Analysis of dissipation and diffusion mechanisms modeled by nonlinear PDEs in developmental biology and quantum mechanics.

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Para Tales... la cuestión no era qué sabemos,
sino cómo lo sabemos.
Aristóteles

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Cuando emprendas tu viaje a Itaca
Pide que el camino sea largo,
Lleno de aventuras, lleno de experiencias.
Pide que el camino sea largo.
Fragmento del poema "Itaca" de Constantin P. Kavafis

Contents

Introducción

Esta tesis se centra en el análisis de algunos aspectos cualitativos relacionados con ecuaciones diferenciales parciales que surgen en la biología del desarrollo y la mecánica cuántica. La idea de fondo que vinculan los diferentes problemas en estudio es el control de esas propiedades de las soluciones relativas a la difusión, la dispersión o disipación en contraste con en dichos modelos físicos considerados. En este espíritu, la Tesis se han abordado y discutido los distintos enfoques del concepto de difusión en mecánica cuántica y la biología, lo que constituye un aspecto crucial en el presente y el futuro del desarrollo de estos campos. Aquí, hemos utilizado diferentes herramientas matemáticas para analizar los objetivos anteriores: el modelado, así como el buen-planteamiento en el marco funcional de los espacios de Sobolev, propiedades dinámicas de las ondas viajeras, las soluciones de entropía, puntos que en el mismo tiempo contribuyen a enriquecer la variedad de temas y contenidos de la tesis.

Vamos a describir brevemente los temas concretos y los resultados de esta tesis. El capítulo 2 está dedicado al modelado de procesos de disipación/difusión cuántica. El marco teórico habitual para este tipo de estudios es el de los sistemas cuánticos abiertos, en los que se analiza la interacción entre el sistema de interés y el ambiente. De esta manera se establece la ecuación maestra que gobierna la evolución temporal del operador de densidad (reducido) ρ de nuestro sistema. Una interpretación cinética de ρ permite asociarle una función de (pseudo-) probabilidad W, cuya evolución temporal responde a una ecuación con término de transporte. En nuestro caso dicha ecuación llevará acoplado un núcleo de Fokker–Planck para describir efectos de disipación. La ecuación de WFP es la siguiente

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x) W + \Theta[V]W = \mathcal{L}_{QFP}[W]\,,$$

con

$$\mathcal{L}_{QFP}[W] = \frac{D_{pp}}{m^2}\Delta_\xi W + 2\lambda \nabla_\xi \cdot (\xi W) + \frac{2D_{pq}}{m}\nabla_x \cdot (\nabla_\xi W) + D_{qq}\Delta_x W\,.$$

La ecuación de WFP puede verse como una generalización del modelo de Caldeira–Leggett [22] (el más comúnmente aceptado que describe efectos de disipación) que está en la forma de Lindblad [69].

Aunque la formulación cinética presenta ventajas respecto al tratamiento de ρ también conlleva algunos inconvenientes: en primer lugar la función W no puede interpretarse como una función de probabilidad con sentido completo ya que puede tomar valores negativos. Por otra parte, la formulación cinética está definida en el espacio de fase, por lo que que el tratamiento es más costoso. Además los fenómenos cuánticos usualmente se describen en términos de una función de onda ψ por lo que es interesante representar los efectos de disipación y difusión en la fomulación de Schrödinger, admitiendo términos no lineales.

Nuestro primer objetivo es establecer un modelo de Schrödinger que represente la misma física que WPF. Para ello interpretaremos la ecuación de continuidad asociada a WFP como resultado de un proceso de difusión gobernada a nivel microscópico por movimiento Browniano, obteniendo la siguiente ecuación de Schrödinger

$$i\alpha\frac{\partial\psi}{\partial t} = -\frac{\alpha^2}{2m}\Delta_x\psi + V\psi + \frac{\alpha^2}{\hbar^2}Q\psi + \Lambda\log(n)\psi + D_{qq}\left(\frac{i\alpha}{2}\frac{\Delta_x n}{n} + m\nabla_x\cdot\frac{J}{n}\right)\psi\,.$$

La no linealidad de esta ecuación de Schrödinger, se reduce a un sólo potencial, el término logarítmico, por medio de una transformación Gauge. Por ello resulta interesante el estudio de la ecuación simplificada ya que la física de ambos problemas es la misma. En el capítulo 3 se estudia la existencia y unicidad de soluciones en todo el espacio de la ecuación de Schrödinger puramente logaritmica.

El resultado principal desarrollado en el capítulo 3 es la prueba de la existencia de una única solución global en tiempo en sentido *mild* en $H^1(\mathbb{R}^3)$, del problema de valores iniciales

$$i\frac{\partial\psi}{\partial t} = -D\Delta\psi + \sigma\log(n)\psi\,, \qquad (t,x)\in[0,\infty)\times\mathbb{R}^3\,, \tag{1}$$

$$\psi(0,x) = \psi_0(x)\,, \qquad \psi_0\in H^1(\mathbb{R}^3)\,, \quad |x|\,n_0\in L^1(\mathbb{R}^3)\,, \tag{2}$$

bajo la única hipótesis de que el momento de inercia inicial $\int_{\mathbb{R}^3}|x|n_0\,dx$ sea finito, este estudio es independiente del signo que acompaña al logarítmo, donde se ha denotado $n_0(x) = n(0,x)$. El principal objetivo consiste en el desarrollo de una teoría matemática del buen planteamiento en todo el espacio en $H^1(\mathbb{R}^3)$, sin ninguna restricción del espacio funcional a fin de evitar la singularidad del potencial logarítmico en el origen ni las condiciones técnicas que permiten garantizar *a priori* la convergencia de la secesión de soluciones aproximadas. El resultado principal es el siguiente teorema

Teorema 1 *Existe una única función*

$$\psi\in L^\infty([0,\infty);H^1(\mathbb{R}^3))\cap C([0,\infty);L^2(\mathbb{R}^3))$$

la cual es solución del problema de valores iniciales (1.1)–(1.2) en un sentido mild.

En el Capítulo 4 se ha lleva a cabo una modificación del efecto de difusión ligado a la ley de Fick, ya que no describe la realidad de los modelos biológicos porque se produce la difusión en todo el espacio de manera instantánea , para aproximarnos a la realidad de este proceso se ha modificado Fick según un término no lineal que aparece por primera vez en [88], también aparece en el marco de transporte de masa óptimo [19].

Una vez llevada acabo esta modificación se han estudiado un tipo de soluciones especiales de las ecuaciones de RD que tiene un papel importante en las aplicaciones, para el caso escalar se denominan ondas viajeras y para el caso de sistema formación de patrones. Dadas las características que las soluciones de ondas viajeras tienen son muy útiles en modelacion en diferentes áreas como invasiones biológicas [24], epidemias [93], crecimiento de tumores [21] . Consideramos el caso escalar de la ecuación modificada con un término de reacción del tipo de Fisher Kolmogorov–PP ($f(u)$) y haremos la clasificación de ondas viajeras según la velocidad de avance del soporte de la solución y la viscosidad.

El principal resultado descrito en el Capítulo 4 de esta memoria da las condiciones para la existencia de soluciones de tipo onda viajera de la ecuación

$$\frac{\partial u}{\partial t} = \nu \partial_x \left(\frac{u \partial_x u}{\sqrt{|u|^2 + \frac{\nu^2}{c^2} |\partial_x u|^2}} \right) + f(u), \qquad u(t=0,x) = u_0(x), \tag{3}$$

Teorema 2 *En términos de un valor de $\sigma^* \leq c$, dependiendo de ν, c, y k, existe un frente de onda que es*

(i) una solución clásica para (4.2), con velocidad de onda $\sigma > \sigma^*$ o $\sigma = \sigma^* < c$;

(ii) una solución de entropía discontinua para (4.2), con velocidad de onda $\sigma = \sigma^* = c$.

La existencia de soluciones de ondas viajeras en el caso para $\sigma < \sigma^*$ es un problema abierto. También, la existencia de otra clase de ondas viajeras tales como pulsos o solitones podrían estudiarse (véase por ejemplo [87], o [44] en otro contexto).

Chapter 1

Introduction

This Thesis is focused on the analysis of some qualitative aspects related to partial differential equations arising in developmental biology and quantum mechanics. The basic idea linking the different problems under study is the scrutiny of those properties of the solutions concerning diffusion, dispersion or dissipation in contrast with the physical inputs of the models considered. In this spirit, the Thesis deals with and discuss the various approaches to the concept of diffusion in quantum mechanics and biology, which constitutes a crucial aspect in the present and the future of the development of both fields. Here, different mathematical tools come together in order to analyze the above general objectives: modeling, interphase fluid flows, well–posedness in the functional framework of Sobolev spaces, dynamic properties of traveling waves, entropy solutions, . . . , that at the same time contribute to enrich the variety of topics and contents of the Thesis.

Let us briefly describe the specific subjects and results of this Thesis. The second chapter is devoted to the modeling of quantum dissipation processes. The theoretical framework supporting this sort of phenomena is that of open quantum systems, which takes into account the interactions among the particle ensemble under study and the environment. This is actually the starting point to derive the master equation governing the temporal evolution of the (reduced) density matrix operator of the system. A kinetic interpretation of this operator allows to construct a pseudo–probability distribution function W in phase space, whose evolution in time is ruled by a quantum–kinetic transport equation in the Wigner picture. In our case, this equation is considered to be supplemented by a Fokker–Planck kernel describing dissipation and diffusion effects. The Wigner–Fokker–Plank (WFP) equation is the following

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \mathcal{L}_{QFP}[W]\,,$$

with

$$\mathcal{L}_{QFP}[W] = \frac{D_{pp}}{m^2}\Delta_\xi W + 2\lambda\nabla_\xi \cdot (\xi W) + \frac{2D_{pq}}{m}\nabla_x \cdot (\nabla_\xi W) + D_{qq}\Delta_x W\,.$$

The WFP equation can be seen as a generalization (written in Lindblad form [69]) of the well–known Caldeira–Leggett dissipative model [22].

Though the kinetic formulation shows some advantages with respect to the mathematical treatment of the density operator it also exhibits some drawbacks, mainly the fact that the Wigner function W cannot be interpreted as a true probability function, since it may take negative values. Our purpose is to represent quantum diffusive effects in the wavefunction approach via nonlinear Schrödinger models.

Our first objective is to establish a Schrödinger model describing the same physics that the WFP equation. To this aim, the continuity equation associated with the WFP equation is interpreted as associated with a diffusion process governed by Brownian motion at a microscopic level (in the sense of Nelsonian stochastic mechanics [81]). We find the following Schrödinger type equation

$$i\alpha\frac{\partial\psi}{\partial t} = -\frac{\alpha^2}{2m}\Delta_x\psi + V\psi + \frac{\alpha^2}{\hbar^2}Q\psi + \Lambda\log(n)\psi + D_{qq}\left(\frac{i\alpha}{2}\frac{\Delta_x n}{n} + m\nabla_x\cdot\frac{J}{n}\right)\psi\,,$$

where the action unit is now $\alpha = 2mD_{qq}$ instead of the Planck constant $\hbar$. This is our main goal in Chapter 2, as well as the development of a numerical code to simulate the dispersive and (anti)dissipative behaviour of solutions.

The family of nonlinearities of this equation is reduced to a single nonlinear potential of logarithmic type by means of an adecquate Gauge transformation. This makes the study of the reduced logarithmic equation particularly interesting, since the physics underlying both problems is the same. In Chapter 3, the existence and uniqueness of solutions to the purely logarithmic Schrödinger equation in whole space is analyzed.

The main result in Chapter 3 concerns the existence of a unique global–in–time *mild* solution in $H^1(\mathbb{R}^3)$ to the following initial–value problem

$$i\frac{\partial\psi}{\partial t} = -D\Delta\psi + \sigma\log(n)\psi\,, \qquad (t,x)\in[0,\infty)\times\mathbb{R}^3\,, \tag{1.1}$$

$$\psi(0,x) = \psi_0(x)\,, \qquad \psi_0\in H^1(\mathbb{R}^3)\,, \quad |x|\,n_0\in L^1(\mathbb{R}^3)\,, \tag{1.2}$$

under the unique hypothesis that the initial inertial momentum $\int_{\mathbb{R}^3}|x|n_0\,dx$, n_0 standing for the initial position density, is finite. This study is independent of the sign (attractive or repulsive) of the nonlinear term. Our main goal consists of developing a mathematical theory for the well–posedness of this problem in $H^1(\mathbb{R}^3)$, without further restrictions neither of the functional space in order to avoid the logarithmic singularity at the origin, nor of the technical conditions that guarantee the convergence of the sequence of approximate solutions. The main result is the following

Theorem 0.1 *There exists a unique function*

$$\psi\in L^\infty([0,\infty);H^1(\mathbb{R}^3))\cap C([0,\infty);L^2(\mathbb{R}^3))$$

that solve the initial value problem (1.1)–(1.2) in a mild sense.

In Chapter 4 we are concerned with the introduction of a correction to the diffusion effects linked to Fick's law in a biological context, so as to avoid that diffusion propagates to the whole space instantaneously. In this spirit, Fick's law is augmented with a nonlinear term first derived in [88], which is also inherent to optimal mass transport processes [19]. Then, we study an especial type of solutions to the model reaction–diffusion equations which are relevant in applications. In the scalar case they are known as traveling waves, while otherwise we call it pattern formation. In virtue of their particular features, these solutions have proved quite useful in modeling biological invasions [24], epidemies [93] or tumor growth [21], among other phenomena stemming from various disciplines. In the scalar case, we consider the equation modified by a reaction term of Fisher–Kolmogorov type, and classify the traveling waves according to the speed of propagation of their supports as well as the viscosity.

The main result of Chapter 4 is concerned with the study of the conditions under which there exist traveling wave solutions of the following equation

$$\frac{\partial u}{\partial t} = \nu \partial_x \left(\frac{u \partial_x u}{\sqrt{|u|^2 + \frac{\nu^2}{c^2}|\partial_x u|^2}} \right) + f(u), \qquad u(t=0,x) = u_0(x), \tag{1.3}$$

Indeed this flux–limited equation, known as relativistic heat equation, is postulated as an alternative to the linear flow given by Fick's equation.

Theorem 0.2 *Given $\sigma^* \leq c$ depending upon ν, c and k, there exists a wave front which is*

(i) a classical solution to Eq. (4.2), with wave speed $\sigma > \sigma^*$ or $\sigma = \sigma^* < c$;

(ii) a discontinuous entropy solution to Eq.(4.2), with wave speed $\sigma = \sigma^* = c$.

The existence of traveling wave solutions for the case $\sigma < \sigma^*$ is an open problem. Also, the existence of other kind of traveling waves such as pulses or solitons is worth to be studied (see for example [87], or [44] in other framework).

Chapter 2

A wavefunction description of stochastic–mechanical Fokker–Planck dissipation: derivation, stationary dynamics and numerical approximation

2.1 Introduction

Modeling of quantum dissipation has experienced a great impulse over recent years mainly due to the scrutiny of system+reservoir structures, which take into account energy transfer from the system to the environment (e.g. semiconductor devices with doped regions as reservoirs that inject electrons into the active regions). This aims to open quantum systems as the physical scenario [36], i.e. a particle interacting dissipatively with an idealized heat bath of harmonic oscillators, the effect of the bath on the particle motion being typically described by the bath temperature and the friction constant after tracing over the reservoir degrees of freedom. Nevertheless, though many nonlinear corrections have been proposed up to now, quantum dissipative interactions are still far from being well understood, mainly in the Schrödinger picture, and still deeper insight on their physical interpretation is needed. One of the best accepted diffusion mechanisms in modern quantum mechanics is the Fokker–Planck scattering kernel when added to Wigner's equation. Remarkably, the Caldeira–Leggett master equation [22] has been succeedingly applied in spite of its mathematical defficiencies, as it does not fit Lindblad's form [69] so as to guarantee positivity of the density matrix operator. Beingthe the quantum Fokker–Planck master equation (QFPME) the most general extension of the pioneering Caldeira–Legett master equation, which models the interaction of a quantum fermionic gas with a thermal bath subject to moderate/high temperatures, in the Wigner quantum–mechanical representation it reads

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x) W + \Theta[V]W = \mathcal{L}_{QFP}[W] \,, \tag{2.1}$$

with

$$\mathcal{L}_{QFP}[W] = \frac{D_{pp}}{m^2}\Delta_\xi W + 2\lambda \nabla_\xi \cdot (\xi W) + \frac{2D_{pq}}{m}\nabla_x \cdot (\nabla_\xi W) + D_{qq}\Delta_x W \,, \tag{2.2}$$

where $W(t,x,\xi)$ is the quasi–probability distibution function associated with a quantum mixture of (complex) states $\psi_k(t,x)$, that is

$$W(t,x,\xi) = \frac{1}{(2\pi)^3}\sum_{k\geq 1}\lambda_k \int_{\mathbb{R}^3} \overline{\psi}_k\left(t, x - \frac{\hbar y}{2m}\right)\psi_k\left(t, x + \frac{\hbar y}{2m}\right) e^{-i\xi\cdot y}\, dy \,,$$

with the λ_k's standing for occupation probabilities, thus satisfying

$$\lambda_k \geq 0 \,, \quad \sum_{k\geq 1}\lambda_k = 1 \,.$$

Here $x, \xi \in \mathbb{R}^3$ are position and momentum coordinates of the electron gas, $\hbar$ is the (reduced) Planck constant,

$$D_{pp} = \eta k_B T \,, \quad D_{pq} = \frac{\eta \Omega \hbar^2}{12\pi m k_B T} \,, \text{ and } D_{qq} = \frac{\eta \hbar^2}{12 m^2 k_B T}$$

are phenomenological constants related to electron–bath interactions, $\lambda = \frac{\eta}{2m}$ is the friction coefficient, m the effective mass of the electrons, η the damping/coupling constant of the bath, Ω the cut–off frequency of the oscillators, k_B the Boltzmann constant, T the bath temperature and where

$$\begin{aligned}\theta_V[W](t,x,\xi) \;&=\; \frac{1}{(2\pi)^3}\int_{\mathbb{R}^6}\frac{i}{\hbar}\left[V\left(t, x + \frac{\hbar y}{2m}\right) - V\left(t, x - \frac{\hbar y}{2m}\right)\right] \\ &\quad \times W(t,x,\xi')e^{-i(\xi-\xi')\cdot y}\, d\xi'\, dy\end{aligned}$$

is a pseudo–differential operator related to the external potential V. In the presence of a purely Ohmic environment (namely, linear coupling in both system and environment coordinates), the QFPME comes out from the Liouville (super-)operator $i\hbar\partial_t \rho = L[\rho]$ after Wignerization, with

$$L[\rho] = [H,\rho] + \lambda[q,\{p,\rho\}] - \frac{i}{\hbar}\Big(D_{pp}\big[q,[q,\rho]\big] + D_{qq}\big[p,[p,\rho]\big] + 2D_{pq}\big[q,[p,\rho]\big]\Big) \,,$$

where q, p are position and momentum operators, $H = -\frac{\hbar^2}{2m}\nabla_q^2 + V(q)$ is the electron Hamiltonian and ρ the reduced density matrix operator, derived in [?, 41] as the Markovian approximation of the originally non–Markovian evolution of the electron in the oscillator bath. Here, the assumptions on the parameters are: (i) the reservoir memory time Ω^{-1} is much smaller than the characteristic time scale of the electrons, (ii) weak coupling: $\lambda \ll \Omega$, and (iii) medium/high temperatures: $\Omega \lesssim \frac{k_B T}{\hbar}$. Notice that the Caldeira–Leggett model is obtained when $D_{pq} = D_{qq} = 0$ is assumed in the QFPME, i.e. in a high temperatures regime. Somehow less restrictive models belonging to the Lindblad class were derived for example in [49] and [95].

2.2 The wavefunction approach

One of the main aspects of quantum–mechanical dissipative theories relies on the presence of a diffusive term in the continuity equation. Indeed, the equation for the position density $n = \int_{\mathbb{R}^3} W(t,x,\xi)\,d\xi$ reads

$$\frac{\partial n}{\partial t} + \nabla_x \cdot J = D_{qq}\Delta_x n\,,$$

which is of Fokker–Planck type. Here, we denoted $J = \int_{\mathbb{R}^3} \xi W(t,x,\xi)\,d\xi$ the electric current density. This equation along with

$$\frac{\partial u}{\partial t} + (u\cdot\nabla_x)u = -\frac{1}{m}\nabla_x V - \frac{\nabla_x\cdot\mathbb{P}}{n} - 2\lambda u - \frac{2D_{pq}}{m}\nabla_x \log(n) + F(n,u)$$

constitute the hydrodynamic system associated with the QFPME, where $u = \frac{J}{n}$ represents the fluid mean velocity, and where $\mathbb{P} = E - nu\otimes u$ is the stress tensor with $E = \int_{\mathbb{R}^3}(\xi\otimes\xi)\,W(t,x,\xi)\,d\xi$ denoting the kinetic energy tensor, while the viscous term

$$F(n,u) = D_{qq}\Big(2(\nabla_x \log(n)\cdot\nabla_x)u + \Delta_x u\Big)$$

stands for the dissipative force. The idea underlying our derivation consists of interpreting the continuity equation in terms of Nelsonian stochastic mechanics. This theory gives a description of quantum mechanics in terms of classical probability densities for particles undergoing Brownian motion with diffusive interactions. In this spirit, the evolution of a particle subject to nondissipative Brownian motion is shown to be equivalent (in the sense of its probability and current density) to that described by Schrödinger's equation [81]. In our context we assume Brownian motion as produced by the dissipative interaction between the electron gas and the thermal environment, the particles thus being subject to the action of forward and backward velocities u_+ and $u_- = u_+ - 2u_0$ respectively, ingentering the continuity equation as

$$\frac{\partial n}{\partial t} + \nabla_x\cdot(nu_\pm) = \pm D_{qq}\Delta_x n\,. \tag{2.3}$$

Here, $u_o = D_{qq}\nabla_x \log(n)$ is the osmotic velocity defined according to Fick's law, that sets the exact balance between the osmotic current nu_o and the diffusion current $D_{qq}\nabla_x n$ and somehow controls the degree of stochasticity of the process. Summing up both forward and backward equations in (2.3) and introducing the current mean velocity

$$v := \frac{1}{2}(u_+ + u_-) = u_+ - u_o\,,$$

it is easy to check that the standard continuity equation of quantum mechanics $\partial_t n + \nabla_x\cdot(nv) = 0$ is recovered. Henceforth we shall use Einstein's convention for summation over repeated indices. By defining the mean backward derivative of the forward velocity as

$$\mathcal{D}_- u_+(t,x) := \frac{\partial u_+}{\partial t} + (u_- \cdot \nabla_x) u_+ - D_{qq}\Delta_x u_+ \,,$$

the momentum equation can be rewritten for u_+ as

$$\mathcal{D}_- u_+ = -\frac{1}{m}\nabla_x V - \frac{\nabla_x \cdot \mathbb{P}_{u_+}}{n} - 2\lambda u_+ - \frac{2D_{pq}}{m}\nabla_x \log(n)\,. \tag{2.4}$$

We now perform time inversion according to the rules [56]

$$t \mapsto -t\,, \quad \frac{\partial z}{\partial t} \mapsto -\frac{\partial z}{\partial t}\,, \quad u_\pm \mapsto -u_\mp\,, \quad \mathcal{D}_\pm \mapsto -\mathcal{D}_\mp\,.$$

Since the internal stress tensor $\mathbb{P}_{u_+}$ is a dynamic characteristic of motion, its divergence changes sign under time inversion. Accordingly, Eq. (2.4) becomes

$$\mathcal{D}_+ u_- = -\frac{1}{m}\nabla_x V + \frac{\nabla_x \cdot \mathbb{P}_{u_+}}{n} + 2\lambda u_- - \frac{2D_{pq}}{m}\nabla_x \log(n)\,, \tag{2.5}$$

where $\mathcal{D}_+ u_- := \frac{\partial u_-}{\partial t} + (u_+ \cdot \nabla_x)u_- + D_{qq}\Delta_x u_-$ is the mean forward derivative of the backward velocity. Subtracting (2.5) from (2.4) yields

$$\frac{\partial (u_o)_j}{\partial t} + v_i \frac{\partial (u_o)_j}{\partial x_i} = \frac{\partial v_j}{\partial x_i}(u_o)_i + D_{qq}\frac{\partial^2 v_j}{\partial x_i^2} - 2\lambda v_j - \frac{1}{n}\frac{\partial (\mathbb{P}_{u_+})_{ji}}{\partial x_i}\,.$$

or equivalently the following law for the stress tensor

$$\frac{\partial (\mathbb{P}_{u_+})_{ji}}{\partial x_i} = D_{qq}(\frac{\partial n}{\partial x_i} + \frac{\partial}{\partial x_i})(\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j}) - 2\lambda n v_j\,.$$

We then sum up (2.4) and (2.5) to get the frictional version of Nelson's stochastic generalization of Newton's law

$$\begin{aligned} \frac{\partial v_j}{\partial t} + v_i \frac{\partial v_j}{\partial x_i} &= - \frac{1}{m}\frac{\partial}{\partial x_j}\big(V + \Lambda \log(n)\big) \\ &- D_{qq}^2 \left[\frac{1}{n}\frac{\partial n}{\partial x_i}\frac{\partial}{\partial x_i}\left(\frac{1}{n}\frac{\partial n}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(\frac{1}{n}\frac{\partial^2 n}{\partial x_i^2}\right)\right]\,, \end{aligned} \tag{2.6}$$

where we have set $\Lambda := 2D_{pq} + \eta D_{qq}$.

The evolution governed by the (general) QFPME and combining Eqs. (2.3) and (2.6) with the relation

$$v = u_+ - 2u_0\,,$$

the equation for u_+

$$\begin{aligned} \frac{\partial (u_+)_j}{\partial t} + (u_+)_i \frac{\partial (u_+)_j}{\partial x_i} &= - \frac{1}{m}\frac{\partial V}{\partial x_j} - \frac{\Lambda}{m}\frac{\partial \log(n)}{\partial x_j} - \frac{2\alpha^2}{\hbar^2}\frac{\partial Q}{\partial x_j} \\ &+ D_{qq}\left[\frac{1}{n}\frac{\partial n}{\partial x_j}(\frac{\partial (u_+)_j}{\partial x_j} - \frac{\partial (u_+)_i}{\partial x_j}) - \frac{\partial^2 (u_+)_i}{\partial x_i \partial x_j}\right] \end{aligned}$$

can be recovered, where we denoted $\alpha = 2mD_{qq}$ and Q holds for Bohm's quantum potential defined by

$$Q = -\frac{\hbar^2}{2m}\frac{\Delta_x\sqrt{n}}{\sqrt{n}} = -\frac{\hbar^2}{4m}\left(\frac{\Delta_x n}{n} - \frac{|\nabla_x n|^2}{2n^2}\right).$$

Under the original assumptions on the parameters we are straightforwardly led to $\alpha \ll \hbar$, which means that the quantum potential effects are drastically relaxed due to the spatial diffussion introduced by the QFPME. As consequence, the D_{qq} term confers 'classical' behaviour to the system at the hydrodynamic level.

Now, after the identification of the velocity as an irrotacional field we get $u_+ = \frac{1}{m}\nabla_x S$, hence

$$\frac{\partial}{\partial x_j}\left(\frac{\partial S}{\partial t} + \frac{1}{m}\frac{\partial S}{\partial x_i}\frac{\partial^2 S}{\partial x_j \partial x_i}\right) = -\frac{\partial}{\partial x_j}\left(V + \frac{2\alpha^2}{\hbar^2}Q + \Lambda\log(n) + D_{qq}\frac{\partial^2 S}{\partial x_i^2}\right),$$

which after integration along x_j yields the following Hamilton–Jacobi type equation for the evolution of S:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left|\nabla_x S\right|^2 = -V - \frac{2\alpha^2}{\hbar^2}Q - \Lambda\log(n) - D_{qq}\Delta_x S + \Xi\,, \qquad (2.7)$$

$\Xi(t)$ being an arbitrary function of time. This along with the continuity equation

$$\frac{\partial n}{\partial t} + \frac{1}{m}\nabla_x\cdot(n\nabla_x S) = D_{qq}\Delta_x n$$

constitute a closed potential–flow quantum hydrodynamic system, thus we may construct an 'envelope' wavefunction which contains the same physical information that the QFPME. Indeed, if we consider

$$\psi = \sqrt{n}\,e^{\frac{i}{\alpha}S} \qquad (2.8)$$

along with the quantization rule $m\oint_L u_+\,dl = 2k\pi$, where k is an integer and L is any closed loop [97], in order to keep ψ single–valued, we are led to the following Schrödinger–like equation accounting for frictional and dissipative effects

$$i\alpha\frac{\partial\psi}{\partial t} = H_\alpha\psi + \frac{\alpha^2}{\hbar^2}Q\psi + \Lambda\log(n)\psi + D_{qq}\left(\frac{i\alpha}{2}\frac{\Delta_x n}{n} + m\nabla_x\cdot\frac{J}{n}\right)\psi\,, \qquad (2.9)$$

where $H_\alpha = -\frac{\alpha^2}{2m}\Delta_x + V$ is the electron Hamiltonian (under the new action unit α, see Section 4 and [32] for details). In this picture, the magnitudes $|\psi|^2$ and $\frac{\alpha}{m}\mathrm{Im}(\overline{\psi}\nabla_{\mathrm{x}}\psi)$ coincide with n and J, respectively. Notice that Ξ has been set to zero in virtue of the gauge $\widetilde{\psi} = e^{i\theta}\psi$. Indeed, Eq. (2.9) is the (nonlinear) equation we postulate in the Schrödinger picture to model the dissipative effects undergone by a quantum particle ensemble in contact with a thermal reservoir. The crossed–diffusion D_{pq}–term (or 'anomalous diffusion'), owing to a linear velocity–dependent frictional force caused by the interaction of the electrons with the dissipative environment, is of logarithmic type [20] (actually, $\log(n)$ can be seen as an expansion of V up to $O(\hbar^2)$ when V is assumed to be the Hartree electrostatic potential solving $\Delta_x V = n$). On the other hand, the position–diffusion D_{qq}–terms contain nonlinearities which form part of a more general family of Schrödinger equations of Doebner–Goldin type [42], which is actually the most general class of nonlinear Schrödinger equations compatible with a Fokker–Planck continuity equation. It is also noticeable that the D_{pp}–term, responsible for the decoherence process, does not contribute to the final form of Eq. (2.9). This is due to the fact that the moment system has been truncated at the level of the momentum equation, while the D_{pp}–contribution is only 'visible' at the next level, i.e. that of the energy equation. However, the role played by D_{pp} is essential for the fulfillment of the uncertainty inequality as well as for the Lindblad form of the QFPME, thus for the positivity preservation of the density matrix operator. Indeed, a sufficient and necessary condition to fit Lindblad's class is that the reservoir parameters be such that the inequality

$$D_{pp}D_{qq} - D_{pq}^2 \geq \frac{\hbar^2\lambda^2}{4}$$

holds.

Remark 1 *In the particular case of the Caldeira–Leggett master equation (i.e. Eq. (2.1)-(2.2) with $D_{pq} = D_{qq} = 0$), our approach gives rise to the following potential–flow quantum hydrodynamic system*

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{1}{m}\nabla_x \cdot (n\nabla_x S) + \frac{h}{2m}\Delta_x n \,, \\ \frac{\partial S}{\partial t} &= -\frac{1}{2m}|\nabla_x S|^2 - V - 2Q - \hbar\lambda\log(n) - \frac{\hbar}{2m}\Delta_x S + \Xi \,. \end{aligned}$$

If we introduce the Madelung wavefunction $\psi = \sqrt{n}\, e^{\frac{i}{\hbar}S}$, its temporal evolution is shown to be ruled by the Schrödinger–like equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi + Q\psi + \hbar\lambda\log(n)\psi + \frac{i\hbar^2}{4m}\frac{\Delta_x n}{n}\psi + \frac{\hbar}{2}\left(\nabla_x \cdot \frac{J}{n}\right)\psi \,, \tag{2.10}$$

with $H = -\frac{\hbar^2}{2m}\Delta_x + V$ standing for the electron Hamiltonian (under the standard action unit $\hbar$), which is analogous to that for the general case by taking $\alpha = \hbar$.

We can also take advantage of the following nonlinear gauge transformation [80]

$$G : \psi \mapsto \Phi = \psi\, \exp\left\{-\frac{i}{2}\log(n)\right\} \,, \tag{2.11}$$

which makes Eq. (2.9) formally equivalent to the (simpler) purely logarithmic Schrödinger equation (see for instance [28, 29, 30, 58])

$$i\alpha\frac{\partial\Phi}{\partial t} = H_\alpha\Phi + \Lambda\log(n)\Phi \,. \tag{2.12}$$

A rigorous proof of this equivalence is being developed in [59] under a more general mapping

$$\mathcal{G} : \psi \mapsto \Phi = |\psi| \, \exp\left\{ \frac{i}{\alpha}\Big(A\log(n) + BS \Big) \right\} ,$$

where A, B are arbitrary real numbers. $\mathcal{G}$ will be shown to be an homeomorphic transformation between both equations in a suitable functional space, thus preserving the physical behaviour. G is easily revealed to enjoy several nice properties (indeed, it preserves the local density and satisfies the Ehrenfest theorem) which allow us to study some aspects of Eq. (2.9) via the logarithmic Schrödinger equation (2.12). A variant of this equation was successfully derived in [66] to describe quantum Langevin processes and has been recently applied to the modeling of different phenomena such as magma transport or capillarity in fluids [38, 37, 67].

2.3 Steady state dynamics

We now explore the free–particle solutions (i.e. $V \equiv 0$) of (2.9) within the thermal equilibrium regimes $J_\psi = \pm D_{qq} \nabla_x n$ (corresponding to vanishing local diffusion current and Fick's law) as well as $J_\psi = 0$, making special emphasis in the dynamics of radial solutions. In the sequel we shall consider a unit system for which $\hbar = m = k_B = 1$. We shall also use the transformation (2.2) to reduce eq. (2.9) to the logarithmic Schrödinger equation. In this system of units, it may written as

$$i\frac{\partial \Phi}{\partial t} = -D_{qq}\Delta_x \Phi + \frac{\Gamma}{2}\log(n)\Phi, \tag{2.13}$$

where $\Gamma = \frac{\Lambda}{Dqq}$. Observe that G is provides $n_\psi = n_\Phi$ (we denote both of them by n), and

$$S_\Phi = S_\psi - D_{qq}\log(n) \, .$$

2.3.1 Vanishing local diffusion current

Firstly assume that the local diffusion current defined by $j_\psi := J_\psi - D_{qq}\nabla_x n$ identically vanishes. According to (2.2) this gives rise to $J_\Phi = 0$, which implies $\nabla_x S_\Phi = 0$ (notice that for $m = 1$, $\nabla_x S_\Phi = \frac{J_\Phi}{n}$). The continuity equation so adopts its simplest form $\partial_t n = 0$, that leads to stationary profiles $n(t, q) = n_0(q)$. In this setting we search for solutions

$$\Phi(t, q) = |\Phi_0(q)| e^{i\nu(t)} \, ,$$

which inserted into (2.12) yield $\nu' = D_{qq}\frac{\Delta_x|\Phi_0|}{|\Phi_0|} - \Gamma\log(|\Phi_0|)$. Differentiating now with respect to time we readily find $\nu'' = 0$, thus $\nu(t) = -\omega t + k$ with $\omega, k \in \mathbb{R}$. Accordingly,

$$\omega = -D_{qq}\frac{\Delta_x|\Phi_0|}{|\Phi_0|} + \Gamma\log(|\Phi_0|) \, . \tag{2.14}$$

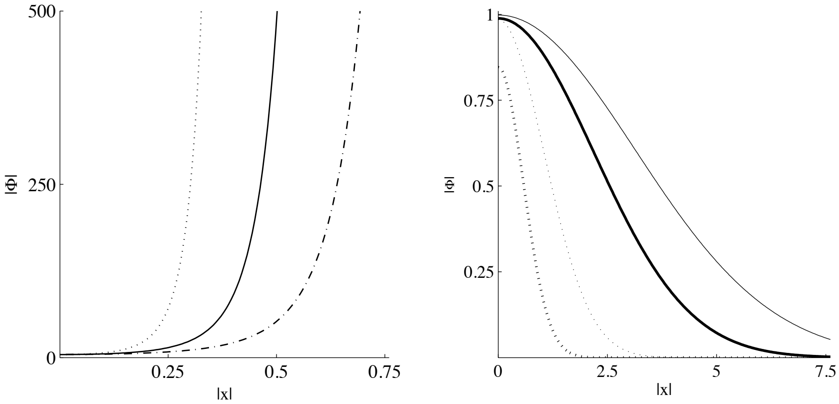

Figure 2.1: Solutions of Eq. (2.14) for high temperatures: $T = 2$, $\Omega = 1$. On the left increasing weak coupling: $\lambda = 0.05$ (dashed), $\lambda = 0.15$ (continuous) and $\lambda = 0.5$ (dashed–pointed) with $V = 0$. And on the right with $V = \omega_0^2 x^2/2:$ $\lambda = 0.05$ and $w_0 = 0.075$ (thin-dashed), $\lambda = 0.25$ and $w_0 = 0.4$ (thick-dashed), $\lambda = 0.05$ and $w_0 = 0.025$ (thin-continuous) and $\lambda = 0.25$ and $w_0 = 0.1$ (thick-continuous) respectively. Note that very different qualitative behaviours are observed depending on the external potencial.

Therefore, the uniparametric family of wavefunctions $\Phi(t,x) = |\Phi_0(x)|e^{-i\omega t}$ are steady state solutions (up to a constant phase factor) of (2.12) with constant density. Now, by applying G^{-1} we are led to the associated stationary profiles of (2.9) given by

$$\psi = |\Phi_0| \exp\big\{i\big(\log(|\Phi_0|) - \omega t\big)\big\}\,.$$

One important feature to be stressed at this point is the absence of Gaussons due to the sign of the logarithmic term (see [35] for a discussion). Indeed, when searching for solutions $\Phi = |\Phi_0|e^{i\nu}$ with $\Phi_0 = e^{A|x|^2+B}$, we are led to

$$\Delta_x|\Phi_0| = (6A + 4A^2|x|^2)e^{A|x|^2+B}\,,$$

so that (2.14) now reads

$$\omega D_{qq} + 6D_{qq}^2 A - \Gamma D_{qq} B = D_{qq}(\Gamma - 4AD_{qq})A|x|^2\,,$$

yielding $A = \frac{\Gamma}{4D_{qq}}$ and $B = \frac{3}{2} + \frac{\omega}{\Gamma}$, which leads to

$$\Phi(t,x) = \exp\{\gamma(x) - i\omega t\} \text{ with } \gamma(x) = \frac{\Gamma}{4D_{qq}}|x|^2 + \frac{\omega}{\Gamma} + \frac{3}{2}\,.$$

Translated into the context of Eq. (2.9) we get

$$\psi = G^{-1}(\Phi) = \exp\big\{\gamma(x) + i(\gamma(x) - \omega t)\big\}\,.$$

It proves also of interest to find nontrivial solutions of (2.12) as functions of the symmetric polynomial $s = x_1 + x_2 + x_3$. As a matter of fact, in considering the ansatz $|\Phi_0(x)| = y(s)$ we can deduce

$$\omega = -3D_{qq}\,\frac{y''}{y} + \Gamma\log(y)\,. \tag{2.15}$$

Now, taking $y(s) = \exp\{Cs^a + D\}$ we are necessarily led to

$$a = 2\,, \quad C = \frac{\Gamma}{12D_{qq}}\,, \quad D = \frac{1}{2} + \frac{\omega}{\Gamma}\,,$$

that gives

$$\Phi = \exp\bigl\{\gamma(s/\sqrt{3}) - i\omega t - 1\bigr\}\,.$$

Hence, the wavefunction profiles

$$\psi(t,q) = \exp\bigl\{\gamma(s/\sqrt{3}) - 1 + i\bigl(\gamma(s/\sqrt{3}) - 1 - \omega t\bigr)\bigr\}$$

satisfy (2.9). To find a relation between y and y' we just multiply (2.15) by yy' and integrate against s to get

$$(y')^2 + \frac{\omega}{3D_{qq}}y^2 - \frac{\Gamma}{6D_{qq}}y^2\bigl(\log(y^2) - 1\bigr) \equiv K_0 \in \mathbb{R}\,.$$

If K_0 is set to zero, then this equation is easily shown to have two saddle points at $(\pm y_0, 0)$ with $y_0 = \exp\{\omega/\Gamma + 1/2\}$. Furthermore, we may remove the parameter ω by introducing the scaling $y = y_0 Y$, which gives rise to the simpler equation

$$(Y')^2 - \frac{\Gamma}{6D_{qq}}Y^2\log(Y^2) = 0\,, \tag{2.16}$$

that now has the saddle points at $(\pm 1, 0)$. We finally investigate the radial (rotationally symmetric) solutions of (2.9). To this aim, consider $|\Phi_0(x)| = \varphi(r)$ with $r = |x|$. Then, $\Delta_x|\Phi_0| = \frac{2}{r}\varphi' + \varphi''$ and (2.14) does become

$$\omega = -D_{qq}\left(\frac{2}{r}\frac{\varphi'}{\varphi} + \frac{\varphi''}{\varphi}\right) + \Gamma\log(\varphi)\,.$$

Using again the scaling $\varphi = y_0\phi$ we find the normalized equation satisfied by the (amplitude of the) radial solutions of (2.9) (see Figs. 2, 3 and 4)

$$\phi'' + \frac{2}{r}\phi' - \frac{\Gamma}{2D_{qq}}\bigl(2\log(\phi) + 1\bigr)\phi = 0\,. \tag{2.17}$$

2.4 Numerical evidence accounting for negative dissipation in the log–law Schrödinger equation

The purpose of this section is to construct numerical solutions of Eq. (2.13) in 1D (wich is gauge-equivalent to Eq. (2.10) acording to the transformation (2.2)) and compare them to the exact ones, which come out after solving the (linear) quantum Fokker–Planck master equation in the free particle and damped harmonic oscillator cases (i.e. Eq. (2.1)–(2.2) with $V = 0$ and $V = \frac{1}{2}\omega_0^2 x^2$, respectively, ω_0 denoting the frequency of the oscillator), namely

$$W_t + \xi W_x = \frac{D_{pp}}{m^2} W_{\xi\xi} + 2\lambda(\xi W)_\xi + \frac{2D_{pq}}{m} W_{\xi x} + D_{qq} W_{xx}\,, \tag{2.18}$$

$$W_t + \xi W_x - \omega_0^2 x W_\xi = \frac{D_{pp}}{m^2} W_{\xi\xi} + 2\lambda(\xi W)_\xi + \frac{2D_{pq}}{m} W_{\xi x} + D_{qq} W_{xx}\,, \tag{2.19}$$

where subscripts of the Wigner function denote the variables with respect to which differentiation is performed here and hereafter. To this aim we still choose a unit system for which $\hbar = m = k_B = 1$ and adapt the discretization procedure introduced in [86] to our context. We start with the presentation of the exact solutions of Eq. (2.19).

2.4.1 Exact solutions of the quantum Fokker–Planck master equation

Using the standard Fourier transform techniques for the calculus of the propagators G_0^{fr} and G_0^{ho} associated with Eqs. (2.18) and (2.19), we obtain the following expressions (see Appendix A in [71] for the details)

$$G_0^{fr,ho}(x,\xi,t) = \frac{1}{2\pi\sqrt{d_{fr,ho}(t)}} \exp\left\{-\frac{c_{fr,ho}(t)}{d_{fr,ho}(t)}x^2 + \frac{b_{fr,ho}(t)}{d_{fr,ho}(t)} m\,x\,\xi - \frac{a_{fr,ho}(t)}{d_{fr,ho}(t)} m^2 \xi^2\right\}\,,$$

where

$$\begin{aligned}
a_{fr}(t) &= \frac{D_{pp}}{4\lambda^2} + D_{qq} + \frac{D_{pq}}{\lambda} + \frac{1-e^{-2\lambda t}}{16\lambda^3}\left(\frac{D_{pp}}{4\lambda}(e^{-2\lambda t} - 3) - 8\lambda D_{pq}\right)\,,\\
b_{fr}(t) &= \frac{1-e^{-2\lambda t}}{4\lambda^2}\left(4\lambda D_{pq} + D_{pp}(1-e^{-2\lambda t})\right)\,,\\
c_{fr}(t) &= \frac{D_{pp}}{4\lambda}(1-e^{-4\lambda t})\,,\\
d_{fr}(t) &= d_{ho}(t) = 4a(t)c(t) - b(t)^2 > 0\,, \quad \forall\, t > 0\,,
\end{aligned}$$

and where

$$
\begin{aligned}
a_{ho}(t) &= \frac{e^{-4\lambda t}}{(\lambda_+ - \lambda_-)^2}\Big\{\hat{a}(t)\big(\lambda_+ e^{\lambda_+ t} - \lambda_- e^{\lambda_- t}\big)^2 + \hat{c}(t)\big(e^{\lambda_+ t} - e^{\lambda_- t}\big)^2 \\
&\quad + \hat{b}(t)\big(\lambda_+ e^{2\lambda_+ t} + \lambda_- e^{2\lambda_- t} - 2\lambda e^{2\lambda t}\big)\Big\}, \\
b_{ho}(t) &= -\frac{e^{-4\lambda t}}{(\lambda_+ - \lambda_-)^2}\Big\{\omega_0^2 \hat{a}(t)\big(\lambda_+ e^{2\lambda_+ t} + \lambda_- e^{2\lambda_- t} - 2\lambda e^{2\lambda t}\big) \\
&\quad + \hat{c}(t)\big(\lambda_- e^{2\lambda_+ t} + \lambda_+ e^{2\lambda_- t} - 2\lambda e^{2\lambda t}\big) \\
&\quad + \hat{b}(t)\Big(2\omega_0^2\big(e^{2\lambda_+ t} + e^{2\lambda_- t}\big) + (\lambda_+ + \lambda_-)^2 e^{2\lambda t}\Big)\Big\}, \\
c_{ho}(t) &= \frac{e^{-4\lambda t}}{(\lambda_+ - \lambda_-)^2}\Big\{\hat{a}(t)\big(e^{\lambda_+ t} - e^{\lambda_- t}\big)^2 + \hat{c}(t)\big(\lambda_+ e^{\lambda_- t} - \lambda_- e^{\lambda_+ t}\big)^2 \\
&\quad + \omega_0^2 \hat{b}(t)\big(\lambda_+ e^{2\lambda_- t} + \lambda_- e^{2\lambda_+ t} - 2\lambda e^{2\lambda t}\big)\Big\}.
\end{aligned}
$$

Here, we denoted $\lambda_\pm = \lambda \pm \sqrt{\lambda^2 - \omega_0^2}$ and

$$
\begin{aligned}
\hat{a}(t) &= \frac{\lambda_+^2}{2\lambda_-}\left[D_{qq} + \frac{\lambda_-}{\omega_0^2}\left(\frac{\lambda_-}{\omega_0^2}D_{pp} + 2D_{pq}\right)\right](e^{2\lambda_- t} - 1) \\
&\quad + \frac{\lambda_-^2}{2\lambda_+}\left[D_{qq} + \frac{\lambda_+}{\omega_0^2}\left(\frac{\lambda_+}{\omega_0^2}D_{pp} + 2D_{pq}\right)\right](e^{2\lambda_+ t} - 1) \\
&\quad - \frac{1}{\lambda}\big(2\omega_0^2 D_{qq} + D_{pp} + 4\lambda D_{pq}\big)(e^{2\lambda t} - 1), \\
\hat{b}(t) &= \frac{1}{\lambda}(2\omega_0^2 D_{qq} + D_{pp} + 4\lambda D_{pq})(e^{2\lambda t} - 1) \\
&\quad - \left(\frac{\omega_0^2}{\lambda_+}D_{qq} + \frac{\lambda_+}{\omega_0^2}D_{pp} + 2D_{pq}\right)(e^{2\lambda_+ t} - 1) \\
&\quad - \left(\frac{\omega_0^2}{\lambda_-}D_{qq} + \frac{\lambda_-}{\omega_0^2}D_{pp} + 2D_{pq}\right)(e^{2\lambda_- t} - 1), \\
\hat{c}(t) &= \frac{\omega_0^2}{2}\left\{\left(\frac{\omega_0^2}{\lambda_+}D_{qq} + \frac{\lambda_+}{\omega}D_{pp} + 2D_{pq}\right)(e^{2\lambda_+ t} - 1)\right. \\
&\quad + \left(\frac{\omega_0^2}{\lambda_-}D_{qq} + \frac{\lambda_-}{\omega_0^2}D_{pp} + 2D_{pq}\right)(e^{2\lambda_- t} - 1) \\
&\quad \left. - \frac{1}{\lambda}(2\omega_0^2 D_{qq} + D_{pp} + 4\lambda D_{pq})(e^{2\lambda t} - 1)\right\}.
\end{aligned}
$$

Then, the unique solution to the initial value problem associated with Eqs. (2.18) and (2.19) (the initial datum being $W(t=0,x,\xi) = W_I(x,\xi)$) is written as

$$
\begin{aligned}
W_{fr,ho} &= \int_{\mathbb{R}^2} G_0^{fr,ho}\Big(t, x - A_z^{fr,ho}(t)z - A_v^{fr,ho}(t)v, m\,\xi - B_z^{fr,ho}(t)z - B_v^{fr,ho}(t)v\Big) \\
&\quad \times W_I(z,v)\,dvdz,
\end{aligned}
$$

where the position and momentum time paths are now given by

$$\begin{aligned} A_z^{fr} &\equiv 1\,, \quad A_z^{ho}(t) = \frac{1}{\lambda_+ - \lambda_-}\left(\lambda_+ e^{-\lambda_- t} - \lambda_- e^{-\lambda_+ t}\right)\,, \\ A_v^{fr}(t) &= \frac{1-e^{-2\lambda t}}{2\lambda}\,, \quad A_v^{ho}(t) = \frac{1}{\lambda_+ - \lambda_-}\left(e^{-\lambda_- t} - e^{-\lambda_+ t}\right)\,, \\ B_z^{fr} &\equiv 0\,, \quad B_z^{ho}(t) = \frac{\omega_0^2}{\lambda_+ - \lambda_-}\left(e^{-\lambda_+ t} - e^{-\lambda_- t}\right)\,, \\ B_v^{fr} &= e^{-2\lambda t}\,, \quad B_v^{ho}(t) = \frac{1}{\lambda_+ - \lambda_-}\left(\lambda_+ e^{-\lambda_+ t} - \lambda_- e^{-\lambda_- t}\right)\,. \end{aligned}$$

We remark that all of the above calculations also make sense in the complex plane whether $\lambda^2 - \omega_0^2 < 0$.

2.4.2 The numerical algorithm

In this paragraph we shall give a short description of the numerical procedure (adapted from that in [86]) employed to approximate the solution to the 1D initial value problem associated with Eq. (2.9) as well as its macroscopic magnitudes, say the energy and local and current densities, and dispersion quantities such as the variance of the wave packet, to be compared with those obtained from the exact Wigner–Fokker–Planck solutions established in the previous section.

Consider the interval $[a, b]$ and the partition associated with the position step $h = (b-a)/N$. Let also $X = \{x_m\}_{1\le m\le N+1}$ and $Y = \{y_n\}_{0\le n\le N-1}$ the meshes for the subsequent evaluations of ψ and $\nabla_x\psi$ respectively, with $x_m = a + h(m-1)$ and $y_n = x_n + h/2 = (x_{n+1} + x_n)/2$, equipped with the following inner products

$$\langle u, v\rangle_X = \sum_{m=0}^{N} \alpha_m \overline{u(x_m)} v(x_m)\,, \quad \langle u, v\rangle_Y = \sum_{n=0}^{N-1} \alpha_m \overline{U(y_n)} A_n v(y_n)\,,$$

where $\alpha = (h, \ldots, h)_{N+1}$ and $A = (h, \ldots, h)_N$. Then, the derivatives (gradient and divergence) can be written as

$$\nabla_D u(y_n) = \sum_{m=1}^{N+1} D_{nm} u(x_m)\,, \quad \nabla_D \cdot U(x_m) = -\frac{1}{\alpha_m}\sum_{n=1}^{N} D_{nm} A_n U(y_n)\,,$$

thus satisfying the essential 'discrete divergence property'

$$\langle u, \nabla_D \cdot V\rangle_X = -\langle \nabla_D u, V\rangle_Y\,.$$

Then, if choosing centered differences $\nabla u(y_n) = \frac{1}{2h}\big(u(x_{n+1}) - u(x_n)\big)$ we are led to

$$D = (D_{nm})_{1\le n\le N, 1\le m\le N+1} = \begin{pmatrix} -\frac{1}{h} & \frac{1}{h} & 0 & 0 & \ldots & 0 \\ 0 & -\frac{1}{h} & \frac{1}{h} & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & -\frac{1}{h} & \frac{1}{h} \end{pmatrix}\,,$$

so that

$$\nabla_D u = D \begin{pmatrix} u(x_1) \\ u(x_2) \\ \vdots \\ u(x_{N+1}) \end{pmatrix},$$

$$\begin{aligned}
\nabla_D \cdot U &= \begin{pmatrix} \frac{1}{\alpha_1} D_{11} & \frac{1}{\alpha_1} D_{21} & \dots & \frac{1}{\alpha_1} D_{N1} \\ \frac{1}{\alpha_2} D_{12} & \frac{1}{\alpha_2} D_{22} & \dots & \frac{1}{\alpha_2} D_{N2} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{1}{\alpha_{N+1}} D_{1(N+1)} & \dots & \dots & \frac{1}{\alpha_{N+1}} D_{N(N+1)} \end{pmatrix} \begin{pmatrix} A_1 U(y_1) \\ A_2 U(y_2) \\ \vdots \\ A_N U(y_N) \end{pmatrix} \\
&= \begin{pmatrix} -\frac{1}{h^2} & 0 & 0 & 0 & \dots & 0 \\ \frac{1}{h^2} & -\frac{1}{h^2} & 0 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \frac{1}{h^2} & -\frac{1}{h^2} & 0 \end{pmatrix} \begin{pmatrix} hU(y_1) \\ hU(y_2) \\ \vdots \\ hU(y_N) \end{pmatrix},
\end{aligned}$$

in such a way that

$$\begin{aligned}
\nabla \cdot U(x_1) &= \frac{1}{h} U(y_1)\,, \quad \nabla \cdot U(x_{N+1}) = -\frac{1}{h} U(y_N)\,, \\
\nabla \cdot U(x_m) &= \frac{1}{h}\big(U(y_m) - U(m-1)\big) \quad \forall\, 2 \leq m \leq N\,, \\
\Delta_D u(x_m) &= \frac{1}{h^2}\big(u(x_{m+1}) - 2u(x_m) + u(x_{m-1})\big)\,, \quad \forall\, 0 \leq m \leq N-1\,.
\end{aligned}$$

Furthermore, we consider

$$\delta_t u^k = \frac{1}{dt}(u^{k+1} - u^k)\,, \quad \mu_t u^k = \frac{1}{2}(u^{k+1} + u^k)\,,$$

where dt denotes the time step. After all this, the discretized version of Eq. (2.9) reads

$$i\delta_t \psi^k + D_{qq} \mu_t \Delta_D \psi^k - \mu_t U^k \mu_t \psi^k = 0\,, \tag{2.20}$$

where we denoted $U(\psi) = 2D_{qq} Q + \frac{1}{2D_{qq}}\big(V + \Lambda \log(n)\big) + \frac{1}{2}\big(iD_{qq}\frac{\Delta_x n}{n} + \nabla_x \cdot \frac{J}{n}\big)$. Equivalently, Eq. (2.20) can be rewritten as

$$\frac{i}{dt}\big(\psi^{k+1} - \psi^k\big) + \frac{D_{qq}}{2}\big(\Delta_D \psi^{k+1} + \Delta_D \psi^k\big) - \frac{1}{4}\big(U^{k+1} + U^k\big)\big(\psi^{k+1} + \psi^k\big) = 0\,. \tag{2.21}$$

To make this finite differences scheme more tractable form a computational viewpoint, we invoke a predictor–corrector procedure $\psi^k \mapsto \psi^{k,1} \mapsto \psi^{k+1}$, where the prediction $\psi^{k,1}$ is obtained from

$$\frac{i}{dt}\big(\psi^{k,1} - \psi^k\big) + \frac{D_{qq}}{2}\big(\Delta_D \psi^{k,1} + \Delta_D \psi^k\big) - \frac{1}{2} U^k \big(\psi^{k,1} + \psi^k\big) = 0\,. \tag{2.22}$$

Then we make

$$U^{k,1} := \frac{1}{2D_{qq}}\big(V + \Lambda\log(n^{k,1})\big)$$

and solve

$$\frac{i}{dt}\big(\psi^{k,2} - \psi^{k}\big) + \frac{D_{qq}}{2}\big(\Delta_D\psi^{k,2} + \Delta_D\psi^{k}\big) - \frac{1}{4}\big(U^{k,1} + U^{k}\big)\big(\psi^{k,2} + \psi^{k}\big) = 0\,. \quad (2.23)$$

to find $\psi^{k+1} := \psi^{k,2}$. It is important to note that the whole scheme presented above is mass–preserving.

To proceed with the calculations, we make use of an algorithm for an efficient multiplication of tridiagonal matrices, in such a way that the predictor step $\psi^{k,1}$ is obtained as a solution to $A_p\psi^{k,1} = B_p\psi^{k}$, with

$$\begin{aligned} A_p &= \begin{pmatrix} A_1d_1 & A_1c_1 & & & \\ A_1a_2 & A_1d_2 & A_1c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & A_1a_N & A_1d_N & A_1c_N \\ & & & A_1a_{N+1} & A_1d_{N+1} \end{pmatrix}, \\ B_p &= \begin{pmatrix} B_1d_1 & B_1c_1 & & & \\ B_1a_2 & B_1d_2 & B_1c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & B_1a_N & B_1d_N & B_1c_N \\ & & & B_1a_{N+1} & B_1d_{N+1} \end{pmatrix}, \end{aligned}$$

while the corrector step stems from the homologous equation $A_c\psi^{k,2} = B_c\psi^{k,1}$, with

$$\begin{aligned} A_c &= \begin{pmatrix} A_2d_1 & A_2c_1 & & & \\ A_2a_2 & A_2d_2 & A_2c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & A_2a_N & A_2d_N & A_2c_N \\ & & & A_2a_{N+1} & A_2d_{N+1} \end{pmatrix}, \\ B_c &= \begin{pmatrix} B_2d_1 & B_2c_1 & & & \\ B_2a_2 & B_2d_2 & B_2c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & B_2a_N & B_2d_N & B_2c_N \\ & & & B_2a_{N+1} & B_2d_{N+1} \end{pmatrix}. \end{aligned}$$

Here, the various coefficients are given by

$$
\begin{aligned}
A_1 d_1 &= \frac{i}{dt} - \frac{D_{qq}}{2h^2} - \frac{1}{2}U_1^k\,, \quad A_1 d_2 = \frac{i}{dt} - \frac{3D_{qq}}{4h^2} - \frac{1}{2}U_2^k\,,\\
A_1 d_N &= \frac{i}{dt} - \frac{3D_{qq}}{4h^2} - \frac{1}{2}U_N^k\,, \quad A_1 d_{N+1}\frac{i}{dt} - \frac{D_{qq}}{2h^2} - \frac{1}{2}U_{N+1}^k\,,\\
A_1 d_n &= \frac{i}{dt} - \frac{D_{qq}}{h^2} - \frac{1}{2}U_n^k \quad \forall\, 3 \le n \le N-1\,,\\
A_1 c_n &= \frac{D_{qq}}{2h^2} \quad \forall\, 1 \le n \le N-1\,, \quad A_1 c_N = \frac{D_{qq}}{4h^2}\,,\\
A_1 a_2 &= \frac{D_{qq}}{4h^2}\,, \quad A_1 a_n = \frac{D_{qq}}{2h^2}\forall\, 3 \le n \le N+1\,,\\
B_1 d_1 &= \frac{i}{dt} + \frac{D_{qq}}{2h^2} + \frac{1}{2}U_1^k\,, \quad B_1 d_2 = \frac{i}{dt} - \frac{3D_{qq}}{4h^2} + \frac{1}{2}U_2^k\,,\\
B_1 d_N &= \frac{i}{dt} + \frac{3D_{qq}}{4h^2} + \frac{1}{2}U_N^k\,, \quad B_1 d_{N+1} = \frac{i}{dt} + \frac{D_{qq}}{2h^2} + \frac{1}{2}U_{N+1}^k\,,\\
B_1 d_n &= \frac{i}{dt} + \frac{D_{qq}}{h^2} + \frac{1}{2}U_n^k \quad \forall\, 3 \le n \le N-1\,,\\
B_1 c_n &= -\frac{D_{qq}}{2h^2} \quad \forall\, 1 \le n \le N-1\,, \quad B_1 c_N = -\frac{D_{qq}}{4h^2}\,,\\
B_1 a_2 &= -\frac{D_{qq}}{4h^2}\,, \quad B_1 a_n = -\frac{D_{qq}}{2h^2}\forall\, 3 \le n \le N+1\,.
\end{aligned}
$$

The matrices A_2 and B_2 are identical by just replacing $\frac{1}{2}U_n^k$ by $\frac{1}{4}\big(U_n^{k,1} + U_n^k\big)$ for all $1 \le n \le N+1$.

We now observe that the discretizations of the Doebner–Goldin terms conforming the nonlinear potential $U(\psi)$ are given by

$$
\big(\log(n)\big)_k = \log(n_k) \quad \forall\, 1 \le k \le N+1\,,
$$

and $V_k = \frac{\omega_0^2}{2}x_k^2$ for all $1 \le k \le N+1$ (in the harmonic oscillator case). On one hand, $\nabla_x\psi$ must be evaluated over the mesh Y, $\nabla_x\psi(y_k) = \frac{1}{h}(\psi_{k+1} - \psi_k)$. On the other hand, as $\psi(y_k)$ is not known, we can aproach it by $\frac{1}{2}(\psi_{k+1} + \psi_k)$.

The simulations of the dissipative behaviour of solutions to the free-particule and harmonic-oscillator logarithmic Schrödinger equation (2.13) are attached at the end of the Chapter.

2.5 Summary and conclusions

In many mathematical and physical situations the Schrödinger picture of quantum mechanics is preferable to the Liouvillian representation, for instance for computational reasons. Indeed, the Wigner function is evaluated in the position–momentum space, which makes the subsequent numerical analysis certainly intricate. Even from an analytical viewpoint, though most PDE techniques are expected to be inhereted from kinetic theory, the fact that the probability distribution (i.e. the Wigner function) can assume negative values constitutes a serious drawback in making things rigorous. In any case, it seems convenient to have an 'equivalent' description of the dissipative Fokker–Planck mechanism, that has proved to give satisfactory results in both the Wigner and the quantum hydrodynamic formulations, in terms of the particle wavefunction. Actually, that is our main purpose and goal here. Starting from the quantum Fokker–Planck master equation, which models the interactions occurring between the electron ensemble under examination and the phonons of a thermal bath in the framework of open quantum systems, we derive a nonlinear dissipative Schrödinger equation which is characterized in an essential way by the presence of a quantum correction of logarithmic type (present in the literature since the seminal works by Kostin [66] and Bialynicki–Birula and Mycielski [20]) as well as of various other nonlinearities that fit the Doebner–Goldin diffusive structure [42]. This equation does retain the same macroscopic local density that the Wigner–Fokker–Planck equation we started with. The derivation follows the fundamental lines of Nelsonian stochastic mechanics [81] combined with Madelung theory [75]. The stationary regime for the new Eq. (2.9) has been widely explored from both an analytical and computational point of view, making especial emphasis on the behaviour of radial solutions and the absence of Gaussons.

Some final remarks on the role played by α are in order. The parameter $\alpha = 2mD_{qq}$ has the dimensions of an action but it is not an universal constant, as it hinges on the particular system under study. Thus, though $\alpha \neq \hbar$ in general it plays the role of $\hbar$ in some sense (see [32] for a wider discussion), confering quantum–mechanical meaning to our wavefunction. If we consider $\psi = \sqrt{n}\, e^{\frac{i}{\hbar}S}$ instead of ψ (cf. (2.8)), the continuity equation and Eq. (2.7) along with the quantization rule lead us to

$$i\hbar\partial_t\psi = H\psi + \left(\frac{2\alpha^2}{\hbar^2} - 1\right) Q\psi + \Lambda\log(n)\psi + D_{qq}\left(\frac{i\hbar}{2}\frac{\nabla_q^2 n}{n} + m\nabla_q \cdot \frac{J}{n}\right)\psi\,, \quad (2.24)$$

that might be simplified into the so–called modular Schrödinger equation with coupling parameter $\kappa = 1 - \frac{\alpha^2}{\hbar^2}$ augmented by a logarithmic nonlinearity

$$i\alpha\partial_t\phi = H_\alpha\phi - \kappa Q\phi + \Lambda\log(n)\phi\,, \quad (2.25)$$

by making use of the gauge transformation

$$g : \psi \mapsto \phi = \psi\, \exp\left\{-\frac{i\alpha}{2\hbar}\log(n)\right\}\,.$$

For $\kappa = 1$ (see [11, 51]), this equation does not admit exponentially confined solutions but it can be derived from a local Lagrangian. Besides, its associated hydrodynamics does not contain quantum effects. As we have already observed, in Eq. (2.7) the effects derived from the action of Q are quite close to be negligible. On the contrary, the choice of ψ as envelope wavefunction still retains this contribution in Eq. (2.25) with $\kappa \simeq 1$. However, taking α as the action unit makes Q not to appear in Eq. (2.12). Since we are mainly interested in the local densities associated with Ψ and ψ, which are identical to each other and also to that stemming from the Wigner function, we are called to focus further analysis on the simpler Eq. (2.9) and its gauge reduction to the purely logarithmic Schrödinger equation (see [59]) . Anyway, both Eqs. (2.9) and (2.24) retain the dissipative effects introduced by the QFPME. Numerical simulations when quantum Fokker–Planck dynamics with negative dissipation is reproduced are performed and compared with the exact results for the free particle and the damped harmonic oscillator cases.

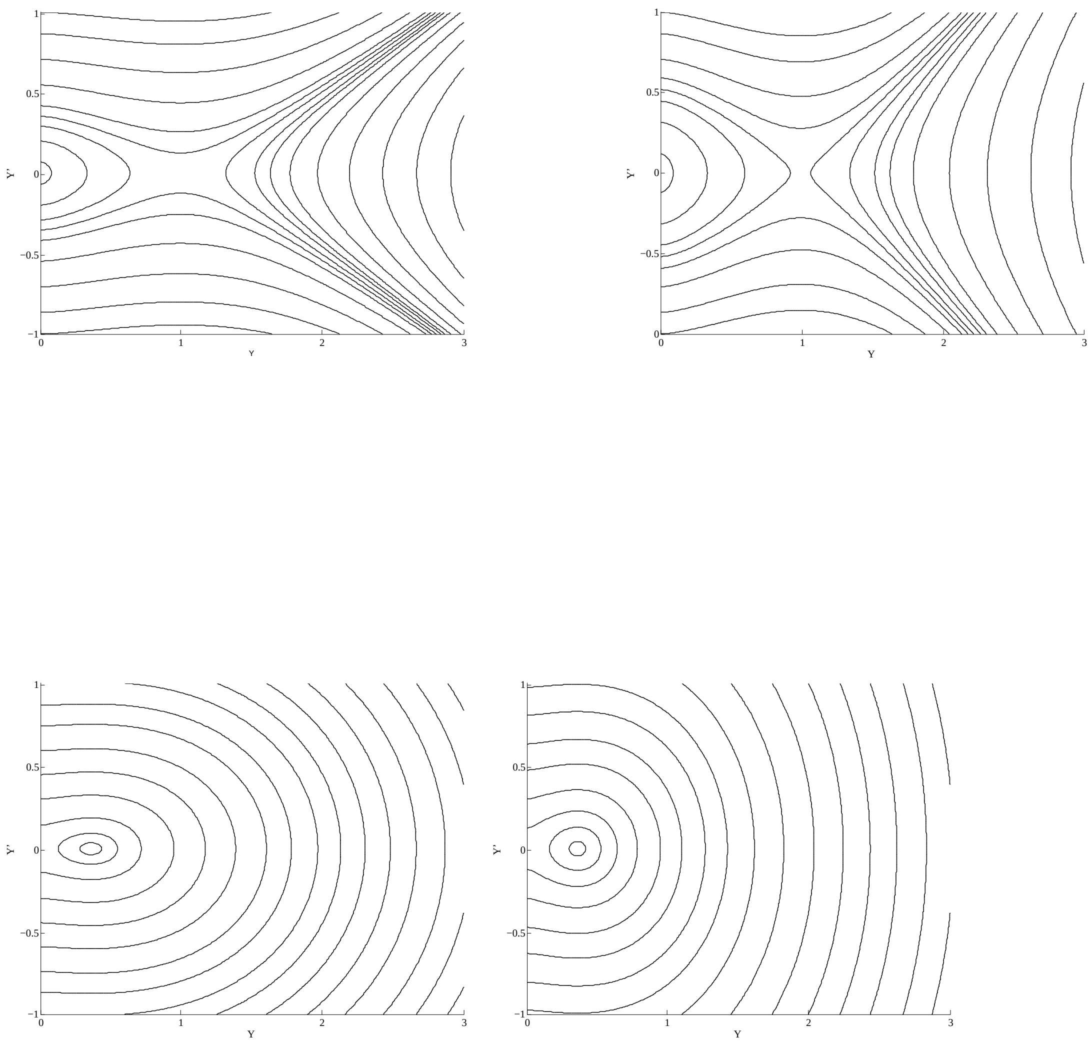

Figure 2.2: Left to right and top to bottom: the first two pictures show the phase portrait of (2.16) for typical high–temperature values of the coefficients (T, Ω, λ) within Dekker's phenomenology [39, 84]: $(2, 1, 0.01)$ and $(2, 1, 0.5)$, respectively. The last two pictures correspond to the opposite sign for the logarithmic term.

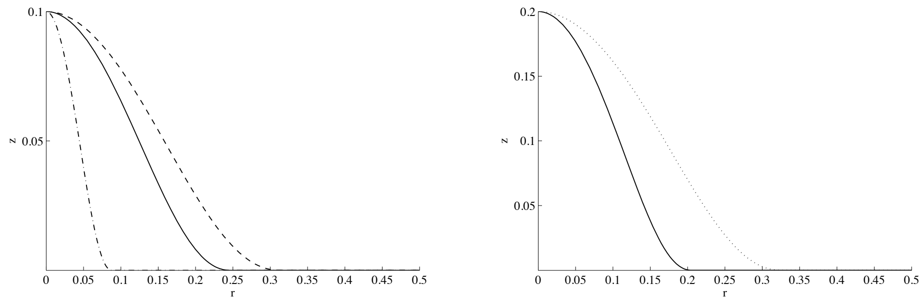

Figure 2.3: Numerical solutions of Eq. (2.17) for high temperatures: $T = 2$, $\Omega = 1$. On the left : $V = 0$ and $\lambda = 0.2$ (dashed), $\lambda = 0.1$ (continuous) and $\lambda = 0.01$ (dashed-points). On the right: $V = w_0^2 x^2/2$, $w_0 = 0.05$ and $\lambda = 0.15$ (dashed), $w_0 = 0.3$ and $\lambda = 0.05$ (continuous) and $w_0 =$. Left to right: initial data ($\phi(0) = 0.1$, $\phi'(0) = 0$) and ($\phi(0) = 0.2$, $\phi'(0) = 0$), respectively.

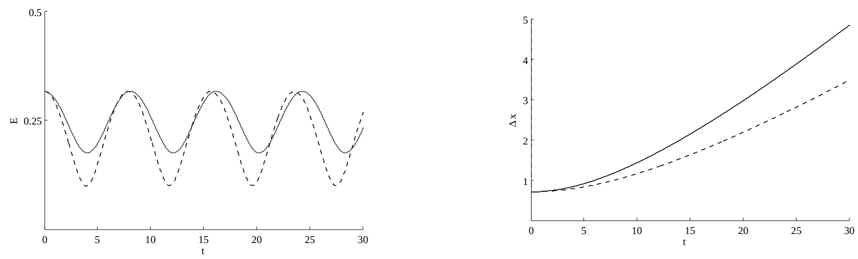

Figure 2.4: Position dispersion of the numerical solutions of Eq. (2.10) for high temperatures: $T = 2$, $\Omega = 1$. On the left : $V = 0$ and $\lambda = 0.1$ (dashed), $\lambda = 0.15$ (continuous). On the right: $V = w_0^2 x^2/2$, $w_0 = 0.5$ and $\lambda = 0.1$ (dashed) and $\lambda = 0.15$ (continuous).

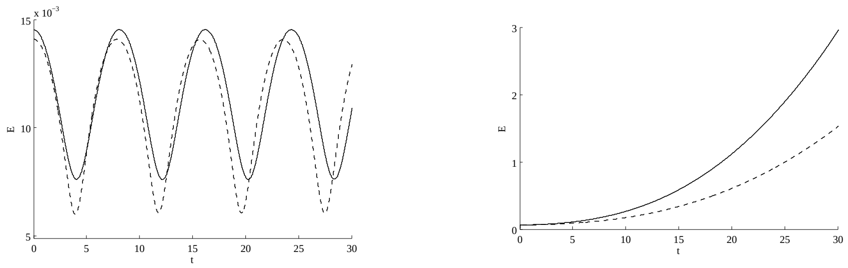

Figure 2.5: Kinetic plus potencial energy of the numerical solutions of Eq. (2.10) for high temperatures: $T = 2$, $\Omega = 1$. On the left : $V = 0$ and $\lambda = 0.1$ (dashed), $\lambda = 0.15$ (continuous). On the right: $V = w_0^2 x^2/2$, $w_0 = 0.5$ and $\lambda = 0.1$ (dashed) and $\lambda = 0.15$ (continuous).

Chapter 3

Global H^1 solvability of the 3D logarithmic Schrödinger equation

3.1 Introduction and main result

The logarithmic Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = -D\Delta\psi + \sigma\log(|\psi|^2)\psi\,, \tag{3.1}$$

$D > 0$ being a diffusion constant (typically $D = \frac{\hbar}{2m}$ where $\hbar$ is the Planck constant and m stands for the electron mass) and $\sigma \in \mathbb{R} \setminus \{0\}$ representing the strength of the (attractive or repulsive) nonlinear interaction, was proposed by Bialynicki–Birula and Mycielski [20] in 1976 as the only nonlinear equation of Schrödinger type accounting for some fundamental aspects of quantum mechanics such as separability of noninteracting subsystems (i.e. a solution of the nonlinear equation for the overall system can be constructed by taking the product of two arbitrary solutions of the nonlinear equations for the subsystems), additivity of the total energy for noninteracting subsystems: $E[\psi_1\psi_2] = E[\psi_1] + E[\psi_2]$, boundedness from below of $E[\psi]$ for a free particle in any number of dimensions, Planck's relation for all stationary states: $E[\psi] = \hbar\omega$ with ω denoting the frequency, Ehrenfest theorem and invariance under the transformation $\psi \mapsto \alpha\psi\exp\big(-i\sigma t\log(|\alpha|^2)\big)$. Nevertheless, they only addressed the case $\sigma < 0$. A derivation of this equation from Nelson's stochastic quantum mechanics [81] was also given by Lemos in [68] (see also [79]). The single sign choice for the logarithmic term first made in [20] and later continued in [27, 28, 29] was owing to the fact that the other sign leads to an energy functional not bounded from below. However, the positive sign for the logarithmic nonlinearity was physically justified by Davidson in [35] as representing a diffusion force within the context of stochastic quantum mechanics. Indeed, by considering slowly varying profiles in the absence of external forces one easily observes that the kinetic contribution $\int_{\mathbb{R}^3} |\nabla\psi|^2\,dx$ is negligible, so that the effective energy operator may be written as

$$E[\psi] = \sigma \int_{\mathbb{R}^3} |\psi|^2 \log(|\psi|^2)\, dx\,. \tag{3.2}$$

This expression is not bounded from below. However, provided $\psi(t,x)$ has its support over a domain Ω with finite measure in configuration space, it is a simple matter to check that (3.2) admits a minimizer.

Various meaningful physical interpretations have been given to the presence of the logarithmic potential $\log(|\psi|^2)$ in the Schrödinger equation. Indeed, it can be understood as the effect of statistical uncertainty or as the potential energy associated with the information encoded in the matter distribution described by the probability density $|\psi(t,x)|^2$. Recently, Eq. (3.1) has proved useful for the modeling of several nonlinear phenomena including capillary fluids [38] and geophysical applications of magma transport [37], as well as nuclear physics [63], Brownian dynamics or photochemistry. From a mathematical viewpoint this model has not apparently raised much interest, although important contributions have been done by Cazenave [27, 28], who showed the existence of stable, localized non-spreading profiles of Gaussian shape (Gaussons), Cazenave and Haraux [29] and by Cid and Dolbeault [30], who established some dispersion and asymptotic stability properties via rescaling techniques. Concerning well–posedness, the global–in–time existence of solutions was studied in [27, §9.3] on a subspace of $H_0^1(\Omega)$, Ω being an arbitrary open domain. Also Jüngel, Mariani and Rial dealt in a recent paper [64] with the local well–posedness in $H^2(\Omega)$ of the Schrödinger equation equipped with a general family of nonlinearities, among them that of logarithmic type. The locality of their result is owing to the strong constraint imposed by working with the functional space

$$X_\delta = \left\{ \psi \in H^2(\Omega) : \operatorname*{ess\,inf}_{x\in\Omega} |\psi(x)| > \delta > 0 \right\}$$

in order to avoid the singularity of the logarithmic potential at the origin. In [70], one of us stressed the relevance of a family of logarithmic Schrödinger equations (of Doebner–Goldin type, see [42]) accounting for diffusion currents in appropriately modeling quantum dissipation ($\sigma > 0$) of an electron ensemble in contact with a heat bath, when viewed as a hydrodynamic or stochastic approach to the so–called Wigner–Fokker–Planck equation (see also [8, 71]). In that context, the logarithmic nonlinearity corresponds to a linear velocity–dependent frictional force caused by the interaction of the particle ensemble with a dissipative environment. Other nonlinear Schrödinger models of logarithmic type have proved interesting in the literature, for instance the Schrödinger–Langevin equation [66] for the description of nonconservative quantum systems or the logarithmic–type and modular corrections introduced by Sabatier in [89]. In the general setting of nonlinear Schrödinger equations, many different well–posedness results can be found in the literature (see for example [26, 52, 73]), but none of them includes the model under study here to the best of our knowledge.

Our aim in this Chapter is to prove the existence of a unique global–in–time mild solution in $H^1(\mathbb{R}^3)$ of the following initial value problem

$$i\frac{\partial\psi}{\partial t} = -D\Delta\psi + \sigma\log(n)\psi\,, \qquad (t,x)\in[0,\infty)\times\mathbb{R}^3\,, \tag{3.3}$$

$$\psi(0,x) = \psi_0(x)\,, \qquad \psi_0\in H^1(\mathbb{R}^3)\,, \quad |x|\,n_0\in L^1(\mathbb{R}^3)\,, \tag{3.4}$$

under the only hypothesis that the initial inertial momentum $\int_{\mathbb{R}^3}|x|n_0\,dx$ is finite, independently of the fact that attractive or repulsive interactions are considered, where $n(t,x) = |\psi(t,x)|^2$ is the charge density and where we denoted $n_0(x) = n(0,x)$. Our main goal consists in developing a mathematical theory of global well–posedness in the whole space consistent in $H^1(\mathbb{R}^3)$, with neither any restriction of the functional space in order to avoid the singularity of the logarithmic potential at the origin nor technical conditions which allow to guarantee *a priori* the convergence of the sequence of approximate solutions. Our main theorem is the following

Theorem 1.3 *There exists a unique function*

$$\psi\in L^\infty([0,\infty);H^1(\mathbb{R}^3))\cap C([0,\infty);L^2(\mathbb{R}^3))$$

which solves the initial value problem (3.3)–(3.4) in a mild sense.

The key points to control the H^1–norm are the Carleman entropy inequality and the logarithmic Sobolev inequality (see (3.14) and (3.21) below) along with the charge and energy conservations. These inequalities allow us to work in the subspace of H^1 given by the functions with bounded inertial momentum (which is a natural condition with straightforward mathematical and physical meanings) instead of the subspace consisting of functions with finite energy (which is mathematically more involved because of the singularity of the potential). Actually, we shall prove that solutions with bounded inertial momentum have finite energy. Our crucial technical goals are the estimates of Lemma 2.2 (i), which do not hold if working only with $H^1(\mathbb{R}^3)$–solutions. For the sake of selfconsistency, we present in detail the regularization process of our initial value problem in H^2 (thus in L^∞) and later use some adequate compactness properties.

We structure this Chapter as follows: In Section 2 we build up a sequence of ε–approximate problems via regularization of the logarithmic nonlinearity, each of them enjoying global $H^2(\mathbb{R}^3)$ solvability. Finally, Section 3 concerns the passage to the limit $\varepsilon\to 0$ via compactness arguments and the uniqueness proof.

3.2 Global well–posedness of a sequence of approximate problems

It is well–known that the Laplace operator is self–adjoint and dissipative on $H^2(\mathbb{R}^3)$, so that $iD\Delta$ generates a unitary group of isometries $U(t) := e^{itD\Delta}$ on

$L^2(\mathbb{R}^3)$ which gives rise to the free Schrödinger propagator. We start by defining the concept of solution to the initial value problem (3.3)–(3.4) we shall deal with.

Definition 2.1 (Mild solution) *Given $T > 0$ and $X = H^1(\mathbb{R}^3)$ or $H^2(\mathbb{R}^3)$, the complex function $\psi \in C(0,T;X)$ is called a mild solution of the logarithmic Schrödinger initial value problem (3.3)–(3.4) if it solves the integral equation*

$$\psi(t,x) = U(t)[\psi_0] - i\sigma \int_0^t U(t-s)\big[\log(n(s))\psi(s)\big]\,ds\,, \tag{3.5}$$

where $U(t)[\psi_0]$ is the solution of the linear Schrödinger equation.

In order to circumvent the singularity of the potential at the origin, we start by constructing a sequence of wave functions ψ_ε which solves an ε–approximate family of problems, consisting in an appropriate regularization of the nonlinear term $\log(n)\psi$ and of the initial data ψ_0.

3.2.1 *A priori* estimates: ε–local existence

For $1 > \varepsilon > 0$, we consider a sequence of initial data $\psi_{\varepsilon,0} \subset H^2(\mathbb{R}^3)$ converging to ψ_0 in $H^1(\mathbb{R}^3)$ such that the total charge and the inertial momentum satisfy

$$\|\psi_{\varepsilon,0}\|^2_{L^2(\mathbb{R}^3)} := Q_\varepsilon \le Q := \|\psi_0\|^2_{L^2(\mathbb{R}^3)}\,, \tag{3.6}$$

and

$$\||x|\, n_{\varepsilon,0}\|_{L^1(\mathbb{R}^3)} := I_\varepsilon(0) \le 2\, I_0 := 2\,\||x|\, n_0\|_{L^1(\mathbb{R}^3)}\,, \tag{3.7}$$

respectively. We then consider the following sequence of approximate initial value problems

$$i\frac{\partial \psi_\varepsilon}{\partial t} = -D\Delta\psi_\varepsilon + \sigma h_\varepsilon(n_\varepsilon)\psi_\varepsilon\,, \qquad (t,x) \in [0,\infty) \times \mathbb{R}^3\,, \tag{3.8}$$

$$\psi_\varepsilon(0,x) = \psi_{\varepsilon,0}(x)\,, \qquad x \in \mathbb{R}^3\,, \tag{3.9}$$

where $n_\varepsilon = |\psi_\varepsilon|^2$ and $h_\varepsilon(r)$ is a smooth function defined on $\mathbb{R}^+_0$. Let us briefly show how this function can be constructed and its main properties.

3.2.2 Approximation of the logarithmic nonlinearity

Consider a function $h_\varepsilon \in C^3_0([0,\infty))$ verifying

$$h_\varepsilon(r) := \begin{cases} \log(2\,\varepsilon/3)\,, & 0 \le r < \varepsilon/2\,, \\ \log(r)\,, & \varepsilon \le r < 1/\varepsilon\,, \\ 0\,, & 2/\varepsilon \le r\,, \end{cases} \tag{3.10}$$

to be extended to $[\varepsilon/2, \varepsilon]$ and $[1/\varepsilon, 2/\varepsilon]$ in such a way that

$$|h_\varepsilon(r)| \le |\log(r)| \quad \forall r > 0\,. \tag{3.11}$$

Then, it is continuously defined in $r = 0$ and obviously approaches $\log(r)$. We now define the accumulation function

$$H_\varepsilon(r) := \int_0^r h_\varepsilon(s)\, ds\,,$$

which shall play a crucial role in defining the potential energy operator. For further comparison of the potential energy of the original problem, $\int_{\mathbb{R}^3} \log(n) n\, dx$, with that of the ε–approximate solutions, we shall derive some simple but useful estimates on $H_\varepsilon(r)$. Taking into account that $h_\varepsilon(r) \geq \log(r)$ if $r < 1/\varepsilon$ and starts decaying to zero afterwards, by simply integrating it becomes a simple matter to observe that

$$r\log(r) - r \leq H_\varepsilon(r) + r^{3/2}\,, \quad r \geq 0\,. \tag{3.12}$$

Using (3.11) and integrating again one can also observe that

$$|H_\varepsilon(r)| \leq |r\log(r)| + r\,, \quad r \geq 0\,. \tag{3.13}$$

Then, from (3.13) we have

$$H_\varepsilon(r) \leq |r\log(r)| + r = -|r\log(r)| + 2|r\log(r)| + r\,, \quad r \geq 0\,,$$

from which, taking into account Carleman's entropy inequality (see [82])

$$|r\log(r)| \leq r\log(r) + |x|r + 2e^{-|x|/4} \tag{3.14}$$

and the fact that $r\log(r) \leq r^{3/2}$ we finally find

$$|r\log(r)| \leq -H_\varepsilon(r) + 2\, r^{3/2} + (1 + 2|x|)r + 4\, e^{-|x|/4}\,, \quad r \geq 0\,. \tag{3.15}$$

These inequalities are far from been optimal and might be easily improved, but are good enough for our purposes here.

3.2.3 ε–local existence

In the sequel, we are intended to apply the standard Pazy's theory to obtain a global mild solution of the approximate problem (3.8)–(3.9) in $H^2(\mathbb{R}^3)$ (see Theorem 6.1.4 in [83]). To this purpose, we first show that the nonlinear term is locally Lipschitz continuous in $H^2(\mathbb{R}^3)$, uniformly on bounded intervals of time, i.e. that the operator

$$\begin{array}{rccc} \Gamma: & C([0,T]; H^2(\mathbb{R}^3)) & \to & C([0,T]; H^2(\mathbb{R}^3)) \\ & \psi & \mapsto & h_\varepsilon(|\psi|^2)\psi \end{array}$$

restricted to

$$B_M := \left\{ \psi \in H^2(\mathbb{R}^3) : \sup_{0\leq t\leq T} \|\psi(t)\|_{H^2(\mathbb{R}^3)} \leq M \right\}$$

is a Lispschitz continuous map for any $T > 0$ and $M > 0$. In the following, C will represent a generic constant eventually depending on T and M, while C_ε will denote a generic constant depending on ε. Also, for the sake of simplicity we shall omit further reference to $\mathbb{R}^3$ when dealing with the functional spaces $L^2(\mathbb{R}^3)$, $H^1(\mathbb{R}^3)$ or $H^2(\mathbb{R}^3)$. We first compute

$$\begin{aligned}\|\Gamma[\psi_1]-\Gamma[\psi_2]\|_{L^2} &\leq \|h_\varepsilon(|\psi_1|^2)(\psi_1-\psi_2)\|_{L^2}+\|\big(h_\varepsilon(|\psi_1|^2)-h_\varepsilon(|\psi_2|^2)\big)\psi_2\|_{L^2}\\ &\leq C_\varepsilon\left(\|\psi_1-\psi_2\|_{L^2}+\big\||\psi_1|^2-|\psi_2|^2\big\|_{L^2}\|\psi_2\|_{L^\infty}\right)\\ &\leq C_\varepsilon(1+2M^2)\|\psi_1-\psi_2\|_{L^2}\,, \end{aligned} \tag{3.16}$$

where we used that $\psi \in B_M$ implies $\|\psi(t)\|_{L^\infty} \leq C\|\psi(t)\|_{H^2} \leq CM$ and the fact that h_ε is a bounded, Lipschitz continuous function (with a Lipschitz constant depending on ε). Concerning the gradients, we argue by adding and subtracting several crossed terms as follows:

$$\begin{aligned}\nabla\Gamma[\psi_1]-\nabla\Gamma[\psi_2] &= 2h'_\varepsilon(|\psi_1|^2)\mathrm{Re}\big(\overline{\psi_1}\nabla\psi_1\big)\psi_1+h_\varepsilon(|\psi_1|^2)\nabla\psi_1\\ &\quad -2h'_\varepsilon(|\psi_2|^2)\mathrm{Re}\big(\overline{\psi_2}\nabla\psi_2\big)\psi_2-h_\varepsilon(|\psi_2|^2)\nabla\psi_2\\ &= 2\big(h'_\varepsilon(|\psi_1|^2)-h'_\varepsilon(|\psi_2|^2)\big)\mathrm{Re}\big(\overline{\psi_1}\nabla\psi_1\big)\psi_1\\ &\quad +2h'_\varepsilon(|\psi_2|^2)\mathrm{Re}\big(\overline{\psi_1}\nabla\psi_1\big)(\psi_1-\psi_2)\\ &\quad +2h'_\varepsilon(|\psi_2|^2)\mathrm{Re}\big(\overline{\psi_1}(\nabla\psi_1-\nabla\psi_2)\big)\psi_2\\ &\quad +2h'_\varepsilon(|\psi_2|^2)\mathrm{Re}\big(\big(\overline{\psi_1}-\overline{\psi_2}\big)\nabla\psi_2)\big)\psi_2\\ &\quad +h_\varepsilon(|\psi_1|^2)(\nabla\psi_1-\nabla\psi_2)\\ &\quad +\big(h_\varepsilon(|\psi_1|^2)-h_\varepsilon(|\psi_2|^2)\big)\nabla\psi_2\,.\end{aligned}$$

Using now that h'_ε is also a bounded, Lipschitz continuous function we can estimate (term by term) the above expression as follows

$$\begin{aligned}\|\nabla\Gamma[\psi_1]-\nabla\Gamma[\psi_2]\|_{L^2} &\leq C_\varepsilon\|\psi_1\|^2_{L^\infty}\|\nabla\psi_1\|_{L^4}\|\psi_1-\psi_2\|_{L^4}\\ &\quad +C_\varepsilon\|\psi_1\|_{L^\infty}\|\nabla\psi_1\|_{L^4}\|\psi_1-\psi_2\|_{L^4}\\ &\quad +C_\varepsilon\|\psi_1\|_{L^\infty}\|\psi_2\|_{L^\infty}\|\nabla\psi_1-\nabla\psi_2\|_{L^2}\\ &\quad +C_\varepsilon\|\psi_2\|_{L^\infty}\|\nabla\psi_2\|_{L^4}\|\psi_1-\psi_2\|_{L^4}\\ &\quad +C_\varepsilon\|\nabla\psi_1-\nabla\psi_2\|_{L^2}\\ &\quad +C_\varepsilon\|\nabla\psi_2\|_{L^4}\|\psi_1-\psi_2\|_{L^4}\\ &\leq C_\varepsilon\|\psi_1-\psi_2\|_{H^2}\,.\end{aligned} \tag{3.17}$$

Finally, for the second order derivatives we compute

$$\begin{aligned}\Delta\Gamma[\psi] &= 4h''_\varepsilon(|\psi|^2)\big(\mathrm{Re}\big(\overline{\psi}\nabla\psi\big)\big)^2\psi+2h'_\varepsilon(|\psi|^2)|\nabla\psi|^2\psi\\ &\quad +2h'_\varepsilon(|\psi|^2)\mathrm{Re}\big(\overline{\psi}\Delta\psi\big)\psi+4h'_\varepsilon(|\psi|^2)\mathrm{Re}\big(\overline{\psi}\nabla\psi\big)\nabla\psi+h_\varepsilon(|\psi|^2)\Delta\psi\,.\end{aligned}$$

Proceeding as for the gradients, we can analogously estimate $\Delta\Gamma[\psi_1]-\Delta\Gamma[\psi_2]$ after adding and subtracting various crossed terms in such a way that all pieces of the whole estimate involve a difference between ψ_1 and ψ_2 or their derivatives. For the reader's convenience, we shall not write up the twenty terms conforming the whole estimate. In spite of that, we just remark that in all of them the factors involving h_ε, h'_ε and h''_ε or ψ_1 and ψ_2 (without derivatives) can be bounded by their L^∞ norm. On the other hand, the gradients of the wave functions can be estimated by their L^4 norms and the laplacians by their L^2 norms, taking into account in the latter case that the rest of factors in these terms belong to L^∞. After all that, we finally get

$$\|\Delta\Gamma[\psi_1] - \Delta\Gamma[\psi_2]\|_{L^2} \leq C_\varepsilon \|\psi_1 - \psi_2\|_{H^2} \,. \tag{3.18}$$

Combining now (3.16), (3.17) and (3.18) we achieve the local Lipschitz continuity of the operator Γ in $H^2(\mathbb{R}^3)$:

$$\sup_{0\leq t\leq T} \|\Gamma[\psi_1] - \Gamma[\psi_2]\|_{H^2} \leq C_\varepsilon \sup_{0\leq t\leq T} \|\psi_1 - \psi_2\|_{H^2}, \quad \forall \psi_1, \psi_2 \in B_M.$$

Then, Pazy's theory applied to (3.8)–(3.9) gives us the existence of a unique mild ε–approximate solution

$$\psi_\varepsilon(t,x) = U(t)\big[\psi_{\varepsilon,0}(x)\big] - i\sigma \int_0^t U(t-s)\big[\Gamma[\psi_\varepsilon(s,x)]\big]\, ds\,, \tag{3.19}$$

defined on $[0, t_{max})$, where t_{max} is the maximal time of existence, which equals infinity if and only if $\|\psi_\varepsilon(t)\|_{H^2}$ does not blow–up in finite time.

3.2.4 *A posteriori* estimates: ε–global existence

The required *a posteriori* estimates and conservation laws for the problem (3.8)–(3.10) before going to the limit $\varepsilon \to 0$ are collected in the following

Lemma 2.1 *Let $T > 0$ and $\psi_\varepsilon \in C(0,T; H^2(\mathbb{R}^3))$ be a mild solution of (3.8)–(3.10). Then, the following properties are fulfilled:*

(i) The total charge is preserved along the evolution, i.e.

$$Q_\varepsilon(t) := \|\psi_\varepsilon(t)\|_{L^2}^2 = Q_\varepsilon(0) := Q_\varepsilon \leq Q\,.$$

(ii) The inertial momentum satisfies the estimate

$$I_\varepsilon(t) := \||x| n_\varepsilon(t)\|_{L^1} \leq C + 2D\sqrt{Q} \int_0^t \|\nabla\psi_\varepsilon(s)\|_{L^2}\, ds\,,$$

where $C > 0$ is a constant only depending upon the initial data.

(iii) $\|n_\varepsilon h_\varepsilon(n_\varepsilon)\|_{L^1} \leq \|n_\varepsilon \log(n_\varepsilon)\|_{L^1} \leq \|\nabla\psi_\varepsilon(t)\|_{L^2}^2 + I_\varepsilon(t) + C.$

(iv) The total energy operator associated with ψ_ε,

$$E_\varepsilon(t) := D\int_{\mathbb{R}^3} |\nabla\psi_\varepsilon(t)|^2\,dx + \sigma\int_{\mathbb{R}^3} H_\varepsilon(n_\varepsilon(t))\,dx\,,$$

is well–defined and preserved along the time evolution, i.e. $E_\varepsilon(t) = E_\varepsilon(0)$ for all $0 < t < T$.

(v) $|\sigma|\,|n_\varepsilon\log(n_\varepsilon)| \le \sigma H_\varepsilon(n_\varepsilon) + 4|\sigma|(|x|n_\varepsilon + n_\varepsilon + n_\varepsilon^{3/2} + e^{-|x|/4})\,.$

Proof. The standard continuity equation linked to (3.8) reads

$$\frac{\partial n_\varepsilon}{\partial t} + \mathrm{div}(j_\varepsilon) = 0\,, \tag{3.20}$$

where $j_\varepsilon = 2D\mathrm{Im}\big(\overline{\psi_\varepsilon}\nabla\psi_\varepsilon\big)$ is the electric current associated with ψ_ε. Assertion (i) is a standard property for Schrödinger models and follows from the continuity equation (3.20) after integrating with respect to the position variable (see also (3.6)), meanwhile (ii) stems from multiplying (3.20) by $|x|$, integrating by parts and using the estimate $\|j_\varepsilon\|_{L^1} \le 2D\sqrt{Q}\|\nabla\psi_\varepsilon(t)\|_{L^2}$ and (3.7).

To prove (iii) we first recall (cf. (3.11)) that $|h_\varepsilon(r)| \le |\log(r)|$ for all $r > 0$, thus the first inequality is inmediately satisfied. For the second inequality we take essential advantage of the following logarithmic Sobolev inequality (see [45, §8])

$$\int_{\mathbb{R}^3} n_\varepsilon\log(n_\varepsilon)(t)\,dx \le \|\nabla\psi_\varepsilon(t)\|_{L^2}^2 + Q_\varepsilon\log(Q_\varepsilon)\,. \tag{3.21}$$

Finally, combining the estimates (3.14) and (3.21) along with (ii) yields (iii).

The total energy operator is well–defined thanks to (3.13), (iii) and (ii), by simply noting that

$$\begin{aligned}|E_\varepsilon(t)| &\le D\|\nabla\psi_\varepsilon(t)\|_{L^2}^2 + |\sigma|\,\|H_\varepsilon(n_\varepsilon(t))\|_{L^1}\\ &\le C\big(\|\psi_\varepsilon(t)\|_{H^1}^2 + \|n_\varepsilon(t)\log(n_\varepsilon(t))\|_{L^1} + Q\big)\,.\end{aligned}$$

The preservation property stated in (iv) follows from a direct computation on (3.8) by using that $\psi_\varepsilon \in H^2$, the relation $H_\varepsilon'(r) = h_\varepsilon(r)$ and the continuity equation (3.20).

Finally, we prove (v) in two steps concerning the two possible cases $\sigma > 0$ and $\sigma < 0$. On one hand, if $\sigma > 0$ we may use (3.14) which along with (3.12) leads to

$$|r\log(r)| \le H_\varepsilon(r) + (1+|x|)r + r^{3/2} + 2e^{-|x|/4}\,,$$

hence to (v) by identifying $r = n_\varepsilon$. On the other hand, if $\sigma < 0$ we just multiply inequality (3.15) times $|\sigma| = -\sigma$ to get (v) after identifying again $r = n_\varepsilon$. □

In the following lemma we collect the precise estimates that will yield the global–in–time existence in H^2 of the ε–approximate mild solutions.

Lemma 2.2 *Let $\psi_\varepsilon \in C(0,T;H^2(\mathbb{R}^3))$ be a mild solution of (3.8)–(3.10). Then, there exist positive constants C_ε (independent of time) and C (independent of time and ε) such that*

(i) $\|\nabla\psi_\varepsilon(t)\|_{L^2}+\|n_\varepsilon \log(n_\varepsilon)(t)\|_{L^1}+\||x|\, n_\varepsilon(t)\|_{L^1} \le Ce^{CT}$, *for all* $t \le T < t_{max}$.

(ii) $\left\|\frac{\partial \psi_\varepsilon}{\partial t}(t)\right\|_{L^2} + \|\Delta\psi_\varepsilon(t)\|_{L^2} \le C_\varepsilon e^{C_\varepsilon T}$, *for all* $t \le T < t_{max}$.

(iii) $\|\psi_\varepsilon(t)\|_{H^2} \le C_\varepsilon e^{C_\varepsilon T}$, *for all* $t \le T < t_{max}$ *and* $t_{max} = \infty$.

Proof. Using Lemma 2.1(v), (iv) and (ii), the following estimate

$$\begin{aligned}
& D\int_{\mathbb{R}^3} |\nabla\psi_\varepsilon(t)|^2\,dx + |\sigma| \int_{\mathbb{R}^3} |n_\varepsilon \log(n_\varepsilon)(t)|\,dx \\
\le\ & E_\varepsilon(t) + 4|\sigma| \int_{\mathbb{R}^3} (|x|n_\varepsilon + n_\varepsilon + n_\varepsilon^{3/2} + e^{-|x|/4})\,dx \\
\le\ & E_\varepsilon(0) + 4|\sigma|\Big(C + 2D\sqrt{Q}\int_0^t \|\nabla\psi_\varepsilon(s)\|_{L^2}^2\,ds + \|\psi_\varepsilon(t)\|_{L^3}^3\Big) \\
\le\ & C\Big(1+\int_0^t \|\nabla\psi_\varepsilon(s)\|_{L^2}^2\,ds\Big) + 4|\sigma|\|\psi_\varepsilon(t)\|_{L^3}^3
\end{aligned}$$

holds. Now, interpolation and Sobolev–Gagliardo–Nirenberg inequalities apply to give

$$\|\psi_\varepsilon(t)\|_{L^3}^3 \le \|\psi_\varepsilon(t)\|_{L^2}^{3/2}\|\psi_\varepsilon(t)\|_{L^6}^{3/2} \le C_{SGN}\, Q^{3/2}\|\nabla\psi_\varepsilon(t)\|_{L^2}^{3/2},$$

thus we deduce

$$\begin{aligned}
& D\|\nabla\psi_\varepsilon(t)\|_{L^2}^2 + |\sigma| \int_{\mathbb{R}^3} |n_\varepsilon \log(n_\varepsilon)(t)|\,dx \\
\le\ & C\Big(1+\int_0^t \|\nabla\psi_\varepsilon(s)\|_{L^2}^2\,ds\Big) + 4|\sigma|C_{SGN}\, Q^{3/2}\|\nabla\psi_\varepsilon(t)\|_{L^2}^{3/2}. \qquad (3.22)
\end{aligned}$$

Finally, applying to (3.22) the following inequality from real analysis

$$r^{3/2} \le \frac{54|\sigma|^3 C_{SGN}^3 Q^{9/2}}{D^3} + \frac{D}{8|\sigma|\, C_{SGN}\, Q^{3/2}}\, r^2, \quad r \ge 0,$$

with $r = \|\nabla\psi_\varepsilon(t)\|_{L^2}$, we conclude

$$\frac{D}{2}\|\nabla\psi_\varepsilon(t)\|_{L^2}^2 + |\sigma|\,\|n_\varepsilon \log(n_\varepsilon)(t)\|_{L^1} \le C\Big(1+\int_0^t \|\nabla\psi_\varepsilon(s)\|_{L^2}^2\,ds\Big).$$

Now, the proof of (i) ends after application of Gronwall's lemma and Lemma 2.1(ii).

We now prove (ii). The regularity of ψ_ε along with (3.8) show that $\partial_t \psi_\varepsilon$ belongs to L^2 but do not provide a control of the norm. However, following [27, §5] we can argue as follows, starting from the mild formulation:

$$\begin{aligned} \psi_\varepsilon(t+h,x) - \psi_\varepsilon(t,x) &= i\int_0^h U(s)[\Delta\psi_{\varepsilon,0}(x)]\,ds \\ &\quad -i\sigma\int_0^h U(t+h-s)\big[\Gamma[\psi_\varepsilon(s,x)]\big]\,ds \\ &\quad -i\sigma\int_0^t U(t-s)\Big[\Gamma[\psi_\varepsilon(s+h,x)] - \Gamma[\psi_\varepsilon(s,x)]\Big]\,ds. \end{aligned}$$

Taking L^2 norms, using that $U(t)$ is an isometry in L^2 in the tree integrals of the right–hand side and the inequality (3.16) for the third term, we guess that

$$\|\psi_\varepsilon(t+h) - \psi_\varepsilon(t)\|_{L^2} \le h\Big(\|\Delta\psi_{\varepsilon,0}\|_{L^2} + C_\varepsilon\Big) + C_\varepsilon\int_0^t \|\psi_\varepsilon(s+h) - \psi_\varepsilon(s)\|_{L^2}\,ds\,.$$

Now, Gronwall's lemma applies to give us the first part of (ii). The second part is now straightforward by noticing that

$$\Delta\psi_\varepsilon = \frac{1}{D}\Big(-i\frac{\partial\psi_\varepsilon}{\partial t} + \sigma h_\varepsilon(n_\varepsilon)\psi_\varepsilon\Big).$$

Finally, (iii) is an inmediate consequence of (i) and (ii) as well as of charge conservation (cf. Lemma 2.1(i)). □

Remark 2 *Notice that, in spite of the fact that a change of sign in the non-linear term of the logarithmic Schrödinger equation (3.3) generates very different dynamics (see [70] for a 1D analysis), the a priori and a posteriori estimates derived in previous sections to finally achieve the $H^1(\mathbb{R}^3)$ existence of mild solutions are all independent of the sign choice.*

3.3 Passing to the limit $\varepsilon \to 0$: Global solvability in $H^1(\mathbb{R}^3)$

We finally find the unique global–in–time solution $\psi(t,x)$ to (3.3)–(3.4) as the limit of the ε–approximate solutions $\psi_\varepsilon(t,x)$ to (3.8)–(3.10), as ε is sent to zero, by means of the following

Theorem 3.4 (Existence) *Let ψ_ε be the mild solution of (3.8)–(3.10). Then, there exists a function $\psi \in L^\infty([0,\infty); H^1(\mathbb{R}^3)) \cap C([0,\infty); L^2(\mathbb{R}^3))$ such that, up to a subsequence,*

(i) ψ_ε converges to ψ as $\varepsilon \to 0$ in $C([0,T]; L^2(\mathbb{R}^3))$ for all $T > 0$,

(ii) $\psi_\varepsilon h_\varepsilon(n_\varepsilon)$ converges to $\psi\log(|\psi|^2)$ as $\varepsilon \to 0$ in $L^2_{loc}([0,\infty) \times \mathbb{R}^3)$,

(iii) ψ is a mild solution of the initial value problem (3.3)–(3.4).

Proof. We start by showing that, for $1 \le p < 6$, the following inequality

$$\|\phi\, h_\varepsilon(|\phi|^2)\|_{L^p(K)} \le \|\phi \log(|\phi|^2)\|_{L^p(K)} \le C(1 + \|\phi\|_{H^1(K)}) \qquad (3.23)$$

holds for any function $\phi \in H^1(K)$ and any bounded domain $K \subset \mathbb{R}^3$. To do that we recall that, according to (3.11), we only need to prove the second inequality. First we split $\phi \log(|\phi|^2)$ into two parts as $\phi \log(|\phi|^2) = \phi \log(|\phi|^2)\Big(\chi_{\{|\phi|<1\}} + \chi_{\{|\phi|\ge 1\}}\Big)$ in such a way that after optimizing we find

$$|\phi \log(|\phi|^2)| \le \frac{2}{e} + C|\phi|^{1+\beta},$$

where β is any positive number. Given that $\phi \in L^q(K)$ for all $1 \le q \le 6$, it is a simple matter to conclude (3.23) via Sobolev imbeddings.

We are now in position to prove (i). The charge conservation established in Lemma 2.1(i) (cf. (3.6)) guarantees the (*a priori*, weak*) convergence of a subsequence of ψ_ε to a function ψ in $L^\infty([0,T]; L^2(\mathbb{R}^3))$ for all $T > 0$. In order to observe that this convergence is actually strong, and thus that $\psi \in C([0,T]; L^2(\mathbb{R}^3))$, we use Aubin's Lemma (see [12] or [82, Lemma 11]). We first note that the momentum bounds established in Lemma 2.2(i) guarantee that for all $R > 0$, we have

$$\int_{|x|>R} |\psi_\varepsilon(t,x)|^2 dx \le \int_{|x|>R} \frac{|x|}{R} |\psi_\varepsilon(t,x)|^2 dx \le \frac{1}{R} C e^{CT}, \qquad \forall t \in [0,T].$$

Then, the arbitrariness of R reduces the problem to prove the convergence only in $C([0,T]; L^2(K))$, K being the ball of radius R. Finally, using the kinetic energy bound showed in Lemma 2.2(i) together with the inequality (3.23) for ψ_ε and the approximated equation (3.8), we deduce that the sequence ψ_ε is bounded in $L^\infty([0,T]; H^1(K))$ and its time derivative $\frac{\partial \psi_\varepsilon}{\partial t}$ is bounded in $L^\infty([0,T]; H^{-1}(K))$. Therefore, a straightforward application of Aubin's Lemma concludes the proof. Moreover, the boundedness of $\nabla\psi_\varepsilon$ directly implies that $\psi \in L^\infty([0,\infty); H^1(\mathbb{R}^3))$.

Let us now prove (ii). We first note that, by according to (3.23), we deduce that

$$\|\psi_\varepsilon h_\varepsilon(|\psi_\varepsilon|^2)\|_{L^2(K)} \le C(1 + \|\psi_\varepsilon\|_{H^1}), \quad \|\psi \log(|\psi|^2)\|_{L^2(K)} \le C(1 + \|\psi\|_{H^1}),$$

for any arbitrary bounded domain $K \subset \mathbb{R}^3$, so they are both in $L^2_{loc}([0,\infty) \times \mathbb{R}^3)$ as stated in (ii). To prove the convergence we observe that the sequence of functions $z \mapsto z h_\varepsilon(|z|^2)$ is uniformly equicontinuous on compact sets (although not uniformly Lipschitz continuous), thus we can deduce via Ascoli–Arzela's theorem that it converges uniformly on compact sets to $z\log(|z|^2)$. Combining this convergence property with (i), we easily deduce that $\psi_\varepsilon h_\varepsilon(n_\varepsilon)$ tends to $\psi \log(|\psi|^2)$

a.e. $(t,x) \in [0,T] \times K$. Using now Egorov's theorem we find that, for any $k \in \mathbb{N}$, there exists a subset $A \subset [0,T] \times K$ with measure $|A| < 1/k$ such that $\psi_\varepsilon h_\varepsilon(n_\varepsilon)$ converges to $\psi \log(|\psi|^2)$ uniformly on $(t,x) \in \big([0,T] \times K\big) \setminus A$. Therefore, there exists $\varepsilon_0 > 0$ such that for any $\varepsilon < \varepsilon_0$ we have

$$\|\psi_\varepsilon h_\varepsilon(|\psi_\varepsilon|^2) - \psi \log(|\psi|^2)\|_{L^2(([0,T]\times K)\setminus A)} \leq \frac{\sqrt{|K|T}}{k}\,.$$

On the other hand, from (3.23) and Hölder's inequality we can compute

$$\|\psi_\varepsilon h_\varepsilon(|\psi_\varepsilon|^2) - \psi \log(|\psi|^2)\|_{L^2(A)} \leq 2C|A|^{1/4} \leq \frac{2C}{k^{1/4}}$$

and conclude that, for any $\varepsilon < \varepsilon_0$, we have

$$\|\psi_\varepsilon h_\varepsilon(|\psi_\varepsilon|^2) - \psi \log(|\psi|^2)\|_{L^2([0,T]\times K)} \leq \frac{\sqrt{|K|T}}{k} + \frac{2C}{k^{1/4}}\,.$$

Now we are done with (ii).

Finally, (i) and (ii) allow us to go to the limit $\varepsilon \to 0$ in the mild formulation (3.19) and show that the limiting wave function ψ is a mild solution of (3.3), which completes the proof. □

Theorem 3.5 (Uniqueness) *Let $\psi_1, \psi_2 \in C([0,\infty); L^2(\mathbb{R}^3))$ be two mild solutions of the initial value problem (3.3)–(3.4). Then $\psi_1 = \psi_2$ a.e., thus the whole sequence of ε–approximate solutions converges to it.*

Proof. We just make a sketch of the proof, since the details can be found in [27]. Take $u, v \in \mathbb{C}$ so that we may assume $0 < |v| < |u|$ without loss of generality. Then, using the inequality

$$\big|\log(|v|) - \log(|u|)\big| \leq \frac{|v-u|}{|v|}$$

along with the identity

$$|\mathrm{Im}(v\overline{u} - u\overline{v})| = |v(\overline{u} - \overline{v}) + \overline{v}(v-u)| \leq 2|v||v-u|,$$

the following result is achieved

$$\left|\mathrm{Im}\Big(\big(v\log(|v|^2) - u\log(|u|^2)\big)(\overline{v} - \overline{u})\Big)\right| \leq 4|v-u|^2. \tag{3.24}$$

Computing now the difference between (3.3) and its conjugate counterpart for ψ_1 and ψ_2 and taking the L^2 product with $(\psi_1 - \psi_2)$, it follows that

$$\frac{d}{dt}\int_{\mathbb{R}^3} |\psi_2 - \psi_1|^2\,dx = 2\sigma \mathrm{Im}\left(\int_{\mathbb{R}^3}\Big(\psi_2\log(|\psi_2|^2) - \psi_1\log(|\psi_1|^2)\Big)\big(\overline{\psi_2} - \overline{\psi_1}\big)\,dx\right).$$

Then, (3.24) with $u = \psi_1$ and $v = \psi_2$ implies

$$\|\psi_2(t) - \psi_1(t)\|_{L^2}^2 \leq 8|\sigma|\int_0^t \|\psi_2(s) - \psi_1(s)\|_{L^2}^2\,ds\,.$$

Uniqueness follows after a straightforward application of Gronwall's lemma. This completes the proof. □

Chapter 4

On the analysis of travelling waves to a nonlinear flux limited reaction–diffusion equation

4.1 Introduction and main results

The aim of this Chapter is to analyze the existence of travelling waves associated to a heterogeneous nonlinear diffusion partial differential equation coupled to a reaction term of Fisher–Kolmogorov–Petrovskii–Piskunov type. The nonlinear diffusion term has been motivated in different contexts and from different points of view (see the pioneering work [88]). Also, it has been deduced in the Monge-Kantorovich's optimal mass transport framework where it is usually called the relativistic heat equation [19] or in astrophysics [77]. The existence and uniqueness of entropy solutions for the nonlinear parabolic flux diffusion was proved in [4], while in [5] the finite speed of propagation was analyzed. The resulting reaction–flux–limited–diffusion system exhibits new properties compared to the classical reaction coupled to the linear diffusion equation, such as the existence of singular travelling waves which opens new perspectives of application to biology or traffic flow frameworks.

Reaction–diffusion systems consist in mathematical models describing the dynamics of the concentration of one or more populations distributed in space under the influence of two processes: local reactions in which the populations interact with each other, and diffusion which provokes the populations to spread out in space. In the context of reaction-diffusion the notion of population can be understood in a wide sense such as particles or concentrations in chemical processes, but also examples can be found in biology (cells, morphogens), geology, combustion, physics and ecology or more recently in computer science or complex systems, see for instance [31, 47, 61, 74, 76, 78, 90, 92, 94]. This fact has motivated the attention by both formal and rigorous work on a variety of applications starting from linear diffusion of type

$$\frac{\partial u}{\partial t} = \nu \, \Delta u + f(u), \qquad u(t=0,x) = u_0(x), \tag{4.1}$$

where ν is the so called diffusion coefficient and f represents the reaction term. Cooperative behavior often stems from diffusive coupling of nonlinear elements and reaction-diffusion equations provide the prototypical description of such systems.

In many applications and in particular in complex systems reaction-diffusion equations often provide a natural mathematical description of these dynamical networks since the elements of the networks are coupled through diffusion in many instances. The correct description of reaction-diffusion phenomena requires a detailed knowledge of the interactions between individuals and groups of individuals. This line of research motivates the study of nonlinear cooperative behavior in complex systems [13], which is a closed subject interconnected with reaction–diffusion systems. There is a wide literature raising the universality of application of reaction–diffusion systems. Nevertheless, there are limitations to the reaction-diffusion description. In biochemical networks constituted by small cellular geometries a macroscopic reaction-diffusion model may be inappropriate. In some circumstances the coupling among elements is not diffusive or the diffusive processes are nonlinear, which will strongly influence the dynamical behavior of the network. In [91] it is proposed a nonlinear degenerate density-dependent diffusion motivated by the fact that there are biological (mating, attracting and repelling substances, overcrowding, spatial distribution of food, social behavior, etc.) and physical (light, temperature, humidity, etc.) factors which imply that the probability is no longer a space-symmetric function, i.e., it looses the homogeneity, and so linear diffusion is not a good approach. This heterogeneity property of the diffusion operator comes from the heterogeneous character of the equation and/or from the underlying domain, we refer also to [16, 17, 14, 15]. The same problems with the universality in the applicability occurs when we have not a mean-field interaction between particles or when the particles are dilute or large with respect to the vessel or the media where they are moving [6, 90]. In these cases the linear diffusion approximation might not be the most appropriate. The above processes probably require to incorporate one or various phenomena not included in linear diffusion such as the finite speed of propagation of matter or the existence of nonsmooth densities (singular travelling waves), for example. The mathematical argument justifying that even if the solution has not compact support the size (mass or concentration, depending on the case dealt with) is very small out of some ball with large radius could be unrealistic because in several applications in biology (morphogenesis) [1, 15, 94, 96], social sciences [13] or traffic flow [18] this kind of situations (solutions with large queues) could activate other processes which is the case, for example, of the biochemical processes inside the cells whose activation depends on the time of exposure as well as on the received concentration of morphogen, see [1]. Then, exploring or modeling new nonlinear transport/diffusion phenomena is an interesting subject not only from the viewpoint of applications but also from a mathematical perspective.

Reaction–diffusion systems have also attracted the attention as prototype models for pattern formation which is, in particular, connected with the study of travelling waves, i.e. solutions of the type $u(t,x) = u(x - \sigma t)$ playing an important role in concrete applications. The problem when considering travelling waves for (4.1) is that the evolution of the support could have an infinite speed of propagation, which would contradict the fact that the speed should not exceed the propagation rate of the real transport process.

Motivated by the above considerations the objective of this Chapter consists in analyzing the existence of travelling waves for the one–dimensional, nonlinear, flux limited reaction–diffusion equation

$$\frac{\partial u}{\partial t} = \nu \partial_x \left(\frac{u \partial_x u}{\sqrt{|u|^2 + \frac{\nu^2}{c^2}|\partial_x u|^2}} \right) + f(u), \qquad u(t=0,x) = u_0(x), \tag{4.2}$$

where ν is the viscosity and c is a constant velocity related to the inner properties of the particles. Why this election for the nonlinear diffusion term? First of all, the solutions to this system have finite speed of propagation as opposite to the linear heat equation, i.e. for an initial data with compact support the velocity of growth of the support of the solution is bounded by c (see [2]). Furthermore, this is an extension of the heat equation in the following sense: rewrite the heat equation as

$$\frac{\partial u}{\partial t} = \nu \frac{\partial}{\partial x}\left[u \frac{\partial}{\partial x} \ln u \right] = \nu \frac{\partial}{\partial x}[u\, v], \tag{4.3}$$

where v is a microscopic velocity. In this form the heat equation can be seen as a transport kinetic equation. The velocity v is determined by the entropy of the system, $S(u) = u \ln u$, and by the concentration u, via the following formula

$$v = \frac{\partial}{\partial x}\left(\frac{S(u)}{u} \right). \tag{4.4}$$

Note that $\frac{S(u)}{u} = \ln u$ is known as the chemical potential. We propose to modify the form of the flux in (4.3) by considering a new microscopic velocity averaged with respect to the line element associated with the motion of the particle, so that the new velocity is given by $\frac{\partial}{\partial v}\sqrt{1+|v|^2} = \frac{v}{\sqrt{1+|v|^2}}$ with

$$v = \frac{\partial_x (S(u)/u)}{\sqrt{1 + [\partial_x (S(u)/u)]^2}}, \tag{4.5}$$

arriving at the flux limited equation (4.2). This implies that the chemical potential is now finite, which is not the case for the linear heat equation. Thus, the velocity for which the concentration or density u is transported depends on the entropy of the system (determining the disorder) as well as on its density under an appropriate measure. This is the situation in which one can think in a traffic flow or in a biological context, for example.

For the reaction term, we will consider one canonical model of Fisher [48] or KPP [65] (for Kolmogorov, Petrovsky and Piskunov) type to analyze travelling waves, called FKPP from now on. For the linear diffusion case, the properties associated with this system are well understood in the homogeneous framework, see for example [9, 10, 48, 65]. The above equation (4.2) with $f = 0$ is known as the relativistic heat equation and is one among the various flux limited diffusion equations used in the theory of radiation hydrodynamics [77].

The term $f(u)$ is written as $uK(u)$, where K is known in biology as the growth rate of the population. The main hypotheses on the FKPP reaction term $K \in C^1([0,1])$ are typically written as

$$\text{(i) } K(1) = 0\,, \qquad \text{(ii) } K'(s) < 0\,,\ s \in (0,1]\,. \tag{4.6}$$

These hypotheses on $K(u)$ have some consequences on $f(u)$ such us $f(0) = f(1) = 0$, $f'(1) < 0$, $f'(0) > 0$, $f > 0$ in $(0,1)$. Hypothesis (i) in (4.6) is a normalization property of the carrying capacity and (ii) represents a saturation of the media when the concentration is increasing. Typical examples of such nonlinearities are $K(s) = k(1-s)$ or $K(s) = k(1-s^2)$, where $k = K(0) = f'(0)$ is a constant related to the growth rate of the (biological) particles, usually called intrinsic growth rate. In [48, 65] it was proved that, under the above assumptions, there is a threshold value $\sigma^* = 2\sqrt{\nu k}$ for the speed σ associated with the linear diffusion system (4.1). Namely, no fronts exist for $\sigma < \sigma^*$, and there is a unique front (up to space or time shifts) for all $\sigma \geq \sigma^*$.

The study of existence and uniqueness of solutions to the flux limited reaction-diffusion equation (4.2) has been done in [2], see also the references therein for a complete study of the "relativistic" heat equation. The natural concept of solution for this problem implies the use of Kruzhkoz's entropy solutions. In fact, in [2] it is proved that for any initial datum $0 \leq u_0 \in L^1(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$, there exists a unique entropy solution u of (4.2) in the N-dimensional case $[0,T) \times \mathbb{R}^N$, for every $T > 0$, such that $u(t=0) = u_0$. In addition, solutions live in a subspace of Bounded Variation functions. Moreover, if $u(t)$, $\bar{u}(t)$ are the entropy solutions corresponding to initial data u_0, $\bar{u}_0 \in (L^\infty(\mathbb{R}^N) \cap L^1(\mathbb{R}^N))^+$, respectively, then

$$\|u(t) - \bar{u}(t)\|_{L^1(\mathbb{R}^N)} \leq e^{t\|f\|_{Lip}} \|u_0 - \bar{u}_0\|_{L^1(\mathbb{R}^N)}\,,\ \forall t \geq 0\,,$$

where $\|f\|_{Lip}$ denotes the Lipschitz constant for f in $[0,1]$. The the existence of entropy solutions to initial data only in in L^∞ was extended in Proposition 3.14 of [2].

One of the most important differences between the linear (4.1) and the nonlinear (4.2) diffusion models emerges, besides the existence theory reported above, in the study of travelling waves. A travelling wave is a solution having a constant profile which moves with constant speed, i.e. a solution of the equation of the form $u(t,x) = u(\xi)$ with $\xi = x - \sigma t$ for some constant σ. The function u is usually called the wave profile and the constant σ is the wave speed. Let us give a simple example that may illustrate the results obtained in this Chapter for (4.2) by means of a simplified reaction-flux–limited-diffusion equation,

$$\partial_t u = \partial_x \left(u \frac{\partial_x u}{|\partial_x u|} \right) + u(1-u)\,, \tag{4.7}$$

which allows us to compute explicit travelling waves. Given (4.7), the equation satisfied by a decreasing wave front profile $u(\xi) = u(x - \sigma t)$ is

$$-\sigma \dot{u} = -\dot{u} + u(1-u)\,.$$

Then, it can be easily proved the existence of a unique, global classical solution given by

$$u_\sigma(\xi) = \frac{1}{e^{-\frac{1}{\sigma-1}\xi} + 1}\,, \quad \xi \in \mathbb{R}\,,$$

only if $\sigma > 1$ up to space or time shifts. Furthermore, the step function $u(\xi) = 1$ if $\xi < 0$ and null otherwise, gives the travelling wave profile of an entropy solution to (4.7) with $\sigma = 1$. Let us observe how regular and discontinuous solutions coexist in this simplified model. To complete the above results see [2].

As in the previous case, we find singular profiles for the travelling waves of (4.2) which to a certain extent constitute the equivalent notion of shock waves in hyperbolic models for traffic flow. On the other hand, there is a wide variety and significant differences for the possible choices of the velocity σ for the travelling wave solutions to the nonlinear reaction–diffusion equations (4.2) with respect to those associated with (4.1).

In this Chapter, we look for a particular kind of travelling waves called *wave front*, determined by a decreasing wave profile $u \in (0,1)$ such that $\lim_{\xi\to-\infty} u(\xi) = 1$, $\lim_{\xi\to\infty} u(\xi) = 0$, verifying (4.2) in a sense specified later. By the degenerate character of the flux limiter if $u \equiv 0$, we split the analysis of the wave front in two steps. For the positive part $u(\xi) > 0\ \forall \xi \in (-\infty, \xi_0)$, we impose that $u \in C^2$ solves the equation in a classical sense. Thus, if $\xi_0 = \infty$ we will have a *classical solution* verifying the equation everywhere in the domain of definition. If $\xi_0 < \infty$, we will see that the null extension of the positive part can be an entropy solution under certain conditions, these solutions being *discontinuous*. The entropy criterium is necessary in this problem since it selects travelling waves of discontinuous type.

Our main result is the following.

Theorem 1.6 *In terms of a value $\sigma^* \le c$, depending on ν, c, and k, there exists a wave front which is*

(i) a classical solution to (4.2), with wave speed $\sigma > \sigma^*$ or $\sigma = \sigma^* < c$;

(ii) a discontinuous entropy solution to (4.2), with wave speed $\sigma = \sigma^* = c$.

Remark 3 *The existence of travelling wave solutions in the case $\sigma < \sigma^*$ is an open problem. Also, the existence of other kind of travelling waves such as those with pulses or soliton-type shape could be explored, see for example [87] or [44] in another context.*

In Section 2 we will analyze the necessary and sufficient condition for the parameters ν, c, and k in order to determine σ^*. The analytical theory dealing with the existence of a solution-set-structure follows from the associated asymptotic initial value problem satisfied by the travelling wave profile. This problem is framed in the analysis of a planar dynamical system where the wave speed σ is a parameter.

Another fundamental property of equation (4.1) concerns the asymptotic speed of spreading and was established in [10]: If $u_0 \geq 0$ is a continuous function in $\mathbb{R}^N$ with compact support and $u_0 \not\equiv 0$, then the solution $u(t,x)$ with initial data $u(t=0,x) = u_0(x)$ spreads out with speed σ^* in all directions as $t \to +\infty$, i.e. $\max_{|x|\leq \sigma t}|u(t,x)-1| \to 0$ for each $\sigma \in [0,\sigma^*)$, and $\max_{|x|\geq \sigma t} u(t,x) \to 0$ for each $\sigma > \sigma^*$. A similar result may fit our context by the control of the bound of the entropy solution in the set $\{x > \sigma\, t\}$ by means of an exponential function with negative exponent (see Proposition 3.4 below).

The Chapter is organized as follows. In Section 2 we pose the asymptotic initial value problem associated with travelling wave solutions and deal with the existence and uniqueness of regular travelling waves. Finally, in Section 3 we analyze the singular wave profiles that can be identified as entropy solutions.

4.2 An equivalent problem for classical travelling waves

As we mentioned before, the aim of this section is to analyze the classical wave front solutions to (4.2).

4.2.1 Travelling wave equations

The existence of a regular travelling wave $u(x-\sigma t)$ of the equation (4.2) leads to the problem of finding a solution of the following equation

$$\nu \left(\frac{u\, u'}{\sqrt{|u|^2 + \frac{\nu^2}{c^2}|u'|^2}} \right)' + \sigma u' + f(u) = 0\,, \tag{4.8}$$

which is defined on $(-\infty, \xi_0)$ and satisfies

$$\lim_{\xi \to -\infty} u(\xi) = 1 \tag{4.9}$$

and

$$u'(\xi) < 0 \text{ for any } \xi \in (-\infty, \xi_0)\,. \tag{4.10}$$

The constant σ is a further unknown of the problem. Let us analyze this asymptotic initial value problem where $f(u) = uK(u)$ and K fulfills (4.6). The following result contributes to deduce the asymptotic value of the derivative of u.

Lemma 2.3 *Let $u : (-\infty, \xi_0) \to (0, 1)$ be a solution of (4.8) that satisfies (4.9)-(4.10). Then,*

$$\lim_{\xi \to -\infty} u'(\xi) = 0\,. \tag{4.11}$$

Proof. Take $\xi_n \to -\infty$ with $\xi_n < \xi_0$. For any fixed $n \in \mathbb{N}$ we use the mean value theorem in the interval $[\xi_n - 1, \xi_n]$ to obtain the existence of a sequence $s_n \in [\xi_n - 1, \xi_n]$ satisfying

$$u'(s_n) = u(\xi_n) - u(\xi_n - 1) \to 0.$$

Then, we integrate (4.8) over $[s_n, \xi_n]$ and analyze the terms of the following equality

$$\int_{s_n}^{\xi_n} \nu \left(\frac{u(\delta)u'(\delta)}{\sqrt{|u(\delta)|^2 + \frac{\nu^2}{c^2}|u'(\delta)|^2}} \right)' d\delta + \int_{s_n}^{\xi_n} \sigma u'(\delta) d\delta + \int_{s_n}^{\xi_n} f(u(\delta)) d\delta = 0\,.$$

The third term

$$\int_{s_n}^{\xi_n} f(u(\delta)) d\delta \to 0\,,$$

since the interval is bounded and the integrand converges uniformly to zero. The second term, using Barrow's rule, is

$$\sigma(u(\xi_n) - u(s_n))$$

that tends to zero because of (4.9). The first term, again from Barrow's rule, takes the form

$$\nu \frac{u(\xi_n)u'(\xi_n)}{\sqrt{|u(\xi_n)|^2 + \frac{\nu^2}{c^2}|u'(\xi_n)|^2}} - \nu \frac{u(s_n)u'(s_n)}{\sqrt{|u(s_n)|^2 + \frac{\nu^2}{c^2}|u'(s_n)|^2}}\,,$$

which tends to zero since $u'(s_n) \to 0$ and

$$\nu \frac{u(\xi_n)u'(\xi_n)}{\sqrt{|u(\xi_n)|^2 + \frac{\nu^2}{c^2}|u'(\xi_n)|^2}} \to 0.$$

Using (4.10) one gets

$$\frac{u(\xi_n)u'(\xi_n)}{\sqrt{|u(\xi_n)|^2 + \frac{\nu^2}{c^2}|u'(\xi_n)|^2}} = \frac{-1}{\sqrt{\frac{1}{|u'(\xi_n)|^2} + \frac{\nu^2}{c^2}\frac{1}{|u(\xi_n)|^2}}}\,,$$

therefore

$$\frac{1}{|u'(\xi_n)|^2} + \frac{\nu^2}{c^2}\frac{1}{|u(\xi_n)|^2} \to \infty\,.$$

As the second term tends to $\frac{\nu^2}{c^2}$, then $\frac{1}{|u'(\xi_n)|^2} \to \infty$ and finally $u'(\xi_n) \to 0$. We have then shown that for any $\xi_n \to -\infty$, $u'(\xi_n) \to 0$. This proves (4.11). □

In a classical framework, looking for travelling wave solutions is equivalent to finding heteroclinic trajectories of a planar system of ODE's which arises from transforming the original problem into travelling wave coordinates (see [48, 65, 91]). The same ideas in the search of travelling waves of (4.2) leads to a system which is not uniquely derived from heteroclinic trajectories. Hence, a more detailed analysis of the phase diagram for the planar system of ODE's is required. Define

$$r(\xi) = -\frac{\nu}{c}\frac{u'(\xi)}{\sqrt{|u(\xi)|^2 + \frac{\nu^2}{c^2}|u'(\xi)|^2}}\,, \tag{4.12}$$

where u is any positive solution of (4.8)–(4.9)–(4.10). Then (u, r) satisfies the first order differential system

$$\left.\begin{aligned} u' &= -\frac{c}{\nu}\frac{|u|\,r}{\sqrt{1-r^2}}\,, \\ r' &= \frac{c}{\nu}\frac{r(r-\frac{\sigma}{c})}{\sqrt{1-r^2}} + \frac{1}{c}K(u)\,. \end{aligned}\right\} \tag{4.13}$$

By using that $u' < 0$, (4.12) yields $r \in (0,1)$. Also, Lemma 2.3 implies $\lim_{\xi\to-\infty} r(\xi) = 0$. As a consequence, the problem of finding a maximal solution of (4.8)–(4.10) is equivalent to look for a solution $(u, r) : (-\infty, \xi_0) \to (0,1)^2$ of (4.13), maximal in $(0,1)^2$, that satisfies

$$\lim_{\xi\to-\infty} u(\xi) = 1, \qquad \lim_{\xi\to-\infty} r(\xi) = 0. \tag{4.14}$$

We now analyze the equilibrium points of the system (4.13) which are $(1, 0)$ and $(0, r^*)$, where $r^* \in (0,1)$ is a possible root of

$$\frac{c}{\nu}\frac{r(r-\frac{\sigma}{c})}{\sqrt{1-r^2}} + \frac{1}{c}k = 0\,, \tag{4.15}$$

with $k = K(0) = f'(0)$. The existence of equilibrium points $(u, r) = (0, r^*)$ will determine the behavior of the solution to (4.13)-(4.14) and consequently of the solution to (4.8)–(4.10). More precisely, we obtain the following result.

Proposition 2.1 *There always exists a solution u of (4.8) that satisfies (4.9) and (4.10). This solution is unique up to a time translation and verifies:*

(i) If there exist no roots $r^* \in (0,1)$ of (4.15), then the existence interval for u can be extended to $(-\infty, \xi_0)$, with $\xi_0 < \infty$, and

$$\lim_{\xi \to \xi_0} u(\xi) > 0, \quad \lim_{\xi \to \xi_0} u'(\xi) = -\infty. \tag{4.16}$$

(ii) If there exist roots of (4.15), then $\xi_0 = \infty$ and u satisfies

$$\lim_{\xi \to \infty} u(\xi) = 0\,. \tag{4.17}$$

As a consequence, this solution is maximal in $\mathbb{R} \times (-1,1)$ and is located in $(0,1)^2$.

To prove Proposition 2.1 we will need two preliminary results describing some properties of r and u.

Lemma 2.4 *Let $-\infty < \xi_0 \leq \infty$ and $(u,r) : (-\infty, \xi_0) \to (0,1)^2$ be a solution of (4.13) that satisfies (4.14). Then, $r'(\xi) > 0$. The same holds true for any extension of (u,r). In particular, the maximal solution (u_M, r_M) associated with (u,r) remains in $(0,1)^2$ and verifies $r'_M(\xi) > 0$.*

We will give the proof of this result at the end of this Section by analyzing in detail the zeros of r' in (4.13) and describing the phase diagram associated with (4.13)-(4.14).

The following result deals with the strict positivity of u.

Lemma 2.5 *Let $(u,r) : (\xi_1, \xi_0) \to (0,1)^2$ be a solution of (4.13), where $-\infty \leq \xi_1 < \xi_0 \leq \infty$ are such that*

$$\lim_{\xi \to \xi_0} r(\xi) = 1\,, \quad r'(\xi) > 0\,.$$

Then

$$\lim_{\xi \to \xi_0} u(\xi) > 0\,.$$

Proof. Denote $(\bar{u}, \bar{r})$ this particular solution. A contradiction argument allows to define $\tilde{u}(r) := \bar{u}(\bar{r}^{-1}(r))$ in an interval $(1-\varepsilon, 1)$ that satisfies

$$z' = \frac{-zr}{r(r - \frac{\sigma}{c}) + \frac{\nu}{c^2} K(\tilde{u}(r))\sqrt{1-r^2}}\,, \quad z(1) = 0\,.$$

If $\frac{\sigma}{c} \neq 1$, this equation is locally Lischitsz-continuous in z and the point $(1,0)$ is regular. Then, by using the uniqueness of the initial value problem z must vanish identically, which is a contradiction. If $\frac{\sigma}{c} = 1$, then the differential equation is singular. However, $\tilde{u}$ is a solution of the differential equation

$$z' = -z\frac{h(r)}{\sqrt{1-r}}$$

With
$$h(r) = \frac{r}{-r\sqrt{1-r} + \frac{\nu}{c^2}K(\tilde{u}(r))\sqrt{1+r}}\,.$$
The term $\frac{h(r)}{\sqrt{1-r}}$ is singular but improperly integrable and the associated differential equation has uniqueness again by arguing via the separated variables theory. □

We are now in a position to prove Proposition 2.1.

4.2.2 Proof of Proposition 2.1

A local analysis of (4.13) gives the following Jacobian matrix in (u, r)
$$J[u,r] = \begin{pmatrix} -\dfrac{c}{\nu}\dfrac{r}{\sqrt{1-r^2}} & -\dfrac{c}{\nu}\dfrac{u}{(1-r^2)^{3/2}} \\[2ex] \dfrac{K'(u)}{c} & -\dfrac{c}{\nu}\dfrac{\frac{\sigma}{c} - 2r + r^3}{(1-r^2)^{3/2}} \end{pmatrix}.$$
Clearly,
$$J[1,0] = \begin{pmatrix} 0 & -\dfrac{c}{\nu} \\[2ex] \dfrac{K'(1)}{c} & -\dfrac{\sigma}{\nu} \end{pmatrix}$$
has two eigenvalues $\lambda_- < 0 < \lambda_+$ (because $K'(1) < 0$) which are given by $\lambda_\pm = -\frac{\sigma}{2\nu} \pm \sqrt{\left(\frac{\sigma}{2\nu}\right)^2 - \frac{K'(1)}{\nu}}$. The local unstable manifold theorem (see [54, 62]) guarantees the existence of a curve with initial condition γ for which the corresponding solution satisfies (4.14). As the slope of the eigenvector corresponding to λ_+ is negative (see Remark 4 for an explicit calculus of the eigenvector) only one branch of $\gamma - \{(1,0)\}$ is locally contained in $(0,1)^2$. Let us take γ maximal in $(0,1)^2$. Then, there exist solutions of (4.13) satisfying (4.14). Uniqueness up to a time translation comes up from the local uniqueness of the branch γ. Now, Lemmata 2.4 and 2.5 can be applied.

From the fact that u' has opposite sign to r we can deduce that u satisfies (4.9) and (4.10). According to the existence of roots of equation (4.15) we will prove the statements, (1) or (2), of Proposition 2.1. Let us choose $(u,r) : (-\infty, \xi_0) \to (0,1)^2$ to be a particular solution of (4.13) satisfying (4.14). Then, Lemma 2.4 implies that the following limit exists
$$\lim_{\xi \to \xi_0} r(\xi) = r_L\,.$$
Let us prove that r_L is a lower bound for any possible root r^* of (4.15), i.e. $r_L \le r^*$. In fact, if $r(\bar{\xi}) = r^*$ for $\bar{\xi} \in (-\infty, \xi_0)$, then (4.6) leads to
$$r'(\bar{\xi}) = \frac{c}{\nu}\frac{r(\bar{\xi})(r(\bar{\xi}) - \frac{\sigma}{c})}{\sqrt{1-r^2(\bar{\xi})}} + \frac{1}{c}K(u(\bar{\xi})) < \frac{c}{\nu}\frac{r(\bar{\xi})(r(\bar{\xi}) - \frac{\sigma}{c})}{\sqrt{1-r^2(\bar{\xi})}} + \frac{1}{c}k = 0\,,$$

which contradicts Lemma 2.4. We focus now on the case in which there exists r^* a root of (4.15). Assume $u < 1$ and $r(\xi) < r^*$ for any $\xi \in (-\infty, \bar{\xi})$. Thus, $0 < r(\xi) < r_L < 1$ and the pair $(u(\xi), r(\xi))$ lives in a compact set for ξ near ξ_0, away from $r = 0$, $r = 1$, and maximal also in $\mathbb{R} \times (-1, 1)$. Global continuation theorems imply $\xi_0 = \infty$.

To prove (4.17) we observe that

$$\lim_{\xi\to\infty} \frac{u'(\xi)}{u(\xi)} = -\frac{c}{\nu} \lim_{\xi\to\infty} \frac{r(\xi)}{\sqrt{1-(r(\xi))^2}} = -\frac{c}{\nu}\frac{r_L}{\sqrt{1-r_L^2}} < 0\,. \tag{4.18}$$

Hence, we can use a Gronwall-type estimate in an interval $(\xi^*, +\infty)$ with ξ^* large enough so that $u'(\xi) \le -\alpha u(\xi)$ holds, where α is a positive constant and $\xi > \xi^*$.

In the case that (4.15) has no roots, let us first prove that $r_L = 1$. Arguing by contradiction (by assuming $r_L < 1$), we can use a similar argument as in the previous case by using r_L instead of r^*. In this way, we will obtain that $\xi_0 = +\infty$, and also (4.17). On the other hand, since r has a limit as ξ goes to $+\infty$, then $r'(\xi_n) \to 0$ up to a subsequence. Using this fact in the second equation of (4.13) we obtain that r_L is a root of (4.15), which contradicts our assumption. Hence, $r_L = 1$ holds and the first equation of (4.13) leads to

$$\lim_{\xi\to\xi_0} \frac{u'(\xi)}{u(\xi)} = -\infty\,. \tag{4.19}$$

Now, we use Lemma 2.5 to show the first part of (4.16). There only remains to prove that $\xi_0 < \infty$. This statement can be achieved by a contradiction argument again. Actually, if $\xi_0 = +\infty$ we get a sequence ξ_n for which $u'(\xi_n) \to 0$, which contradicts (4.19). □

Remark 4 *It is possible to follow very precisely the track of the solution of (4.13) starting from the point* $(u, r) = (0, 1)$. *Denote* $r = \tilde{r}(u)$ *the smallest root of*

$$\frac{1}{K(u)}\frac{c^2}{\nu}\left(\frac{\sigma}{c} - \tilde{r}(u)\right) = \frac{\sqrt{1-(\tilde{r}(u))^2}}{\tilde{r}(u)}\,, \qquad u \in (0,1)\,.$$

The eigenfunction associated with the eigenvalue $\lambda_+ = -\frac{\sigma}{2\nu} + \sqrt{\left(\frac{\sigma}{2\nu}\right)^2 - \frac{K'(1)}{\nu}}$, *defined at the beginning of the proof of Proposition 2.1, determines the local unstable manifold and is defined by* $\left(c\frac{\sigma+\sqrt{-4K'(1)\nu+\sigma^2}}{2K'(1)\nu}, 1\right)$. *On the other hand, it is easy to check that the following identity*

$$\lim_{u\to 1} \tilde{r}(u) = \frac{\nu}{c\,\sigma}K'(1)$$

holds. Then, $\left(1, \frac{\nu}{c\,\sigma}K'(1)\right)$ *is the tangent vector to the solution curve* $r = \tilde{r}(u)$. *Comparing the slopes of the above vectors leads to the following unrestricted inequality*

$$\frac{2K'(1)\nu}{c(\sigma + \sqrt{-4K'(1)\nu + \sigma^2})} > \frac{\nu}{c\,\sigma}K'(1)\,.$$

Therefore, the curve $r = \tilde{r}(u)$ *starting at* $u = 1$ *verifies that* $r'|_{u=1} < 0$.

4.2.3 Existence of roots for (4.15)

To conclude the section we describe the existence of roots in (4.15) depending on σ, c, ν and $k = K(0)$. This problem is equivalent to find zeros of the equation

$$\frac{c^2}{\nu k}\left(\frac{\sigma}{c} - r\right) = g(r)\,, \quad r \in (0,1)\,, \tag{4.20}$$

where g is defined as

$$g(r) = \frac{\sqrt{1-r^2}}{r}\,,$$

which is a decreasing function with a pole at $r = 0$. The left–hand side is a decreasing linear function that touches the r–axis at $\frac{\sigma}{c}$ with slope $-\frac{1}{k}\frac{c^2}{\nu}$. So, when

$$\frac{\sigma}{c} > 1 \tag{4.21}$$

there exists at least one root of (4.20), see Figure 4.1 (first two cases). Define $\tilde{r}$ as the smallest root of (4.20) in $(0,1)$.

Let us now focus our attention on the case

$$\frac{\sigma}{c} \leq 1. \tag{4.22}$$

Now, the existence of roots of (4.20) depends on $\frac{\sigma}{c}$ as well as on the slope $-\frac{c^2}{\nu}\frac{1}{k}$ of the straight line in the left–hand side of (4.20). Let us prove that for a range of values $m = \frac{c^2}{\nu}\frac{1}{k}$, there exists $\sigma^* = \sigma^*(m)$ such that for every $\frac{\sigma}{c} \in (\frac{\sigma^*}{c}, 1)$ there exists a root of (4.20). Note that $g'(r)$ has a unique maximum in $(0,1)$, around it the function is inceasing and then decreasing, verifying $g'(r) \leq -\frac{3\sqrt{3}}{2} = g'(\sqrt{2/3})$ and $\lim_{r\to 0} g'(r) = \lim_{r\to 1} g'(r) = -\infty$. Then, if $-m \leq -\frac{3\sqrt{3}}{2}$, we can claim that there exist roots in $(0,1)$ of the equation

$$g'(r) = -m\,. \tag{4.23}$$

In fact, when the inequality is strict, i.e. $-m < -\frac{3\sqrt{3}}{2}$, there are two roots in $(0,1)$ while there is only one if the equality is fulfilled, see Figure 4.1. Let us denote $\tilde{r}$ the smallest real root of (4.20), $\tilde{r} \in (0, \sqrt{2/3})$. Consider the intersection $\tilde{\delta}$ of the tangent to g at $\tilde{r}$ with the abscissa, which has the expression

$$\tilde{\delta} = \tilde{\delta}\,(m) = \tilde{r} - \frac{g(\tilde{r})}{g'(\tilde{r})} = 2\tilde{r} - \tilde{r}^3. \tag{4.24}$$

Clearly, we have that for any $\frac{\sigma}{c} \geq \tilde{\delta}\,(m)$ the equation (4.20), with $m = \frac{c^2}{\nu}\frac{1}{k}$, has at least one root in $(0,1)$. To analyze the case $\frac{\sigma}{c} < 1$ we will check the range of values m for which $\tilde{\delta}\,(m) \leq 1$. By using (4.24) we deduce that $\tilde{\delta}\,(m) \leq 1$ if and only if $\tilde{r} \leq \frac{\sqrt{5}-1}{2}$ or, according to (4.23),

$$m \geq \left(\frac{1+\sqrt{5}}{2}\right)^{\frac{5}{2}}. \tag{4.25}$$

In conclusion, under condition (4.25) there exists a root of (4.20) in $(0,1)$, for every $\frac{\sigma}{c} \geq \tilde{\delta}\,(m)$.

Define $\sigma^*(m)$ as follows

$$\frac{\sigma^*(m)}{c} = \begin{cases} \tilde{\delta}(m), & \text{when } m \geq \left(\frac{1+\sqrt{5}}{2}\right)^{\frac{5}{2}}, \\ 1, & \text{otherwise.} \end{cases} \tag{4.26}$$

Then, we have proved the following result

Proposition 2.2 *There exists a solution of (4.15) in $r \in (0,1)$ if and only if $\sigma > \sigma^*$ or $\sigma = \sigma^* < c$, where σ^* is defined by (4.26).*

As a consequence, combining Propositions 2.2 and 2.1 allows to deduce the existence of a classical solution in Theorem 1.6.

4.2.4 Proof of Lemma 2.4

In order to prove Lemma 2.4, let us provide a description of the positive invariant set associated with the flux defined by the planar system (4.13). The values (u, r) for which $r' = 0$ are defined by the equation

$$K(u) = -\frac{c^2}{\nu}\frac{r(r-\frac{\sigma}{c})}{\sqrt{1-r^2}}\,. \tag{4.27}$$

The roots of this equation can be equivalently obtained as the intersections between $g(r) = \frac{\sqrt{1-r^2}}{r}$ and the straight line $-\frac{c^2}{K(u)\nu}\left(r - \frac{\sigma}{c}\right)$. The straight line is determined by the point $\left(\frac{\sigma}{c}, 0\right)$ and the slope $-\frac{c^2}{K(u)\nu}$, where only the last one depends on u. Using (4.6), we have that the slope is a decreasing function of u verifying

$$-\infty < -\frac{c^2}{K(u)\nu} \leq -\frac{c^2}{K(0)\nu} = -\frac{c^2}{k\nu}, \qquad u \in [0,1).$$

Our purpose now is to describe the function $\tilde{r}(u)$, which is defined by the smallest root of (4.27) for σ, c and ν fixed. We will prove that he number of these roots as well as their existence depend on the value $\frac{\sigma}{c}$. Simple calculus gives that the tangent to g passing by $(\frac{\sigma}{c}, 0)$ satisfies

$$r\left(2 - r^2\right) = -\frac{g(r)}{g'(r)} + r = \frac{\sigma}{c}.$$

The maximum value of the function $r\left(2 - r^2\right)$, reached at $\sqrt{2/3}$, is $8/(3\sqrt{6})$. The value of $\frac{\sigma}{c}$ in relation to 1 and $8/(3\sqrt{6})$ will determine the different cases. In Figure 4.1 the curved lines describe the function $g(r)$ while the straight lines represent the function $\frac{1}{K(u)}\frac{c^2}{\nu}\left(\frac{\sigma}{c} - r\right)$.

In the first case (left–hand side in Figure 4.1), $\frac{\sigma}{c} \geq 8/(3\sqrt{6})$, the straight lines have an unique intersection with the curve $g(r)$ and consequently $\tilde{r}(u)$ is uniquely

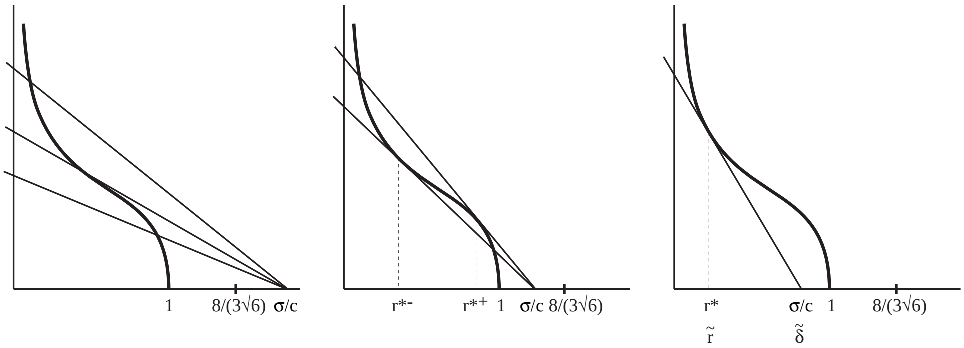

Figure 4.1: The curved lines represent the function $g(r)$ and the straight lines the functions $\frac{c^2}{\nu K(u)}\left(\frac{\sigma}{c}-r\right)$ for different values u.

determined and is a decreasing function. The second case (central picture in Figure 4.1) corresponds to $1<\frac{\sigma}{c}<8/(3\sqrt{6})$. It is easy to check that again $\tilde{r}(u)$ is uniquely determined and is a decreasing function which has the shape given in Figure 4.2 in terms of the two critical values r^{*+} and r^{*-}. Finally, the third case $0\le\frac{\sigma}{c}\le 1$ is represented by the picture in the right–hand side of Figure 4.1. The function $\tilde{r}(u)$ has the same monotonicity and well–definition properties that in the previous cases, but now the critical value r^* determines the range of definition. The analysis represented in Figure 4.1 leads to the complete definition of $\tilde{r}(u)$.

Let us now prove that the region

$$S=\left((u,r)\in(0,1)^2,\left\{\begin{array}{ll}0<r<\tilde{r}(u), & \text{if } \tilde{r}(u) \text{ is defined,}\\ 0<r<1, & \text{otherwise}\end{array}\right.\right) \tag{4.28}$$

is positively invariant. In order to prove the positive invariance of S we will describe the flux at the boundary. First, we observe that the segment $\{(u,r),\ 0\le r<1,\ u=0\}$ at the left–hand side of the square $(0,1)^2$ is invariant, which prevents the solutions to escape through it. Every point of the segment $\{(u,r),\ 0<u<1,\ r=0\}$ at the bottom of the square $(0,1)^2$ has an strict incoming flux because the vector field is vertical through this segment. The arrow coming from the corner $(u,r)=(1,0)$ corresponds to the discussion about the eigenvector for the local unstable manifold theorem in Remark 4. The solid lines in Figure 4.2 correspond to the curves $\tilde{r}(u)$ and satisfy that the vertical components of the flux are zero because $r'=0$ while $u'<0$. The dashed lines corresponding to the slopes in the curves $\tilde{r}(u)$ are also incoming points since $u'<0$ there. Then, in Figure 4.2 we have plotted the phase diagram (slope field) of the planar system (4.13), $(u,r):(-\infty,\xi_0)\to(0,1)^2$ with boundary conditions (4.14) and (4.17). Therefore, we have proved that if there exists $\bar{\xi}$ such that $(u(\bar{\xi}),r(\bar{\xi}))\in S$, then $(u(\xi),r(\xi))\in S$, for any $\xi\ge\bar{\xi}$.

We shall be done with the proof once we prove the existence of a sequence of values $\bar{\xi}_n$ such that $\bar{\xi}_n\to-\infty$ and $(u(\bar{\xi}_n),r(\bar{\xi}_n))\in S$. Using (4.14), we can deduce the existence of a sequence $\bar{\xi}_n\to-\infty$ for which $r'(\bar{\xi}_n)>0$. Now, we observe that

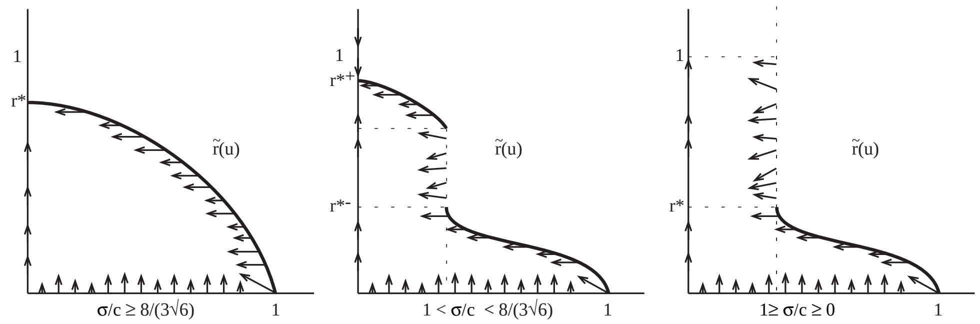

Figure 4.2: Description of the positive invariant regions S in terms of the curves $\tilde{r}(u)$.

the graphic of $\tilde{r}(u)$ splits $(0,1)\times(0,r^*)$ into two components characterized by $r' > 0$ or $r' < 0$. Since $(u(\bar{\xi}_n), r(\bar{\xi}_n)) \to (1,0)$, then $(u(\bar{\xi}_n), r(\bar{\xi}_n)) \in S \cap (0,1)\times(0,r^*)$ for n large enough. □

4.3 Entropy solutions and consequences

In this section we deal with the study of discontinuous traveling waves. So far ad authors know, there is no previous literature reporting on the existence of singular traveling waves. In this case it is necessary to use the notion of entropy solution for this equation, which has been introduced in [2].

The main result of this section is the following Theorem about existence of singular travelling wave solutions.

Theorem 3.7 *Assume $\sigma = \sigma^* = c$. Then, there exists a discontinuous entropy travelling wave solution of (4.2).*

The existence of entropy, travelling wave solutions if $\sigma < \sigma^*$ is an open problem.

Define

$$v(t,x) = \begin{cases} u(x-\sigma t), & x-\sigma t < \xi_0, \\ 0, & \text{otherwise}, \end{cases} \qquad (4.29)$$

where $\sigma \le \sigma^*$ and $u : (-\infty, \xi_0) \to (0,1)$, $\xi_0 < \infty$, is a solution of (4.8) given by Proposition 2.1. (4.16) implies that v is discontinuous.

It is not trivial to prove that some of these functions v are entropy solutions. This follows from the next two results.

Lemma 3.6 *Any solution of (4.8) satisfying (4.9)–(4.10) is log-concave in $(-\infty, \xi_0)$.*

Proof. To see that $\log(v(\xi))$ is concave, it is enough to prove that $\frac{v'(\xi)}{v(\xi)}$ is decreasing. Using the system (4.13) we have

$$\frac{v'(\xi)}{v(\xi)} = -\frac{c}{\nu}\frac{r(\xi)}{\sqrt{1-r(\xi)^2}}\,.$$

The result follows from Lemma 2.4, since the function $r \to \frac{r}{\sqrt{1-r^2}}$, $r \in (0,1)$, is strictly increasing. □

The following Proposition characterizes the entropy solutions. The proof follows the same lines of Proposition 6.6 in [3], where a similar result was obtained in the case of compact support solutions for the equation without the reaction FKPP term. Thus, combining Theorem 3.4 and Proposition 6.6 in [3] together with the null flux at infinity for non–compact support solutions and Proposition 3.15 in [2] we have

Proposition 3.3 *Let $v : [0,T) \times \mathbb{R} \to [0,1)$ and $\Omega = supp(v(0,\cdot))$ be such that for any $t \in [0,T)$:*

(i) $supp(v(t,\cdot)) = \overline{\Omega_t}$, where $\Omega_t = \Omega + B(0, ct)$.

(ii) $v \in C^2(\Omega_t)$ and satisfies the differential equation (4.2).

(iii) $v(t,x)$ has a vertical contact angle at the boundary of Ω_t, for any $t \in (0,T)$.

(iv) $v(t,x)$ is log-concave in Ω_t.

Then, v is an entropy solution.

This result allows to select an entropy solution v from those defined by (4.29). Properties (ii) and (iv) of Proposition 3.3 are satisfied by any v, but only when $\sigma = \sigma^* = c$ the statement (i) holds, i.e. $supp(v) = \Omega(t)$. Moreover, we conclude the proof of Theorem 3.7 by proving that, in this case, v has a vertical contact angle at the boundary of $\Omega(t)$, and therefore (iii) is also satisfied.

The following result can be deduced directly from Proposition 2.1. We give here a more explicit behavior of the vertical angle near ξ_0.

Lemma 3.7 *Let u be a discontinuous travelling wave for $\sigma = \sigma^* = c$. Then, the vertical angle near ξ_0 is of order $(\xi_0 - \xi)^{-\frac{1}{2}}$.*

Proof. Our starting point is system (4.13). By using Lemma 2.5 we can assure, when $\sigma \leq \sigma^*$, that there exists a constant $\alpha_\sigma > 0$ and ξ_0 such that $u(\xi_0) = \alpha_\sigma$ and $r(\xi_0) = 1$. In the case $\sigma = \sigma^* = c$, (4.13) leads to

$$r' = \frac{1}{c}K(u) - \frac{c}{\nu}r\frac{\sqrt{1-r}}{\sqrt{1+r}}\,.$$

Clearly $r'(\xi_0) = \frac{1}{c}K(\alpha_\sigma) < \infty$. An expansion of $r(\xi)$ in Taylor series around ξ_0 allows to find $r(\xi) = 1 + \frac{1}{c}K(\alpha_\sigma)(\xi - \xi_0) + O((\xi - \xi_0)^2)$. Now, combining this expression with the equation for u and integrating between ξ_0 y ξ, $0 < \xi_0 - \xi \ll 1$, we obtain

$$-\log(u(\xi_0)) + \log(u(\xi)) = \frac{c}{\nu}\frac{2}{\left(2\frac{1}{c}K(\alpha_\sigma)\right)^{\frac{1}{2}}}(\xi_0 - \xi)^{\frac{1}{2}} - \frac{c}{\nu}\left(\frac{K(\alpha_\sigma)}{2c}\right)(\xi_0 - \xi)^{\frac{3}{2}}\,.$$

Neglecting higher–order terms we find $u(\xi) = \alpha_\sigma e^{\frac{2}{\left(2\frac{1}{c}K(\alpha_\sigma)\right)^{\frac{1}{2}}}(\xi_0-\xi)^{\frac{1}{2}}}$ or

$$u(\xi) = \alpha_\sigma + \alpha_\sigma \frac{2}{\left(2\frac{1}{c}K(\alpha_\sigma)\right)^{\frac{1}{2}}}(\xi_0 - \xi)^{\frac{1}{2}}\,, \qquad \text{for } 0 < \xi_0 - \xi \ll 1\,,$$

after Taylor expansion. □

Remark 5 *Since classical solutions are in particular entropy solutions, the existence of travelling waves for $\sigma \geq \sigma^*$ is completed. The existence of an entropy solution for $\sigma < \sigma^*$ is an open question, we can only assure that the corresponding function v, defined by (4.29), is not an entropy solution. This follows from the fact established in Theorem 3.9 of [2], that the support of any log-concave solution moves with speed c while the support of $v(t,\cdot)$ moves with $\sigma < c$.*

Remark 6 *The existence of travelling waves having different profiles from wave fronts is also an open question. It can be proved that no more classical (C^2) wave fronts exist. The authors conjecture that no more entropy travelling wave solution will exist, but it is likely to be a much harder problem.*

To conclude this section we propose an application of the travelling wave solutions with $\sigma^* < c$ that allows to bound entropy solutions.

Proposition 3.4 *Let $u_0 : \mathbb{R} \to [0,1)$ be a measurable function with compact support and* ess sup$(u_0) < 1$. *Let $u(t,x)$ be an entropy solution of (4.2) with initial data u_0. Then,*

$$\text{ess sup}_{x\in\mathbb{R}}(u(t,x)) < 1$$

and for any $c > \sigma > \sigma^*$ there exist positive constants α and β not depending on σ such that

$$\text{ess sup}_{|x|>\sigma t} u(t,x) \leq \alpha e^{-\beta(\sigma-\sigma^*)t}.$$

In addition, if $\sigma > c$ we have

$$\text{ess sup}_{|x|>\sigma t} u(t,x) = 0$$

for large t.

Proof. Let $v^*(t,x) = u^*(x - \sigma^* t)$ be a C^2 travelling wave solution of (4.2) defined by Theorem 1.6. Then, we can take a translation of u^*, still denoted u^* for simplicity, such that $u^*(\xi) \geq u_0(\xi)$. A comparison principle for entropy solutions, see Theorem 3.8 in [2], leads to

$$u(t,x) \leq u^*(x - \sigma^* t), \quad \text{a.e. } (t,x) \in \mathbb{R}^2.$$

On the other hand, for a classical travelling wave there exist positive constants α and β such that

$$u(\xi) \leq \alpha e^{-\beta\xi}\,, \quad \xi \in \mathbb{R}\,.$$

This upper estimate is a consequence of the fact that u^* is uniformly bounded and $\lim_{\xi\to\infty} \frac{(u^*(\xi))'}{u(\xi)}$ is strictly negative as pointed out in (4.18). Hence, we find

$$u(t,x) \leq u^*(x - \sigma^* t) \leq \alpha e^{-\beta(x-\sigma^* t)}, \quad \text{a.e. } (t,x) \in \mathbb{R}^2. \tag{4.30}$$

Assuming now that $x > \sigma\, t$, we deduce from (4.30) the inequality

$$u(t,x) \leq \alpha e^{-\beta(\sigma-\sigma^*)t}, \quad \text{a.e. } (t,x) \in \mathbb{R}^2,\ x > \sigma\, t. \tag{4.31}$$

In the case $x < -\sigma\, t$ we can argue in a similar way by using a classical travelling wave $\tilde{u}^*(\sigma^* t - x)$ such that $u_0(\xi) < \tilde{u}^*(-\xi)$.

The second assertion follows by a comparison argument with the singular travelling wave defined by (4.29). □

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