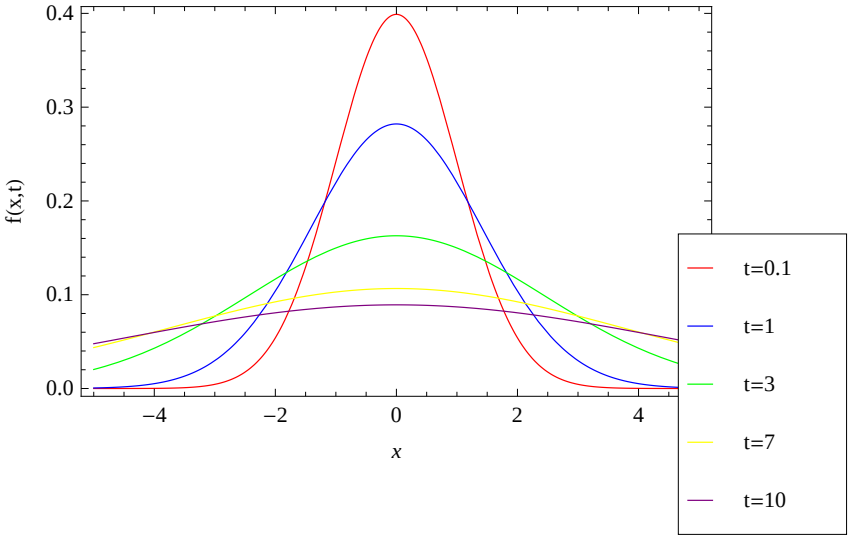

Figure 2.4: The solution 2.94) of the FDE (2.87) in one spatial dimension for $\alpha = 1$ and for different values of t.

Laplace transformed version (2.84) and transforms it to Fourier space as well. The initial condition, which is also in this case considered to be $f(\mathbf{x}, t = 0) = \delta(\mathbf{x})$, reduces to a constant in Fourier space. The result is a simple ananalytic expression for the transformed pdf

$$\hat{\tilde{f}}(\lambda, k) = \frac{1}{\lambda + \lambda^{1-\alpha} D k^2}\,, \tag{2.95}$$

calculated for one spatial dimension. The mean squared displacement is calculated as the second derivative with respect to k in the limit $k \to 0$.

$$\mathrm{LT}\left[\left\langle \mathbf{X}^2 \right\rangle_f\right] = \lim_{k\to 0}\left(\frac{\partial^2}{\partial k^2}\hat{\tilde{f}}(\lambda, k)\right) = \frac{2D}{\lambda^{1+\alpha}}\,. \tag{2.96}$$

Inverse Laplace transformation then yields

$$\left\langle \mathbf{X}^2 \right\rangle_f = \frac{2Dt^\alpha}{\Gamma(1+\alpha)} \tag{2.97}$$

(see [6]). The sublinear dependence on time is verified. As a result it is obvious that the exponent that stems from the derivation of the function $\tilde{p}(s, \lambda)$ originally, which is equal to the characteristic exponent of the according Lévy distribution, is equal to the characteristic exponent, α, concerning anomalous diffusion.

2.10 The continuous time random walk

Equation (2.87) can also be derived from another model, which is very common and often applied concerning modelling of anomalous transport in general. In section 2.5 the random time scale was inflected directly into the diffusion equation. In contrast to that one can also start the discussion of anomalous transport on the level of Brownian

motion. Thinking of particles that perform some kind of random movement, like the ones Robert Brown observed, where this zitterbewegung is interrupted by random waiting times. Of course the RW model then fails to describe the behaviour of these particles, so another model or an extension of the RW model is needed. The continouos time random walk (CTRW) model yields this extension. In 1965 it was first developed by Elliott W. Montroll and George H. Weiss [29]. Since then it has been applied to various kinds of systems for it is capable of describing both, super- and subdiffusion. The extension of the RW lies in the assumption that also the number of steps a particle performes in a given time duration is a random variable. Consequently the CTRW is referred to as a renewal process subordinated to a RW.

The distribution underlying the motion of these particles is a function of both, the displacements Δx and the waiting times τ. Let us name it $\xi(\Delta x, \tau)$. In this connection an important approximation has to be inflected. Intuitively one would say that jump length and waiting time should be corellated. But taking the RW model, where jumps are considered to reach only the neighbouring positions, as a basis, one assumes waiting times and displacements to be uncorrelated. The CTRW model is hence also characterised as decoupled. The joint probability factorises

$$\xi(\Delta x, \tau) = h(\Delta x)\Psi(\tau)\,. \tag{2.98}$$

To simplify the procedure, let space be discrete and one dimensional once more. The distribution of a particle can then be established in the following way

$$f(x,t) = \sum_{n=0}^{\infty} p_n(t) h_n(x) \tag{2.99}$$

where $p_n(t)$ again counts the number of renewals, so in this case the number of random displacements, for a given time interval $[0,t]$ and $h_n(x)$ assigns each time step with a random displacement, see [9]. It is already known from the renewal theory (see sec.2.8). Applying both Fourier and Laplace transform to expression (2.99) yields

$$\hat{\tilde{f}}(k,\lambda) = \sum_{n=0}^{\infty} \left(\tilde{\Psi}(\lambda)\right)^n \frac{1-\tilde{\Psi}(\lambda)}{\lambda} \left(\hat{h}(k)\right)^n\,, \tag{2.100}$$

with $\hat{h}_n(k) = \left(\hat{h}(k)\right)^n$ (see sec. 2.6). The infinite sum can be evaluated due to the fact that pdf's as well as their characteristic functions are always equal to or less than one. Accordingly the given expression is an infinite geometric series converging to

$$\hat{\tilde{f}}(k,\lambda) = \frac{1-\tilde{\Psi}(\lambda)}{\lambda} \frac{1}{1-\hat{h}(k)\tilde{\Psi}(\lambda)} \tag{2.101}$$

This is the famous Montroll-Weiss equation bearing the solution of the decoupled CTRW model. The inverse transformation yields the solution in physical time and space. For waiting times, which are exponentially decreasing , the resulting CTRW is a Markov process, whereas in case of waiting time distributions exhibiting a power-law tail, which applies to distributions with an infinite mean value and standard deviation, the Markovian property is violated [9]. Moreover, it is the central equation for all phenomenons

of anomalous transport, because also superdiffusion is included. If we apply the right asymptotic behaviour for $\hat{h}(k)$ as well as for $\tilde{\Psi}(\lambda)$, the FDE (2.87), which was derived in the last section, emerges. For large values of x, which again corresponds to small values of k, a suitable approximation reads

$$\hat{h}(k) \approx 1 - \sigma^2 k^2 \tag{2.102}$$

assuming the mean value $\langle X \rangle_h$ to be zero with the standard deviation being σ. The reason for taking the asymptotic behaviour for the two characteristic functions is that a diffusion limit will be necessary (cf. sec. 2.3). The asymptotic approximation for the waiting time distribution was already evaluated in terms of the renewal theory

$$\tilde{\Psi}(\lambda) \approx 1 - \lambda^\alpha \,, \tag{2.103}$$

including the constant into the variable. Insertion of (2.102) and (2.103) into (2.101) yields the specific Montroll-Weiss equation

$$\hat{\tilde{f}}(k,\, \lambda) = \lambda^{\alpha-1} \frac{1}{\lambda^\alpha - \lambda^\alpha \sigma^2 k^2 + \sigma^2 k^2} \,. \tag{2.104}$$

Now a diffusion limit with $(\lambda, k) \to (0{,}0)$ provides

$$\hat{\tilde{f}}(k, \lambda) = \frac{\lambda^{\alpha-1}}{\lambda^\alpha + D_\alpha k^2} \,, \tag{2.105}$$

which is a consequence of the Tauberian theorems (cf. [9, 12]). D_α is the fractional version of the diffusion constant. In the following I will go on omitting the α. The inverse Fourier and Laplace transform of expression (2.105) again yield the FDE (2.87).

The CTRW model and the method of subordination particularly allow for a generalisation of the master equation, which was derived before (sec. 2.2). That sounds a bit mysterious due to the fact that we are dealing with non-Markovian processes. It is again due to the before introduced system time. One can again consider the process to be a Markovian one and describe it via a master equation in the system time, see [9]. It reads

$$\frac{\partial}{\partial t} P(x,t) = \int_0^t \mathrm{d}t' \sum_{x \neq x'} \big(w(x|\, x', t') P(x', t - t') - w(x'|\, x, t') P(x, t - t') \big) \tag{2.106}$$

which can also be expressed in terms of the time kernel for the case of a decoupled CTRW

$$\frac{\partial}{\partial t} P(x,t) = \int_0^t \mathrm{d}t' Q(t - t') \sum_{x \neq x'} \big(w(x|\, x') P(x', t') - w(x'|\, x,) P(x, t') \big) \,, \tag{2.107}$$

with space being one dimensional and discrete. The further generalisation is easily provided by replacing the sum by an integral.

2.11 Remark about the initial condition

This thesis is exclusively concerned with initial conditions that have the form of δ-peaks. Moreover, the solutions, which were presented so far, were all constituted with the condition $f(\mathbf{x}, t = 0) = \delta(\mathbf{x})$. Nevertheless, it is easy to generalise them at least on initial conditions that are not located at $\mathbf{x} = \vec{0}$. The general solution of each differential equation can always be given in terms of the according Greens function. A particular solution can then be constituted as the convolution of the Greens function with the initial condition. Concerning the solutions given so far it is therefore simple to establish the Greens function

$$f(\mathbf{x}\,,t) = \int_{-\infty}^{\infty} \mathrm{d}^3x' G(\mathbf{x} - \mathbf{x}'\,,t)\delta(\mathbf{x}') = G(\mathbf{x}\,,t)\,. \tag{2.108}$$

In this case it is equal to the solution. Another initial condition that will be treated is $f(\mathbf{x}\,,t = 0) = \frac{1}{2}\left(\delta(\mathbf{x} - \mathbf{x}_0) - \delta(\mathbf{x} + \mathbf{x}_0)\right)$. One is consequently able to express the solution for this initial condition in terms of the given solution. It appears to be

$$f_{\mathrm{new}}(\mathbf{x}\,,t) = \frac{1}{2}\left(f(\mathbf{x} - \mathbf{x}_0\,,t) - f(\mathbf{x} + \mathbf{x}_0\,,t)\right) \tag{2.109}$$

3 Reaction-diffusion equations with normal diffusion

Chapter two is going to deal with normal diffusive reaction-diffusion equations and especially with the Fisher-Kolmogorov-Petrovskii-Piskunov and the Zeldovich equation. The first section will give a short introduction into this topic, outlining the general form of normal diffusive reaction-diffusion equations and their applications to different systems. In the second and third section the two mentioned equations will be discussed in terms of linear stability analysis. In the fourth section general properties of nonlinear reaction-diffusion equations will be mentioned. The important distinction of pulled and pushed fronts will be outlined, a quite general expression for the asymptotic front speed of the solutions of nonlinear reaction-diffusion equations will be derived and also the case of stationary fronts will be explained. An account similar to this section is found in [20]. Section 3.5 will demonstrate an option to evaluate the so called linear spreading speed. This velocity can be calculated in terms of the linearised system and appeares to be the asymptotic propagating speed of solutions of the Fisher-Kolmogorov-Petrovskii-Piskunov equation. The method of calculating this speed was taken from [39]. In the last section of this chapter a method to approximate the two equations of interest will be described. The singular perturbation approximation will be used to evaluate solutions, which exhibit the asymptotic features of the two equations exactly. A detailed account on this technique of approximation is found in [34].

3.1 General Form

Reaction-diffusion equations (RDE) play a significant role not only in chemistry and in physics. Often they display different phenomenons of pattern formation that arise in biological, ecologic or sociological systems, as well. Concerning these phenomenons they can and are often used as model equations. The Fisher-Kolmogorov-Petrovskii-Piskunov (FKPP) equation, which will be one of the main subjects of this thesis, was originally derived to simulate propagation of a gene in a population [15]. The Zeldovich equation was originally used as a model for flame propagation [40]. Both of them are today being exploited in different fields of sciences. In general reaction-diffusion equations are partial differential equations, similar to the diffusion equations, additionally exhibiting a deterministic reaction term. In the case of normal diffusion they have the following form

$$\frac{\partial}{\partial t}\mathbf{c}(\mathbf{x},t) = \mathbf{R}(\mathbf{c}) + D\Delta_{\mathbf{x}}\mathbf{c}(\mathbf{x},t). \tag{3.1}$$

In this context $\mathbf{c}$ cannot be regarded as a pdf anymore. Due to the reactions space has to be interpreted as something discrete, where one spatial position has to be regarded as a compartement which is small enouch that reactions take place. The equation can, depending on the number of different reactants, also be a system of equations.

Therefore, $\mathbf{c}$ can be interpreted as a concentration vector in the context of chemical reactions, with its dimensionality accounting for the number of different reactants. But that would essentially restrict the individual constitutents to the interval [0,1]. In many non-chemical applications also this interpretation cannot be adopted. Throughout this thesis I will refer to $\mathbf{c}$ as the order parameter if the interpretation that it takes only values ϵ [0,1] fails. $\mathbf{R}(\mathbf{c})$ denotes the reaction term. In this thesis the FKPP and Zeldovich equation will be discussed. Both of them are one dimensional, concerning the function c, exposing a nonlinear reaction term. At first a discussion in terms of linear stability analysis shall be provided. All of the plots that will be shown were evaluated for one spatial dimension. The according discussions shall be be conducted assuming space to be one dimensional as well.

3.2 Linear stability analysis of the FKPP equation

The FKPP equation is one of the easiest nonlinear RDE's. Accordingly, it has no general solution but its behaviour for different classes of initial conditions was extensively investigated. There are also different forms of it available concerning control parameters in the reaction term. The FKPP equation, I have been working on, reads

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = c(\mathbf{x},t)(1-c(\mathbf{x},t)) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,, \tag{3.2}$$

with $0 < c < 1$. The reaction kinetics may also be regarded as the time evolution neglecting the diffusion. The fixed points are then figured out by examining $R(c)$. A simple method is calculating the potential and finding the fixed points as maxima or minima respectively. The potential in general is given as follows

$$V(c) = -\int_{c_0}^{c} \mathrm{d}c' R(c') \tag{3.3}$$

One finds that the system has one stable fixed point at $c = 1$, the minimum, and an unstable one at $c = 0$, the maximum. To perform a linear stability analysis the reaction kinetics is linearised via Taylor expansion in the vicinity of the fixed points. The reaction term near the unstable fixed point reads

$$R(c) = c \tag{3.4}$$

Consequently the according linearised FKPP equation is given as

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = c(\mathbf{x},t) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,. \tag{3.5}$$

This equation is easily attributed to the diffusion equation via the transformation $c = \mathrm{e}^t\tilde{c}$, with $\tilde{c}$ being a Gaussian for the initial condition $c(\mathbf{x}, t = 0) = \delta(\mathbf{x})$

$$c(\mathbf{x},t) = \frac{1}{\sqrt{4D\pi t}}\mathrm{e}^{t-\frac{\mathbf{x}^2}{4Dt}}\,. \tag{3.6}$$

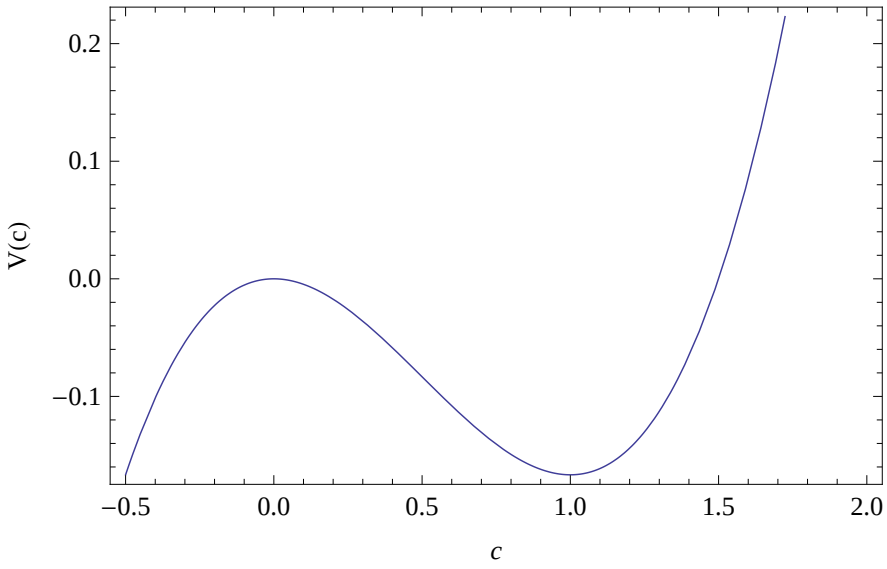

Figure 3.1: The potential attached to the reaction kinetics of the FKPP equation.

Figure 3.2 shows the rising of the initial condition , which is due to the linearised reaction term. Going a bit away from the initial position one sees that for the different values of time, the differences are equal, the distances of the flanks as well as their shape is approximately equal. The flanks are consequently interpreted as so-called reaction fronts propagating to both sides of the initial position $x = 0$. These fronts are typical for

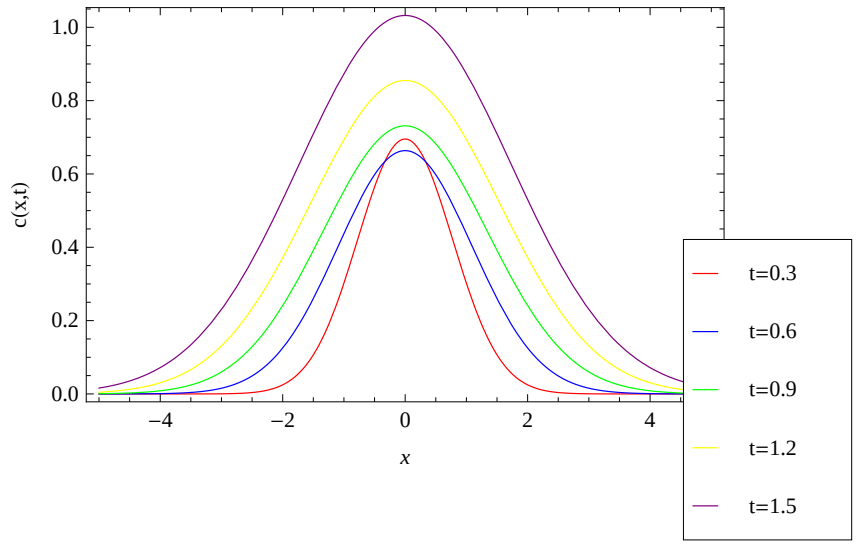

Figure 3.2: Solution of the linearised FKPP equation (3.5) near the fixed point $c = 0$, with $D = 1$.

many nonlinear RDE‘s especially for the FKPP equation. In the vicinity of the stable

fixed point $c = 1$ the linearised rection term reads

$$R(c) = 1 - c = -\overline{c}\,, \tag{3.7}$$

where $\overline{c}$ is the deviation from the stable fixed point. As for the value of the concentration it has to be positive and equal to or less than one. The corresponding linearised RDE is assembled to

$$\frac{\partial}{\partial t}\overline{c}(\mathbf{x},t) = -\overline{c}(\mathbf{x},t) + D\Delta_{\mathbf{x}}\overline{c}(\mathbf{x},t)\,. \tag{3.8}$$

The equation is again reduced to the diffusion equation via the transformation

$$\overline{c} = \mathrm{e}^{-t}\tilde{c} \tag{3.9}$$

where $\tilde{c}$ solves the diffusion equation. The full solution, which shall be investigated, can then be established to

$$c(\mathbf{x},t) = 1 - \frac{1}{\sqrt{4D\pi t}}\mathrm{e}^{-t-\frac{\mathbf{x}^2}{4Dt}}\,. \tag{3.10}$$

Figure 3.3 shows that for a deviation in the vicinity of $c = 1$ the density returns to this state in a short time. Taking both plots of the linearised FKPP equation into account,

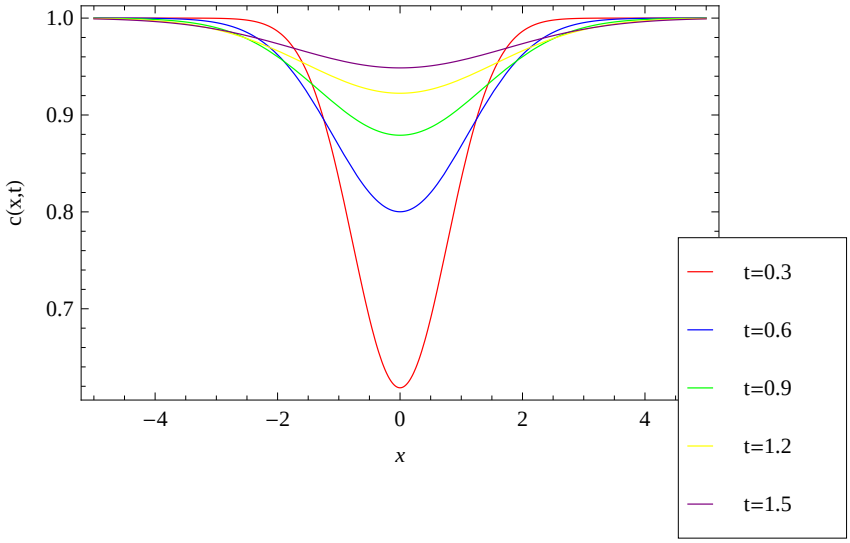

Figure 3.3: Solution of the linearised FKPP equation (3.8) near the fixed point $c = 1$, with $D = 1$.

one expects reaction fronts running from a domain, where the system is already in the stable state, into a domain where it is in the unstable state.

3.3 Linear stability analysis of the Zeldovich equation

Also for the Zeldovich equation there is a number of different forms available. The one I was working on provides a reaction term with one external control parameter

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = \varepsilon c(\mathbf{x},t)\left(\varepsilon - c(\mathbf{x},t)^2\right) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,. \tag{3.11}$$

One important difference in comparison to the FKPP equation is that the order parameter c cannot be regarded as a concentration any more. In this case it can also be negative. Its linear stability analysis is quite similar to the one for the FKPP equation. Nevertheless the control parameter has an influence on the potential which is given as

$$V(c) = -\varepsilon\frac{1}{2}c^2 + \frac{1}{4}c^4\,. \tag{3.12}$$

The interesting case is the one with two stable and one unstable fixed point. For the

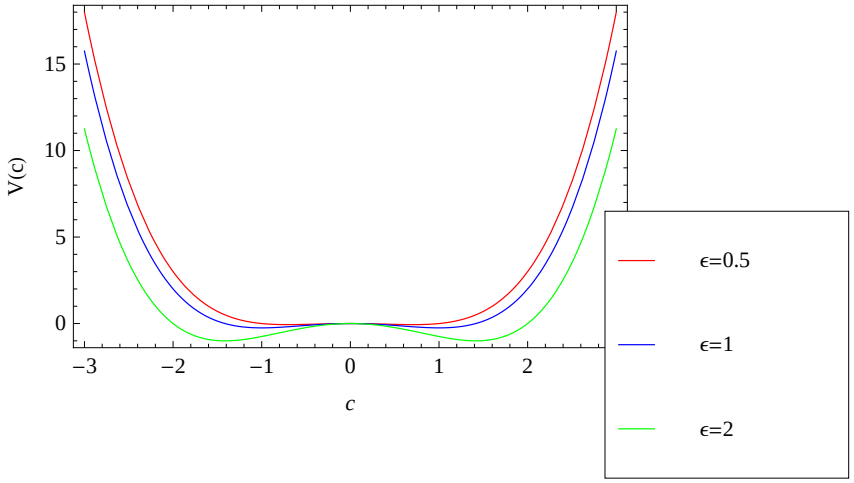

Figure 3.4: The potential (3.12) concerning the reaction kinetics of the Zeldovich equation for different values of ε.

value $\varepsilon = 0$ there is a bifurcation. So the further discussion will only concern with the cases $\varepsilon > 0$. The two stable stationary states are located at $c = \pm\sqrt{\varepsilon}$, the unstable one again at $c = 0$. Therefore, the interesting interval, in which the behaviour of the solutions of this equation shall be discussed, is $c\ \epsilon\ [-\sqrt{\varepsilon},\sqrt{\varepsilon}]$. In the vicinity of the unstable fixed point the linearised reaction kinetics reads

$$R(c) = \varepsilon c\,. \tag{3.13}$$

The linearised Zeldovich equation is then derived to

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = \varepsilon c(\mathbf{x},t) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,. \tag{3.14}$$

Similar to the procedure that was applied in the last section, this equation is attached to the diffusion equation via the transformation

$$c = \mathrm{e}^{\varepsilon t}\tilde{c}\,. \tag{3.15}$$

In this case it is more interesting to evaluate the behaviour for a slightly different initial condition. So let us consider the condition $\tilde{c}(\mathbf{x}, t=0) = \frac{1}{2}(\delta(\mathbf{x}-\mathbf{x}_0) - \delta(\mathbf{x}-\mathbf{x}_0))$. The solution then appears to be

$$c(\mathbf{x},t) = \frac{\mathrm{e}^{\varepsilon t}}{\sqrt{16D\pi t}}\left(\mathrm{e}^{-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4Dt}} - \mathrm{e}^{-\frac{(\mathbf{x}+\mathbf{x}_0)^2}{4Dt}}\right). \tag{3.16}$$

Due to the chosen initial condition we see a static inflexion point, dividing the plot into one half plane where the function c is exclusively negative and one where it is positive (see fig. 3.5). The symmetry of the function is apparently governed by the initial condition. The plot shows a point symmetry where the central point lies between the two initial peaks, which is in this case the position $x = 0$. Varying the parameter

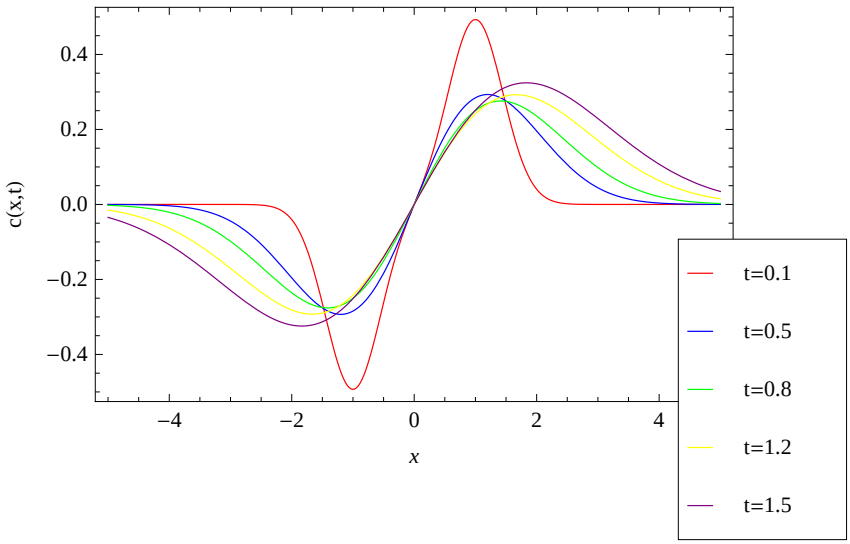

Figure 3.5: Solution of the linearised Zeldovich equation (3.14) near the fixed point $c = 0$, with $D = 1$, $x_0 = 1$ and $\varepsilon = 1$.

ε the influence of diffusion and reaction can be acconted for separately (see fig. 3.6). Choosing a smaller value for this control parameter the peaks in the very beginning, so for small values of t, become steeper. The broadening of the initial condition is, therefore, interpreted as a result of the reaction term. Also the rising of the solution after the initial peaks have decreased is obviously due to the reaction term. It is fater for larger values of the control parameter. In the vicinity of the stable states, the reaction term appears to be

$$R(c)_\pm = -2\varepsilon\left(c - \mp\sqrt{\varepsilon}\right) = -2\varepsilon\bar{c}_\pm\,, \tag{3.17}$$

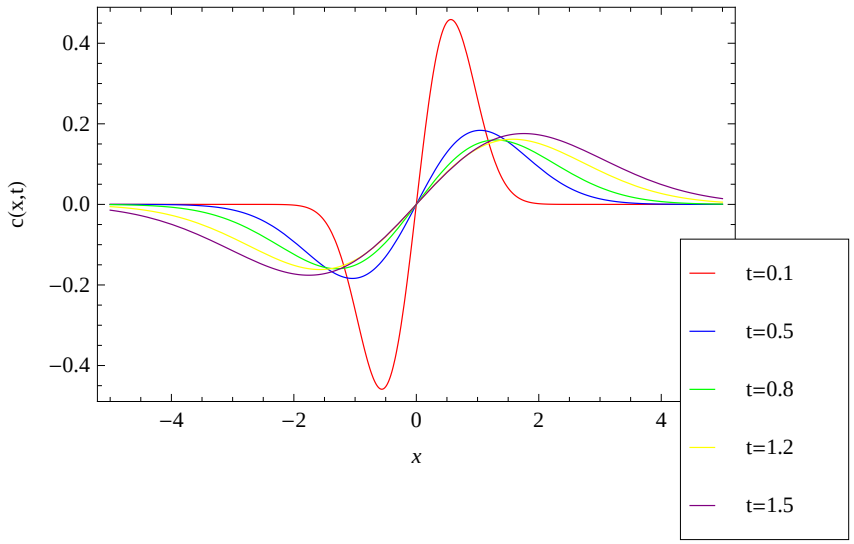

Figure 3.6: Solution of the linearised Zeldovich equation (3.14) near the fixed point $c = 0$, with $D = 1$, $x_0 = 1$ and $\varepsilon = 0.5$.

where $\bar{c}_\pm$ is the deviation from the positive and for the negative stable stationary state respectively. Near these fixed points the Zeldovich equation can be linearised to

$$\frac{\partial}{\partial t}\bar{c}_\pm(\mathbf{x},t) = -2\varepsilon\bar{c}_\pm(\mathbf{x},t) + D\Delta_\mathbf{x}\bar{c}_\pm(\mathbf{x},t)\,. \tag{3.18}$$

The solutions for both signs are again attributed to the diffusion equation with the transformations

$$\bar{c}_\pm = \mathrm{e}^{-2\varepsilon t}\tilde{c}_\pm\,, \tag{3.19}$$

with $\tilde{c}_\pm$ being Gaussian distributions. In this case the initial conditions have to be taken as singular δ-peaks pointing in different directions, which is due to the interval, c was defined on in the beginning. The full solution in the vicinity of the stable stationary state $c = \sqrt{\varepsilon}$ reads

$$c(\mathbf{x},t) = \sqrt{\varepsilon} - \frac{1}{\sqrt{4D\pi t}}\mathrm{e}^{-2\varepsilon t - \frac{\mathbf{x}^2}{4Dt}}\,, \tag{3.20}$$

and in the case of $c = -\sqrt{\varepsilon}$ it is given as

$$c(\mathbf{x},t) = -\sqrt{\varepsilon} + \frac{1}{\sqrt{4D\pi t}}\mathrm{e}^{-2\varepsilon t - \frac{\mathbf{x}^2}{4Dt}}\,. \tag{3.21}$$

The behaviour in the vicinity of the two stable states is at least qualitatively the same as the according behaviour of the linearised FKPP equation (see fig. 3.7). Choosing different values for ε also varies the position of the fixed point. The relaxation to the stable fixed point is accelerated by enlarging the control parameter. Accordingly the interpretation seems apparent that on both sides of the inflexion point (see fig. 3.5 and 3.6) propagating fronts arise, running away from $x = 0$, whereas at this position a static domain wall evolves. Finally the reaction term may be seen as the force driving the inhomogenities, whereas diffusion has the effect of balancing. If the initial condition is

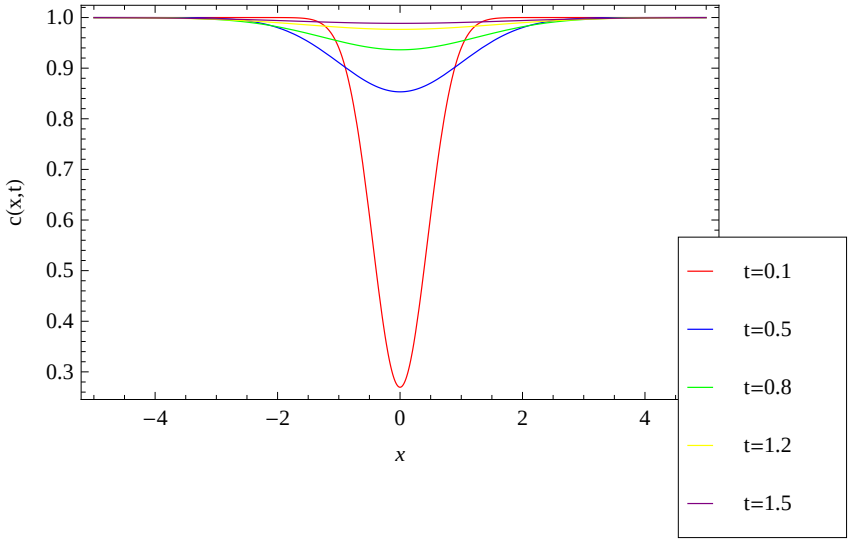

Figure 3.7: Solution of the linearised Zeldovich equation (3.18) near the fixed point $c = \sqrt{\varepsilon}$, with $D = 1$ and $\varepsilon = 1$.

chosen to be a singular δ-peak in the vicinity of $c = 0$, consequently a front of the form as shown for the FKPP equation arises.

3.4 Propagating fronts in nonlinear reaction-diffusion systems

Both the FKPP equation as well as the Zeldovich equation can be represented by the general form that was mentioned before

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = R(c) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,, \tag{3.22}$$

with $R(c)$ being the nonlinear reaction term, which is of the form

$$R(c) = \varepsilon c - c^n\,. \tag{3.23}$$

Thus, their behaviour can be discussed in a more general account. Let us claim that

$$R(0) = R(\sqrt{\varepsilon}) = 0\,, \tag{3.24}$$

$$\left[\frac{\partial}{\partial c}R(c)\right]_{c=0} > 0\,, \tag{3.25}$$

$$[R(c)]_{c\epsilon[0,\sqrt{\varepsilon}]} \geq 0\,, \tag{3.26}$$

which can be applied to both equations. A typical solution of equation (3.22) is then as already mentioned a propagating front also often referred to as waves of transition from an unstable state. The subject has been widely investigated at first in the mathematical [14] later on also in the physical society [4,26] with various applications in other sciences.

In a rigorous mathematical treatment of the given general form of a nonlinear RDE Aronson and Weinberger [2] could show that these propagating fronts always relax to a unique shape and velocity if the initial condition can be considered as sufficiently localised [39]. Depending on the particular form of the nonlinearities, there are different forms of front behaviour. In case of the propagating fronts there are the so-called pulled and the pushed fronts. For the pulled ones the front velocity can be figured out in terms of the linearised system. The system is "pulled" by the linear dynamics. In the pushed case the front propagation is driven by the nonlinearities. Typically the velocity, which is calculated via linearising about the unstable state, the linear spreading speed, gives the lower bound for the velocity the front is translating with asymptotically. Therefore, in the pushed case it moves with a larger velocity than the linear spreading speed. Another important class of RDE's are the so-called bistable systems. The Zeldovich equation can be regarded as such a system if it is analysed in the interval $[-\sqrt{\varepsilon},\sqrt{\varepsilon}]$. They exhibit two stable and an unstable fixed point. They arise in many phenomena where some kind of switching process is provided (see [40]). Therefore, the application to the process of flame propagation is obvious. In these cases trigger or switching waves are found as possible solutions. For the reaction kinetics of the form of Zeldovich equation I was working on, a stationary front is expected, which is due to the symmetry of the according potential. The assumption that the front has asymptotically a constant velocity can be exploited for serious simplifications. Let us therefore assume space to be one dimensional. The former PDE can then be transformed into an ordinary differential equation (ODE). For large values of t it can, thus, be claimed that

$$D\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}c(\xi) + R(c) + v\frac{\mathrm{d}}{\mathrm{d}\xi}c(\xi) = 0\,, \tag{3.27}$$

with $\xi = x - vt$ and $c(x,t) \to c(\xi)$, which is sometimes referred to as front ansatz. There is a continuos spectrum of solutions of this ODE for different front velocities with the linear spreading speed as a minimum (see for example [1]). The question is not only what the solution is looking like but mainly which front velocity is selected under certain initial or boundary conditions. An evaluation about what establishes this constant front velocity can be determined in terms of the auxiliary function

$$F(c) = \int_{c_0}^{c} \mathrm{d}c' R(c')\,. \tag{3.28}$$

In terms of this function the front velocity takes the form

$$v = \frac{F(c(\xi\to\infty)) - F(c(\xi\to-\infty))}{\int_{-\infty}^{\infty}\mathrm{d}\xi\left(\frac{\mathrm{d}c}{\mathrm{d}\xi}\right)^2} \tag{3.29}$$

(see [14]). Assuming that the system is in the unstable stationary state for $\xi \to -\infty$ and in the stable stationary state for $\xi \to \infty$ or vice versa one can at least get an idea of the direction in a certain case. In the case of the bistable system it is consequently assumed to be in one of the stable states for $\xi \to -\infty$ and in the other for $\xi \to \infty$ respectively. Consequently it is clear that the fronts evolving in the case of the bistable

Zeldovich equation are static [20].

3.5 The linear spreading speed

A really important value in connection with front propagtion is the linear spreading speed. So let us have a closer look at the first plot of the linear stability analysis, concerning the FKPP equation (see fig. 3.2). Going a bit away from the initial position one sees that the fronts plotted for different but equivalent time steps seem to reach equal distances. One then chooses a point on the flank of the front going to the right where the density has a constant value (see fig. 3.8). Let us name the value C with the chosen positions $x_C(t)$. Asymptotically the position $x_C(t)$ travels with a constant velocity v^*, the linear spreading speed, so that

$$v^* = \lim_{t\to\infty} \frac{\mathrm{d}x_C}{\mathrm{d}t} \,. \tag{3.30}$$

So the question arises how this velocity can be calculated? Let us, for the first, get back

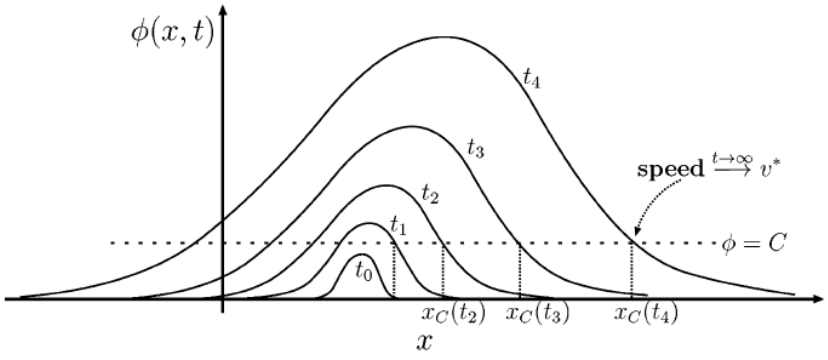

Figure 3.8: A propagating front evolving in the linearised regime (taken from [39]).

to the linearised equation in the vicinity of $c = 0$ (eq. (3.5)). The Fourier transform of the solution, let space be one dimensional, is given as

$$\hat{c}(k,t) = \int_{-\infty}^{\infty} \mathrm{d}x c(x,t) \mathrm{e}^{-\mathrm{i}kx} \,. \tag{3.31}$$

Then the ansatz

$$\hat{c}(k,t) = \bar{c}(k) \mathrm{e}^{-\mathrm{i}\omega(k)t} \tag{3.32}$$

yields the dispersion relation of Fourier modes. With the state $c = 0$ being linearly unstable, it is clear that $\mathrm{Im}(\omega(k)) > 0$ for a certain range of k-values. The particular equation is encoded in the dispersion relation. Let us consequently assume that $\omega(k)$ is an analytic function of k in the complex k-plane. The inverse transform of the solution reads

$$c(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \bar{c}(k) \mathrm{e}^{\mathrm{i}(kx - \omega(k)t)} \,. \tag{3.33}$$

At this point the importance of the initial condition is quite observable. In the given expression it is the $\bar{c}(k)$, which is the Fourier transform of the initial condition. I will continue only facing the initial condition $c(x, t = 0) = \delta(x)$, which makes its Fourier transform a constant independent of k. Thus, the investigation of the integral gets much easier. Let us now assume that this linear spreading speed v^* exists and is finite so that it makes sense to interpret the solution in a co-moving frame with

$$x \to \xi = x - v^* t \,. \tag{3.34}$$

Within this frame the front should asymptotically keep its shape. Substituting v^* into the inverse transformation results in

$$c(\xi, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \bar{c}(k) \mathrm{e}^{\mathrm{i}k\xi - \mathrm{i}(\omega(k) - v^* k)t} \,. \tag{3.35}$$

To determine v^* self-consistently one analyses when this expression neither leads to exponential growth nor to decay in the limit $t \to \infty$. Because of this large-time limit one then performs a so-called saddle-point approximation (for a rigorous treatment see [12]). On the contour of integration one is looking for the value of k where the expression $\omega(k)t - v^* k t$ varies least in terms of k. The integral is dominated by the contribution from the region near this point, the linear spreading point k^*. This saddle-point is then given by

$$\left[\frac{\mathrm{d}\left(\omega(k) - v^* k\right)}{\mathrm{d}k}\right]_{k=k^*} = 0 \,. \tag{3.36}$$

So that

$$\left[\frac{\mathrm{d}\omega(k)}{\mathrm{d}k}\right]_{k=k^*} = v^* \,. \tag{3.37}$$

Therefore, the argument that expression (3.35) should not grow or decay exponentially, results in the condition

$$\mathrm{Im}(\omega(k^*)) - v^* \mathrm{Im}(k^*) = 0 \Rightarrow v^* = \frac{\mathrm{Im}(\omega(k^*))}{\mathrm{Im}(k^*)} \,. \tag{3.38}$$

For the linearised system v^* is then easily calculated. The Fourier transform of equation (3.5) leads to the dispersion relation

$$\omega(k) = \mathrm{i}\left(1 - Dk^2\right) \,. \tag{3.39}$$

As the linear spreading speed has to be a real number, one obtains $\mathrm{Im}(k^*) = \mathrm{i}k^* = \pm\frac{1}{\sqrt{D}}$ and, therefore, reaches

$$v^* = \pm 2\sqrt{D} \tag{3.40}$$

for the two fronts evolving on both sides of the initial condition. This way of calculating the linear spreading speed was taken from [39]. In the case of the FKPP equation it was shown, with structural stability arguments [32, 39], that the selected front velocity is the linear spreading speed.

3.6 The singular perturbation approximation

An option to get approximate solutions for the FKPP and the Zeldovich equation under normal diffusion is the singular perturbation approximation (SPA) [34]. The advantage of this technique is that nonlinear equations can be replaced by a quickly converging hierarchy of linear equations. To begin with let us apply this technique to the FKPP equation

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = c(\mathbf{x},t)(1-c(\mathbf{x},t)) + D\Delta_{\mathbf{x}}c(\mathbf{x},t)\,. \tag{3.41}$$

Simplifying equation (3.41), let us take D to be one. It is transformed with the substitution $c = \frac{\phi}{1+\phi}$ and the result being

$$\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \phi(\mathbf{x},t) + \Delta_{\mathbf{x}}\phi(\mathbf{x},t) - \frac{2\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t)\right)^2}{1+\phi(\mathbf{x},t)}\,. \tag{3.42}$$

As I already mentioned, c is in this case a concentration and therefore defined on the interval [0,1], which transforms to $\phi \in [0,1]$. The nonlinearity on the rhs is neglected, so that this equation can be solved. Thus, the concentration in terms of this approximation, c_0, fulfils the equation

$$\frac{\partial}{\partial t}c_0(\mathbf{x},t) = c_0(\mathbf{x},t)(1-c_0(\mathbf{x},t)) + \Delta_{\mathbf{x}}c_0(\mathbf{x},t) + \frac{2\left(\nabla_{\mathbf{x}}c_0(\mathbf{x},t)\right)^2}{1-c_0(\mathbf{x},t)}\,, \tag{3.43}$$

where

$$\frac{2\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t)\right)^2}{\left(1+\phi(\mathbf{x},t)\right)^3} = \frac{2\left(\nabla_{\mathbf{x}}c_0(\mathbf{x},t)\right)^2}{1-c_0(\mathbf{x},t)}\,. \tag{3.44}$$

The exact solution of the FKPP equation is then decomposed $c = c_0 + \theta_0$, where the correction term θ_0 solves the equation

$$\frac{\partial}{\partial t}\theta_0(\mathbf{x},t) = \left(1-2c_0(\mathbf{x},t)\right)\theta_0(\mathbf{x},t) - \left(\theta_0(\mathbf{x},t)\right)^2 + \Delta_{\mathbf{x}}\theta_0(\mathbf{x},t) - \frac{2\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t)\right)^2}{\left(1+\phi(\mathbf{x},t)\right)^3}\,. \tag{3.45}$$

This θ_0 is then again replaced by two auxiliary functions, $\theta_0 = c_1 + \theta_1$, with c_1 solving the linear part of the equation. The approximate solution at the nth level of iteration is given as

$$c(\mathbf{x},t) \approx \sum_{k=0}^{n} c_k(\mathbf{x},t)\,. \tag{3.46}$$

Consequently the zeroth order approximation can be expressed in terms of the auxiliary function ϕ, which solves an equation similar to a linearised FKPP equation. The solution is

$$\phi(\mathbf{x},t) = \frac{1}{\sqrt{4\pi t}}\mathrm{e}^{t-\frac{\mathbf{x}^2}{4t}}\,. \tag{3.47}$$

Due to the transformation that was inflected the front shows a saturation. Figure 3.10 shows the evolution of fronts propagating into the unstable state $c = 0$, leaving the system in the stable state $c = 1$ homogenously. For the given situation the linear spreading speed can be figured out with the help of the prosedure presented in section 3.5. Due to the choice of the diffusion constant it is evaluated to be two. Studying the

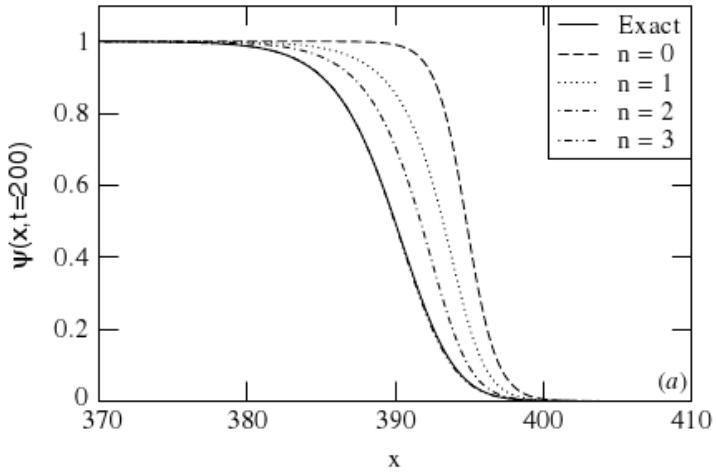

Figure 3.9: Convergence of the SPA concerning the FKPP equation, (taken from [34]).

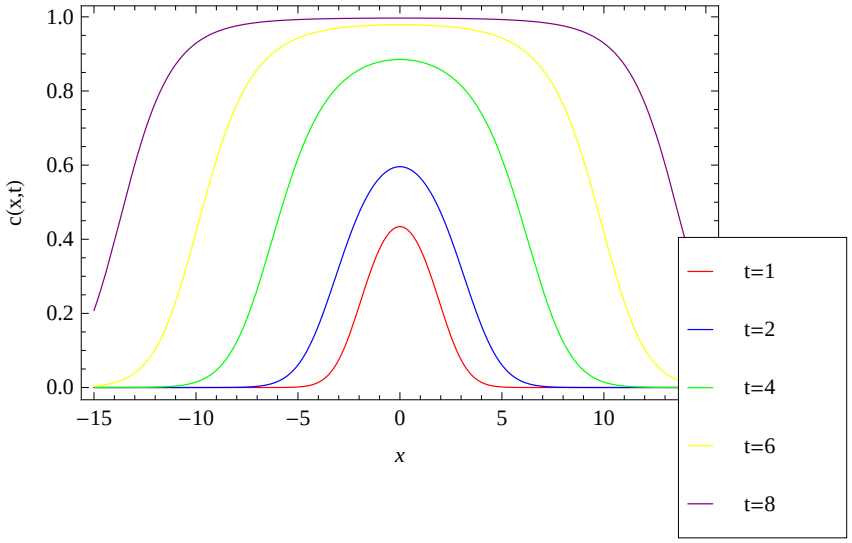

Figure 3.10: Behaviour of the zeroth order approximation of the FKPP equation (eq. (3.43))for small values of t.

front behaviour for large values of t (fig. 3.11), leads to the conclusion that this linear spreading speed is the one which is selected asymptotically. This is also in accordance with the asymptotic behaviour Aronson and Weinberger evaluated for localised initial conditions [2]. The relaxation to this asymptotic behaviour can also be evaluated in terms of the SPA. It proofs to be

$$v \approx 2 - \frac{d}{2t}\,, \tag{3.48}$$

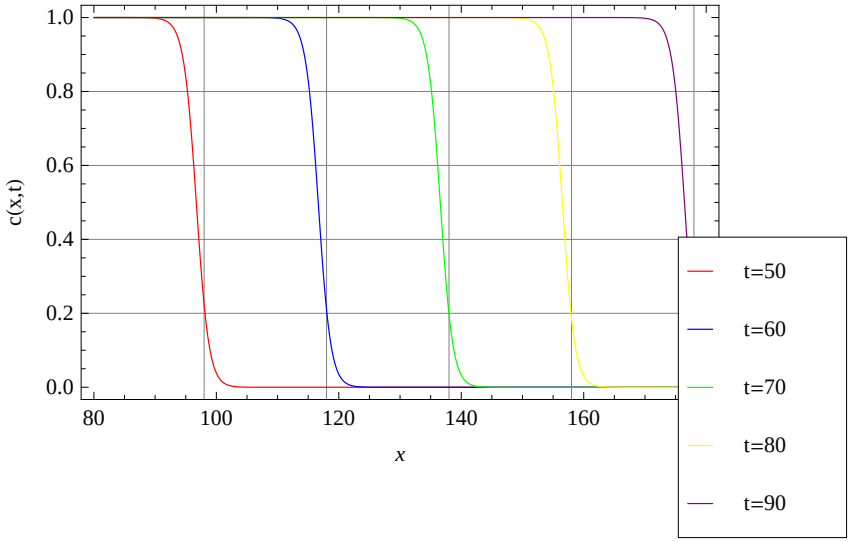

Figure 3.11: Behaviour of the zeroth order approximation of the FKPP equation (eq. (3.43))for large values of t, the grid lines have a distance of 20 units of length.

where d is the dimensionality of space [34]. This is not fully in line with the analytic result achieved by Bramson who evaluated

$$v \approx 2 - \frac{3}{2t} \tag{3.49}$$

for the one dimensional case [3]. In the the zeroth order approximation there is no relaxation observable, which can be evaluated by simple counting arguments (see fig. 3.12) A similar approach can be chosen to approximate the Zeldovich equation (see [34]). Therefore, it is better to simplify the Zeldovich equation due to some trivial scaling arguments. The Zeldovich equation which will be discussed reads

$$\frac{\partial}{\partial t} c(\mathbf{x}, t) = c(\mathbf{x}, t) - c(\mathbf{x}, t)^2 + D\Delta_{\mathbf{x}} c(\mathbf{x}, t)\,. \tag{3.50}$$

This is provided by the substitutions $c \to \frac{c}{\sqrt{\varepsilon}}, t \to \frac{t}{\varepsilon}$ and $D \to \frac{D}{\varepsilon}$. Another transformation applied to the function again leads to a hierarchy of linear equations. In this case the transformation reads

$$c = \frac{\phi}{\sqrt{1+\phi^2}}\,. \tag{3.51}$$

The condition $c \in [-1,1]$ transforms to $\phi \in [-1,1]$, which is due to the simplification of the former Zeldovich equation. The linearised zeroth order term is given as

$$\frac{\partial}{\partial t} \phi(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \Delta_{\mathbf{x}} \phi(\mathbf{x}, t)\,. \tag{3.52}$$

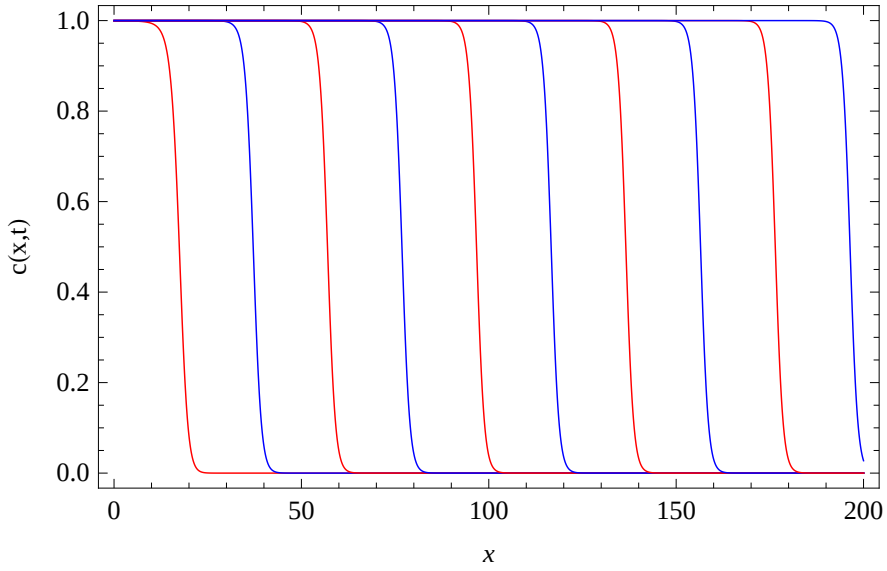

Figure 3.12: Relaxation of the zeroth order approximation of the FKPP equation (eq. (3.43)). The fronts were evaluated for $t = n \times 10$ each.

To investigate the evolution of a static domain wall the initial condition is in this case $\phi(\mathbf{x}, t = 0) = \frac{1}{2}(\delta(\mathbf{x} - \mathbf{x}_0) - \delta(\mathbf{x} + \mathbf{x}_0))$. The according solution is as follows

$$\phi(\mathbf{x}, t) = \frac{\mathrm{e}^t}{\sqrt{16\pi t}} \left(\mathrm{e}^{-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4t}} - \mathrm{e}^{-\frac{(\mathbf{x}+\mathbf{x}_0)^2}{4t}} \right) . \tag{3.53}$$

Actually the previously claimed static domain wall proofs to evolve (fig. 3.13). The external control parameter ε varies the stationary states as well as the time scale of relaxation (cf. fig. 3.14 and fig. 3.13). The process of relaxation is decelerated by enlarging the order parameter (cf. fig. 3.13 and fig. 3.14). The relaxation process as a whole proofs to follow an exponential. This can be seen if the spatial derivative at the point $x = 0$ is plotted versus time. The logarithmic plot shows the dependence on the control parameter ε (see fig. 3.15). As the zeroth order SPA does not allow for investigations of the relaxation to a uniform front in case of the FKPP equation, it may be doubted that the relaxation to a stationary front, concerning the Zeldovich equation, can be investigated in this order of approximation. Nevertheless, the observed dependence on ε should at least qualitatively apply for the full nonlinear system, as well. The scaling of t with ε stays the same for all orders of approximation.

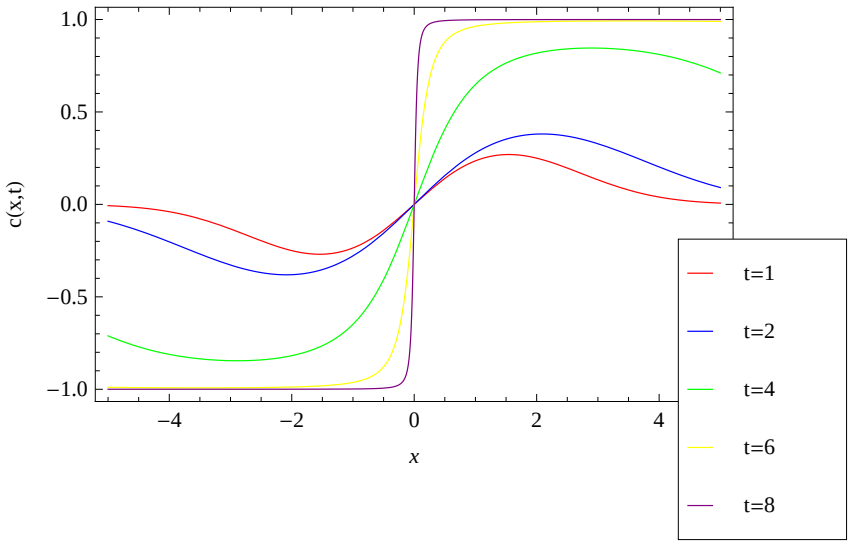

Figure 3.13: Behaviour of the zeroth order approximation of the Zeldovich equation (expr. (3.53)), with $\varepsilon = 1$.

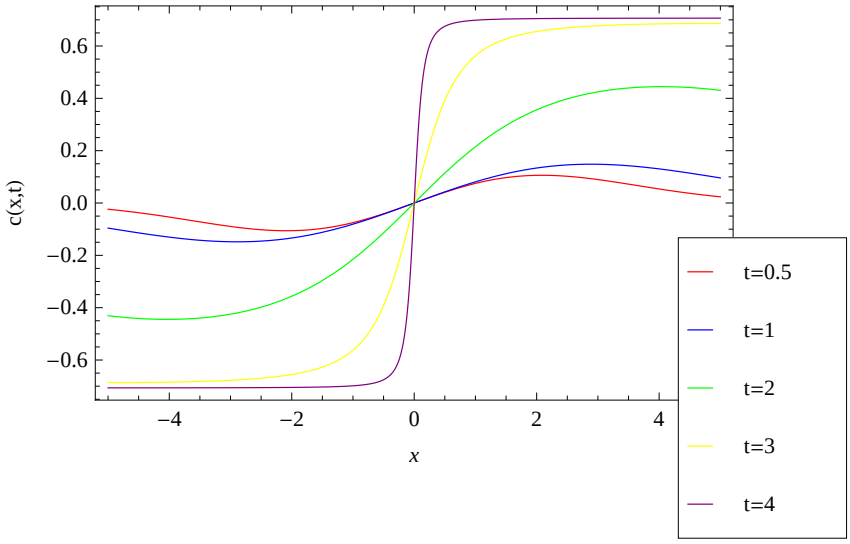

Figure 3.14: Behaviour of the zeroth order approximation of the Zeldovich equation (expr. (3.53)), with $\varepsilon = 0.5$.

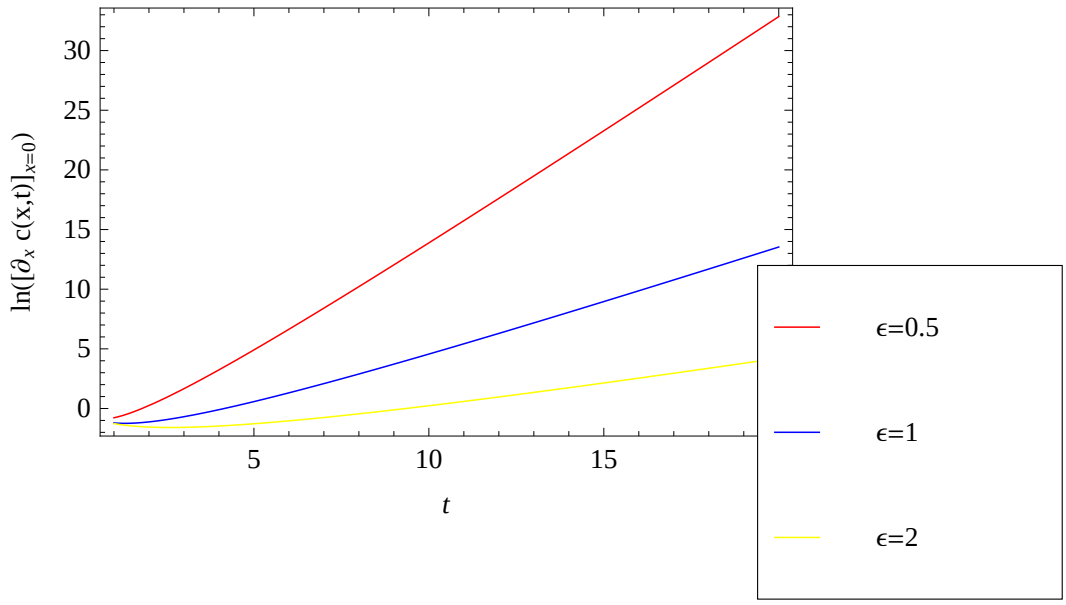

Figure 3.15: The dependence of the relaxation process on ε, concerning the zeroth order SPA for the Zeldovich equation.

4 Subdiffusive reaction-diffusion equations

The fourth chapter is going to deal with subdiffusive reaction-diffusion equations. In the first section a way to derive subdiffusive reaction-diffusion equations will be introduced starting from a generalised master equation. A general form of subdiffusive reaction-diffusion equation will be established. This method of derivation was taken from [8]. In the second section the subdiffusive Fischer-Kolmogorov-Petrovskii-Piskounov and Zeldovich equation will be derived. In section 4.3 and 4.4 a discussion of these subdiffusive equations in terms of linear stability analysis will be carried out. In section 4.5 the attempt will be made to extend the singular perturbation approximation, which was introduced in 3.6, to the the subdiffusive Fischer-Kolmogorov-Petrovskii-Piskounov equation. In section 4.6 a formula to predict the asymptotic front velocities, which the approximate system exhibits, will be derived leading to a transcendental equation. In section 4.7 solutions for different values of the characteristic exponent α will be shown by means of three dimensional graphics. Furthermore, they will be compared to the corresponding velocities of the approximate system, which is derived in 4.5. In section 4.8 a treatment, which is similar to the ones used in 4.5 and 3.6, will be carried out to approximate the subdiffusive Zeldovich equation. Some graphic examples will be shown and finally the last section of this chapter will provide a comparison of the relaxation to the characteristic domain walls, concerning the Zeldovich equation, taking account for different values of α and different initial conditions. In all of the sections from section 4.3 on to the end of this chapter the comparison to the corresponding equations in the normal diffusive domain will be present to secure that in the limit $\alpha \to 1$ the normal diffusive behaviour can be restored.

4.1 General form

RDE‘s in general as well as diffusion equations both, anomalous and normal, have a wide range of application as mentioned before. RDE‘s are also used in connection with processes where the Brownian nature of the random movement is not as evident as in the case of the Zitterbewegung of suspended particles in a fluid. So considering for example the spread of genes in a population [15], what is the argument for taking the diffusion as to be normal? Considering the different systems in which subdiffusion is observed, different scenarios under which subdiffusive RDE‘s could arise, come to mind. To set up such an equation let us once again consider the FDE (2.87), which was derived in the first chapter

$$\frac{\partial}{\partial t}\mathbf{c}(\mathbf{x},t) = D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}\tau Q(t-\tau)\mathbf{c}(\mathbf{x},\tau)\,. \tag{4.1}$$

Here the alternative form is given, with $Q(\tau)$ being the time kernel. This form of the FDE has the advantage that it is easily adapted to subdiffusive RDE's. To reach the FDE with the Riemann-Liouville fractional derivative, the convolution has to be exploited by means of Laplace transformation, which is not generally possible if a reaction term comes into play. The most intuitive way to go on would be taking a given normal RDE and replacing the diffusion term by the convolution integral

$$\frac{\partial}{\partial t}\mathbf{c}(\mathbf{x},t) = \mathbf{R}(\mathbf{c}) + D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}\tau Q(t-\tau)\mathbf{c}(\mathbf{x},\tau)\,. \tag{4.2}$$

In this formulation the reaction term is obviously not influenced by the emergence of subdiffusion and vice versa. Here the convolution integral could also be given in terms of fractional calculus. There were attempts to solve subdiffusive RDE's like the FKPP equation [11] or systems of subdiffusive RDE's [22], which were derived in that way. But they do not describe the situation adequatly. In some cases they even show violations of mass conservation, see [8, 37]. The right way to achieve a subdiffusive RDE, or at least one that does not show these inconsistencies, is to implicate the reaction term into the diffusion integral. Due to the memory effect of the time kernel the comlete past of the order parameter $\mathbf{c}$ has to be taken into account, which of course also holds true for the reactions that took place. To see where this implication stems from and to derive a general form of a subdiffusive RDE let us start with the generalised master equation, which can be assembled in the following way. At first it is essential to introduce a spatial scale on which the reactions occur. So let us partition space into small compartments denoted by an index i with a second index α identifying the chemical reactants. Accordingly, $\mathbf{c}$ is interpreted as a local density or a state vector. The reaction rate and therefore the evolution due to reaction for each compartment and reactant reads

$$\dot{c}_{i,\alpha} = R_\alpha(c_{i,\alpha})\,. \tag{4.3}$$

Transitions in terms of the master equation shall only be allowed between neighbouring compartments and take place simultaneously. The state vector $\mathbf{c}$, thus, includes both information about the chemical species and the particle number of each for each compartment. The master equation reads

$$\begin{aligned}\frac{\partial}{\partial t}P(\mathbf{c},t) = -\frac{\partial}{\partial \mathbf{c}}\mathbf{R}(\mathbf{c})P(\mathbf{c},t) + \int_0^t \mathrm{d}\tau Q(t-\tau)\int \mathrm{d}\mathbf{c}' \\ \times \int \mathrm{d}\mathbf{c}''\left[w(\mathbf{c}|\mathbf{c}') - \delta(\mathbf{c}-\mathbf{c}')\right]\delta\left(\mathbf{c}' - \mathbf{G}(\mathbf{c}'',t-\tau)\right)P(\mathbf{c}'',\tau)\end{aligned} \tag{4.4}$$

(see [8]). The reaction rate apparently is included into the integral. $\mathbf{G}(\mathbf{c},t)$ is the solution of the reaction kinetics, with $\mathbf{c}$ playing the role of an initial condition. In this context the desired subdiffusive RDE can be considered as an evolution equation for the mean value of the state vector

$$\mathbf{C} = \int \mathrm{d}\mathbf{c}\mathbf{c}P(\mathbf{c},t)\,. \tag{4.5}$$

Claiming $P(\mathbf{c},t)$ to be a slowly varying function in terms of $\mathbf{c}$, the evolution of the mean value $\mathbf{C}$ can be established

$$\frac{\partial}{\partial t}\mathbf{C} = \int \mathrm{d}\mathbf{c}\mathbf{R}(\mathbf{c})P(\mathbf{c},t) + \int_0^t \mathrm{d}\tau Q(t-\tau) \times \left[\int \mathrm{d}\mathbf{c}\int \mathrm{d}\mathbf{c}'\mathbf{c}w(\mathbf{c}|\mathbf{G}(\mathbf{c}',t-\tau))P(\mathbf{c}',\tau) - \int \mathrm{d}\mathbf{c}'\mathbf{G}(\mathbf{c}',\,t-\tau)P(\mathbf{c}',\tau)\right]. \quad (4.6)$$

Then a mean-field approximation is applied which means

$$\int \mathrm{d}\mathbf{c}H(\mathbf{c})P(\mathbf{c},t) \approx H(\mathbf{C})\,. \quad (4.7)$$

As a consequence the general form of a reaction diffusion equation is obtained

$$\frac{\partial}{\partial t}\mathbf{c}(\mathbf{x}),t) = \mathbf{R}(\mathbf{c}) + D\Delta_{\mathbf{x}}\int_0^t \mathrm{d}\tau Q(t-\tau)\mathbf{G}(\mathbf{c}(\mathbf{x}),\tau),t-\tau) \quad (4.8)$$

in the proper diffusion limes, where $\mathbf{C}$ was again replaced by $\mathbf{c}$. Here was, once more, a Taylor expansion to the second order evaluated, which leads to the spatial derivative. This procedure is similar to the one performed in section 2.2. In the following all plots concerning different solutions of the two subdiffusive RDE's will be given for one spatial dimension.

4.2 Arranging the subdiffusive RDE's

Due to the comparatively simple nonlinearities of the two considered RDE's, the solutions of the reaction terms, the function $G(c,t)$ for both of them, are easy to evaluate. Both reaction terms are nonlinear ODE's, which can be interpreted as particular forms of the so-called Bernoulli differential equation. According to a trivial substitution the reaction kinetics can be transformed to achieve linear ODE's. Let us take the FKPP equation as an example. The nonlinear equation

$$\dot{c} = c(1-c) \quad (4.9)$$

has to be solved. Therefore, one at first multiplies with $-\frac{1}{c^2}$, which leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{c}\right) = -\frac{1}{c} + 1\,. \quad (4.10)$$

Now the mentioned subsitution $y = \frac{1}{c}$ is applied, with the result

$$\dot{y} = -y + 1\,, \quad (4.11)$$

and the solution

$$y(t) = (y_0 - 1)\mathrm{e}^{-t} + 1\,. \quad (4.12)$$

Therefore, the solution of the reaction kinetics reads

$$c(t) = \frac{1}{\left(\frac{1}{c_0} - 1\right) \mathrm{e}^{-t} + 1}\,, \tag{4.13}$$

with the substituted initial condition $y_0 = \frac{1}{c_0}$. The solution as it has to be inserted into the subdiffusive RDE, must have the function $c(\mathbf{x},t')$ as the initial condition, ressembling the past of the density in the subdiffusive equation. It is accordingly established to

$$G(c(\mathbf{x},t'),t-t') = \frac{c(\mathbf{x},t')}{\left(1-\mathrm{e}^{-(t-t')}\right) c(\mathbf{x},t') + \mathrm{e}^{-(t-t')}}\,. \tag{4.14}$$

The FKPP equation is finally reached

$$\frac{\partial}{\partial t} c(\mathbf{x},t) = c(\mathbf{x},t)(1-c(\mathbf{x},t)) + D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t-t') \frac{c(\mathbf{x},t')}{\left(1-\mathrm{e}^{-(t-t')}\right) c(\mathbf{x},t') + \mathrm{e}^{-(t-t')}}\,. \tag{4.15}$$

An equivalent procedure for the Zeldovich equation can be performed. This time the substitution $y = \frac{1}{c^2}$ is used. This leads to two solutions, with different signs

$$c(t) = \pm \sqrt{\frac{\varepsilon}{\left(\frac{\varepsilon}{(c_0)^2} - 1\right) \mathrm{e}^{-2\varepsilon t} + 1}}\,. \tag{4.16}$$

The function G is assembled to

$$G(c(\mathbf{x},t'),t-t') = \pm \sqrt{\frac{\varepsilon}{\left(\frac{\varepsilon}{(c_0)^2} - 1\right) \mathrm{e}^{-2\varepsilon(t-t')} + 1}}\,, \tag{4.17}$$

with the subdiffusive Zeldovich equation

$$\frac{\partial}{\partial t} c(\mathbf{x},\,t) = \varepsilon c(\mathbf{x},\,t) - c(\mathbf{x},\,t)^3 \pm D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t-t') \sqrt{\frac{\varepsilon}{(\frac{\varepsilon}{c(\mathbf{x},t')^2} - 1)\mathrm{e}^{-2\varepsilon(t-t')} + 1}}\,. \tag{4.18}$$

In the following the subdiffusive RDE with the postive sign will be examined. The problems the minus sign brings about will become obvious later on.

4.3 Linear stability analysis of the FKPP equation

To begin with, let us evaluate the behaviour of this subdiffusive RDE (eq. (4.15)) in the linearised regime, as already done in the normal diffusive case. The two fixed points of the subdiffusive FKPP equation are the same as before. The unstable fixed point is $c = 0$, the stable one $c = 1$. The linearised reaction kinetics in the vicinity of the unstable stationary state is as follows

$$R(c) = c\,, \tag{4.19}$$

with the solution

$$G(c_0, t) = c_0 \mathrm{e}^t \,. \tag{4.20}$$

So the linearised FKPP equation reads

$$\frac{\partial}{\partial t} c(\mathbf{x}, t) = c + D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t - t') c(\mathbf{x}, t') \mathrm{e}^{t - t'} \,. \tag{4.21}$$

This can be attributed to the solution of the FDE via the transformation $c(\mathbf{x}, t) = \tilde{c}(\mathbf{x}, t)\mathrm{e}^t$. The full solution appeares to be

$$c(\mathbf{x}, t) = \frac{\mathrm{e}^t}{\sqrt{4Dt^\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(1 - \frac{\alpha}{2}(k+1))} \left(\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}} \right)^k \tag{4.22}$$

in terms of the series expansion of the Fox function (cf. sec. 2.8). Figure 4.1 shows that

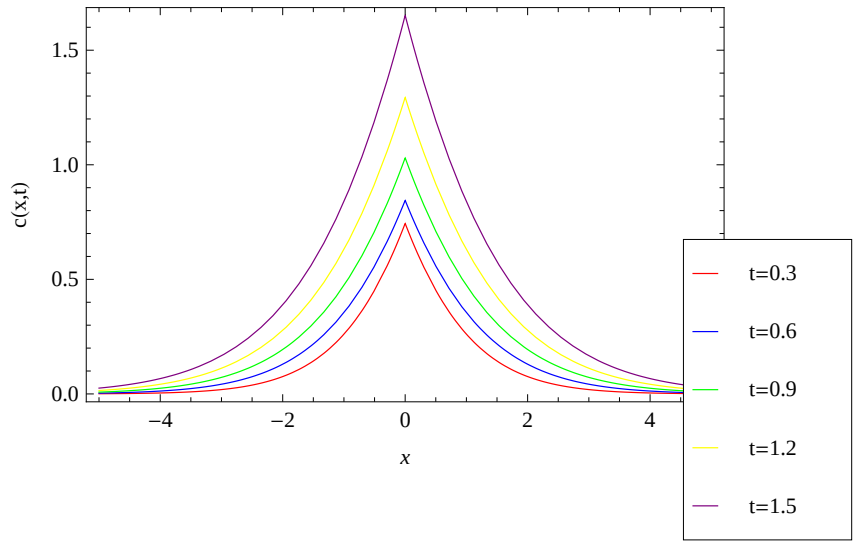

Figure 4.1: Solution of the linearised FKPP equation (eq. (4.21)) for small values of t, with $D = 1$ and $\alpha = 0.5$.

also in this case fronts of equal shape evolve. Neverteless, the speed of propagation is slower than it was concerning the linearised regime under normal diffusion. The rising of the peak at $x = 0$ is faster in the subdiffusive case (cf. fig. 4.1, fig. 3.2). The effect of balancing inhomogenities by diffusion is obviously decelarated in the latter case. The flanks of the function c get steeper with decreasing values α and in the limit $\alpha \to 1$ the normal diffusive case is restored (cf. fig. 4.2, 3.2). In figure 4.2 the plot for $t = 0.3$ was left out. On the plotting interval, concerning the spatial coordinate x, the series expansion for $t = 0.3$ does not converge.

In the same manner the equation in the vicinity of the stable state is derived. The linearised reaction kinetics in the vicinity of the stable state is derived to

$$R(c) = 1 - c = -\overline{c} \,. \tag{4.23}$$

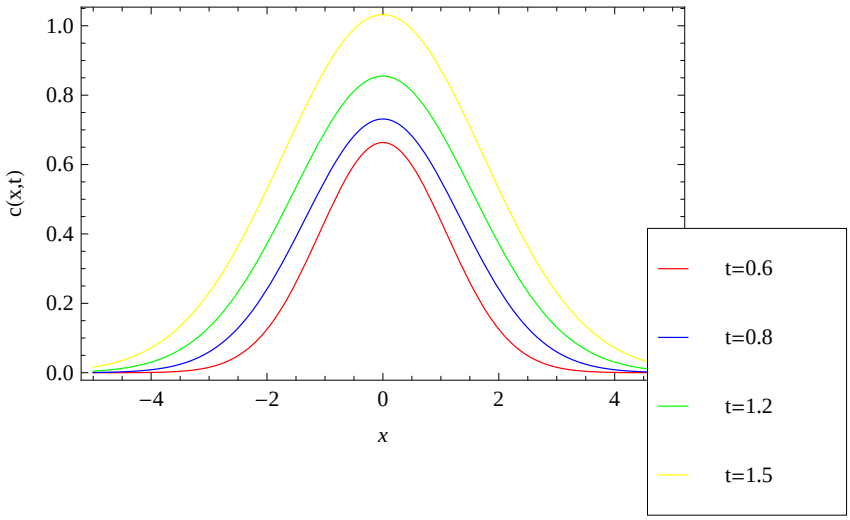

Figure 4.2: Solution (4.22) of the linearised FKPP equation (eq. (4.21)) for small values of t, with $D = 1$ and $\alpha = 1$.

Therfore, with the solution

$$G(\overline{c}_0, t) = \overline{c}_0 \mathrm{e}^{-t}\,, \tag{4.24}$$

the linearised equation can be derived to

$$\frac{\partial}{\partial t}\overline{c}(\mathbf{x},t) = -\overline{c}(\mathbf{x},t) + D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t-t')\overline{c}(\mathbf{x},t')\mathrm{e}^{-(t-t')}\,. \tag{4.25}$$

The solution can again be expressed in terms of the solution of the FDE. This time the according transformation is $\overline{c}(\mathbf{x},t) = \tilde{c}(\mathbf{x},t)\mathrm{e}^{-t}$, with the full solution

$$c(\mathbf{x},t) = \mathrm{e}^{-t}\left(\mathrm{e}^{t} - \frac{1}{\sqrt{4Dt^{\alpha}}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(1-\frac{\alpha}{2}(k+1))}\left(\frac{|x|}{\sqrt{Dt^{\alpha}}}\right)^k\right)\,. \tag{4.26}$$

Comparison of figure 4.3 to figure 3.3 shows that the process of relaxation to a homogeneous state is decelerated because of subdiffusion. Again the effect of balancing inhomogenities is retarded (see also discussion in sec. 3.3). Considering figure 4.1 and figure 4.3 the interpretation is again that fronts arise, propagating into the unstable stationary state and leaving the system in the system in the stationary state homogenously.

4.4 Linear stability analysis of the Zeldovich equation

The linearised reaction kinetics of the Zeldovich equation (4.18) in the vicinity of the unstable stationary state $c = 0$ reads

$$R(c) = \varepsilon c\,, \tag{4.27}$$

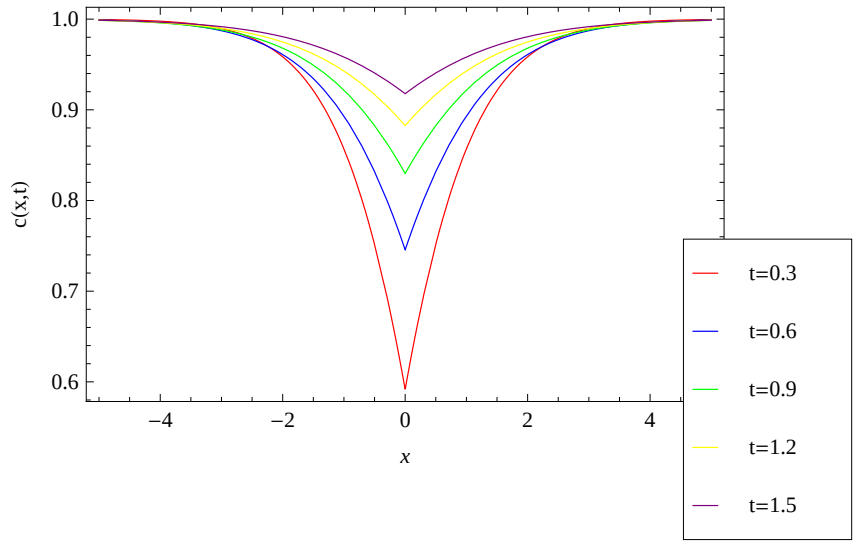

Figure 4.3: Solution (4.26)of the linearised FKPP equation (4.25) for small values of t, with $D = 1$ and $\alpha = 0.5$.

with the solution

$$G(c_0, t) = c_0 \mathrm{e}^{\varepsilon t} \,. \tag{4.28}$$

Therefore, the linearised subdiffusive Zeldovich equation, concerning the unstable fixed point, is established to

$$\frac{\partial}{\partial t} c(\mathbf{x}, t) = \varepsilon c + D \Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t - t') c(\mathbf{x}, t') \mathrm{e}^{\varepsilon (t - t')} \,. \tag{4.29}$$

Attaching equation (4.29) to the FDE via the transformation $c = \tilde{c}\mathrm{e}^{\varepsilon t}$ and accounting for the initial condition $c(\mathbf{x}, t = 0) = \frac{1}{2} \left(\delta(\mathbf{x} - \mathbf{x}_0) - \delta(\mathbf{x} + \mathbf{x}_0) \right)$, finally yields the solution

$$c(\mathbf{x}, t) = \frac{\mathrm{e}^{\varepsilon t}}{\sqrt{16 D t^\alpha}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(1 - \frac{\alpha}{2}(k+1))} \left(\frac{1}{\sqrt{D t^\alpha}} \right)^k \left(|\mathbf{x} - \mathbf{x}_0|^k - |\mathbf{x} + \mathbf{x}_0|^k \right) \,, \tag{4.30}$$

again in terms of the series expansion of the according Fox function. Figure 4.4 shows also in the case of subdiffusion a stationary inflexion point between the two initial. The rising of the peaks with time is faster than it was in the normal diffusive case (cf. fig. 3.5). Figure 4.5 shows that the evolution of the front is faster for larger values of the parameter ε. So again the effect of diffusion is the balancing of inhomogenities, which is retarded in the subdiffusive regime, so for smaller values of the characteristic exponent. The effect of the reaction term is to drive the growth of the inhomogenities, which is enhanced by the choice of larger values of ε. In the limit $\alpha \to 1$. the behaviour again ressembles the normal diffusive behaviour in the linearised regime. Here again the plot for $t = 0.1$ was left out. It does not converge on the considered interval. In the vicinity of the two stable stationary states $c = \pm\sqrt{\varepsilon}$ the Zeldovich equation can be derived in

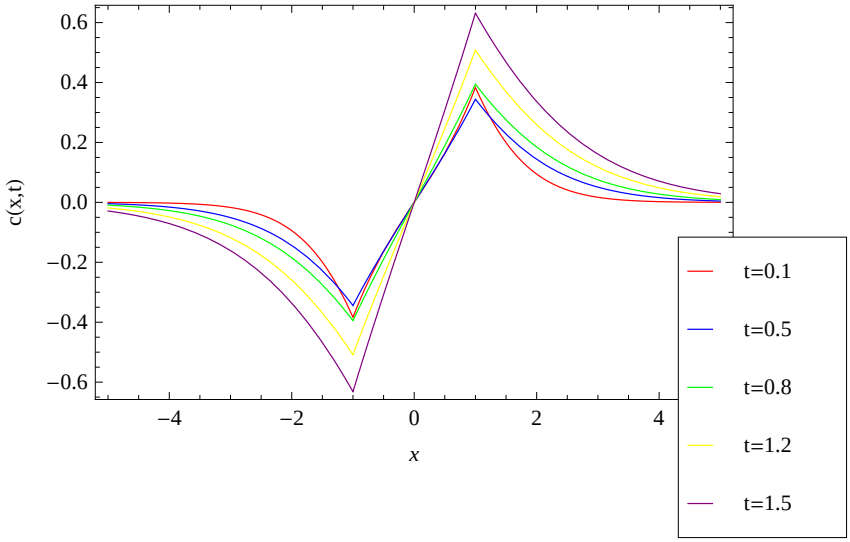

Figure 4.4: Solution (4.30) of the linearised Zeldovich equation (4.29) for small values of t, with $D = 1$, $\varepsilon = 1$, $x_0 = 1$ and $\alpha = 0.5$.

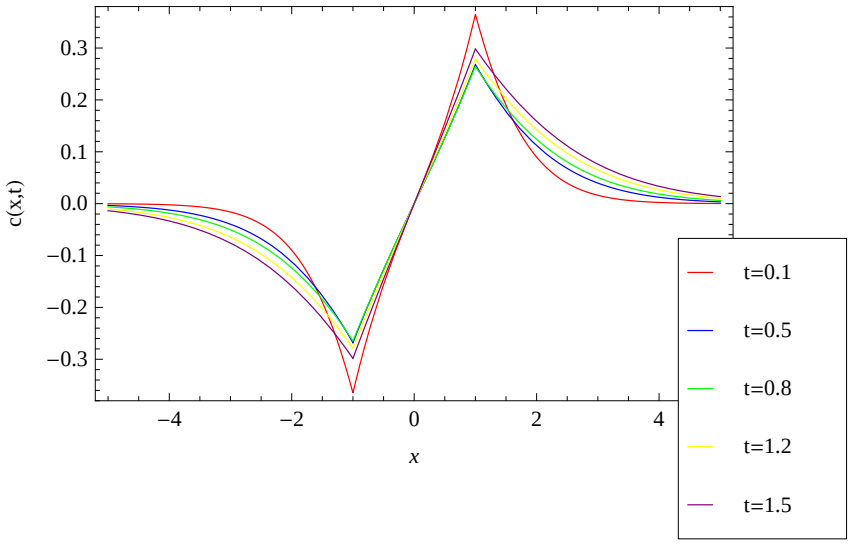

Figure 4.5: Solution (4.30) of the linearised Zeldovich equation (4.29) for small values of t, with $D = 1$, $\varepsilon = 0.5$, $x_0 = 1$ and $\alpha = 0.5$.

the same way as it was done before. Due to the linearised reaction kinetics

$$R(c)_\pm = -2\varepsilon \left(c \mp \sqrt{\varepsilon}\right) = -2\varepsilon \bar{c}_\pm \,, \tag{4.31}$$

with the solution for $\bar{c}_+$ being

$$G(\bar{c}_0, t) = \bar{c}_0 \mathrm{e}^{-2\varepsilon t} \,. \tag{4.32}$$

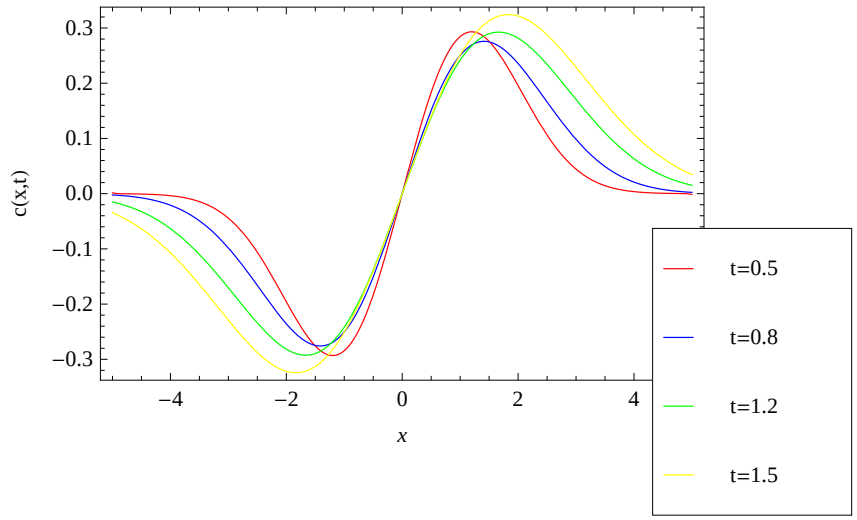

Figure 4.6: Solution (4.30) of the linearised Zeldovich equation (4.29) for small values of t, with $D = 1$, $\varepsilon = 0.5$, $x_0 = 1$ and $\alpha = 1$.

The solution in the case of the minus sign is the same, abandoning the different initial conditions. The Zeldovich equation in the vicinity of the stable fixed points $c = \sqrt{\varepsilon}$ reads

$$\frac{\partial}{\partial t} c_{\pm}(\mathbf{x}, t) = -2\varepsilon \left(c_{\pm}(\mathbf{x}, t) \mp \sqrt{\varepsilon} \right) + D \int_0^t \mathrm{d}t' Q(t - t') \mathrm{e}^{-2\varepsilon(t-t')} c_{\pm}(\mathbf{x}, t') \,. \tag{4.33}$$

The solution is attached to the FDE via the transformation

$$\bar{c}_{\pm} = \tilde{c}_{\pm} \mathrm{e}^{-2\varepsilon t} \,. \tag{4.34}$$

The full solution is, therefore, assembled to

$$c_{\pm}(\mathbf{x}, t) = \mathrm{e}^{-2\varepsilon t} \frac{1}{\sqrt{4Dt^{\alpha}}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(1 - \frac{\alpha}{2}(k+1))} \left(\frac{|x|}{\sqrt{Dt^{\alpha}}} \right)^k \pm \sqrt{\varepsilon} \,. \tag{4.35}$$

Figure 4.7 shows the relaxation to the stationary fixed point, which can be varied by choosing different values of ε (cf. expr. 4.35). The growing of inhomogenities near the stationary inflexion point $x = 0$ in case of the linearised equation (4.29) and the relaxation to the stationary fixed points $\pm\sqrt{\varepsilon}$ in case of equation (4.33), result in the conclusion that a stationary domain wall evolves for the exact equation. The plot for the solution in the vicinity of $c = \sqrt{\varepsilon}$ is of course similar to figure 4.7 reflected at the x-axes.

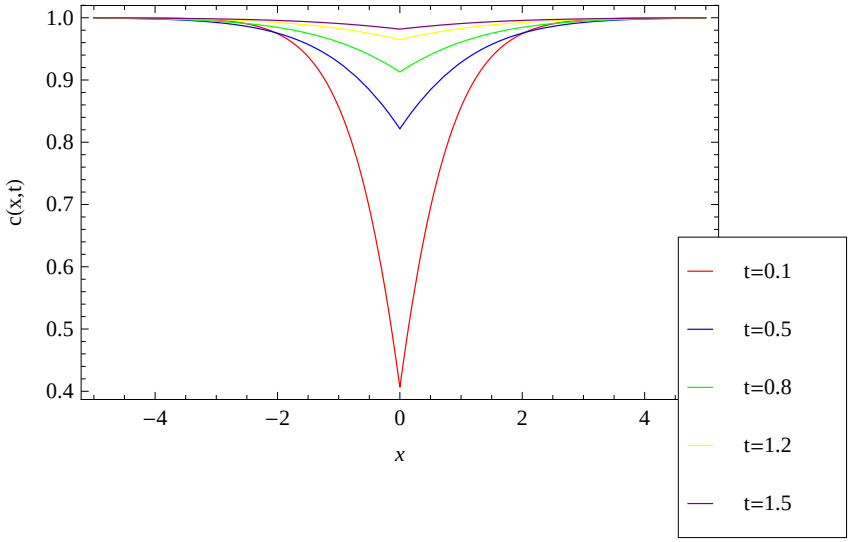

Figure 4.7: Solution (4.35) of the linearised Zeldovich equation (4.33) in case of the positive sign for small values of t, with $D = 1$, $\varepsilon = 1$ and $\alpha = 0.5$.

4.5 Application of the singular perturbation approximation to the FKPP equation

The transformation, that was exploited to establish the zeroth order of the SPA concerning the normal FKPP equation in section 3.6, can also be applied to the according subdiffusive RDE, which shall be done in the following section. It yields the opportunity to achieve a first approximation for the full nonlinear regime and, thus, an idea of what the nonlinear solution of this subdiffusive RDE looks like. So let us take the full nonlinear subdiffusive FKPP equation (4.15) into account

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = c(\mathbf{x},t)(1-c(\mathbf{x},t)) + D\Delta_{\mathbf{x}}\int_0^t \mathrm{d}t' Q(t-t')\frac{c(\mathbf{x},t')}{\left(1-\mathrm{e}^{-(t-t')}\right)c(\mathbf{x},t')+\mathrm{e}^{-(t-t')}}\,. \tag{4.36}$$

Now, as done before in section 3.6, the transformation

$$c(\mathbf{x},t) = \frac{\phi(\mathbf{x},t)}{1+\phi(\mathbf{x},t)} \tag{4.37}$$

is employed. Consequently, as $c \in [0,1]$, the same must hold for ϕ, too. Its temporal derivative reads

$$\dot{c}(\mathbf{x},t) = \frac{\dot{\phi}(\mathbf{x},t)}{(1+\phi(\mathbf{x},t))^2}\,. \tag{4.38}$$

With the transformed solution of the reaction kinetics

$$\frac{c(\mathbf{x},t')}{\left(1-\mathrm{e}^{-(t-t')}\right)c(\mathbf{x},t')+\mathrm{e}^{-(t-t')}} = \frac{\phi(\mathbf{x},t')}{\left(\phi(\mathbf{x},t')+\mathrm{e}^{-(t-t')}\right)} \tag{4.39}$$

the spatial derivative reads

$$\Delta_{\mathbf{x}}\left(\frac{c(\mathbf{x},t')}{\left(1-\mathrm{e}^{-(t-t')}\right)c(\mathbf{x},t')+\mathrm{e}^{-(t-t')}}\right) = \frac{\left(\Delta_{\mathbf{x}}\phi(\mathbf{x},t')\right)^2\mathrm{e}^{t-t'}}{\left(1+\mathrm{e}^{t-t'}\phi(\mathbf{x},t')\right)^2} - \frac{2\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t')\mathrm{e}^{t-t'}\right)^2}{\left(1+\mathrm{e}^{t-t'}\phi(\mathbf{x},t')\right)^3}\,. \quad (4.40)$$

Thus, the full FKPP equation takes the form

$$\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \phi(\mathbf{x},t) + D\int_0^t \mathrm{d}t'\mathrm{Q}(t-t')\left(\frac{1+\phi(\mathbf{x},t)}{1+\mathrm{e}^{t-t'}\phi(\mathbf{x},t')}\right)^2 \times\left(\Delta_{\mathbf{x}}\phi(\mathbf{x},t')\mathrm{e}^{t-t'} - \frac{2\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t')\mathrm{e}^{t-t'}\right)^2}{1+\mathrm{e}^{t-t'}\phi(\mathbf{x},t')}\right)\,. \quad (4.41)$$

Now one further reduction of this equation is provided by the transformation

$$\phi = \psi\mathrm{e}^t\,, \quad (4.42)$$

with the result

$$\frac{\partial}{\partial t}\psi(\mathbf{x},t) = D\int_0^t \mathrm{d}t'Q(t-t')\left(\frac{1+\mathrm{e}^t\psi(\mathbf{x},t)}{1+\mathrm{e}^t\psi(\mathbf{x},t')}\right)^2 \times\left(\Delta_{\mathbf{x}}\psi(\mathbf{x},t') - \frac{2\left(\nabla_{\mathbf{x}}\psi(\mathbf{x},t')\right)^2\mathrm{e}^t}{1+\mathrm{e}^t\psi(\mathbf{x},t')}\right)\,. \quad (4.43)$$

So now we need an approximation to gain a linear integral term. The nonlinearities under the integral rule at least an analytical result out. So at first the last term under the integral is neglected, which is similar to what was done in the procedure of SPA in section 3.6. But afterwards the integral term is still nonlinear due to the factor

$$\left(\frac{1+\mathrm{e}^t\psi(\mathbf{x},t)}{1+\mathrm{e}^t\psi(\mathbf{x},t')}\right)^2\,. \quad (4.44)$$

That is a consequence of the nonlocality in time and, thus, of the memory effect of subdiffusion. Assuming this term to be unity would terminally yield a solvable approximation of the FKPP equation. It seems to be convenient for large values of t. Nevertheless, taking into consideration that t' is subject of integration, it appeares to be problematic. So let us assume that $Q(t-t') \sim \frac{1}{(t-t')^{1-\alpha}}$ (cf. section 2.8). So the time kernel drives back the contributions of the integral where the difference $t-t'$ is large. Therefore, in case of large values of t, the contributions from regions where the approximation does not hold can be regarded as small. Moreover, we can expect to have a good approximation to describe the asymptotic behaviour of equation (4.15). A realistic description of the behaviour in the beginning, concerning the full FKPP

equation, will probably be difficult to dissolve within this approximation. Considering that also the zeroth order SPA for the normal diffusive FKPP is not able to dissolve effects of relaxation (cf. section 3.6 fig. 3.12) that would not be surprising if we got along without this further approximation. So let us go on with this linearisation. The auxiliary function ψ is then a solution of the FDE

$$\frac{\partial}{\partial t}\psi(\mathbf{x},t) = D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t-t')\psi(\mathbf{x},t') \tag{4.45}$$

or written in terms of the fractional derivative

$$\frac{\partial}{\partial t}\psi(\mathbf{x},t) = D_0 \mathrm{D}_t^{1-\alpha}\Delta_{\mathbf{x}}\psi(\mathbf{x},t')\,. \tag{4.46}$$

Note that due to the transformation employed in the beginning of this section the original pdf is given as

$$c(\mathbf{x},t) = \frac{\psi(\mathbf{x},t)\mathrm{e}^t}{1+\psi(\mathbf{x},t)\mathrm{e}^t}\,. \tag{4.47}$$

The solution can again be established in terms of a Fox function with

$$\psi(\mathbf{x},t) = \frac{1}{\sqrt{4Dt^\alpha}}\mathrm{H}_{1,1}^{1,0}\left[\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}}\middle|\begin{matrix}\left(1-\frac{\alpha}{2},\frac{\alpha}{2}\right)\\(0,1)\end{matrix}\right]\,, \tag{4.48}$$

with the already mentioned series expansion (2.94). So in the end the approximation is nothing more than inserting the solution of the FDE into the solution evaluated for the zeroth order of SPA, concerning normal diffusion. Asymptotically, so for large values of t, the second approximation of assuming expression 4.44 to be one is reasonable so that the solution can be regarded as the zeroth order of SPA, concerning subdiffusion. Figure

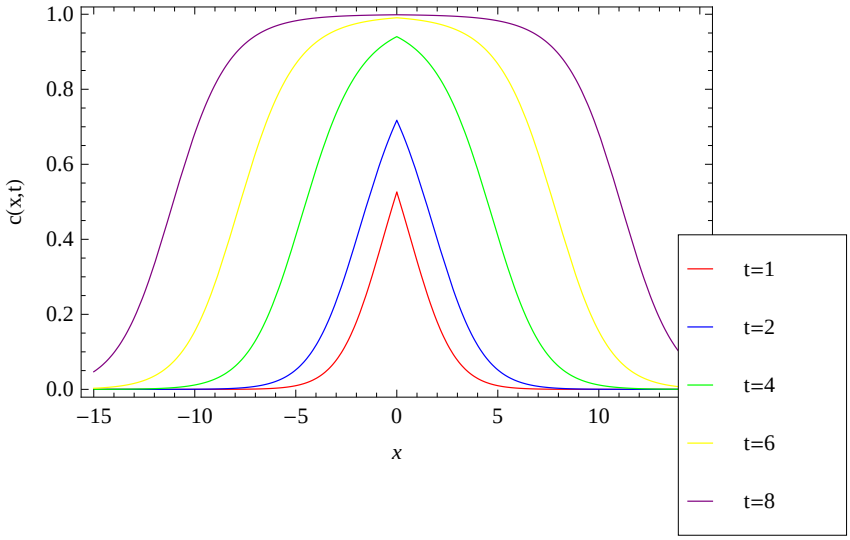

Figure 4.8: Approximate solution of the subdiffusive FKPP equation (4.15) for small values of t, with $D = 1$ and $\alpha = 0.5$.

4.8 shows the rising of two fronts invading the unstable stationary state on both sides of the initial position. So this property is seen to apply at least for the approximate system under subdiffusion, as well. Due to the apparently instantanious relaxation to a uniform front under the given approximation, the front in the subdiffusive case with $\alpha = 0.5$ seems to be slower (cf. fig. 4.8, fig. 3.10). This dependence of the front velocity

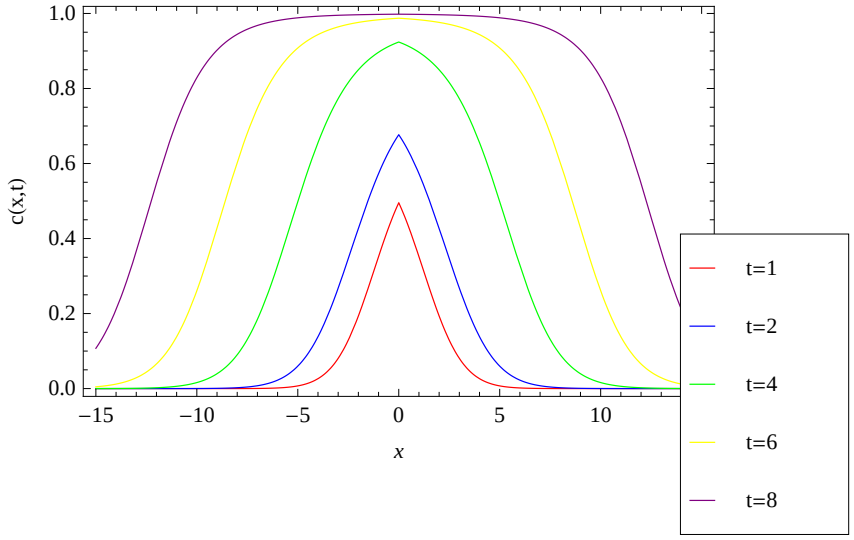

Figure 4.9: Approximate solution of the subdiffusive FKPP equation (4.15) for small values of t, with $D = 1$ and $\alpha = 0.7$.

on the characteristic exponent α seems to be confirmed by figure 4.9. Figure 4.10 shows

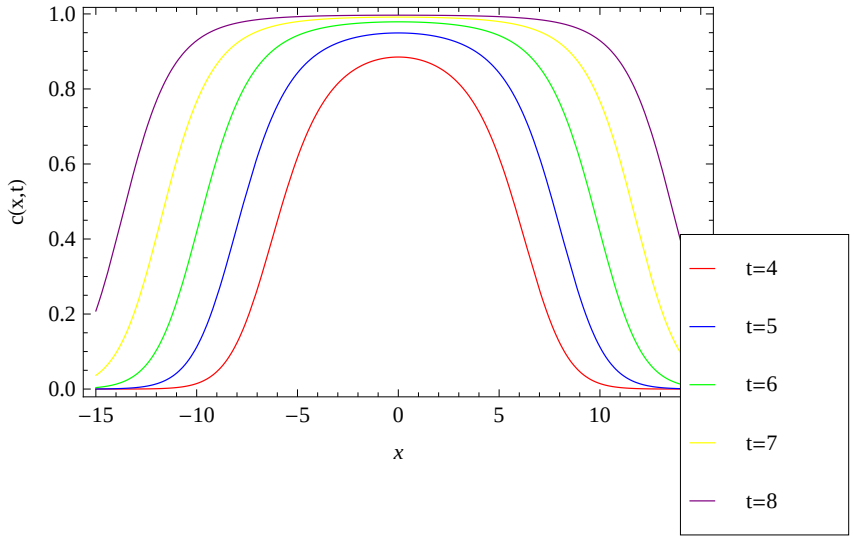

Figure 4.10: Approximate solution of the subdiffusive FKPP equation (4.15) for small values of t, with $D = 1$ and $\alpha = 1$.

that also here the normal diffusive case can be restored (cf. fig. 3.10). The time steps,

for which the plots were evaluated, were adjusted to the need of having a converging solution, considering the given spatial interval.

4.6 The linear spreading speed in the subdiffusive regime

One of the main issues this thesis is concerned with is the question if there is a uniform translating front also observable for the subdiffusive FKPP equation. For the normal diffusive regime it can be shown that the front always relaxes to a uniform shape and velocity. Moreover, in the case of the normal diffusive FKPP equation it can be illustrated, with structural stability arguments (see sec. 3.5), that this velocity is the linear spreading speed, which can be evaluated only taking the linearised system into account. If a higher asymptotic velocity is selected, considering pushed fronts, this is always due to higher order nonlinear terms in the reaction kinetics. In section 4.5 it was shown, within the claimed approximations, that also in the subdiffusive regime the evolution of a uniform front can be observed. This raises the question if the selected velocity, for given characteristic exponents, could also be predicted in terms of the linearised system. As a result of the temporal integration the subdiffusive RDE's are affected with, the procedure to evaluate the linear spreading speed, described in section 3.5, has to be adapted to the situation. The adaption I performed was mainly enforced by a so called leading edge linearisation carried out by Froemberg, Schmidt-Martens, Sokolov and Sagués [18]. Assuming space to be one dimensional, the ansatz

$$c(x,t) = c_0 \mathrm{e}^{-\lambda(x-vt)} \tag{4.49}$$

is applied to the linearised FKPP equation (4.21), which leads to

$$\lambda v c_0 \mathrm{e}^{-\lambda(x-vt)} = c_0 \mathrm{e}^{-\lambda(x-vt)} + D\lambda^2 \int_0^t \mathrm{d}t' Q(t-t') c_0 \mathrm{e}^{-\lambda(x-vt')} \mathrm{e}^{t-t'} \,. \tag{4.50}$$

Then the substitution $t - t' = \tau$, with $\mathrm{d}t' = -\mathrm{d}\tau$ yields

$$\lambda v = 1 + D\lambda^2 \int_0^t \mathrm{d}\tau Q(\tau) c_0 \mathrm{e}^{-\lambda v \tau} \mathrm{e}^{\tau} \,, \tag{4.51}$$

reducing the term as much as possible. Now the asymptotic behaviour of equation (4.51) shall be evaluated. Therefore, the limit $t \to \infty$ is performed. As a result, the integral term can be interpreted as a Laplace transformation. The time kernel $Q(\tau)$ can then be expressed explicitly (see sec. 2.8 eq. 2.91). Accordingly equation (4.51) reduces to

$$\lambda v = 1 + D\lambda^2 \left(\lambda v - 1\right)^{1-\alpha} \,. \tag{4.52}$$

The linear spreading speed can be found as the minimal speed solving equation (4.52) under the condition $\lambda \, \epsilon \, \mathbb{R}$. As equation (4.52) is transcendental a good way to find solutions is a three dimensional plot. Another form of the equation is easier to plot

$$D = \frac{\left(\lambda v - 1\right)^{\alpha}}{\lambda^2} =: f(\lambda, v, \alpha) \,. \tag{4.53}$$

The front velocity for certain values of D can then be pointed out as the penetration point of the function with the plane, concerning D, which is minimal in terms of v. A good test to get an idea if this evaluation leads to reasonable results is to investigate the limit $\alpha \to 1$. Figure 4.11 shows that the normal diffusive case is restored, $v^* = 2$. The

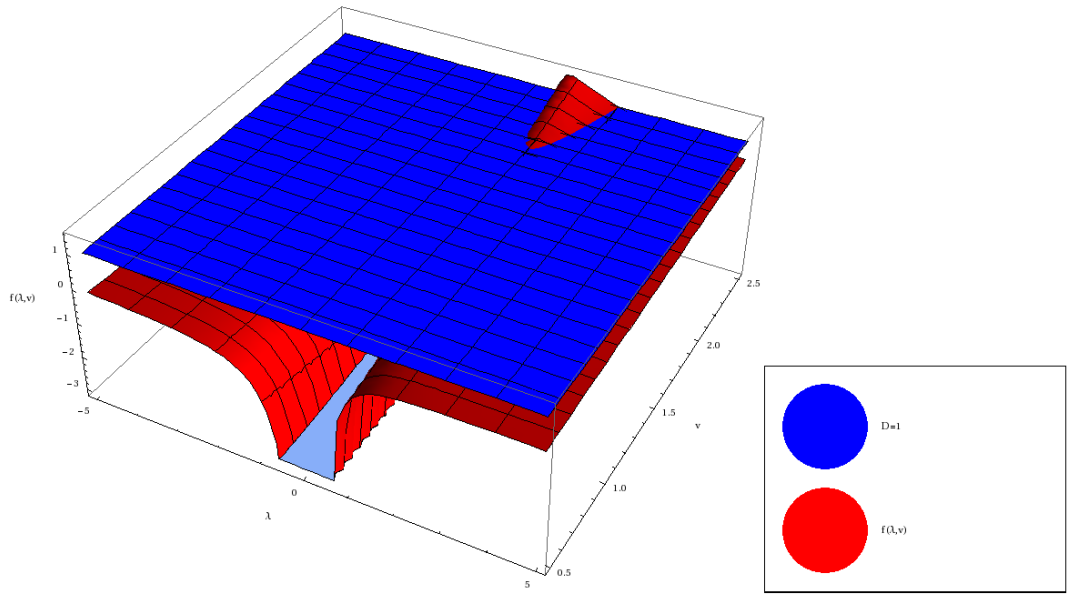

Figure 4.11: Transcendental equation (4.53) plotted versus λ and v, with $\alpha = 1$, the blue plane denotes $f(\lambda,v) = D = 1$, the gridlines concerning the v-axes have a distance of 0.1 units of velocity each.

minimal value of v under the condition of λ being a real number, turns out to be the one where only a single value for this parameter is possible, this applies for all choices of α. For $\alpha = 1$ it is easy to show that $v^* = 2$ is the result of $\lambda = 1$.

4.7 Front velocity of the FKPP equation

The front velocities for different values of α shall be evaluated in terms of the following asymptotic approximation of the Fox function [28]

$$\psi(\mathbf{x},t) \sim \frac{1}{\sqrt{4\pi D t^\alpha}} \sqrt{\frac{1}{2-\alpha}} \left(\frac{2}{\alpha}\right)^{\frac{1-\alpha}{2-\alpha}} \left(\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}}\right)^{-\frac{1-\alpha}{2-\alpha}} \times \exp\left(-\frac{2-\alpha}{2}\left(\frac{\alpha}{2}\right)^{\frac{\alpha}{2-\alpha}} \left(\frac{|\mathbf{x}|}{\sqrt{Dt^\alpha}}\right)^{\frac{1}{1-\frac{\alpha}{2}}}\right). \tag{4.54}$$

The solutions are given in terms of the transformation (4.47). The front velocity for

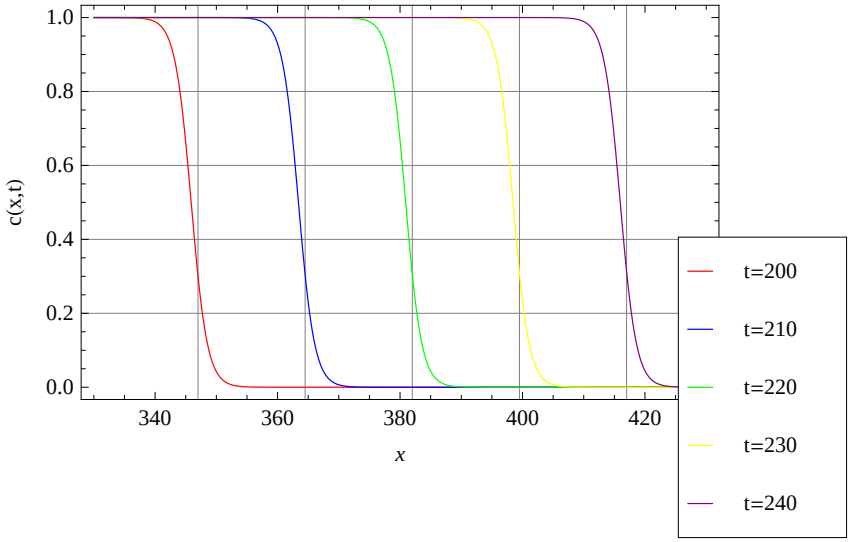

Figure 4.12: Front velocity in the case of $\alpha = 0.5$ and $D = 1$, the grid lines have equal distances of 17.5 units of length each.

the case of $\alpha = 0.5$ is evaluated to $v \approx 1.75$ (see fig. 4.12). The three dimensional plot was turned (fig. 4.13) in this case. One is looking "from above" on the $(D = 1)$-plane. In this way it is easier to estimate the minimal value for v. It is a bit larger than the approximate speed of the front (fig. 4.12) and can be read off to $v^* \approx 1.8$. Nevertheless, a numerical investigation shows that linear spreading speed for the given value of the characteristic exponent is $v^* \approx 1.755$. In the case of $\alpha = 0.7$ the front speed can be approximated to $v \approx 1.9$ And also this time the minimal speed gained by equation (4.53) for $D = 1$, the linear spreading speed, is a bit larger than the one that is selected asymptotically. In this case it is read off to $v^* \approx 1.95$. Also here a numerical investigation confirms that the asymptotic speed of the front evaluated for the approximated FKPP equation is closer to the linear spreading speed calculated via equation (4.53) than figure 4.15 shows. The investigation comes to the result $v^* \approx 1.91$. Terminally figure 4.16 shows that also in the case of asymptotic front velocities the normal diffusive result is restored, $v \approx 2$.

4.8 Application of the singular perturbation approximation to the Zeldovich equation

For the subdiffusive Zeldovich equation the method of SPA shall also be exploited. Here again the following Zeldovich equation will be examined

$$\frac{\partial}{\partial t}c(\mathbf{x},t) = c(\mathbf{x},t) - c(\mathbf{x},t)^3 \pm D\Delta_{\mathbf{x}} \int_0^t \mathrm{d}t' Q(t-t') \sqrt{\frac{1}{(\frac{1}{c(\mathbf{x},t')^2} - 1)\mathrm{e}^{-2(t-t')} + 1}}\,. \quad (4.55)$$

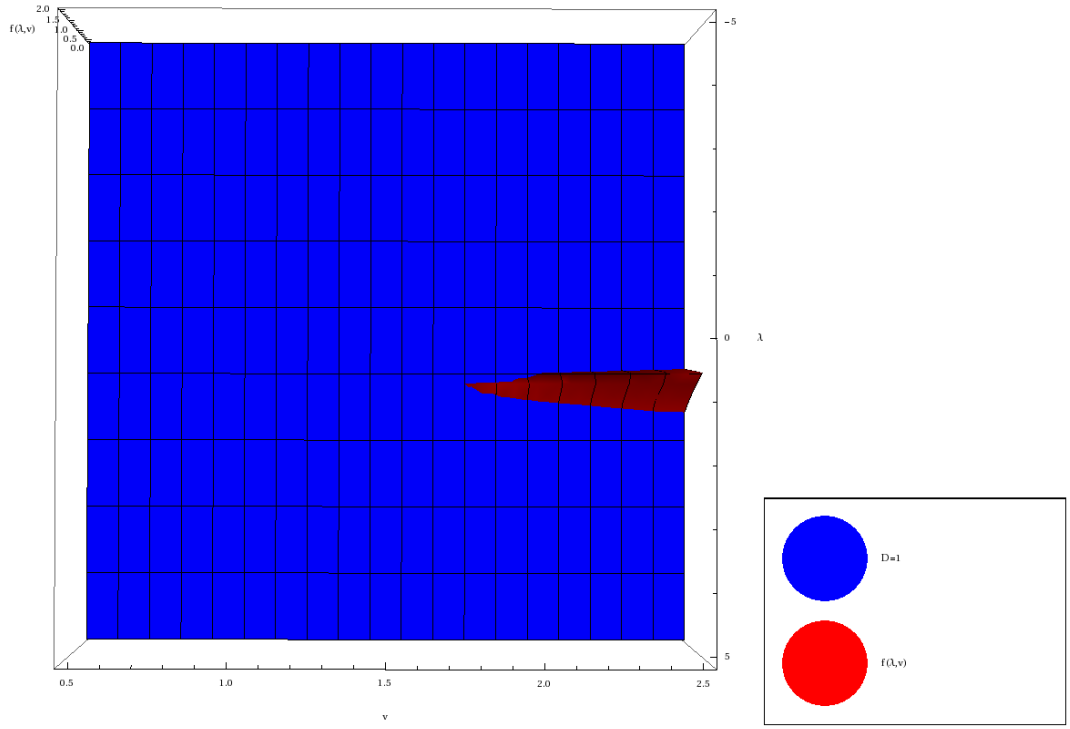

Figure 4.13: Transcendental equation (4.53) plotted versus λ and v, with $\alpha = 0.5$, the blue plane denotes $f(\lambda,v) = D = 1$, the gridlines concerning the v-axes have a distance of 0.1 units of velocity each.

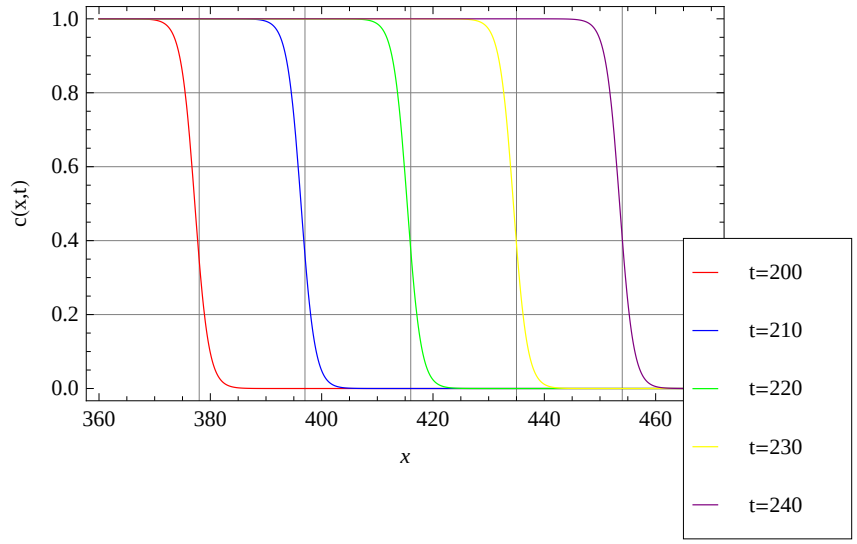

Figure 4.14: Front velocity in the case of $\alpha = 0.7$ and $D = 1$, the grid lines have equal distances of 19 units of length each.

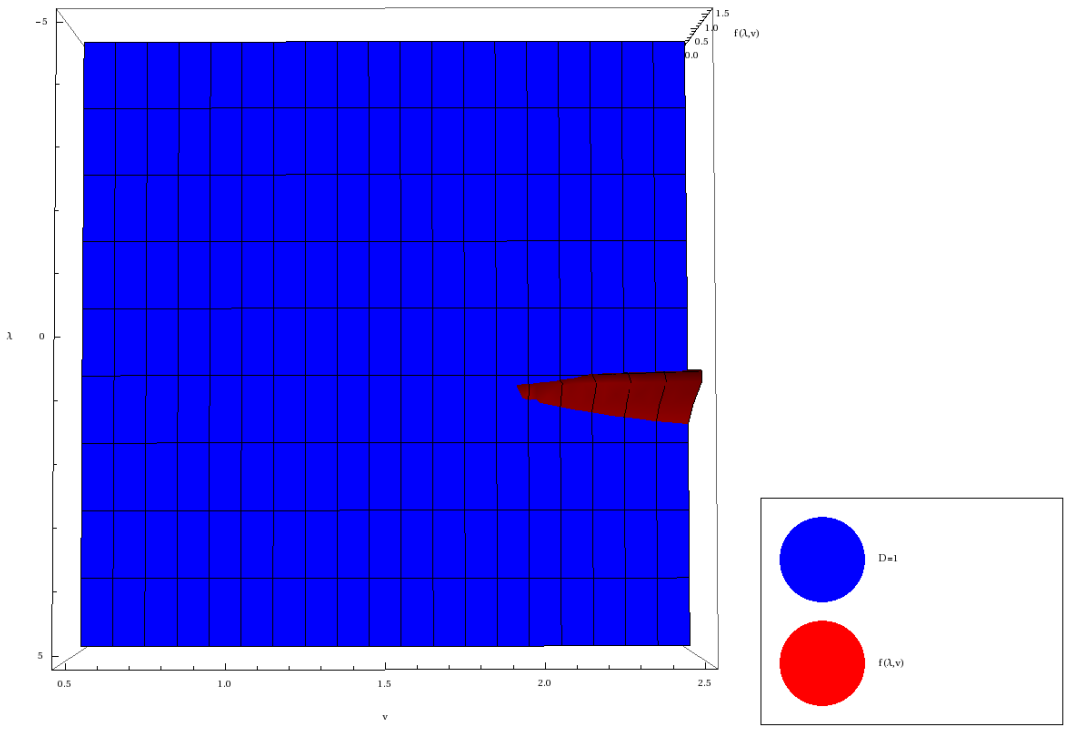

Figure 4.15: Transcendental equation (4.53) plotted versus λ and v, with $\alpha = 0.7$, the blue plane denotes $f(\lambda,v) = D = 1$, the gridlines concerning the v-axes have a distance of 0.1 units of velocity each.

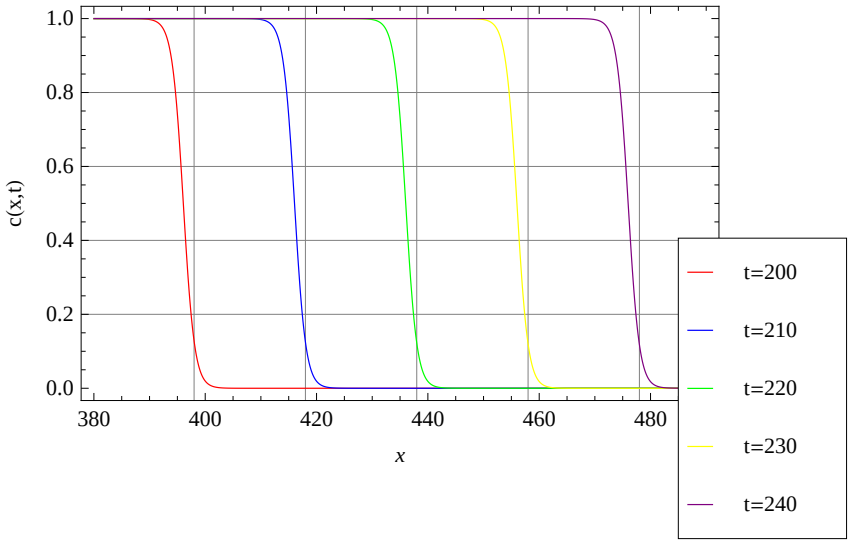

Figure 4.16: Front velocity in the case of $\alpha = 1$ and $D = 1$, the grid lines have equal distances of 20 units of length each.

The changeover is easy to perform due to simple scaling arguments (see sec. 3.6). Now the following transformation is put into effect

$$c(\mathbf{x},t) = \frac{\phi(\mathbf{x},t)}{\sqrt{1+\phi(\mathbf{x},t)^2}}\,. \tag{4.56}$$

In this case the function ϕ can also be negative. It is defined on the same interval as c. The temporal derivative appeares to be

$$\dot{c}(\mathbf{x},t) = \frac{\dot{\phi}(\mathbf{x},t)}{\left(\sqrt{1+\phi(\mathbf{x},t)^2}\right)^3}\,. \tag{4.57}$$

The function G (see section 4.1) transforms to

$$\frac{1}{\sqrt{\left(\frac{1}{c(\mathbf{x},t')}-1\right)\mathrm{e}^{-2(t-t')}+1}} = \frac{\phi(\mathbf{x},t')}{\sqrt{\mathrm{e}^{-2(t-t')}+\phi(\mathbf{x},t')}}\,, \tag{4.58}$$

with the spatial derivative

$$\begin{aligned}\Delta_{\mathbf{x}}&\frac{\phi(\mathbf{x},t')}{\sqrt{\mathrm{e}^{-2(t-t')}+\phi(\mathbf{x},t')}}\\ &= \frac{\Delta_{\mathbf{x}}\phi(\mathbf{x},t')\mathrm{e}^{t-t'}}{\left(1+\mathrm{e}^{2(t-t')}\phi(\mathbf{x},t')\right)^{\frac{3}{2}}} - \frac{3\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t')\right)^2\phi(\mathbf{x},t')\mathrm{e}^{3(t-t')}}{\left(1+\mathrm{e}^{2(t-t')}\phi(\mathbf{x},t')\right)^{\frac{5}{2}}}\,.\end{aligned} \tag{4.59}$$

Thus, the transformed Zeldovich equation can be assembled to

$$\begin{aligned}\frac{\partial}{\partial t}\phi(\mathbf{x},t) = \phi(\mathbf{x},t) \pm \int_0^t \mathrm{d}t' Q(t-t') &\left(\sqrt{\frac{1+\phi(\mathbf{x},t)^2}{1+\left(\mathrm{e}^{t-t'}\phi(\mathbf{x},t')\right)^2}}\right)^3\\ &\times\left(e^{t-t'}\Delta_{\mathbf{x}}\phi(\mathbf{x},t') - \frac{3\mathrm{e}^{3(t-t')}}{1+\left(\mathrm{e}^{(t-t')}\phi(\mathbf{x},t`)\right)^2}\phi(\mathbf{x},t')\left(\nabla_{\mathbf{x}}\phi(\mathbf{x},t')\right)^2\right)\,.\end{aligned} \tag{4.60}$$

In analogy to the procedure of section 4.5, another transformation is applied

$$\phi = \psi\mathrm{e}^t\,, \tag{4.61}$$

which yields the following expression

$$\begin{aligned}\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \pm\int_0^t \mathrm{d}t' Q(t-t') &\left(\sqrt{\frac{1+\left(\mathrm{e}^t\psi(\mathbf{x},t)\right)^2}{1+\left(\mathrm{e}^t\psi(\mathbf{x},t')\right)^2}}\right)^3\\ &\times\left(\Delta_{\mathbf{x}}\psi(\mathbf{x},t') - \frac{3\left(\nabla_{\mathbf{x}}\psi(\mathbf{x},t')\mathrm{e}^t\right)^2\psi(\mathbf{x},t')}{1+\left(\mathrm{e}^t\psi(\mathbf{x},t`)\right)^2}\right)\,.\end{aligned} \tag{4.62}$$

Now the situation is similar to the one in section 4.5 at the stage of equation (4.43). Due to the transformation the reaction term is completely contained in the integrand. Again an approximation has to be made to avoid the nonlinearities. So let us at first neglect the last term on the rhs under the integral, which is analogous to the SPA performed in the case of the normal diffusive Zeldovich equation (section 3.6). There is still the term

$$\left(\sqrt{\frac{1+\left(\mathrm{e}^t\psi(\mathbf{x},t)\right)^2}{1+\left(\mathrm{e}^t\psi(\mathbf{x},t')\right)^2}}\right)^3 , \tag{4.63}$$

avoiding the approximate equation to be solved. The further approximation, which shall be claimed, is analogous to the one that was assumed in section 4.5. Let us claim expression (4.63) to be one, which yields a linearised integral term. The transformed Zeldovich equation, therefore, reduces to the FDE

$$\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \pm D_0 \mathrm{D}_t^{1-\alpha}\Delta_{\mathbf{x}}\psi(\mathbf{x},t)\,. \tag{4.64}$$

The solution is again constituted in terms of the initial condition $\psi(\mathbf{x},t=0) = \frac{1}{2}\left(\delta(\mathbf{x}-\mathbf{x}_0)-\delta(\mathbf{x}+\mathbf{x}_0)\right)$. Hence, it can be established in terms of a Fox function. Taking account of the positive sign only, it reads

$$\begin{aligned}\psi(\mathbf{x},t) = &\frac{1}{\sqrt{16Dt^\alpha}}\mathrm{H}_{1,1}^{1,0}\left[\frac{|\mathbf{x}-\mathbf{x}_0|}{\sqrt{Dt^\alpha}}\middle|\begin{matrix}\left(1-\frac{\alpha}{2},\frac{\alpha}{2}\right)\\(0,1)\end{matrix}\right]\\ &-\frac{1}{\sqrt{16Dt^\alpha}}\mathrm{H}_{1,1}^{1,0}\left[\frac{|\mathbf{x}+\mathbf{x}_0|}{\sqrt{Dt^\alpha}}\middle|\begin{matrix}\left(1-\frac{\alpha}{2},\frac{\alpha}{2}\right)\\(0,1)\end{matrix}\right] .\end{aligned} \tag{4.65}$$

It can be investigated in terms of the series expansion (see sec 2.8). At this stage it becomes clear that the negative sign has to be neglected. Substituting the negative sign into the diffusion constant leads to a complex solution. Note that the solution of the approximate Zeldovich equation in this case is assembled as follows

$$c = \frac{\mathrm{e}^t\psi}{\sqrt{1+\left(\mathrm{e}^t\psi\right)^2}}\,. \tag{4.66}$$

Figure 4.17 shows the rising of a stationary front in terms assumptions. The evolution of this front is accelerated by the effect of subdiffusion (cf. fig. 3.13). Considering $\varepsilon = 0.5$, the relaxation is accelerated further, which is not surprising. The control parameter varies the time scale, which is inversely proportional to ε (see sec. 3.6). Terminally also here (fig. 4.19) the result of the SPA for the normal diffusive case is restored.

4.9 Comment on the relaxation to a stationary front

Concerning once again with the evolution of a stationary front, a comparison of relaxation for the zeroth order SPA for normal diffusion with the claimed approximation for the subdiffusive regime shall be evaluated. Although the relaxation cannot be taken account of realistically for the full nonlinear regime by means of this approximation, a

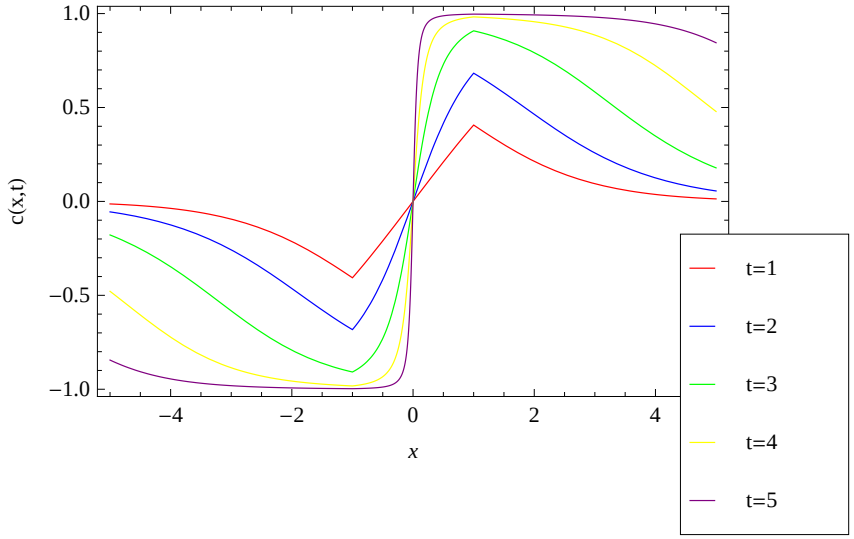

Figure 4.17: Approximate solution of the subdiffusive Zeldovich equation (4.18), with $D = 1$, $x_0 = 1$, $\varepsilon = 1$ and $\alpha = 0.5$.

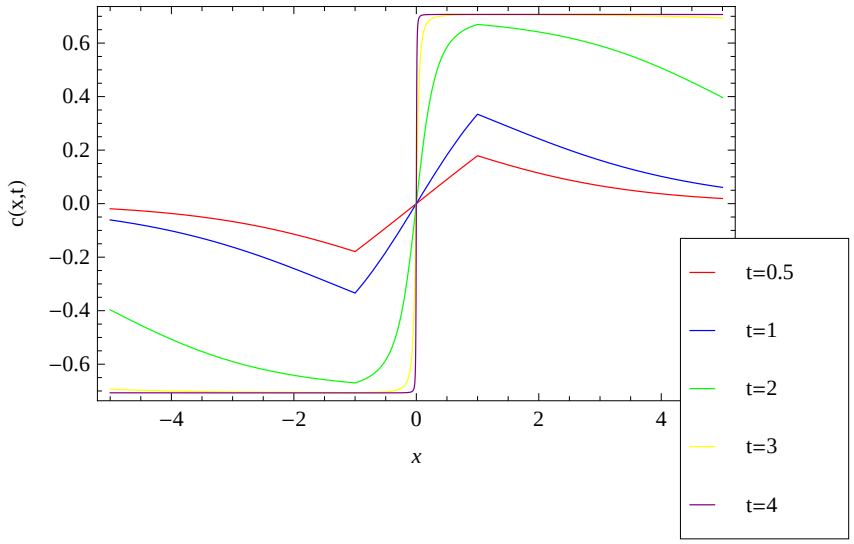

Figure 4.18: Approximate solution of the subdiffusive Zeldovich equation (4.18), with $D = 1$, $x_0 = 1$, $\varepsilon = 0.5$ and $\alpha = 0.5$.

comparison is possible. Comparing figure 4.17 to figure 4.18, it becomes obvious that balancing of inhomogenities, which is slower in the subdiffusive regime (see fig. 4.20), results in the different relaxation characteristics for different values of α. A good value to determine the relaxation to the stationary fronts is the spatial derivative at the position where the domain wall arises. Figure 4.17, as an example, shows that this derivative grows with time. Figure 4.21 shows that, too. The logarithmic plot of the spatial derivative of the function at position $x = 0$ shows that the relaxation to a domain wall follows an exponential for all values of the characteristic exponent. The smaller the value of α

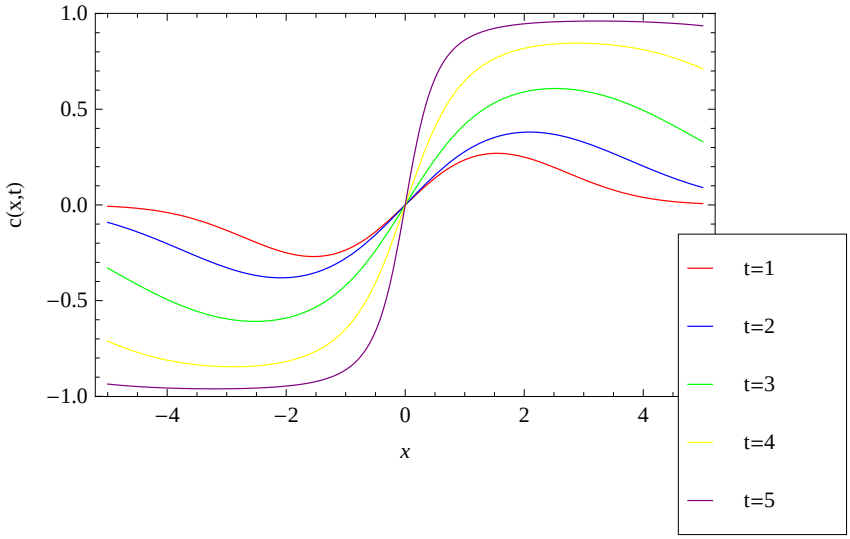

Figure 4.19: Solution of the subdiffusive Zeldovich equation (4.18) in terms of SPA for small values of t, with $D = 1$, $x_0 = 1$, $\varepsilon = 1$ and $\alpha = 1$.

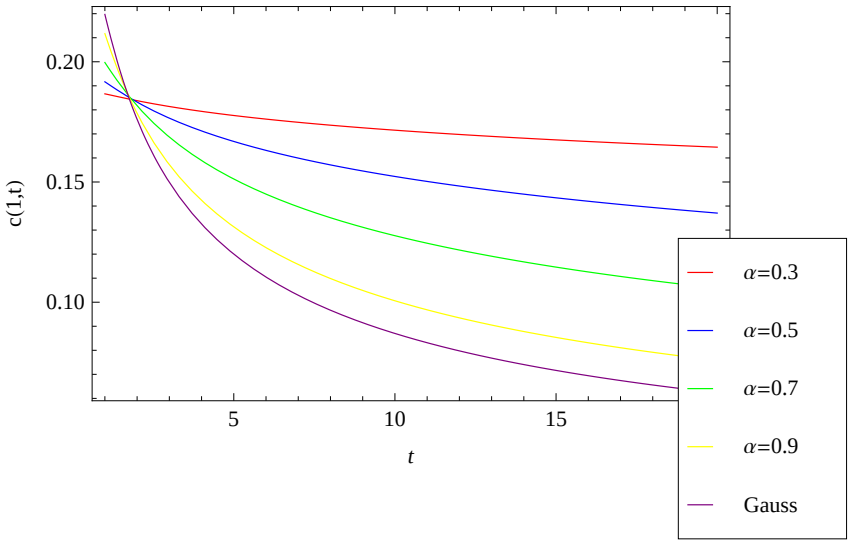

Figure 4.20: Temporal behaviour of the solutions of the FDE (2.87) at position $x = 0$ for different values of α in comparison to the according Gaussian.

is chosen, the faster is the evolution of the stationary front. The value ε, representing the control parameter that varies the time scale, is for the following investigation not interesting. It clearly has an effect on the evolution of the domain wall, but this is already understandable by only taking into account that scaling this parameter into the other variables and parameters leads to $t \to \frac{t}{\varepsilon}$ (cf. sec. 3.6). The smaller the value of ε is chosen the faster will be the relaxation to the stationary front. Therefore, to ease up the following discussion it is assumed to be one. In the given context another control parameter becomes interesting. The parameter that determines the position of the two

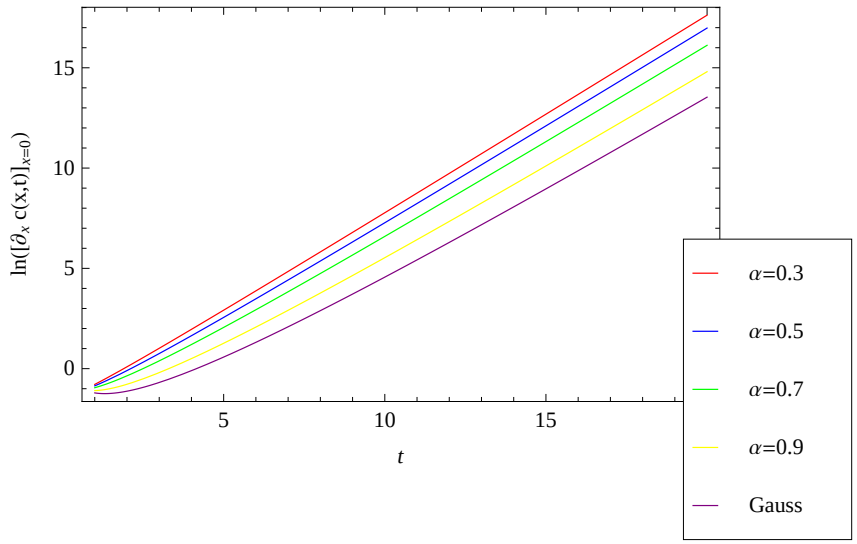

Figure 4.21: Evolution of a domain wall in terms of the natural logarithm of the spatial derivative at position $x = 0$ as a function of t, with $D = 1$, $x_0 = 1$, $\varepsilon = 1$, for different values of α.

initial peaks, and so their distance, for the considered initial conditions. For all plots of the stationary fronts shown before, it was always chosen $x_0 = 1$. So if we choose x_0 to be larger than one, will the domain wall still evolve faster in the subdiffusive regime? Figure 4.22 shows that, for $x_0 = 3$ the relaxation in case of $\alpha = 0.3$ is still fastest but

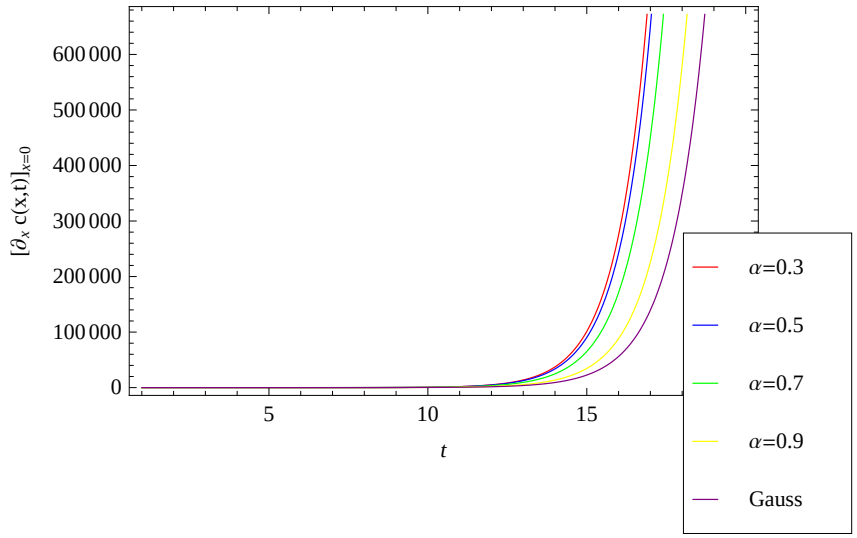

Figure 4.22: Evolution of a domain wall in terms of the spatial derivative at position $x = 0$ as a function of t, with $D = 1$, $x_0 = 3$, $\varepsilon = 1$, for different values of α.

relaxation in the case of $\alpha = 0.5$ is nearly as fast as that. Figure 4.23 shows that for

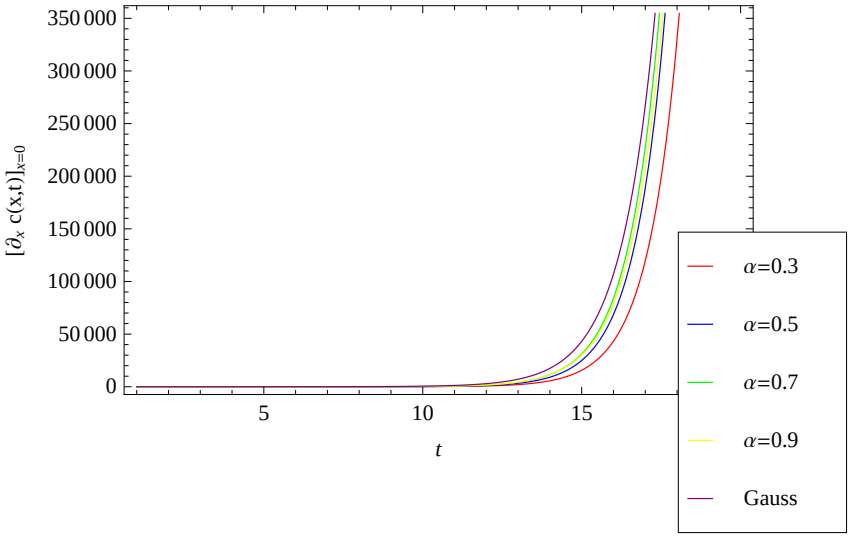

Figure 4.23: Evolution of a domain wall in terms of the spatial derivative at position $x = 0$ as a function of t, with $D = 1$, $x_0 = 6$, $\varepsilon = 1$, for different values of α.

$x_0 = 6$ the former order is turned upside down finally. So the effect subdiffusion has on the evolution of these domain walls strongly depends on the distance of the two initial peaks. Comparing the case of $\alpha = 0.5$ to normal diffusion, initial peaks that are sufficiently near to each other lead to a faster relaxation in the case of subdiffusion, whereas from a distance of approximately 10 units of length on the domain wall arises faster in the normal diffusive regime. One can, therefore, interprete that for small distances the domain wall directly evolves out of the initial conditions. In this case the retardation of balancing inhomogenities accelerates the relaxation. This effect increases with decreasing α. In contrast to that, for large distances at first propagating fronts on both sides of the x-axes arise, which collide at the position $x = 0$. Consequently the faster front propagation in the normal diffusive case is the reason, why the relaxation to domain walls is faster in the normal diffusive regime if x_0 is large enough. Under the given approximation the front velocities the two fronts select before they meet is again the linear spreading speed, which is larger in the normal diffusive case. It is the same that was evaluated for the FKPP equation for normal diffusion as well as for subdiffusion (see eq. (4.29) and eq. (3.14)).

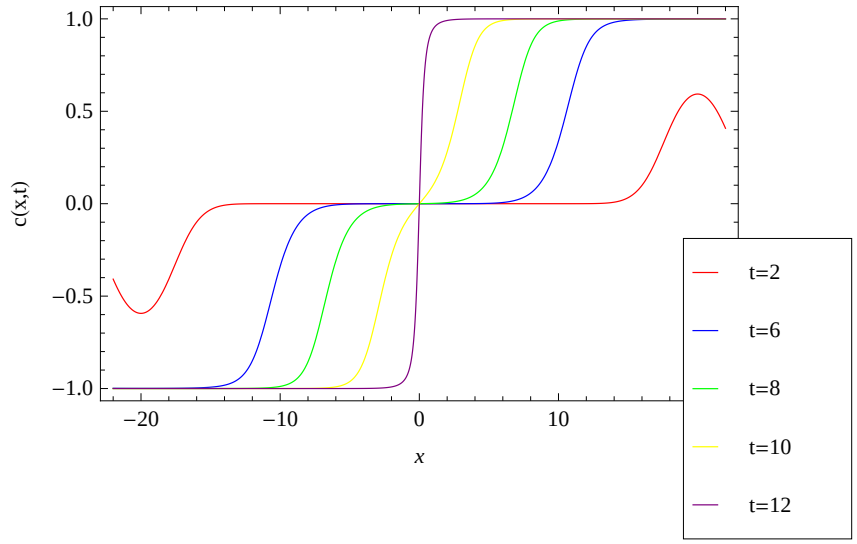

Figure 4.24: Two fronts colliding in the normal diffusive case, with $D = 1$, $x_0 = 20$, $\varepsilon = 1$.

5 Summary and conclusions

This thesis dealt with subdiffusive reaction-diffusion equations and especially with the question of how their characteristic features differ from the characteristics of their normal diffusive counterparts. The Fisher-Kolmogorov-Petrovskii-Piskounov equation as well as the Zeldovich equation were the two examples I was engaged with. As an explanation of subdiffusion in general, the second chapter gave an outline of how diffusion is described physically and how the changeover to anomalous and especially subdiffusion can be performed. Terms that are important in this context were explained such as the Markov property (sec. 2.2), which is violated in case of subdiffusion. The master equation was introduced (sec. 2.2) and its generalisation on processes where the Markov property does not hold was shortly outlined (sec. 2.10). Moreover, the conversion of the diffusion equation via the method of subordination into the fractional diffusion equation was demonstrated (sec. 2.9). The importance of the central limit theorem with its further generalisation was mentioned and the theorem itself was introduced (sec. 2.8). The application of a special form of Lévy distributions to the problem of finding a distribution for the waiting times was elucidated and its importance concerning the method of subordination was claryfied (sec. 2.8). Furthermore, the model Einstein used to describe Brownian motion and diffusion, the random walk model, was explained (sec. 2.3) and its generalisation taking account of anomalous diffusion was introduced (sec. 2.10).

Reaction-diffusion equations providing a normal diffusion term were introduced in the third chapter. A discussion of the two equations, referred to before, was performed in terms of linear stability analysis to get an understanding of their qualitative behaviour (sec. 3.2 and sec. 3.3). A discussion of nonlinear reaction-diffusion equations was outlined and characteristics like the evolution of propagating or stationary fronts were explained (sec. 3.4). The important differentiation of pulled and pushed propagating fronts was mentioned. A central value in this context, the linear spreading speed, was derived (sec. 3.5). For the Fisher-Kolmogorov-Petrovskii-Piskounov equation it was evaluated and declared to be the asymptotic propagation velocity. In the last section of chapter three (sec. 3.6) the singular perturbation approximation was introduced, and applied to both, the Fisher-Kolmogorov-Petrovskii-Piskounov equation as well as the Zeldovich equation. The zeroth order of this approximation was performed, plotted, and compared to the characteristics described before.

The main contributions of my own work were arranged in the last chapter. I also evaluated the concrete examples and plots in chapter three (sec. 3.2, sec. 3.3, sec. 3.6) on my own but they were not entirely new. Reaction-diffusion equations exhibiting subdiffusion were introduced within a general formula in section 4.1. The way to deal with this formula was presented afterwards and the two subdiffusive equations were derived (sec. 4.2). In the following two sections (sec. 4.3 and sec. 4.4) again a discussion in terms of linear stability analysis was carried out. In two quite technical sections (sec. 4.5 and sec. 4.8) the singular perturbation approximation, which was explained in

section 3.6, was applied to the subdiffusive versions of the Fisher-Kolmogorov-Petrovskii-Piskounov and Zeldovich equation. A linearised equation for both of them was deduced with the help of two approximations. Due to these approximations comparison to the zeroth order of singular perturbation approximation concerning the normal diffusive equations could be conducted.

Coming back to the aim of this thesis, the questions raised in the introduction concerning the Fisher-Kolmogorov-Petrovskii-Piskounov equation (4.15) were:

1. Does the solution of the subdiffusive Fisher-Kolmogorov-Petrovskii-Piskounov equation also converge to a uniform front?

2. Is there a simple method available to predict the asymptotic velocity in the subdiffusive regime?

Speaking in terms of the assumed approximations (see sec. 4.5), the answer to the first question is yes, asymptotically uniform fronts can be seen to arise (fig. 4.8, 4.9, and also 4.12, 4.14). Taking into account that the zeroth order of singular perturbation approximation proofed to describe the asymptotic behaviour exactly in the case of the normal diffusive equation (see sec. 3.6), this strongly suggests the existence of uniform fronts for the exact equation in the subdiffusive regime, as well.

The answer to the second question is also yes, the front velocity, which is selected asymptotically, can be predicted quite well. In the subdiffusive domain something similar to the linear spreding speed was calculated (cf. sec. 3.5 and sec. 4.5). The different velocities that were predicted via this method coincide with the asymptotic velocities which are selected by the approximate solutions of the subdiffusive Fisher-Kolmogorov-Petrovskii-Piskounov equation (fig. 4.12 and fig. 4.14), neglecting small deviations. Figure 5.1 demonstrates this. The red dots stem from elementary numerical evaluations that had to be made to gain the velocities from the transcendental equation (4.53) – in the cases where only a red dot is visible the coincidence is complete in terms of the resolution of this plot. The argument that this should also hold for the exact subdiffusive Fisher-Kolmogorov-Petrovskii-Piskounov equation is the same as before. The zeroth order of singular perturbation approximation in the normal diffusive regime shows the same velocity selection as the exact equation. The linear spreading speed, $v^* = 2$, is the one which is selected asymptotically. The approximations assumed to reduce the subdiffusive counterpart entail a similar description for large values of t that also includes normal diffusion, for $\alpha = 1$. Finally, the convergence to a uniform front seems to be determined by the reaction kinetics, whereas the front velocity depends on the diffusivity, which means on the characteristic exponent α, as well.

The questions that were raised in case of the Zeldovich equation (eq. (4.18)) were:

1. Does a domain wall arise?

2. How is the dependence of the evolution of such a domain wall on the exponent α to be characterised?

The answer to the first question is again yes, a domain wall arises also in the subdiffusive regime, speaking in terms of the approximations that were made in section 4.8 (see fig. 4.17, 4.18). This property, which the full system has concerning normal diffusion, can

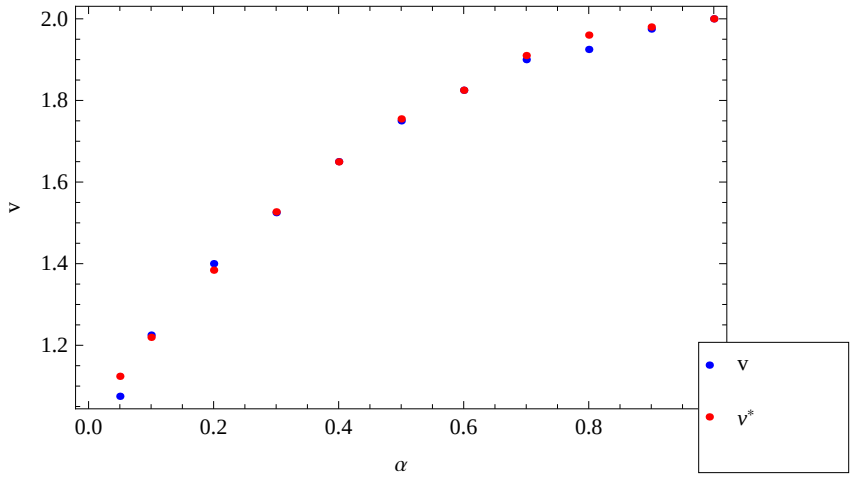

Figure 5.1: Front velocities of the approximate FKPP equation (4.15) and corresponding solutions of the transcendental equation (4.53), for $D = 1$ and different values of α.

already be investigated considering the zeroth order of singular perturbation approximation (see sec. 3.6, fig. 3.13). The approximations that were assumed to deal with the subdiffusive equation are asymptotically similar to the singular perturbation approximation of the zeroth order(see sec. 4.8) and also here the case of normal diffusion is included for $\alpha = 1$. Therefore the conclusion is that the evolution of stationary domain walls is also a characteristic feature of the exact subdiffusive Zeldovich equation.

The answer to the second question is twofold. Assuming the two initial peaks to have a large distance, the domain wall developes from two propagating fronts that collide (see sec. 4.9). In this case relaxation is faster in the normal diffusive domain, which is the result of the larger propagating velocity (cf. 4.23). The dependence of these velocities on the characteristic exponent is the same that was evaluated for the Fisher-Kolmogorov-Petrovskii-Piskounov equation. In this case the speed of relaxation to a domain wall can be interpreted as an asymptotic property, which ascertaines the assumed approximations to be realistic. Therefore, the conclusion is that also for the full equations, the subdiffusive and the normal diffusive Zeldovich equation, the speed of relaxation is governed by the diffusivity. Assuming the initial peaks to be near to each other, the approximations lead to the conclusion that the speed of relaxation is larger in the subdiffusive domain. The changeover to the behaviour described above, takes place approximately for initial conditions with two peaks that have a distance of more than 10 units of length (cf. fig. 4.23 and fig. 4.22). In this case the relaxation takes place after short times (see fig. 3.13 and fig. 4.17). Both, the singular perturbation approximation (sec. 3.6) as well as the approximation used in section 4.8, do not seem to be reasonable approximations for this case. These results can only be backed up by the discussion in terms of linear stability analysis (sec. 3.3 and sec. 4.4). Also here the corresponding plots (fig. 3.5 and fig. 4.4) show that the rising of the inhomogenities, which is due to the linearised reaction kinetics (see eq. 3.14 and eq. 4.29), is faster in the subdiffusive regime. The retarded balancing of inhomogenities concerning subdiffusion

(see fig. 4.20) was explained to be the reason for this.

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Erklärung zur Diplomarbeit

Hiermit versichere ich, diese Arbeit selbständig angefertigt und keine weiteren Hilfsmittel außer den angegebenen verwendet zu haben.

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