On some nonlinear partial differential equations for classical and quantum many body systems

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Declaration

This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except where specifically indicated in the text.

Daniel Marahrens

I dedicate this thesis to my parents Sigrid and Friedrich Marahrens for their limitless love, encouragement, and support

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Abstract

This thesis deals with problems arising in the study of nonlinear partial differential equations arising from many-body problems. It is divided into two parts: The first part concerns the derivation of a nonlinear diffusion equation from a microscopic stochastic process. We give a new method to show that in the hydrodynamic limit, the particle densities of a one-dimensional zero range process on a periodic lattice converge to the solution of a nonlinear diffusion equation. This method allows for the first time an explicit uniform-in-time bound on the rate of convergence in the hydrodynamic limit. We also discuss how to extend this method to the multi-dimensional case. Furthermore we present an argument, which seems to be new in the context of hydrodynamic limits, how to deduce the convergence of the microscopic entropy and Fisher information towards the corresponding macroscopic quantities from the validity of the hydrodynamic limit and the initial convergence of the entropy.

The second part deals with problems arising in the analysis of nonlinear Schrödinger equations of Gross–Pitaevskii type. First, we consider the Cauchy problem for (energy-subcritical) nonlinear Schrödinger equations with subquadratic external potentials and an additional angular momentum rotation term. This equation is a well-known model for superfluid quantum gases in rotating traps. We prove global existence (in the energy space) for defocusing nonlinearities without any restriction on the rotation frequency, generalizing earlier results given in the literature. Moreover, we find that the rotation term has a considerable influence in proving finite time blow-up in the focusing case. Finally, a mathematical framework for optimal bilinear control of nonlinear Schrödinger equations arising in the description of Bose–Einstein condensates is presented. The obtained results generalize earlier efforts found in the literature in several aspects. In particular, the cost induced by the physical work load over the control process is taken into account rather then often used L^2– or H^1–norms for the cost of the control action. We prove well-posedness of the problem and existence of an optimal control. In addition, the first order optimality system is rigorously derived. Also a numerical solution method is proposed, which is based on a Newton type iteration, and used to solve several coherent quantum control problems.

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Nomenclature

General Notation

$x_n \rightharpoonup x$ Weak convergence of the sequence $(x_n)_{n\in\mathbb{N}}$ to x

$x_n \to x$ Strong convergence of the sequence $(x_n)_{n\in\mathbb{N}}$ to x

$L^p(\mathbb{R}^d)$ The space of Lebesgue–integrable functions whose absolute value raised to the p–th power has finite integral

$H^k(\mathbb{R}^d)$ The Sobolev space $W^{k,2}(\mathbb{R}^d)$

$W^{k,p}(\mathbb{R}^d)$ The Sobolev space of k-times weakly differentiable functions with derivatives in $L^p(\mathbb{R}^d)$

$\dot{W}^{k,p}(\mathbb{R}^d)$ The homogeneous Sobolev space of degree n

$L^p_t L^q_x$ Short-hand for $L^p(0,T;L^q(\mathbb{R}^d))$, the space of functions that are L^p–integrable in t and L^q–integrable in x

$\langle\cdot,\cdot\rangle$ An inner product, or an integration of a function with respect to a measure. More generally, a duality pairing

Hydrodynamic Limits

$\mathbb{T}^d_N$ The discrete torus

x, y, z Microscopic variables, i.e. sites in $\mathbb{T}^d_N$

$x \sim y$ Denotes the fact that $x, y \in \mathbb{T}^d_N$ are neighbours, i.e. $|x-y| = 1$

$\mathbb{T}^d$ The continuous torus $\mathbb{R}^d/\mathbb{Z}^d$

u Macroscopic variables, i.e. positions $u \in \mathbb{T}^d$

X_N The state space of the discrete particle system

η, ξ Particle configurations in X_N

α_η^N The empirical measure

$\delta_{x/N}$ The Dirac distribution centered at $x/N \in \mathbb{T}^d$

H The function space of the limit equation

$\alpha_\eta^{N,\epsilon}$ The mollified empirical measure

$\delta_{x/N}^{(\epsilon)}$ The mollified Dirac distribution centered at $x/N \in \mathbb{T}^d$ (a Dirac sequence with respect to ϵ)

$\mathfrak{s}, \mathfrak{r}$ Multi-indices in $\mathbb{N}^d$

$P(X_N)$ Space of probability measures on X_N

$C_b^k(\mathbb{R})$ Uniformly bounded k-times differentiable functions on $\mathbb{R}$ with uniformly bounded derivatives

$C_b(X_N)$ Space of bounded continuous functions on X_N with supremum norm

$\mathcal{M}_+(\mathbb{T}^d)$ The set of positive Radon measures on the torus

f^N, f_0^N, f_t^N Functions in $C_b(X_N)$; usually densities with respect to some measure in $P(X_N)$

μ, ν Probability measures

μ^N, ν^N Probability measures on the state space X_N

f, f_0, f_t Functions in (a subset of) H

$H^N(\mu|\nu)$ Microscopic relative entropy of two probability measures μ and ν

$\mathcal{D}^N(\mu|\nu)$ Microscopic Fisher information corresponding to $H^N(\mu|\nu)$

H^∞ Entropy of the limit equation

$\mathcal{D}^\infty$ Fisher information of the limit equation

ν_ρ^N The Gibbs measure with average density ρ

Ψ, Φ Observables in $C(H)$

φ A test function in $C(\mathbb{T}^d)$

ρ, ϱ Different densities $\rho, \varrho \in [0, \infty)$

S_t^∞ Semigroup of the limit equation

S_t^N Semigroup of the particle process

T_t^N Dual semigroup of S_t^N of the particle process on $C_b(X_N)$

T_t^∞ Pullback semigroup of S_t^∞ on the level of observables

$DS_t^\infty, DT_t^\infty, D\Psi$ Derivatives in the sense of linearizations, cf. Def. 2.4.16

Schrödinger Equations

ψ A wave function, solution to a (nonlinear) Schrödinger equation

$U(x)$ An external potential

$V(x)$ A control potential

$W(t,x)$ A time-dependent potential

λ The proportionality factor in front of nonlinearity

σ The exponent of nonlinearity of Gross-Pitaevskii type

$\alpha(t)$ A time-dependent control parameter

Ω The angular velocity vector of a rotation

L The quantum angular momentum operator

E_0 The energy without angular momentum

E_Ω The energy of the NLS with rotation

L_Ω The ensemble-average of the angular momentum

Σ The energy space of solutions

Σ^m The higher-order energy space

$S(t)$ The unitary semigroup of a linear Schödinger equation

A An observable

J The objective functional

γ_1, γ_2 Cost parameters appearing in J

$\mathcal{J}$ The reduced objective functional

$P(\psi, \alpha)$ The operator of a nonlinear Schrödinger equation

φ The solution to the adjoint equation

$\mathcal{J}'(\alpha)$ The (Gâteaux-)derivative of $\mathcal{J}(\alpha)$ with respect to α

$F(t,s)$ The propagator of the adjoint equation

Chapter 1

Introduction

The theory of partial differential equations (PDE) is one of the main research areas in mathematics and has applications in many disciplines, among them physics, engineering, economics, and chemistry. While the fundamental laws of nature as discovered by Isaac Newton, Albert Einstein, Erwin Schrödinger, Werner Heisenberg, and many others, can be expressed as differential equations, there is a plethora of models describing nature in terms of a partial differential equation, which cannot yet be justified from first principles. Often these models are obtained by considering systems of many interacting entities (in gases on the order of 10^{26} particles), where the entities can be comprised of anything from classical particles in gases to pedestrians within crowds. These systems inherently possess two scales, a microscopic one and a macroscopic one. While it is usually fairly simple to establish the microscopic laws, it is impossible to solve them for most many body systems, making a purely microscopic description infeasible. Fortunately, we are not interested in the properties of every single entity (henceforth called particle). Instead it often suffices to know certain macroscopic, measurable quantities like the density, the temperature, or the velocity. One of the important challenges of science lies in the derivation of macroscopic, effective PDE models for these macroscopic quantities when only the microscopic laws of interaction are known. In the many body systems under consideration in this thesis, this effective description is accurate in the limit of infinitely many particles. An important step in the study of scaling limits of interacting particle systems usually consists in showing that correlations (between particles or occupation numbers) vanish in the limit. This allows one to replace the interactions between different particles by a self-consistent field according to a mean-field theory. These self-consistent fields imply that the limit equation is in general nonlinear. The analysis of nonlinear partial differential equations is in and of itself an important field of study. In this thesis we will show how to obtain a limit description from a class of microscopic dynamics and investigate two problems related to a particular limit system, the nonlinear Schrödinger equation.

Part I of this thesis deals with the rigorous derivation of a macroscopic PDE descrip-

tion from a microscopic stochastic particle dynamics. The derivation of limit descriptions from stochastic interacting particle systems has a long history that can be traced back to Ludwig Boltzmann. Since a rigorous approach is so far only feasible for simple models, we concentrate on a well-studied interacting particle system, the zero range process on a domain with periodic boundary conditions. The zero range process is a stochastic jump process consisting of discrete particles on a lattice, where particles only interact if they occupy the same lattice site. The macroscopic limit for the zero range process in the hydrodynamic scaling, i.e. large time and space scales, is well-known and has been shown to hold in [36] and [86], using different methods. Our contribution to the hydrodynamic limit, presented in Chapter 2, is a new approach that allows us to obtain an explicit rate of convergence which holds uniform in time. This approach is based on a Duhamel–type formula in the space of observables, here taken to be the space of continuous functions of the state space. Furthermore, we present an argument which seems to be new in the context of hydrodynamic limits, which allows to establish the convergence of the microscopic entropy and Fisher information to their macroscopic versions.
In Part II, we consider the nonlinear Schrödinger equation, which in a special (cubic) case is obtained in a scaling limit of the Schrödinger equation for infinitely many Bosonic particles (Bose-Einstein condensation) [28]. Here the microscopic scale is given by the scattering length of the interaction potential, which must be macroscopically small for the particle correlations to vanish in the limit of infintely many particles. The nonlinear Schrödinger equation has received a lot of attention in mathematical physics not only as a model for ultra-cold dilute atomic gases, but also for nonlinear optics and shallow water waves. From the mathematical point of view, it is a dispersive semilinear equation exhibiting many interesting phenomena such as the existence of solitons, scattering, blow-up, and global existence in different parameter ranges. In this thesis we concentrate on two problems for the nonlinear Schrödinger equation. First we consider in Chapter 3 a nonlinear Schr "odinger equation with an angular momentum rotation term which has been used in the physics literature as a model for Bose-Einstein condensates in a rotating trap. We investigate local and global existence in the usual parameter ranges, i.e. local existence for energy-subcritical nonlinearities, and global existence for mass-subcritical or defocusing nonlinearities. Furthermore we deduce conditions on the existence of blow-up solutions by a virial argument (following Glassey's approach [32]).
As a second application, in Chapter 4 we consider the optimal control problem corresponding to the nonlinear Schrödinger equation. The experimental control of quantum systems described by linear and nonlinear Schrödinger equations has applications in microscopic magnetic-field imaging, atom interferometry, and quantum computing, to name but a few examples. In many applications, one is not interested in controlling the whole state of the system but only a few observables. In order to guarantee well-posedness of the control problem, we restrict ourselves to minimizing a certain objective functional

consisting of the observable quantity we want to minimize and a “regularizing” cost term. Thus we propose a mathematical framework for optimal control of nonlinear Schrödinger equations through an external potential, where the objective functional is given by the expected value of the observable with the H^1–norm of the energy as regularizing term. In our example, the external potential depends on the control parameter only through its amplitude, whereas its general shape is fixed. The choice of the H^1–norm of the energy has the advantage that it penalizes large oscillations which are typically found for cost terms involving the L^2–norm. Furthermore it has a direct physical interpretation as the L^2–norm of the power, i.e. the time–derivative of the energy.
In the rest of this introduction, I will give a brief mathematical exposition of the results obtained in this thesis.

1.1 Quantitative uniform hydrodynamic limits

The zero range process on the discrete torus is an stochastic interacting particle system on the lattice $\mathbb{T}_N^d = \{1, \dots, N\}^d$ with state space $X_N = \mathbb{N}^{\mathbb{T}_N^d}$, i.e. $\eta \in X_N$ is the particle configuration with $\eta(x)$ particles at each site $x \in \mathbb{T}_N^d$. Particles are randomly distributed over the lattice and perform a jump process, jumping to neighbouring sites at a rate that only depends on the number of particles at the original site, see Figure 1.1. The distribution of particle configurations at each time $t > 0$ is a probability measure $\mu_t^N \in P(X_N)$, where $P(X_N)$ is the set of probability measures on X_N. Let us denote by $C_b(X_N)$ the space of uniformly bounded, continuous functions and the integral of a function $f^N \in C_b(X_N)$ with respect to the measure $\mu^N \in P(X_N)$ by

$$\langle \mu^N, f^N \rangle = \int_{X_N} f^N(\eta); d\mu^N(\eta).$$

Then the evolution of the state $\mu_t^N \in P(X_N)$ of the particle process, given an initial distribution $\mu_0^N \in P(X_N)$, is determined by

$$\frac{d}{dt}\langle \mu_t^N, f^N \rangle = \langle \mu_t^N, G^N f^N \rangle \qquad \text{for all } f^N \in C_b(X_N),$$

where the generator $G^N : C_b(X_N) \to C_b(X_N)$ satisfies

$$G^N f^N(\eta) = N^2 \sum_{x \sim y \in \mathbb{T}_N^d} g(\eta(x))\big(f^N(\eta^{x,y}) - f^N(\eta)\big). \tag{1.1}$$

Here the sum over $x \sim y$ is over all sites $x, y \in \mathbb{T}_N^d$ that are neighbours, i.e. $|x - y| = 1$, and $\eta^{x,y}$ is the state of the particle system after one particle has jumped from x to y.

Explicitly it holds that

$$\eta^{x,y}(z) = \begin{cases} \eta(x) - 1 & \text{if } z = x, \\ \eta(y) + 1 & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases}$$

In this thesis, we shall assume that the jump rates are not degenerate and satisfy a monotonicity condition which corresponds to uniform ellipticity of the limit equation. A

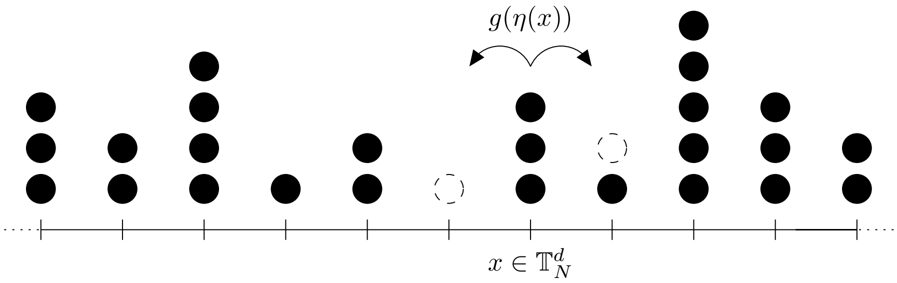

Figure 1.1: The microscopic model. A particle jumps from a site x with $\eta(x)$ particles to a randomly chosen neighbouring site at a rate $g(\eta(x))$.

measure $\nu^N \in P(X_N)$ is invariant under the evolution of the zero range process if

$$\langle \nu^N, G^N f^N \rangle = 0 \quad \text{for all } f^N \in C_b(X_N).$$

We shall see in Chapter 2 that there exists a family of invariant (and translation-invariant) measures ν_ρ^N, indexed by their mean density $\rho \geq 0$, for which the occupation numbers $\eta(x)$, $x \in \mathbb{T}_N^d$, are mutually independent. The average jump rate under the law of ν_ρ^N is a smooth function $\sigma : [0, \infty) \to [0, \infty)$, i.e.

$$\langle \nu_\rho^N, g(\eta(x)) \rangle = \sigma(\rho).$$

If we assume the process to equilibrate locally, we can expect the densities to converge locally by a law of large numbers and the densities $f_t(u)$ at macroscopic points $u \in \mathbb{T}^d$ to change according to a partial differential equation. The limit equation is the filtration equation

$$\partial_t f_t(u) = \Delta \sigma(f_t(u)) \text{ for all } t > 0,\ u \in \mathbb{T}^d, \tag{1.2}$$

where $f_t : \mathbb{T}^d \to [0, \infty)$ denotes the particle density at time t. Here we shall only consider uniformly elliptic limit equations, i.e. $\sigma'(\rho) \geq \delta > 0$ for all $\rho \geq 0$.

The scaling factor N^2 in the definition (1.1) of G^N yields a (macroscopic) time scale and is related to the fact that the limit equation is a second order PDE. In order to get a continuum description via a partial differential equation, we also need to scale space by embedding the discrete torus into the continuous (macroscopic) torus $\mathbb{T}_N^d \subset \mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$

via $x \mapsto x/N \in \mathbb{T}^d$. Thus the microscopic spatial scale is N^{-1}, whereas the microscopic time scale is N^2. This implies a macroscopically visible displacement of particles through the non-zero variance of the jumps, since by symmetry the mean displacement of the particles vanishes. If the number of particles remains roughly constant with respect to N, we expect that the average density $N^{-1}\sum_{x\in\mathbb{T}_N^d}\eta(x)$ does not scale with N. The zero range process has only one conserved quantity, the total number of particles, and hence the particle density is the only macroscopic information which we can expect to retain in the limit as $N \to \infty$. We measure particle densities via the empirical measure

$$\alpha_\eta^N(du) = \frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\eta(x)\delta_{\frac{x}{N}}(du),$$

where δ_u is the Dirac mass at $u \in \mathbb{T}^d$. The convergence of local particle densities can be quantified in terms of weak convergence of the empirical measure. Thus we test α_η^N with a function $\varphi \in C(\mathbb{T}^d)$ and expect convergence of the resulting random variable $\langle \alpha_\eta^N, \varphi\rangle$ under the law μ_t^N. Assuming that the initial data are compatible and f_t solves (1.2), it

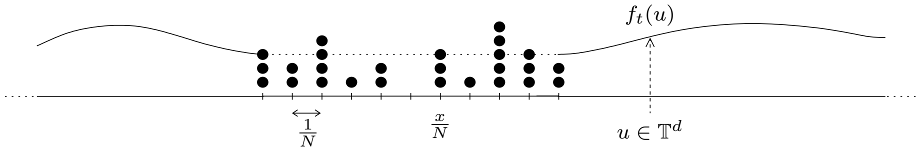

Figure 1.2: Embedding $\mathbb{T}_N^d$ into $\mathbb{T}^d$ yields lattice sites of distance $1/N$. In the limit, we obtain a limit density f_t.

holds that

$$\lim_{N\to\infty}\mathbb{P}_{\mu_t^N}\big(|\langle\alpha_\eta^N,\varphi\rangle - \langle\varphi, f_t\rangle| > \delta\big) = 0, \tag{1.3}$$

where $\mathbb{P}_{\mu_t^N}(\mathcal{A})$ denotes the probability of the event $\mathcal{A}$ under μ_t^N, i.e. $\langle\mu_t^N, \chi_{\mathcal{A}}\rangle$, where $\chi_{\mathcal{A}}$ is the characteristic function of $\mathcal{A}$. Figure 1.2 gives an idea of the microscopic scaling (in space) and the local particle densities. The proof of this result was given in [36] for the Ginzburg-Landau model with Kawasaki dynamics, which is a closely related model. Their proof holds for the zero range process with only minor modifications, see for instance [47]. Further results are available in the literature, e.g. the relative entropy method [86] which shows convergence of the relative entropy with respect to local equilibrium states and can probably be extended to give an explicit rate of convergence - however there is no reason to expect the convergence to be uniform in time. Let us also mention that there exists a result [34] for the Ginzburg-Landau model with Kawasaki dynamics with (almost) explicit rate of convergence which can be extended to hold uniformly in time - however it is not yet clear how to extend this result to the zero range process. Our contribution to the theory is a new approach to quantify the rate of convergence and make it uniform in time.

Specifically, letting $F \in C_b^2(\mathbb{R})$, we prove the convergence

$$\Big| \langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle\big) \rangle - F\big(\langle f_t, \varphi\rangle_{L^2}\big) \Big| \leq CN^{-\beta} \tag{1.4}$$

for some $\beta > 0$, uniformly in $t > 0$. This implies the convergence in probability in (1.3) upon choosing F to be an approximation of an indicator function with support on a translation of $(-\epsilon, \epsilon)$. Even though the particle trajectories diverge as $t \to \infty$, the dissipative properties of the system motivate the uniform convergence: As $t \to \infty$, the system relaxes to an invariant measure, for which the hydrodynamic limit holds. Our approach seems to be fairly flexible and we hope that it can be applied to more complex problems. It was originally developed by Mischler and Mouhot [67] to derive an explicit uniform rate of convergence of a jump process towards the (homogeneous in space) Boltzmann equation. Let us now present the idea of this approach. First, without worrying about regularity, we set

$$\Psi(f) = F(\langle f, \varphi\rangle)$$

for any function or distribution f on $\mathbb{T}^d$. The function Ψ can be turned into a function of the empirical measure by employing the map π^N defined by

$$(\pi^N \Psi)(\eta) = \Psi(\mu_\eta^N) \text{ for all } \eta \in X_N.$$

Furthermore we can define a limit semigroup on functions on $\mathbb{T}^d$ via the pushforward

$$T_t^\infty \Psi(f) = \Psi(f_t),$$

where f_t solves the filtration equation (1.2) with initial datum f_0. Employing this notation, we can estimate the hydrodynamic limit (1.4) by

$$\Big| \langle \mu_0^N, (T_t^N \pi^N \Psi)(\eta) - (\pi^N T_t^\infty \Psi)(\eta)\rangle \Big| + \Big| \langle \mu_0^N, T_t^\infty \Psi(\alpha_\eta^N) - T_t^\infty \Psi(f_0)\rangle \Big|.$$

If the initial data converge in an appropriate sense, we can estimate the second term by a stability estimate on the limit equation corresponding to contractivity of the semigroup T_t^∞. The idea that allows us to estimate the first term is as follows. Just like T_t^N has a generator G^N, so, too, the limit semigroup T_t^∞ has a generator (time-derivative) G^∞. Then we obtain that

$$\begin{aligned} \pi^N(T_t^\infty \Psi) - T_t^N(\pi^N \Psi) &= \int_0^t \frac{d}{ds}\big(T_{t-s}^N \pi^N T_s^\infty \Psi\big)\, ds \\ &= \int_0^t T_{t-s}^N\big(\pi^N G^\infty - G^N \pi^N\big) T_s^\infty \Psi \, ds. \end{aligned}$$

We will provide a consistency estimate for the difference $\pi^N G^\infty - G^N \pi^N$ and use stability results to transport this convergence along the evolution of the limit equation which is given by T_s^∞. This will allow us to obtain a uniform explicit rate of convergence.
Finally we shall present a new argument which allows one to prove convergence of the microscopic entropy to a macroscopic entropy. Let $f_\infty = \int_{\mathbb{T}^d} f_0(u)\, du$ be the constant towards which the macroscopic density equilibrates due to the dissipation. The microscopic entropy with respect to the invariant measure $\nu_{f_\infty}^N$ is given by

$$H^N(\mu_t^N|\nu_{f_\infty}^N) = \int_{X_N} \log\left(\frac{d\mu_t^N}{d\nu_{f_\infty}^N}(\eta)\right) d\mu_t^N(\eta).$$

It holds that

$$\frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) + \int_0^t 4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\, ds \leq \frac{1}{N^d} H^N(\mu_0^N|\nu_{f_\infty}^N), \tag{1.5}$$

where

$$\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N) = \langle \nu_{f_\infty}^N, \sqrt{\frac{d\mu_t^N}{\nu_{f_\infty}^N}} G^N \sqrt{\frac{d\mu_t^N}{\nu_{f_\infty}^N}} \rangle$$

is the microscopic Fisher information. Variational formulae are readily available for both the entropy and the Fisher information which allow us to prove that

$$\liminf_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) \geq H_\infty(f_t), \text{ where} \tag{1.6}$$
$$H_\infty(f_t) = \int_{\mathbb{T}^d}\int_{f_\infty}^{f_t(u)} \log\sigma(\rho)\, d\rho\, du$$

is the macroscopic entropy and

$$\liminf_{N\to\infty} \frac{4}{N^{d-2}} \mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N) \geq \mathcal{D}_\infty(f_t), \text{ where} \tag{1.7}$$
$$\mathcal{D}_\infty(f_t) = \int_{\mathbb{T}^d} \frac{|\nabla\sigma(f_t(u))|^2}{\sigma(f_t(u))}\, du$$

is the macroscopic Fisher information. Differentiation of $H_\infty(f_t)$ in time yields

$$H_\infty(f_t) + \int_0^t \mathcal{D}_\infty(f_s)\, ds = H_\infty(f_0) \tag{1.8}$$

Now, let us assume that the initial microscopic entropy converges to the initial macroscopic entropy, i.e.

$$\lim_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) = H_\infty(f_t). \tag{1.9}$$

Collecting the relations (1.5)-(1.9), we obtain that

$$\lim_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) = H_\infty(f_t) \text{ and}$$
$$\lim_{N\to\infty} \int_0^t 4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\, ds = \int_0^t \mathcal{D}_\infty(f_s)\, ds$$

Note that in Chapter 2 we shall use an equivalent formulation of $H_\infty(f_t)$ in order to prove the above inequality on the limit inferior of the microscopic entropy.

1.2 The nonlinear Schrödinger equation

In Part II, we shall consider the nonlinear Schrödinger equation (NLS), by which we mean the partial differential equation

$$i\partial_t\psi(t,x) = -\frac{1}{2}\Delta\psi(t,x) + U(x)\psi(t,x) + \lambda|\psi(t,x)|^{2\sigma}\psi(t,x)$$

for all $(t,x) \in \mathbb{R}\times\mathbb{R}^d$. Here $i = \sqrt{-1}$, $\lambda \in \mathbb{R}$ and $\sigma \geq 0$ are two parameters describing the nonlinearity, and $V : \mathbb{R}^d \to \mathbb{R}$ is an external potential. As mentioned before, at least in the cubic case $\sigma = 1$, this equation can be obtained from the usual (linear) Schrödinger equation in the limit of infinitely many bosons. In the cubic case, the equation is also known as Gross-Pitaevskii equation. The NLS conserves mass and energy

$$M = \|\psi\|^2_{L^2(\mathbb{R}^d)}, \qquad E = \int_{\mathbb{R}^d} \left(\frac{1}{2}|\nabla\psi|^2 + \frac{\lambda}{\sigma+2}|\psi|^{2\sigma+2} + U|\psi|^2\right) dx.$$

One of the interesting features of this equation is the occurrence of blow-up in certain parameter regimes. Let us quickly discuss some aspects of the existence theory for the NLS without external potential, i.e. $U = 0$. In this thesis, we will look for solutions in the energy space, i.e. the space where the energy is finite. Since it holds that $H^1(\mathbb{R}^d) \subset L^{2\sigma+2}(\mathbb{R}^d)$ if $\sigma < 2/(d-2)$, a good choice for the energy space is $H^1(\mathbb{R}^d)$, where the contribution of the nonlinearity to the energy can be estimated by the contribution of the linear part. This is further motivated by the observation that the NLS is semilinear, i.e. the nonlinear part only involves derivatives of the solution ψ which are of lower order than the whole PDE. Hence it is convenient to treat the nonlinearity as a perturbation of the linear part. To this end, let $S(t) = e^{\frac{i}{2}\Delta t}$ denote the semigroup of the free Schrödinger equation

$$i\partial_t\psi(t,x) = -\frac{1}{2}\Delta\psi(t,x).$$

The mild form of the NLS with initial datum $\psi(t=0,x) = \psi_0(x)$ then becomes

$$\psi(t) = S(t)\psi_0 - i\lambda \int_0^t S(t-s)|\psi(s)|^{2\sigma}\psi(s)\, ds$$

where we have set $\psi(t) = \psi(t,\cdot)$ for ease of notation. If $\sigma = 0$, there is of course global existence. Similar to ordinary differential equations, we can look for mild solutions as fixed points of an appropriately defined map. Local existence is then shown by smoothing properties of the linear part of the equation combined with (Sobolev) embeddings in order to control the nonlinear part. The free Schrödinger equation is not dissipative and does not possess the strong smoothing effects of the heat equation, but its dispersive nature accords us with weaker decay estimates, the so-called Strichartz estimates. These can indeed be used to prove local existence in the energy space $H^1(\mathbb{R}^d)$ if $\sigma < 2/(d-2)$. These local solutions can be continued until the $H^1(\mathbb{R}^d)$–norm of the solution diverges. In the special case of a positive nonlinearity $\lambda \geq 0$, the energy is the sum of two positive quantities. Since the energy is also conserved, both quantities are indeed bounded and in particular, the L^2–norm of the gradient of the solution is uniformly bounded in time. Since the mass $\|\psi\|_{L^2(\mathbb{R}^d)}$ is conserved as well, we conclude that there exists a global solution if $\lambda \geq 0$. Let us now consider the case $\lambda < 0$. A quick calculation yields the virial identity

$$\begin{aligned}\frac{d^2}{dt^2}\int_{\mathbb{R}^d} x^2|\psi(t,x)|^2\, dx &= \int_{\mathbb{R}^d}\left(|\nabla\psi(t,x)|^2 + \lambda\frac{d\sigma}{\sigma+1}|\psi(t,x)|^{2\sigma+2}\right) dx\\ &= 2E + \int_{\mathbb{R}^d}\lambda\frac{d\sigma-2}{\sigma+1}|\psi(t,x)|^{2\sigma+2}\, dx.\end{aligned}$$

Hence if $\sigma \geq d/2$ and $E < 0$, the (positive) integral on the left hand side is bounded by an inverted parabola, which is not possible for all times. Note that it can also be shown that the solution is global if $\sigma < d/2$, whatever the sign of λ. To summarize, local existence holds in the following case:

- initial datum in the energy space $\psi \in H^1(\mathbb{R}^d)$ and energy-subcritical nonlinearity $\sigma < 2/(d-2)$

and global existence holds if additionally

- defocusing nonlinearity $\lambda \geq 0$, or
- mass-subcritical nonlinearity $\sigma < d/2$.

Otherwise, blow-up solutions exist. The described situation generally remains the same in the presence of an external potential U, provided this potential satisfies certain regularity properties, e.g. $|U(x)| \leq C|x|^2$ is subquadratic. In Chapter 3, we shall investigate the NLS with an additional angular momentum term, which describes a rotating Bose-Einstein condensate. In Chapter 4, we consider an optimal control problem for the NLS. Our results are summarized in the next two subsections.

1.2.1 Existence theory with an angular momentum rotation term

The NLS with angular momentum rotation term is the partial differential equation

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + U(x)\psi + \lambda|\psi|^{2\sigma}\psi - \Omega\cdot L\psi, \quad (t,x)\in\mathbb{R}\times\mathbb{R}^3,$$

where $\lambda\in\mathbb{R}$, $\sigma\geq 0$, and U subquadratic. The angular momentum rotation term is given by a angular velocity vector $\Omega\in\mathbb{R}^3$ and the angular momentum $L=-ix\wedge\nabla$, where $\wedge$ denotes the cross product in $\mathbb{R}^3$. This equation also makes sense in two dimensions, where the plane of rotation is the space $\mathbb{R}^2$. In fact, the two-dimensional NLS is usually obtained as an approximation of the three-dimensional NLS in the case of a strongly confining potential (a disc-shaped condensate). Hence we shall consider both cases $d=2,3$. So far this equation has only been considered in [37, 38] for the special case where U is a harmonic trapping potential with frequency exactly equal to $|\Omega|$. In the present setting, the energy space is $\Sigma=\{\psi\in H^1(\mathbb{R}^d) : x\psi\in L^2(\mathbb{R}^d)\}$. Using Strichartz estimates for the linear part including the rotation term, we find that local existence in Σ holds in the usual case $\sigma<2/(d-2)$ (i.e. $sigma<\infty$ if $d=2$). The same methods also allow us to deduce global existence if $\sigma<2/d$ is mass-subcritical. In order to obtain global existence in the defocusing case $\lambda>0$, we change into a rotating coordinate system. Let $X(t,x)$ denote the vector obtained from rotating x around the axis Ω by an angle of $-|\Omega|t$, then the wave function $\tilde{\psi}$ in the new coordinates $X(t,x)$ solves

$$i\partial_t\tilde{\psi} = -\frac{1}{2}\Delta\tilde{\psi} + U(X(t,x))\tilde{\psi} + \lambda|\tilde{\psi}|^{2\sigma}\tilde{\psi}.$$

This is a NLS with time-dependent potential and as such can be treated as in [18], where global existence has been shown to hold in the presence of time-dependent potentials if $\lambda>0$. Furthermore we present two variants of Glassey's virial identity to deduce existence of blow-up if $\lambda<0$. These conditions are stricter than the above conditions due to Glassey, but coincide in the symmetric or rotation-less case. We finish the chapter on the NLS with angular momentum rotation term with a discussion of numerical simulations, where we emphasize how the change of coordinates $X(t,X)$ can be employed to simplify numerical treatment of the equation.

1.2.2 Optimal control of nonlinear Schrödinger equations

The optimal control problem we shall consider is given by

$$J_* = \inf_{\tilde{\psi},\tilde{\alpha}} J(\tilde{\psi}, \tilde{\alpha}) \quad \text{where}$$

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + U(x)\psi + \lambda|\psi|^{2\sigma}\psi + \alpha(t)V(x)\psi, \quad x \in \mathbb{R}^d, t \in \mathbb{R}, \text{ and} \tag{1.10}$$

$$J(\psi, \alpha) = \langle \psi(T, \cdot), A\psi(T, \cdot)\rangle^2_{L^2(\mathbb{R}^d)} + \gamma_1 \int_0^T (\dot{E}(t))^2 \, dt + \gamma_2 \int_0^T (\dot{\alpha}(t))^2 \, dt,$$

with $\lambda \geq 0$, $\sigma < 2/(d-2)$, external potential U, control potential V, and subject to initial data

$$\psi(0, \cdot) = \psi_0 \in \Sigma, \quad \alpha(0) = \alpha_0 \in \mathbb{R}.$$

Here A is an observable, i.e. an operator with domain in $L^2(\mathbb{R}^d)$, $\gamma_1 > 0$ and $\gamma_2 \geq 0$ are two cost parameters, and $E(t)$ is the energy corresponding to the NLS (1.10). In this problem, the energy is not constant due to the presence of variations in the control parameter $\alpha(t)$. The above optimal control problem models an experimenter trying to achieve a certain value for an observable of a condensate (without loss of generality, this value is set to zero) by manipulating the amplitude of an external field, e.g. a field induced by a laser. The cost term models the cost of absorbing variations in total energy stored in the condensate. Note that the underlying NLS implies the following expression for the cost term involving γ_1:

$$\gamma_1 \int_0^T (\dot{E}(t))^2 \, dt = \gamma_1 \int_0^T (\dot{\alpha}(t))^2 \left(\int_{\mathbb{R}^d} V(x)|\psi(t, x)|^2 \, dx \right)^2 \, dt.$$

The optimal control problem is well-posed with $\gamma_2 = 0$ if the potential $V(x)$ is strictly bounded away from zero. On the other hand if this is not the case, it becomes necessary to set $\gamma_2 > 0$. Even in the case $\lambda = 0$, this is a bilinear control problem since the term $\alpha(t)V(x)\psi(t, x)$ is linear in both the control and the wave function, making this optimal control problem highly nonlinear. In our analysis of this optimal control problem, we first show the existence of at least one minimizer $(\alpha^*, \psi^*) \in H^1(0, T) \times W(0, T)$, where $W(0, T)$ denotes an appropriate function space for the solutions to the NLS. We prove this result by the direct method, i.e. we consider a minimizing sequence (α_n, ψ_n) and use boundedness of the functional $J(\psi_n, \alpha_n)$ in order to obtain bounds on the sequence in order to obtain a (weak) limit point (α^*, ψ^*). By going to the limit in the NLS, we then show that (α^*, ψ^*) is itself a solution to the NLS and finally conclude by lower-semicontinuity of J that (α^*, ψ^*) is indeed a minimizer.

In a next step, we characterize minimizers by deriving a system of equations that must be satisfied at critical points. This system can be formally derived using the Lagrangian

$$\mathfrak{L}(\psi, \alpha, \varphi) = J(\psi, \alpha) - \langle \varphi, P(\psi, \alpha) \rangle_{L_t^2 L_x^2},$$

where $P(\psi, \alpha) = 0$ denotes the NLS, i.e.

$$P(\psi, \alpha) = i\partial_t \psi + \frac{1}{2}\Delta\psi - U(x)\psi - \lambda|\psi|^{2\sigma}\psi - \alpha(t)V(x)\psi.$$

Formally, a minimum of J over (ψ, α) under the constraint $P(\psi, \alpha) = 0$ is a minimum of the unconstrained Lagrangian over (ψ, α, φ) and we expect

$$\big(D_\psi \mathfrak{L}(\psi, \alpha, \varphi), D_\alpha \mathfrak{L}(\psi, \alpha, \varphi), D_\varphi \mathfrak{L}(\psi, \alpha, \varphi)\big) = 0.$$

This is a system of three equations, the third one $D_\varphi \mathcal{L} = 0$ one being the NLS, and the other two identifying a critical α and φ. Of course, there is not reason to expect any solution to this critical system to be unique, corresponding to the lack of convexity of our optimal control problem. The usual way to make this argument rigorous requires the use of an implicit function theorem. However, due to the lack of regularity properties of the Schrödinger operator, we could not make this approach work in the fully nonlinear case $\lambda > 0$ and instead we derive the derivative of a reduced functional $\mathcal{J}(\alpha) = J(\psi(\alpha), \alpha)$ directly, where $\psi(\alpha)$ is the solution to the NLS with control α. In order to handle this differentiability problem, we restrict ourselve to cases where $\sigma \in \mathbb{N}$. The condition $\sigma < 2/(d-2)$ then implies $d \leq 3$, which are of course the most relevant cases in physics. Finally, we present some numerical experiments based on a Newton–type method in order to illustrate our optimal control problem.

Part I

Quantitative uniform in time hydrodynamic limits

Chapter 2

A quantitative perturbative approach to hydrodynamic limits

The work in this part has been carried out in collaboration with Clément Mouhot.

2.1 Introduction

We shall consider the problem of hydrodynamic limits for interacting particle systems on a lattice. The problem is to show that under an appropriate scaling of time and space, the local particle densities of a stochastic lattice gas converge to the solution of a partial differential equation. The goal of this work is to provide a fairly general framework allowing us to prove a hydrodynamic limit with an explicit uniform in time rate of convergence. We will present our method using as an example the zero range process for which a hydrodynamic limit is well-known and the limit equation is given by a nonlinear diffusion equation. Our method is inspired by the work [67] on propagation of chaos for the Boltzmann equation, see also [66] for an announcement and summary of the work.

To make our notions precise, we need to introduce some notation. We consider a particle process on the discrete torus

$$\mathbb{T}_N^d = \{1, \dots, N\}^d$$

and consider particle configurations as elements in

$$X_N := \mathbb{N}^{\mathbb{T}_N^d},$$

the *state space* for the zero range process. The lattice $\mathbb{T}_N^d$ can be thought of as a discrete approximation of the d-dimensional Torus

$$\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$$

with periodic boundary conditions $x + e \equiv x$ for all $x \in \mathbb{T}^d$ and $e \in \mathbb{Z}^d$. Variables in the discrete torus $\mathbb{T}_N^d$ are called *microscopic* and denoted by x, y, z, whereas variables in the continuous torus $\mathbb{T}^d$ are called *macroscopic* and denoted by u. In fact, we embed $\mathbb{T}_N^d$ in $\mathbb{T}^d$ via

$$\mathbb{T}_N^d \ni x \mapsto \tfrac{x}{N} \in \mathbb{T}^d.$$

This embeds the microscopic variables $x \in \mathbb{T}_N^d$ to the macroscopic variables $u \in \mathbb{T}^d$. Hence the macroscopic distance between sites of the lattice is N^{-1}. In general, we will denote particle configurations in X_N by the letters η or ξ. The interacting particle system is given by a stochastic process and we let $P(X_N)$ be the set of probability (Radon) measures over the state space. For any initial measure $\mu_0^N \in P(X_N)$ we obtain a unique measure $\mu_t^N \in P(X_N)$ describing the state of the process at a later time t. This also yields a semigroup $(S_t^N)_{t\geq 0}$ on $P(X_N)$, which is given by $\mu_t^N = S_t^N \mu_0^N$ for all $t \geq 0$. The semigroup S_t^N is a Feller-semigroup uniquely determined by its generator, see [54]. The generator is a map $G^N : C_b(X_N) \to C_b(X_N)$ and satisfies

$$\frac{d}{dt}\langle \mu_t^N, f^N\rangle = \langle \mu_t^N, G^N f^N\rangle, \tag{2.1}$$

where we have denoted by $\langle \cdot, \cdot \rangle$ the integral of a continuous function with respect to a measure. Equivalently, this is the duality pairing between (Radon) measures and continuous functions. Thus G^N can also be thought of as the generator of the dual semigroup on $C_b(X_N)$. Here we consider

$$G^N f^N(\eta) = N^2 \sum_{x, y\sim x} g(\eta(x)) \left[f^N(\eta^{x,y}) - f^N(\eta)\right] \tag{2.2}$$

for each $f^N \in C_b(X_N)$, where $\eta^{x,y}$ is the configuration of the particle system after one particle has jumped from site x to y and where $y \sim x$ whenever x and y are neighbours. To be precise, $\eta^{x,y}$ is given by

$$\eta^{x,y}(z) = \begin{cases} \eta(x) - 1 & \text{if } z = x, \\ \eta(y) + 1 & \text{if } z = y, \\ \eta(z) & \text{otherwise.} \end{cases}$$

In order for the process to remain in the state space X_N, we always demand $g(0) = 0$. The *jump rate* $g : \mathbb{N} \to [0, \infty)$ can be thought of as describing the interactions of particles

occupying the same site. Since the jump rate on a given site only depends on the number of particles at that particular site, this process is called *zero range process*. A special case is the case of linear g, where the particles perform independent random walks on the lattice. The factor N^2 in the definition of the generator G^N corresponds to a time scale. Thus we consider a hydrodynamic limit under *diffusive scaling*, i.e. the microscopic spatial variables scale with N and time with N^2.
We will show that, under diffusive scaling, the zero range process is well approximated by the solution $f_t : \mathbb{T}^d \to [0, \infty)$ to the *filtration equation*

$$\partial_t f_t(u) = \Delta\sigma(f_t(u)) \qquad t \in [0, \infty), u \in \mathbb{T}^d. \tag{2.3}$$

We shall have to specify the space H of solutions to our limit partial differential equation. Throughout this chapter, H will be a subspace of the space $\mathcal{M}_+(\mathbb{T}^d)$ of positive Radon measures on the torus. Recall that the space of Radon measures can be defined as the dual space of continuous functions. Let us make precise the notion of convergence of the particle process. Given a particle configuration $\eta \in X_N$, the particle densities are given by the *empirical measure*

$$\alpha_\eta^N := \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)\delta_{\frac{x}{N}} \in \mathcal{M}_+(\mathbb{T}^d). \tag{2.4}$$

Thus we have defined an embedding

$$\alpha^N : X_N \to \mathcal{M}_+(\mathbb{T}^d), \quad \eta \mapsto \alpha_\eta^N,$$

which allows us to compare solutions to the particle system with the solutions $f_t \in H \subseteq \mathcal{M}_+(\mathbb{T}^d)$ to the partial differential equation. Furthermore let f_t be the solution to the filtration equation given an initial density f_0. The goal is to show that the empirical measure (2.4) possesses an asymptotic density profile $f_t(\cdot)$. By this we mean that for any smooth function $\varphi : \mathbb{T}^d \to \mathbb{R}$, it holds that

$$\lim_{N\to\infty} \mathbb{P}_{\mu_t^N} \left(|\langle \alpha_\eta^N, \varphi\rangle - \langle f_t, \varphi\rangle| > \epsilon \right) = 0 \tag{2.5}$$

for all $t \geq 0$ and $\epsilon > 0$. Furthermore we want to specify the rate of convergence explicitly. Here $\mathbb{P}_{\mu^N}(\mathcal{A})$ denotes the probability corresponding to the (measurable) set $\mathcal{A}$ under the probability measure $\mu^N \in P(X_N)$. In other words,

$$\mathbb{P}_{\mu^N}(\mathcal{A}) = \int \chi_{\mathcal{A}}(\eta)\, d\mu^N(\eta),$$

where $\chi_{\mathcal{A}}$ denotes the characteristic function of the set $\mathcal{A}$. In the following, we shall denote the expectation of a measurable function f^N with respect to a probability measure

$\mu^N \in P(X_N)$ by

$$\mathbb{E}_{\mu^N}[f^N(\eta)] = \langle \mu^N, f^N \rangle = \int f^N(\eta)\, d\mu^N(\eta).$$

A measure μ^N is called *invariant* (or equilibrium) measure, if

$$\langle \mu^N, G^N f^N \rangle = 0 \qquad \text{for all } f^N \in C_b(X_N),$$

cf. equation (2.1). A convenient family of invariant measures is given by the *grand-canonical* (or Gibbs) measures, i.e. the measures

$$\nu_\rho^N(\eta) = \prod_{x \in \mathbb{T}_N^d} \frac{\sigma(\rho)^{\eta(x)}}{g(\eta(x))!\; Z(\sigma(\rho))}, \tag{2.6}$$

where Z is the *partition function* of the zero range process, $\rho \geq 0$, and

$$g(n)! := g(1)g(2)\cdots g(n) \;\text{ with }\; g(0)! := 1.$$

The partition function is defined as

$$Z(\rho) = \sum_{n=0}^{\infty} \frac{\rho^n}{g(n)!} \tag{2.7}$$

and the function $\sigma(\rho)$ is chosen such that

$$\langle \nu_\rho^N, \eta(0) \rangle = \rho.$$

We shall elaborate on the construction of σ in Section 2.4. Since the number of particles is conserved and the process has no other conserved quantities, another important set of invariant measure is given by the *canonical measures*

$$\nu^{N,K}(\eta) = \nu_\rho^N\big(\eta \mid \textstyle\sum_x \eta(x) = K\big), \tag{2.8}$$

which are the grand-canonical measures conditioned on hyperplanes of constant number of particles. Note that this definition is independent of $\rho > 0$. Since the equilibrium ν_ρ^N is made up of independent random variables, we expect the convergence (2.5) to hold if we can show that the process is in equilibrium $\nu_{f_t(u)}^N$ locally around $u \in \mathbb{T}^d$ with average density $f_t(u)$.

The organization of this chapter is as follows. First we present some previous results in Section 2.2. In Section 2.3, we present our method with the help of the particularly easy case of independent random walks. Section 2.4 contains our main result, the hydrodynamic limit for the zero range process in one dimension with an explicit estimate on the rate of convergence. Section 2.5 contains an argument, which is new in the context of hydrodynamic limits, that allows us to prove convergence of the microscopic entropy if the entropy converges initially. In Section 2.6 we prove an important ingredient in our proof, the so-called replacement lemma. The replacement lemma is not new, see [36], but we include its proof for the sake of completeness and in order to derive an explicit bound on the rate of convergence in the replacement lemma. We also mention that our slightly modified version of the replacement lemma shows convergence with respect to an L^2–norm instead of the usual L^1–norm. Finally, in Section 2.7, we discuss a strategy, which is work in progress, how to extend our result to the multi-dimensional case. Throughout this chapter, any constant C should be understood to be *generic*, i.e. it can change from line to line and only depends on the "general" parameters of the problem - this should be clear from context.

2.2 Previous results

Using the notation introduced in Section 2.1, we now consider the general zero range process on $\mathbb{T}_N^d$ given by generator (2.2). Let us make the following assumptions on the rate function $g : \mathbb{N} \to [0, \infty)$.

Assumption 1. *(i)* Non-degeneracy*: Assume that g satisfies $g(0) = 0$ and $g(n) > 0$ for all $n > 0$.*
(ii) Lipschitz-property*: We require that g is Lipschitz continuous with*

$$0 \leq |g(n + 1) - g(n)| \leq g^* < +\infty$$

for all $n \in \mathbb{N}$.
(iii) Spectral gap*: We also assume that there exist $n_0 > 0$ and $\delta > 0$ such that*

$$g(n) - g(j) \geq \delta$$

for any $j \in \mathbb{N}$ and $n \geq j + n_0$.
(iv) Attractivity*: Let the jump rate g be monotonously increasing, i.e.*

$$g(n + 1) \geq g(n)$$

for all $n \in \mathbb{N}$.

Remark 2.2.1. Let us comment on the different parts of Assumption 1: Part (i) is essential to avoid degeneracies of the particle system. We need the spectral gap property

(iii) in order to prove an explicit uniform in time rate of convergence, since it allows us to quantify the local relaxation to equilibrium of the particle system as well as the global convergence to equilibrium on the level of the limit equation. It implies in particular that $g(n) \geq g_0 n$ with $g_0 > 0$. The attractivity (iv) is important to obtain moment–bounds on the particle system, see Subsection 2.6.1. The question of moment bounds is still an open problem in its absence. Assumption (ii) is used at several points in the proof, but could possibly be replaced using the uniform moment bounds originating from assumption (iv) - however, it would affect our strategy to prove the regularity result in several dimensions, see Section 2.7.

In the context of the zero range process with diffusive scaling, two very well-known methods of proving a hydrodynamic limit are the *entropy method* due to Guo, Papanicolaou, and Varadhan [36], see Theorem 2.2.2, and the *relative entropy method* due to Yau [86], see Theorem 2.2.3. For an extensive account of these methods in the context of zero range process, see [47].
In order to proceed, we need one more definition. Let $\mu, \nu \in P(X_N)$ be two probability measures. Then the *relative entropy* of μ relative to ν is defined as

$$H^N(\mu|\nu) = \int_{X_N} \log\big(\tfrac{d\mu}{d\nu}\big) d\mu \tag{2.9}$$

whenever μ is absolutely continuous with respect to ν. The relative entropy is connected to the Fisher information

$$\mathcal{D}^N(\mu|\nu) = \int_{X_N} \sqrt{\tfrac{d\mu}{d\nu}} G^N \sqrt{\tfrac{d\mu}{d\nu}} d\nu. \tag{2.10}$$

The entropy method can be summarized in the following theorem. Note that we have not taken great care to optimize the assumptions. The proofs under the assumptions given below can be found in [47].

Theorem 2.2.2 (Guo, Papanicolaou, Varadhan)**.** *Assume (i) and (ii) of Assumption 1 as well as $g(n) \geq g_0 n$ for some $g_0 > 0$ and let $\mu_0^N \in P(X_N)$ and $f_0 \in L^\infty(\mathbb{T}^d)$ such that*

$$\lim_{N\to\infty} \mathbb{P}_{\mu_0^N}\big(|\langle \alpha_\eta^N, \varphi\rangle - \langle f_0, \varphi\rangle| > \epsilon\big) = 0,$$

for every continuous function $\varphi \in C(\mathbb{T}^d)$ and every $\epsilon > 0$. Furthermore we assume that the initial data satisfy the bounds

$$H^N(\mu_0^N|\nu_\rho^N) \leq CN^d \qquad \text{and} \qquad \Big\langle \mu_0^N, \frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d} \eta(x)^2 \Big\rangle \leq C$$

for some $\rho > 0$ and a constant $C < +\infty$.

Then, for every $t \geq 0$, every continuous function $\varphi \in C(\mathbb{T}^d)$, and every $\epsilon > 0$, it holds that

$$\lim_{N\to\infty} \mathbb{P}_{\mu_t^N}\big(|\langle \alpha_\eta^N, \varphi\rangle - \langle f_t, \varphi\rangle| > \epsilon\big) = 0,$$

where f_t is the unique weak solution to (2.3) *and μ_t^N solves* (2.1) *with Cauchy datum μ_0^N.*

Thus the entropy method yields propagation of the hydrodynamic profile. The relative entropy method by Yau, on the other hand, concerns the conservation of a stronger notion. In analogy to (2.6), we define a *local Gibbs measure* with macroscopic profile $f_t \in C(\mathbb{T}^d)$ by

$$\nu_{f_t(\cdot)}^N(\eta) = \prod_{x\in\mathbb{T}_N^d} \frac{\sigma(f_t(\frac{x}{N}))^{\eta(x)}}{g(\eta(x))!\ Z(\sigma(f_t(\frac{x}{N})))}. \tag{2.11}$$

This measure has the property that it is locally (in infinitesimal macroscopic neighbourhoods where f_t is constant) in equilibrium with a macroscopic non-equilibrium profile f_t as $N \to \infty$. The relative entropy method then yields the following theorem.

Theorem 2.2.3 (Yau). *Assume (i) and (ii) of Assumption 1 as well as that the partition function $Z(\cdot)$ is finite on all $[0,\infty)$, e.g. $g(n) \geq g_0 n$ for some $g_0 > 0$. Furthermore, assume that the solution f_t to* (2.3) *satisfies $f_t \in C^2(\mathbb{T}^d)$ and let $\mu_t^N \in P(X_N)$ solve* (2.1). *Finally assume that initially at $t = 0$, the relative entropy $H^N(\mu_0^N|\nu_{f_0(\cdot)}^N)$ vanishes in the limit, i.e.*

$$\lim_{N\to\infty} \frac{1}{N^d} H^N\big(\mu_0^N|\nu_{f_0(\cdot)}^N\big) = 0.$$

Then it holds that

$$\lim_{N\to\infty} \frac{1}{N^d} H^N\big(\mu_t^N|\nu_{f_t(\cdot)}^N\big) = 0 \tag{2.12}$$

for every $t \geq 0$.

Note that the convergence of the relative entropy (2.12) implies that μ_t^N has profile f_t, i.e.

$$\lim_{N\to\infty} \mathbb{P}_{\mu_t^N}\big(|\langle \alpha_\eta^N, \varphi\rangle - \langle \varphi, f_t\rangle| > \epsilon\big) = 0.$$

Thus the convergence of the relative entropy can be thought of as a stronger notion of the hydrodynamic limit. Yau's relative entropy method shows that this stronger notion is conserved by the evolution.

Remark 2.2.4. It appears that using a quantitative replacement lemma, see Section 2.6, this result can be translated to a quantitative result of the form

$$H^N\big(\mu_t^N|\nu_{f_t(\cdot)}^N\big) \leq Ce^{\gamma^{-1}t} H^N\big(\mu_0^N|\nu_{f_0(\cdot)}^N\big) + tr(N),$$

where $\lim_{N\to\infty} r(N) = 0$ if γ is sufficiently small, and $r(N)$ can be made explicit (although, to our knowledge, such a result has never been published). Thus it seems that a quantitative estimate on the rate of convergence is available in the stronger form of the hydrodynamic limit given by the convergence of the entropy relative to the local Gibbs state. However, this convergence is not uniform in time, since γ might be very small. Therefore even if one manages to prove exponential decay in time of the relative entropy $H^N\left(\mu_t^N|\nu^N_{f_t(\cdot)}\right) \le Ce^{-\lambda t}$, e.g. by employing a logarithmic Sobolev inequality, it is still not possible to conclude uniform in time convergence if $\lambda < \gamma^{-1}$. In the context of the zero range process, the following logarithmic Sobolev inequality holds [27, 59]:

$$H^N(\mu|\nu^{N,K}) \le CN^2\mathcal{D}^N(\mu|\nu^{N,K}) \tag{2.13}$$

uniformly in N, K, and $\mu \in P(X_N)$, where we recall that $\nu^{N,K}$ denotes the canonical measure (2.8). Logarithmic Sobolev inequalities are very effective tools to describe concentration of measure and have been employed widely starting with the works [5, 33].

For a related model, the Ginzburg-Landau model with Kawasaki dynamics, there exists an additional method due to Grunewald, Otto, Villani, and Westdickenberg [34], who prove a logarithmic Sobolev inequality and hydrodynamic limit based on a coarse-graining of the state-space. In principle, it should be possible to extend their method to obtain a uniform rate of convergence. On the other hand, it is not clear how to extend the method to the zero range process and how to obtain uniform-in-time convergence.

2.3 A toy model: independent random walks

In order to demonstrate our method, let us consider the especially simple case where $g(n) = n$. Then all the particles perform random walks independently of each other. The invariant measures ν_ρ^N are now given by the Poisson distribution

$$\nu_\rho^N(\eta) = \prod_{x\in\mathbb{T}_N^d} e^{-\rho}\frac{\rho^{\eta(x)}}{\eta(x)!}.$$

Note that $\langle \nu_\rho^N, \eta(x)\rangle = \rho$ and hence $\sigma(\rho) = \rho$ in (2.6) in this case. We want to show that in the sense of Theorem 2.2.2, as the number N of sites in the lattice $\mathbb{T}_N^d$ approaches infinity, the particle system is approximated by the heat equation

$$\partial_t f_t = \Delta f_t. \tag{2.14}$$

Here we consider the heat equation in the space of positive Radon measures

$$H = \mathcal{M}_+(\mathbb{T}^d).$$

It is clear that we have a well-established theory for strong solutions for the heat equation with continuous initial data $\omega \in C(\mathbb{T}^d)$. Denote the corresponding semigroup on $C(\mathbb{T}^d)$ by $S_t^\infty \omega$. We define solutions in H via

$$\langle S_t^\infty f, \omega\rangle_{H,C(\mathbb{T}^d)} = \langle f, S_t^\infty \omega\rangle_{H,C(\mathbb{T}^d)} \tag{2.15}$$

for all $f \in H, \omega \in C(\mathbb{T}^d)$. Note that indeed $S_t^\infty f$ stays a positive measure by the maximum principle. Thus the solution f_t to the heat equation (2.14) with initial datum $f \in H$ is given by $f_t = S_t^\infty f$. Let us denote by $C_b^k(\mathbb{R})$ the space of uniformly bounded and k times continuously differentiable functions on $\mathbb{R}$ with uniformly bounded derivatives. The main result of this section is the following theorem, detailing a hydrodynamic limit with explicit and uniform-in-time rate of convergence.

Theorem 2.3.1 (Hydrodynamic limit for independent random walks)**.** *Let $F \in C_b^2(\mathbb{R})$, $\varphi \in C^3(\mathbb{T}^d)$, and M_1 be given. There exists a constant $C < +\infty$ depending only on the dimension d, such that for all $N \in \mathbb{N}$, $f_0 \in H$, $f_0^N \in P(X_N)$ such that the average density is bounded, i.e.*

$$\Big\langle \mu_0^N, \frac{1}{N^d} \sum_{x\in\mathbb{T}_N^d} \eta(x)\Big\rangle \le M_1,$$

it holds that

$$\Big\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle\big) - F\big(\langle f_t, \varphi\rangle\big)\Big\rangle \le \frac{C}{N} M_1 \|F'\|_{C^1}\big(\|\nabla\varphi\|_{C^2} + \|S_1^\infty \nabla\varphi\|_{H^n}\big) + \|F'\|_{L^\infty}\|\varphi\|_{C^3} \sup_{\substack{\omega\in C^3(\mathbb{T}^d)\\ \|\omega\|_{C^3}\le 1}} \big\langle f_0^N, \langle \alpha_\eta^N - f_0, \omega\rangle\big\rangle \tag{2.16}$$

uniformly for all $t \ge 0$. Here n denotes the smallest integer greater than $2 + d/2$, f_t is given by the solution to the heat equation $\partial_t f_t = \Delta f_t$, and μ_t^N is given by the evolution of the particle process, i.e. a system of independent random walks.

Theorem 2.3.1 yields convergence to the hydrodynamic limit under the condition that the initial data are compatible. If f_0 is continuous, it is straightforward to construct an initial particle distribution μ_0^N for which the initial convergence holds. Indeed let $f_0 \in C(\mathbb{T}^d)$, $f_0 \ge 0$, be given. Then we consider the product measure $\nu_{f_0(\cdot)}^N$ introduced in (2.11), i.e.

$$\nu_{f_0(\cdot)}^N(\eta) = \prod_{x\in\mathbb{T}_N^d} e^{-f_0(\frac{x}{N})} \frac{f_0(\frac{x}{N})^{\eta(x)}}{\eta(x)!}$$

for all $x \in \mathbb{T}_N^d$. Under the law $\mu_0^N := \nu_{f_0(\cdot)}^N$, the term $\langle \alpha_\eta^N, \omega\rangle$ converges in mean to $\langle f_0, \omega\rangle$ and one can show that

$$\sup_{\substack{\omega \in C^3(\mathbb{T}^d) \\ \|\omega\|_{C^3} \leq 1}} \left\langle f_0^N, \langle \alpha_\eta^N - f_0, \omega\rangle \right\rangle \leq \frac{C}{\sqrt{N}}. \tag{2.17}$$

This can be deduced from an application of the law of large numbers and the central limit theorem, also see the proof of Corollary 2.4.9. Under μ_0^N, the average density is bounded by $\|f_0\|_{L^\infty}$. Hence we arrive at the following corollary.

Corollary 2.3.2. *Let $F \in C_b^2(\mathbb{R})$, $\varphi \in C^3(\mathbb{T}^d)$, and $f_0 \in C(\mathbb{T}^d)$ be given. Then there exists a constant $C < +\infty$ and a $f_0^N \in P(X_N)$ for all $N \in \mathbb{N}$, such that*

$$\left\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle\big) - F\big(\langle f_t, \varphi\rangle\big)\right\rangle \leq \frac{C}{\sqrt{N}}$$

for all $N \in \mathbb{N}$, where f_t is given by the solution to the heat equation $\partial_t f_t = \Delta f_t$ and μ_t^N is given by a system of independent random walks.
In other words, $\alpha_\eta^N \rightharpoonup^* f_t$ in distribution (in law) as $N \to \infty$ where the symbol $\rightharpoonup^*$ denotes weak- convergence for measures in $P(X_N)$.*

Let us make several comments.

Remarks 2.3.3. (1) The rate of convergence $\mathcal{O}(1/\sqrt{N})$ is the optimal rate appearing in the law of large numbers for sums of independent random variables, similarly to the estimate (2.17). Hence we see that the largest contribution to the error in the hydrodynamic limit for independent random walks comes from the approximation of the initial datum f_0 by the initial particle distribution f_0^N, since this error is typically $\mathcal{O}(1/\sqrt{N})$.
(2) As we have seen, the restriction that $\langle \mu_0^N, N^{-d}\sum \eta(x)\rangle \leq M_1$ in Theorem 2.3.1 is hardly any restriction and usually follows from the convergence of the initial data.
(3) The function

$$\Psi \in C_b(H) \text{ given by } \Psi(f) = F\left(\langle f, \varphi\rangle\right) \text{ for all } f \in H$$

thus satisfies $\langle \mu_t^N, \Psi(\alpha_\eta^N)\rangle \to \Psi(f_t)$ as $N \to \infty$ under the assumptions of Corollary 2.3.2.
(4) Here we have the convergence of the empirical measures in distribution. This sense of convergence is the same as found in the literature on hydrodynamic limits for interacting particle systems, but it is different in spirit from the convergence result found in [67], from where our method of proof was inspired. In contrast to ours, the result in [67] pertains convergence of the marginals of μ_t^N. An analogous result in our setting would be the convergence of marginals of μ_t^N to the corresponding marginals of $\nu_{f_t(\cdot)}^N$, where $\nu_{f_t(\cdot)}^N$ denotes as above the local Gibbs measure (2.11). In [47], a result of this kind is called

strong conservation of local equilibrium. Indeed it seems likely that a result like this could be deduced using a similar approach.

(5) Convergence in distribution of the random variable $J_N := \langle \alpha_\eta^N, \varphi \rangle$ to the deterministic result $J := \langle f_t, \varphi \rangle$ implies convergence in probability, cf. Theorem 2.2.2, as follows. Let $\epsilon > 0$ be arbitrary and note that

$$\begin{aligned}\mathbb{P}_{\mu_t^N}(|J_N - J| > \epsilon) &\le \mathbb{P}_{\mu_t^N}(J_N > J + \epsilon) + \mathbb{P}_{\mu_t^N}(J_N < J - \epsilon) \\ &\le \mathbb{E}_{\mu_t^N}[F_\epsilon(J_N)] + \mathbb{E}_{\mu_t^N}[\tilde{F}_\epsilon(J_N)]\end{aligned}$$

where F_ϵ and $\tilde{F}_\epsilon$ are smooth approximations from above of the indicator functions of $[J + \epsilon, +\infty)$ and $(-\infty, J - \epsilon]$, respectively, such that $F_\epsilon(J) = 0 = \tilde{F}_\epsilon(J)$. Under the assumptions of Corollary 2.3.2, the right hand side converges as $N \to \infty$ with an explicit, ϵ-dependent rate.

(6) Consider the embedding

$$\pi_P^N : P(X_N) \to P(H)$$

given by $\langle \pi_P^N f^N, \Phi \rangle = \langle f^N, \Phi(\alpha_\eta^N) \rangle$ for all $\Phi \in C_b(H)$. Returning to the map $\Psi \in C_b(H)$, defined in (3), let us mention that the convergence

$$\langle \mu_t^N, \Psi(\alpha_\eta^N) \rangle - \Psi(f_t) \to 0$$

can also be rewritten as

$$\langle \pi_p^N(\mu_t^N), \Psi \rangle - \langle \delta_{f_t}, \Psi \rangle \to 0,$$

or, equivalently, $\pi_P^N(\mu_t^N) \rightharpoonup^* \delta_{f_t}$ in $P(H)$, at least insofar as Ψ given in (3) can represent all of $C_b(H)$.

(7) The choice of a norm for the convergence of the initial data, here given by the dual of the C^3–norm, is rather flexible. Since the heat equation is a contraction in many spaces, e.g. in C^k or H^k, for $k \in \mathbb{N}$, we could use (the dual space of) any of these spaces, provided φ is regular enough and the Dirac distribution δ lies in the dual space. Later, in Section 2.4, we shall use the H^{-1}–norm, dual to the H^1–norm, to measure the convergence of the initial data. Here this is not possible since the Dirac delta is not an element of $H^{-1}(\mathbb{T}^d)$ if $d > 1$.

Before proceeding with the proof of Theorem 2.3.1, let us collect some semigroups related to the evolution of the particle system and the limit equation. We cannot compare the semigroups of the particle system on $P(X_N)$ and of the limit equation on H directly. Instead we will compare them on the *level of observables* by considering dual spaces.

Particle system: We already defined the semigroup S_t^N on $P(X_N)$. Let T_t^N denote the semigroup on $C_b(X_N)$ that is dual to S_t^N, i.e. the semigroup given by

$$\langle \mu^N, T_t^N f^N \rangle = \langle S_t^N \mu^N, f^N \rangle$$

for all $\mu^N \in P(X_N)$, $f^N \in C_b(X_N)$. Thus the generator of T_t^N in $C_b(X_N)$ is given by G^N in (2.2) with $g = \mathrm{id}_{\mathbb{N}}$.

Limit equation: Recall the definition (2.15) of the limit semigroup S_t^∞ on H. Next we define a pullback semigroup T_t^∞ on $C_b(H)$ corresponding to the solution of the limit partial differential equation S_t^∞ via

$$T_t^\infty \Psi(f) = \Psi(S_t^\infty f)$$

for all $\Psi \in C_b(H)$, $f \in H$, and $t \geq 0$.

Thus we get a collection of semigroups

$$\begin{aligned} S_t^N : P(X_N) \to P(X_N) \quad &\text{with dual} \quad T_t^N : C_b(X_N) \to C_b(X_N), \\ S_t^\infty : H \to H \quad &\text{with pullback} \quad T_t^\infty : C_b(H) \to C_b(H). \end{aligned}$$

Note that for a general nonlinear limit equation, the operator S_t^∞ will not be linear but the semigroup T_t^∞ will be linear.

Instead of comparing the semigroup S_t^N on $P(X_N)$ and the semigroup S_t^∞ on H, we shall compare the two semigroups T_t^N on $C_b(X_N)$ and T_t^∞ on $C_b(H)$. To this end let us define an embedding

$$\pi^N : C_b(H) \to C_b(X_N), \quad \Psi \mapsto \pi^N \Psi = (\eta \mapsto \Psi(\alpha_\eta^N)). \tag{2.18}$$

We shall need to identify the time-derivative of T_t^∞ for a special class of functions in $C_b(H)$ which are of special importance for our version of the hydrodynamic limit, see Theorem 2.3.1. These functions are all functions $\Psi \in C_b(H)$ such that

$$\Psi(f) = F(\langle f, \varphi \rangle) \tag{2.19}$$

for some $F \in C_b^1(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$, c.f. Remark 2.3.3 (3). Here we speak of time-derivative instead of generator, because even though it is possible to prove that T_t^∞ induces a C_0–semigroup of contractions on a suitable subspace of $C_b(H)$, we shall not do so here.

Before we prove the hydrodynamic limit, Theorem 2.3.1, let us state and prove two lemmas on the discrete particle system and the limit equation. Both lemmas will be used in the proof of the hydrodynamic limit. The first lemma concerns the stability of the limit partial differential equation.

Lemma 2.3.4 (Stability)**.** *Let $F \in C_b^1(\mathbb{R})$ and $\varphi \in C^3(\mathbb{T}^d)$, and define Ψ as in equation* (2.19).
(i) *Then for all $t \geq 0$, there exists $\varphi_t \in C^3(\mathbb{T}^d)$ such that*

$$T_t^\infty \Psi(f) = F\left(\langle f, \varphi_t\rangle\right) \tag{2.20}$$

for all $f \in H$. Furthermore φ_t satisfies

$$\|\varphi_t\|_{C^3} \leq \|\varphi\|_{C^3}. \tag{2.21}$$

(ii) *For any $t \geq 0$, it holds*

$$|T_t^\infty \Psi(f_2) - T_t^\infty \Psi(f_1)| \leq \|F'\|_{L^\infty} \|\varphi\|_{C^3} \sup_{\substack{\omega \in C^3(\mathbb{T}^d) \\ \|\omega\|_{C^3} \leq 1}} \langle f_2 - f_1, \omega\rangle$$

for all $f_1, f_2 \in H$.

Proof. (i) Since S_t^∞ was constructed on H by duality, it holds that $\langle S_t^\infty f, \varphi\rangle = \langle f, S_t^\infty \varphi\rangle$. Hence the choice $\varphi_t = S_t^\infty \varphi$ yields (2.20). Since $\varphi \in C^3(\mathbb{T}^d)$, the function $D^{\mathfrak{s}}\varphi_t$, where $\mathfrak{s}$ is any multi-index such that $|\mathfrak{s}| \leq 3$, solves the heat equation with initial datum $D^{\mathfrak{s}}\varphi$. Now the maximum principle yields $\varphi_t \in C^3(\mathbb{T}^d)$ with estimate (2.21).
(ii) Using the notation and results of part (i) of this lemma, it is not difficult to see that

$$|\Psi(S_t^\infty f_2) - \Psi(S_t^\infty f_1)| = |F(\langle f_2, \varphi_t\rangle) - F(\langle f_1, \varphi_t\rangle)| \leq \|F'\|_{L^\infty} \big|\langle f_2 - f_1, \varphi_t\rangle\big|,$$

which implies the result. □

The stability result yields that the form (2.19) is preserved by the flow T_t^∞, since

$$T_t^\infty \Psi(f) = F\big(\langle f, S_t^\infty \varphi\rangle\big) \langle f, S_t^\infty \varphi\rangle,$$

where $S_t^\infty \varphi \in C^3(\mathbb{T}^d)$. For such functions $\Psi \in C_b(H)$, its time-derivative is given in the next lemma.

Lemma 2.3.5. *Let $F \in C_b^1(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$, and define Ψ as in equation* (2.19)*. Then its derivative $G^\infty T_t^\infty$ at time $t \geq 0$ is given by*

$$G^\infty T_t^\infty \Psi(f) := \frac{d}{dt} T_t^\infty \Psi(f) = F'\left(\langle f, \varphi_t\rangle\right) \langle f, \Delta\varphi_t\rangle$$

for all $f \in H$, where $\varphi_t = S_t^\infty \varphi$. Note that at time $t = 0$, the derivative is to be understood as the right-hand derivative (as $t \searrow 0$) only.

Proof. By definition of weak solutions to the heat equation, see (2.15), it holds that

$$\frac{d}{dt}\langle S_t^\infty f, \varphi\rangle = \langle S_t^\infty f, \Delta\varphi\rangle.$$

The chain rule yields

$$\frac{d}{dt}T_t^\infty \Psi(f) = \frac{d}{dt}\Psi(S_t^\infty f) = F'(\langle S_t^\infty f, \varphi\rangle)\langle S_t^\infty f, \Delta\varphi\rangle.$$

Hence

$$\frac{d}{dt}T_t^\infty \Psi(f) = F'(\langle f, \varphi_t\rangle)\langle f, \Delta\varphi_t\rangle$$

by the stability result, Lemma 2.3.4. □

Remark 2.3.6. (1) Note that we can write formally

$$F'\left(\langle f, \varphi\rangle\right)\langle \tilde{f}, \varphi\rangle = D\Psi(f)(\tilde{f}),$$

where $D\Psi(f) : H \to \mathbb{R}$ denotes the derivative of $\Psi : H \to \mathbb{R}$ with respect to $f \in H$. Indeed, it holds that

$$|\Psi(f_2) - \Psi(f_1) - D\Psi(f_1)(f_2 - f_1)| \leq \|F''\|_{L^\infty(\mathbb{R})}|\langle f_2 - f_1, \varphi\rangle|^2,$$

which can be understood as differentiability in H, if H is equipped with weak-* convergence, cf. Section 2.4.
(2) Note that it is possible to prove that the semigroup T_t^∞ is a C_0–semigroup of contractions with generator G^∞ on an appropriate subspace of $C_b(H)$, but we just need its time-derivative as obtained in Lemma 2.3.5 for the particular maps Ψ given by (2.19), since the form of Ψ is conserved in the special case of random walks. In order to keep the function spaces involved simple, we shall not prove the C_0–semigroup property.

In order to prove a uniform in time hydrodynamic limit, we need some results on the decay of solutions to the heat equation in the spirit of a spectral gap. Let $\dot{H}^n(\mathbb{T}^d)$ denote the *homogeneous Sobolev space* of degree n, i.e. the space of functions such that

$$\|f\|_{\dot{H}^n}^2 := \sum_{|\mathfrak{s}|=n}\int_{\mathbb{T}^d}|D^{\mathfrak{s}}f|^2\, du$$

is finite.

Lemma 2.3.7 (Spectral gap). *For all $\varphi \in C(\mathbb{T}^d)$ and $t > 0$, the solution $S_t^\infty\varphi$ to the heat equation is in $C^\infty(\mathbb{T}^d)$. Furthermore there exist positive, finite constants c and C such that*

$$\|\nabla S_{t+1}^\infty\varphi\|_{C^2} \leq C\|\nabla S_{t+1}^\infty\varphi\|_{\dot{H}^n} \leq C\|\nabla S_1^\infty\varphi\|_{\dot{H}^n}e^{-t}$$

for all $t \geq 0$ *and* $n > 2 + d/2$.

Proof. The regularization property of the heat equation is classical. Hence $h := \nabla S_1^\infty \varphi \in \dot{H}^n(\mathbb{T}^d)$ for $n > 2 + d/2$ and in Fourier space it holds that

$$\|\nabla S_{t+1}^\infty \varphi\|_{\dot{H}^n}^2 = \sum_{\zeta \in \mathbb{Z}^d} |\hat{h}(\zeta)|^2 |\zeta|^{2n} e^{-2\zeta^2 t} \leq \sum_{\zeta \in \mathbb{Z}^d} |\hat{h}(\zeta)|^2 |\zeta|^{2n} e^{-2t} \leq \|\nabla S_1^\infty \varphi\|_{\dot{H}^n}^2 e^{-2t}.$$

Furthermore a standard Sobolev embedding and Poincaré's inequality yield

$$\|\nabla S_{t+1}^\infty \varphi\|_{C^2} \leq C \|\nabla S_{t+1}^\infty \varphi\|_{\dot{H}^n}$$

since $n > 2 + d/2$ and the integral of gradient over the torus vanishes. □

The next lemma yields closeness of the time-derivatives G^N and G^∞.

Lemma 2.3.8 (Consistency)**.** *Let* $F \in C_b^2(\mathbb{R})$ *and* $\varphi \in C^3(\mathbb{T}^d)$*, and define* Ψ *as in equation* (2.19)*. Furthermore assume that the average density is bounded, i.e.*

$$\left\langle \mu_0^N, N^{-d} \textstyle\sum_x \eta(x) \right\rangle \leq M_1.$$

Then there exists a constant $C < +\infty$ *depending only on the dimension* d *such that*

$$\left| \left\langle \mu_t^N, \left(G^N \pi^N - \pi^N G^\infty \right) \Psi \right\rangle \right| \leq C M_1 \|\nabla \varphi\|_{C^2} \|F'\|_{C^1} \frac{1}{N}$$

for all $t \geq 0$.

Proof. Let $I := \left\langle \mu_t^N, G^N \pi^N \Psi \right\rangle$ denote one of the two terms we want to estimate. In view of the expression for the particle generator (2.2) with $g = \mathrm{id}_{\mathbb{N}}$, it holds that

$$I = \left\langle \mu_t^N, N^2 \sum_{x, y \sim x} \eta(x) \{ (\pi^N \Psi)(\eta^{x,y}) - (\pi^N \Psi)(\eta) \} \right\rangle.$$

By definition (2.18) of π^N, we obtain that

$$I = \left\langle \mu_t^N, N^2 \sum_{x, y \sim x} \eta(x) \{ \Psi(\alpha_{\eta^{x,y}}^N) - \Psi(\alpha_\eta^N) \} \right\rangle.$$

Let $\mathcal{R}_1$ be the error term given by

$$\mathcal{R}_1 = \left\langle \mu_t^N, N^2 \sum_{x, y \sim x} \eta(x) \left(\Psi(\alpha_{\eta^{x,y}}^N) - \Psi(\alpha_\eta^N) - D\Psi(\alpha_\eta^N)(\alpha_{\eta^{x,y}}^N - \alpha_\eta^N) \right) \right\rangle,$$

where $D\Psi$ is defined in Remark 2.3.6. Then it holds that

$$I = \mathcal{R}_1 + \left\langle \mu_t^N, N^2 \sum_{x,y\sim x} \eta(x) F'\left(\langle \alpha_\eta^N, \varphi\rangle\right) \langle \alpha_{\eta^{x,y}}^N - \alpha_\eta^N, \varphi\rangle \right\rangle.$$

Definition (2.4) of the empirical measure then yields

$$\begin{aligned} I &= \mathcal{R}_1 + \left\langle \mu_t^N, F'\left(\langle \alpha_\eta^N, \varphi\rangle\right) N^{2-d} \sum_{x,y\sim x} \eta(x) \langle \delta_{\frac{y}{N}} - \delta_{\frac{x}{N}}, \varphi\rangle \right\rangle \\ &= \mathcal{R}_1 + \left\langle \mu_t^N, F'\left(\langle \alpha_\eta^N, \varphi\rangle\right) N^{-d} \sum_{x\in\mathbb{T}_N^d} \eta(x) \Delta_N \varphi(\tfrac{x}{N}) \right\rangle \end{aligned}$$

where

$$\Delta_N f(x) = N^2 \sum_{e\in\mathbb{Z}^d:|e|=1} \left(f(x+\tfrac{e}{N}) - f(x)\right) \tag{2.22}$$

denotes the discrete Laplacian. Replacing the discrete Laplacian with its continuous version yields that

$$I = \mathcal{R}_1 + \mathcal{R}_2 + \left\langle \mu_t^N, F'\big(\langle \alpha_\eta^N, \varphi\rangle\big) \langle \alpha_\eta^N, \Delta\varphi\rangle \right\rangle$$

with an error term

$$\mathcal{R}_2 = \left\langle \mu_t^N, F'\big(\langle \alpha_\eta^N, \varphi\rangle\big) \langle \alpha_\eta^N, \Delta_N\varphi - \Delta\varphi\rangle \right\rangle.$$

Hence the expression for G^∞, Lemma 2.3.5, yields

$$\begin{aligned} I = \left\langle \mu_t^N, G^N \pi^N \Psi \right\rangle &= \mathcal{R}_1 + \mathcal{R}_2 + \left\langle \mu_t^N, F'\left(\langle \alpha_\eta^N, \varphi\rangle\right) \langle \alpha_\eta^N, \Delta\varphi\rangle \right\rangle \\ &= \mathcal{R}_1 + \mathcal{R}_2 + \left\langle \mu_t^N, \pi^N G^\infty \Psi(\alpha_\eta^N) \right\rangle. \end{aligned}$$

In order to finish the proof of Lemma 2.3.8, we just need to bound the error terms $\mathcal{R}_1$ and $\mathcal{R}_2$.

First we bound $\mathcal{R}_1$. Setting

$$G(\tau) = \Psi\left(\alpha_\eta^N + \tau(\alpha_{\eta^{x,y}}^N - \alpha_\eta^N))\right)$$

yields

$$G'(\tau) = F'\left(\langle \alpha_\eta^N + \tau(\alpha_{\eta^{x,y}}^N - \alpha_\eta^N), \varphi\rangle\right) \langle \alpha_{\eta^{x,y}}^N - \alpha_\eta^N, \varphi\rangle$$

and

$$G''(\tau) = F''\left(\langle \alpha_\eta^N + \tau(\alpha_{\eta^{x,y}}^N - \alpha_\eta^N), \varphi\rangle\right) \langle \alpha_{\eta^{x,y}}^N - \alpha_\eta^N, \varphi\rangle^2.$$

The mean value theorem yields

$$G(1) - G(0) - G'(0) = 1/2G''(\xi)$$

for some $\xi \in (0,1)$. Consequently $|\mathcal{R}_1|$ is bounded by

$$|\mathcal{R}_1| \leq \frac{1}{2}\|F''\|_{L^\infty}\Big\langle \mu_t^N, N^2 \sum_{x\sim y} \eta(x) \left\langle \alpha^N_{\eta^{x,y}} - \alpha^N_\eta, \varphi \right\rangle^2 \Big\rangle.$$

For each fixed $x \in \mathbb{T}_N^d$ it holds that

$$N^2 \sum_{y\,\text{s.t.}\,y\sim x} \langle \alpha^N_{\eta^{x,y}} - \alpha^N_\eta, \varphi\rangle^2 = \frac{N^2}{N^{2d}} \sum_{y\,\text{s.t.}\,y\sim x} \left(\varphi(\tfrac{y}{N}) - \varphi(\tfrac{x}{N})\right)^2 \leq \frac{2^d}{N^{2d}}\|\nabla\varphi\|^2_{L^\infty},$$

where the factor 2^d stems from the number of neighbours y of x. Hence the error is bounded by

$$\mathcal{R}_1 \leq \frac{2^{d-1}}{N^d}\|F''\|_{L^\infty}\|\nabla\varphi\|_{L^\infty}\Big\langle \mu_t^N, \frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\eta(x)\Big\rangle.$$

Since the number of particles is conserved under the evolution, the last of these factors yields

$$\Big\langle \mu_t^N, \frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\eta(x)\Big\rangle = \Big\langle \mu_0^N, \frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\eta(x)\Big\rangle \leq M_1,$$

and hence $|\mathcal{R}_1| \leq CM_1\|F'\|_{C^1}\|\nabla\varphi\|_{L^\infty}N^{-1}$. Finally, a Taylor expansion yields

$$\|\Delta_N\varphi - \Delta\varphi\|_{L^\infty} \leq \|\Delta\varphi\|_{C^1}\frac{1}{N}$$

and therefore $|\mathcal{R}_2| \leq CM_1\|F'\|_{L^\infty}\|\Delta\varphi\|_{C^1}N^{-1}$. □

Using the Lemmas 2.3.4 to 2.3.8, we can prove the hydrodynamic limit.

Proof of Theorem 2.3.1. Let Ψ be as defined in equation (2.19). Then the term to be estimated is

$$\left\langle \mu_t^N, F\left(\langle \alpha_\eta^N, \varphi\rangle\right)\right\rangle - F\left(\langle f_t, \varphi\rangle\right) = \left\langle S_t^N\mu_0^N, \Psi\big(\alpha_\eta^N\big) - \Psi\big(S_t^\infty f_0\big)\right\rangle.$$

Consequently the definitions of T_t^N and T_t^∞ yield

$$\left\langle S_t^N\mu_0^N, \Psi\left(\alpha_\eta^N\right) - \Psi\left(S_t^\infty f_0\right)\right\rangle = \left\langle \mu_0^N, T_t^N\Psi\big(\alpha_\eta^N\big) - T_t^\infty\Psi(f_0)\right\rangle.$$

Note here that T_t^N acts on $\Psi(\alpha_\eta^N)$ through η. Recalling the definition (2.18) of π^N, we need to bound the term

$$\Big|\left\langle \mu_0^N, T_t^N\pi^N\Psi - T_t^\infty\Psi(f_0)\right\rangle\Big|.$$

The triangle inequality and (2.18) yield

$$\begin{aligned}
&\Big|\big\langle \mu_0^N, T_t^N \pi^N \Psi - T_t^\infty \Psi(f_0)\big\rangle\Big| \\
&\le \big|\big\langle \mu_0^N, T_t^N(\pi^N \Psi) - \pi^N(T_t^\infty \Psi)\big\rangle\big| + \big|\big\langle \mu_0^N, (T_t^\infty \Psi)\big(\alpha_\eta^N\big) - (T_t^\infty \Psi)(f_0)\big\rangle\big| \\
&=: \mathcal{T}_1 + \mathcal{T}_2.
\end{aligned}$$

Since Ψ as defined in (2.19) satisfies

$$\frac{d}{dt} T_t^\infty \Psi(f) = G^\infty T_t^\infty \Psi(f),$$

it follows

$$\frac{d}{ds}\big(T_s^N \pi^N T_{t-s}^\infty(\eta)\big) = T_s^N G^N \pi^N T_{t-s}^\infty \Psi(\eta) - T_s^N \pi^N G^\infty T_{t-s}^\infty \Psi(\eta).$$

Consequently, it holds that

$$\begin{aligned}
\mathcal{T}_1 &= \big|\big\langle \mu_0^N, T_t^N \pi^N \Psi - \pi^N T_t^\infty \Psi\big\rangle\big| \\
&\le \int_0^t \big|\langle S_s^N \mu_0^N, (G^N \pi^N - \pi^N G^\infty)(T_{t-s}^\infty \Psi)\rangle\big| \; ds.
\end{aligned}$$

Note that $T_{t-s}^\infty \Psi$ is of the form (2.19) with F and φ_{t-s} as given in Lemma 2.3.4 on stability. Hence Lemma 2.3.8, which regards consistency, yields

$$\mathcal{T}_1 \le \frac{CM_1}{N} \|F'\|_{C^1} \int_0^t \|\nabla \varphi_{t-s}\|_{C^2} \; ds.$$

If we split up the above integral into the contributions $t \le 1$ and $t > 1$, Lemma 2.3.7 yields

$$\mathcal{T}_1 \le \frac{CM_1}{N} \|F'\|_{C^1} \big(\|\nabla \varphi\|_{C^2} + \|S_1^\infty \nabla \varphi\|_{H^n}\big).$$

For the second term $\mathcal{T}_2$, Lemma 2.3.4, (ii) yields

$$\mathcal{T}_2 \le \|F'\|_{C^1} \|\varphi\|_{C^3} \sup_{\substack{\omega \in C^3(\mathbb{T}^d) \\ \|\omega\|_{C^3} \le 1}} \Big\langle \mu_0^N, \big|\langle \alpha_\eta^N - f_0, \omega\rangle\big| \Big\rangle,$$

which completes the proof of the hydrodynamic limit. □

Remark. The term $\mathcal{T}_1$ is a measure for the difference between the discrete and the continuous semigroups along the empirical measure, whereas $\mathcal{T}_2$ measures the evolution under the limit equation of the distance between the initial empirical measure and the initial macroscopic datum.

This is reminiscent of the results in numerical analysis, where the convergence of a numerical scheme usually requires a consistency and a stability estimate.

2.4 Hydrodynamic limit for zero range processes

In this section we shall apply the method outlined in Section 2.3 using the example of independent random walks to prove a hydrodynamic limit for the zero range process with an explicit bound on the rate of convergence. Throughout we require Assumption 1 to hold. Furthermore, in this section we demand $d = 1$. This restriction on the dimension of the problem is necessary only for the propagation of the regularity, Lemma 2.4.13. In order to emphasize the generality of our approach, we shall still denote the dimension by d, and understand $d = 1$. We shall see that indeed Lemma 2.4.13 is the only result where we explicitly need $d = 1$ - assuming a corresponding result in higher dimensions, our method implies the hydrodynamic limit with an explicit, uniform-in-time rate of convergence in d dimensions. In Section 2.7, we shall discuss work in progress on how to achieve this.

We shall show that in the sense of Theorem 2.3.1, as the number N of sites in the lattice $\mathbb{T}_N^d$ approaches infinity, the empirical measure converges to the solution of the limit partial differential equation, specifically the filtration equation

$$\partial_t f_t = \Delta\sigma(f_t)$$

for the nonlinearity $\sigma : [0, \infty) \to [0, \infty)$ appearing in (2.6). The nonlinearity is explicitly given as follows: let $Z : [0, \lambda^*) \to \mathbb{R}$ be the *partition function* of the zero range process given by (2.7), with λ^* denoting the radius of convergence of $Z(\cdot)$. Assumption 1 (iii) in fact yields $\lambda^* = +\infty$, since the assumption implies $g(n) \geq \tilde{\delta} n$ for some $\tilde{\delta} \leq \delta/n_0$.
The density function as a function of the *fugacity* λ is given by

$$R(\lambda) = \lambda\partial_\lambda \log(Z(\lambda)) = \frac{1}{Z(\lambda)} \sum_{n\geq 0} \frac{n\lambda^n}{g(n)!}. \tag{2.23}$$

This is a smooth function $R : [0, \infty) \to \mathbb{R}$. It is not hard to prove, see [47], that R strictly monotonously increasing with $\lim_{\lambda\to\infty} R(\lambda) = \infty$. Then $\sigma : [0, \infty) \to [0, \infty)$ is well-defined as its inverse function. Thus ν_ρ^N, as defined in (2.6), is an invariant and translation-invariant product measure with density

$$\langle \nu_\rho^N , \eta(x)\rangle = \rho.$$

Furthermore its average jump rate satisfies

$$\langle \nu_\rho^N , g(\eta(x))\rangle = \sigma(\rho).$$

The Lipschitz continuity of the rate function implies that $\sigma(\rho)$ is also Lipschitz continuous with constant g^*, see [47]. The second assumption implies that $g(n) \geq \tilde{\delta} n$ and hence

$\inf_\rho \sigma(\rho)/\rho > 0$. Therefore it is impossible to obtain a porous medium equation, e.g. $\sigma(\rho) = \rho^m$, $m > 1$, in this limit. Indeed Assumption 1 yields

Lemma 2.4.1. *It holds that*

$$0 < \inf_{\rho \geq 0} \sigma'(\rho) \leq \sup_{\rho \geq 0} \sigma'(\rho) < +\infty. \tag{2.24}$$

For the higher derivatives of order $j \geq 2$, there exist constants $C_j < +\infty$ such that

$$\sigma^{(j)}(\rho) \leq C_j(1 + \rho^{j-1}) \tag{2.25}$$

for all $\rho \geq 0$ and $j \geq 2$.

Proof. The upper bound in (2.24) is well-known and can be proved by coupling two measures ν_ρ^N and $\nu_{\tilde{\rho}}^N$, cf. [47]. We obtain the lower bound corresponding to ellipticity of (2.3) by a formula expressing σ' through the variation of the number of particles, see [52]. Let us start by proving (2.25) in the case $j = 2$. This second order bound can be seen from

$$\sigma''(\rho) = -\frac{R''(\sigma(\rho))\sigma'(\rho)}{R'(\sigma(\rho))^2} = -R''(\sigma(\rho))\sigma'(\rho)^3, \tag{2.26}$$

since σ and R are inverse to each other, i.e. $R(\sigma(\rho)) = \rho$. Recall that

$$R(\lambda) = \lambda \partial_\lambda \log Z(\lambda).$$

Assumption 1 yields that

$$\delta^j \leq Z^{(j)}(\lambda)/Z(\lambda) \leq (g^*)^j$$

is bounded for all j–th order derivatives with $j \geq 0$. Therefore it holds that

$$\frac{d^j}{d\lambda^j} R(\lambda) = \lambda \frac{d^j}{d\lambda^j} \log Z(\lambda) + j\lambda \frac{d^{j-1}}{d\lambda^{j-1}} \log Z(\lambda) \leq C(1 + \lambda)$$

and consequently setting $\lambda = \sigma(\rho) \leq g^* \rho$ yields $\sigma''(\rho) \leq C(1 + \rho)$. Iterating, we see that with each derivative of (2.26), we pick up another power of ρ. □

Remark 2.4.2. The rather naive estimates on the higher derivatives can be significantly improved using the estimates found in [52].

Since the limit partial differential equation does not allow measure-valued weak solutions, we consider solutions in

$$H := L^\infty(\mathbb{T}^d).$$

Note that in particular $H \subset L^2(\mathbb{T}^d)$. We shall also work a lot in the weak space $H^{-1}(\mathbb{T}^d)$. Let us recall its definition and a few basic facts in the following remark.

Remark 2.4.3 (The weak space $H^{-1}(\mathbb{T}^d)$)**.** Set

$$\mathcal{H}^1(\mathbb{T}^d) := \left\{ f \in H^1(\mathbb{T}^d) \mid \int_{\mathbb{T}^d} f(u)\, du = 0 \right\}$$

and let $H^{-1}(\mathbb{T}^d)$ denote its dual space, i.e. the space of linear bounded maps $\mathcal{H}^1(\mathbb{T}^d) \to \mathbb{R}$. It follows that

$$-\Delta : \mathcal{H}^1(\mathbb{T}^d) \to H^{-1}(\mathbb{T}^d),\ f \mapsto -\Delta f$$

is an isomorphism, where $(-\Delta)^{-1} f$ corresponds to the weak solution to the Poisson equation on $\mathbb{T}^d$, i.e.

$$\langle \nabla(-\Delta)^{-1} f, \nabla \tilde{f} \rangle = \langle f, \tilde{f} \rangle$$

for all $\tilde{f} \in \mathcal{H}^1(\mathbb{T}^d), f \in H^{-1}(\mathbb{T}^d)$. Thus we set

$$\|f\|_{H^{-1}}^2 := \langle f, (-\Delta)^{-1} f \rangle$$

for all $f \in H^{-1}(\mathbb{T}^d)$. In Fourier space, this norm is given by

$$\|f\|_{H^{-1}}^2 = \sum_{\zeta \in \mathbb{Z}^d \setminus \{0\}} \frac{1}{|\zeta|^2} |\hat{f}(\zeta)|^2.$$

This norm is indeed equivalent to the usual H^{-1}–operator norm, e.g. it holds that

$$\langle \tilde{f}, f \rangle_{L^2} \leq \|\nabla f\|_{L^2} \|\tilde{f}\|_{H^{-1}} \tag{2.27}$$

for all $f \in \mathcal{H}^1(\mathbb{T}^d)$ and $\tilde{f} \in L^2(\mathbb{T}^d)$. A slightly complicating factor is the fact that the H^{-1}–norm vanishes for constants, i.e. members of $H^{-1}(\mathbb{T}^d)$ are only uniquely identified up to constants. It directly follows that (2.27) also holds for all $f \in H^1(\mathbb{T}^d)$ as soon as $\tilde{f} \in L^2(\mathbb{T}^d)$ satisfies $\int_{\mathbb{T}^d} \tilde{f}(u)\, du = 0$. It also holds that

$$\|f\|_{H^{-1}} \leq C \|f\|_{L^2}$$

for all $f \in H^{-1}(\mathbb{T}^d)$, which can be seen as a variant of the Poincaré inequality.

In the almost linear case, when (2.24) holds, the theory of weak solutions to equation (2.3) is stated in the following lemma.

Lemma 2.4.4 (Weak solutions to the filtration equation)**.** *For every $f_0 \in H$, the filtration equation* (2.3) *possesses a unique weak solution $f_t \in H$, $t \in [0, \infty)$, in the sense that*

$$\int_0^\infty \int_{\mathbb{T}^d} \big(f_t(u) \partial_t \omega(t,u) + \sigma(f_t(u)) \Delta \omega(t,u) \big)\, du dt + \int_{\mathbb{T}^d} f_0(u) \omega(0,u)\, du = 0$$

for all $\omega \in C^1([0,\infty); C^2(\mathbb{T}^d))$ with compact support in $[0,\infty) \times \mathbb{T}^d$. The solution $f =$

$(f_t)_{t\in[0,\infty)}$ *also satisfies*

$$f \in L^2(0,\infty; H^1(\mathbb{T}^d)) \cap H^1(0,\infty; H^{-1}(\mathbb{T}^d)) \subset C([0,\infty); L^2(\mathbb{T}^d)).$$

In particular

$$\frac{d}{dt}\langle f_t, \varphi\rangle = \langle \sigma(f_t), \Delta\varphi\rangle \tag{2.28}$$

for all $t \geq 0$ *and all* $\varphi \in C^2(\mathbb{T}^d)$.

Proof. Starting from smooth solutions in $C^\infty(\mathbb{T}^d)$, cf. Ladyzhenskaya [51], it is classical to construct a weak solutions, see for example [83] or [47, Appendix 2]. The maximum principle shows that the semigroup S_t^∞ conserves the $L^\infty(\mathbb{T}^d)$–norm, i.e.

$$\|S_t^\infty f_0\|_{L^\infty} \leq \|f_0\|_{L^\infty}.$$

Therefore it holds that $S_t^\infty : H \to H$. The solution is unique, cf. the stability estimates of Lemma 2.4.12. Furthermore it holds that

$$\frac{d}{dt}\|f_t\|_{L^2}^2 = -2\int_{\mathbb{T}^d} \sigma'(f_t)|\nabla f_t|^2\, du,$$

whence S_t^∞ conserves the $L^2(\mathbb{T}^d)$–norm and

$$\int_0^T \int_{\mathbb{T}^d} |\nabla f_t|^2\, dudt \leq C\int_0^T \int_{\mathbb{T}^d} \sigma'(f_t)|\nabla f_t|^2\, dudt \leq C\|f_0\|_{L^2}^2.$$

is bounded. It follows that $f = (f_t)_{t\geq 0} \in L^2(0,\infty; H^1(\mathbb{T}^d))$. The filtration equation $\partial_t f_t = \Delta\sigma(f_t)$ consequently yields $(\partial_t f_t)_{t\geq 0} \in L^2(0,\infty; H^{-1}(\mathbb{T}^d))$ and therefore

$$f \in L^2(0,\infty; H^1(\mathbb{T}^d)) \cap H^1(0,\infty; H^{-1}(\mathbb{T}^d)).$$

Interpolation, see Theorem 3 in §5.9.2 of [29], then yields $f \in C([0,\infty); L^2(\mathbb{T}^d))$. Now the weak form of the filtration equation yields equation (2.28) for all $\varphi \in C^2(\mathbb{T}^d)$ and almost all $t \geq 0$. Since f is continuous in time with values in $L^2(\mathbb{T}^d)$, this equation indeed extends to all $t \geq 0$. $\square$

Before we can proceed with the statement of the hydrodynamic limit and its proof, we need to introduce a last bit of notation.

Definition 2.4.5. We say that two configurations $\eta, \zeta \in X_N$ satisfy

$$\eta \leq \zeta$$

if $\eta(x) \le \zeta(x)$ for all $x \in \mathbb{T}_N^d$. A function $f^N \in C_b(X_N)$ is said to be *monotonous* if

$$f^N(\eta) \le f^N(\zeta)$$

for all $\eta \le \zeta$. Given two probability measures $\mu, \nu \in P(X_N)$, we say that μ is *bounded* by ν, written

$$\mu \le \nu,$$

if it holds that $\langle \mu, f^N \rangle \le \langle \nu, f^N \rangle$ for all monotonous $f^N \in C_b(X_N)$.

Furthermore the empirical measure as defined in (2.4) is not regular enough to give sense to $\Delta\sigma(\alpha_\eta^N)$. Hence we shall measure particle densities of the configuration $\eta \in X_N$ of the discrete system via the mollified empirical measure

$$\alpha_\eta^{N,\epsilon} := \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \delta_{\frac{x}{N}}^{(\epsilon)} \in H, \tag{2.29}$$

where

$$\delta_0^{(\epsilon)} = \frac{1}{\epsilon^d} \chi(\tfrac{\cdot}{\epsilon}) \in H \tag{2.30}$$

is an approximation of the dirac distribution and $\delta_u^{(\epsilon)}$ its translation by $u \in \mathbb{T}^d$. We let $\chi \in C_0^\infty(\mathbb{R}^d)$ have compact support in, for example, $(-1/2, 1/2)^d$. Since we are working on the torus, $\chi(u/\epsilon)$ should be understood in $\mathbb{T}^d$, e.g. by taking its periodization $\sum_{z \in \mathbb{Z}^d} \chi((u+z)/\epsilon)$.

2.4.1 The hydrodynamic limit

The following theorem is our main result, detailing a hydrodynamic limit with an explicit rate of convergence in one dimension.

Theorem 2.4.6 (Hydrodynamic limit for zero range processes)**.** *Assume $d = 1$ and let $F \in C_b^2(\mathbb{R})$, $\varphi \in C^3(\mathbb{T}^d)$, $k > (d+2)/2$, $C_H > 0$, and $\rho > 0$ be given. Then there exists a rate of convergence $r_{\mathrm{HL}}(\epsilon, N)$ with polynomial dependence on ϵ and N, whose exponents only depend on k (and d), such that the following hydrodynamic limit holds. For all $t \ge 0$, $N \in \mathbb{N}$, $1/N < \epsilon < 1$, $f_0 \in H$, and $\mu_0^N \in P(X_N)$ such that the entropy and the measure itself are bounded relative to the grand-canonical measure ν_ρ^N, i.e.*

$$H^N\big(\mu_0^N | \nu_\rho^N\big) \le C_H N^d \qquad \text{and} \qquad \mu_0^N \le \nu_\rho^N,$$

it holds that there exists a rate of convergence $r_{\mathrm{HL}}(\epsilon, N)$ *such that*

$$\begin{aligned}(2.31)\quad \big\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle_{L^2}\big) - F\big(\langle f_t, \varphi\rangle_{L^2}\big)\big\rangle \le r_{\mathrm{HL}}(\epsilon, N) \\ + \|F'\|_{L^\infty}\|\varphi\|_{L^\infty}\left\langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^1}\right\rangle\end{aligned}$$

where f_t *is given by the solution to the filtration equation* (2.3) *and* μ_t^N *is given by the zero range process, as detailed above. For all* $T > 0$*,* $\varrho > 0$*, and* $0 \le 2l + 1 \le N$*, the rate of convergence* $r_{\mathrm{HL}}(\epsilon, N)$ *is bounded by*

$$\begin{aligned}C\|F\|_{C^2}(1 + \|\varphi\|_{C^3} + \|\varphi\|_{H^1}^2)\Big(T\epsilon^{-(d+4)((1+\frac{d}{2})\frac{2k^2+k}{2k+2}+kd)-d(1-\frac{\theta}{2})}N^{1-\theta(d+1)} \\ + T^{\frac12}\epsilon^{-\frac{4+d}{2}}N^{-2} + \epsilon + e^{-cT}N^{2+d}\epsilon^{-2d} + T^{\frac12}r_{\mathrm{RL}}(\varrho, l, \epsilon, N)\Big)\end{aligned}$$

for some finite, positive constants c *and* C *depending only on* d*,* k*,* C_H*, and* ρ*. Here* $\theta = \theta(k) = (2k - d - 2)/(2k + 2)$ *and the additional rate function* $r_{\mathrm{RL}}(\varrho, l, \epsilon, N)$ *is bounded by*

$$\big(N^{-\frac12}l^{\frac12} + \epsilon^{\frac12}l^{\frac14}\big)\varrho l^{\frac{d}{4}} + \varrho l^{-\frac{d}{4}} + \varrho^{-\frac14} + \frac{l}{\epsilon N}.$$

It stems from the replacement lemma, Lemma 2.4.19.

Remark 2.4.7. Thus we see that the contributions to the hydrodynamic limit can be divided into three parts. The first term describes the propagation of the initial error due to the approximation of f_0 by the discrete particle configurations at time $t = 0$ and the other two are errors coming from stability properties of the limit equation and an error term due to the replacement lemma, respectively. The replacement lemma is an older result, appearing first in [36].

Note that the choice of the density ρ in the assumption regarding the Gibbs measure ν_ρ^N is a slightly arbitrary. Indeed, if the relative entropy

$$\frac{1}{N^d}H^N(\mu_0^N|\nu_\rho^N) \le C$$

is bounded, then so is

$$\frac{1}{N^d}H^N(\mu_0^N|\nu_{\tilde\rho}^N) \le C(\tilde\rho)$$

for any $\tilde\rho > 0$. Furthermore, if $\|f_0\|_{L^\infty} \le \rho$, the local Gibbs measure (2.11) satisfies

$$\nu_{f_0(\cdot)}^N \le \nu_\rho^N$$

and this choice for μ_0^N satisfies the bound on the entropy as well. The rate here is much slower than the rate for independent random walks, given in Theorem 2.3.1. This is mainly due to the fact that we shall need to replace the rate function g with its local average via a replacement lemma.

Remark 2.4.8. We can replace the term estimating the compatibility of the initial data by a slightly modified version. Under the assumptions of Theorem 2.4.6, its proof also yields

$$\begin{aligned}&\big\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle_{L^2}\big) - F\big(\langle f_t, \varphi\rangle_{L^2}\big)\big\rangle \\ &\le r_{\mathrm{HL}}(\epsilon, N) + \|F'\|_{L^\infty}\|\varphi\|_{H^1}\big\langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{H^{-1}}\big\rangle \\ &\qquad + \|F'\|_{L^\infty}\big|\textstyle\int_{\mathbb{T}^d}\varphi(u)\,du\big|\big\langle \mu_0^N, \big|N^{-d}\sum_x \eta(x) - \int_{\mathbb{T}^d} f_0(u)\,du\big|\big\rangle.\end{aligned}$$

This is a consequence of the following variant of the basic H^{-1}–stability estimate in Lemma 2.4.12:

$$\|\tilde f_t - \tilde f_\infty - f_t + f_\infty\|_{H^{-1}} \le \|\tilde f_0 - \tilde f_\infty - f_0 + f_\infty\|_{H^{-1}} + C|\tilde f_\infty - f_\infty|,$$

where $f_\infty = \int_{\mathbb{T}^d} f_t(u)du$ is the (constant) integral of the solution f_t and likewise for $\tilde f_\infty$. The above estimate of the hydrodynamic limit can be useful if we only have information about the H^{-1}–convergence of the initial data and some information on the number of particles of the zero range process. For example, we might require that there exists some $N_0 \in \mathbb{N}$ such that

$$\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\eta(x) = \int_{\mathbb{T}^d} f_0(u)\,du$$

holds μ_0^N–almost surely for all $N \ge N_0$. Of course, this is only possible if the integral $\int_{\mathbb{T}^d} f_0(u)du$ is an integer. The convergence of $\alpha_\eta^{N,\epsilon}$ in $H^{-1}(\mathbb{T}^d)$ is more favourable in terms of powers of ϵ than the convergence in $L^1(\mathbb{T}^d)$. On the other hand, the initial data converges much faster in general than the bounds we can give for $r_{\mathrm{HL}}(\epsilon, N)$, so it will not matter much in which norm we measure the convergence of the initial data, see the proof of Corollar 2.4.9 below.

As before Theorem 2.4.6 yields convergence to the hydrodynamic limit, conditional on convergence of the initial data.

Corollary 2.4.9. *Assume $d = 1$ and let $F \in C_b^2(\mathbb{R})$, and $\varphi \in C^3(\mathbb{T}^d)$ be given. Then for all $N \in \mathbb{N}$ and $f_0 \in C^1(\mathbb{T}^d)$, there exists a $\mu_0^N \in P(X_N)$ such that it holds*

$$\big\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle_{L^2}\big) - F\big(\langle f_t, \varphi\rangle_{L^2}\big)\big\rangle \le CN^{-\kappa}$$

for some $\kappa > 0$, e.g. any $\kappa < 1/6700$ works. Here μ_t^N is given by the zero range process and f_t by the solution to the corresponding filtration equation $\partial_t f_t = \Delta\sigma(f_t)$.
In other words, if η is distributed according to law μ_t^N, then $\alpha_\eta^N \rightharpoonup^* f_t$ in distribution as $N \to \infty$.

Remarks 2.4.10. (1) The statements (3)-(6) of Remark 2.3.3 remain valid and relevant to this case.
(2) The condition $H^N(\mu_0^N|\nu_\rho^N) \le CN^d$ is quite useful in connection with the so-called *entropy inequality*. This inequality states that for all $\gamma > 0$, $f \in C_b(X_N)$ and any two probability measures $\mu, \nu \in P(X_N)$, it holds that

$$\langle \mu, f\rangle \le \frac{1}{\gamma}\Big(H^N(\mu|\nu) + \log\langle \nu, \exp(\gamma f)\rangle\Big). \tag{2.32}$$

For example, if we set $f(\eta) = \sum_x \eta(x)$, $\mu = \mu_0^N$, and $\nu = \nu_\rho^N$ in estimate (2.32), we obtain that

$$\langle \mu_0^N, N^{-d}\textstyle\sum_x \eta(x)\rangle \le \dfrac{1}{\gamma}\Big(N^{-d}H^N(\mu_0^N|\nu_\rho^N) + \log\langle \nu_\rho^N, \exp(\gamma\eta(0))\rangle\Big),$$

since ν_ρ^N is a product measure. Thus we obtain a bound on the average particle density

$$\langle \mu_0^N, N^{-d}\sum_{x\in\mathbb{T}_N^d} \eta(x)\rangle \le C.$$

Note here that the infinite radius of convergence $\rho^* = +\infty$ of the partition function $Z(\cdot)$ yields finite exponential moments

$$\langle \nu_\rho^N, \exp(\gamma\eta(0))\rangle = \frac{Z(\rho e^\gamma)}{Z(\rho)} < +\infty$$

for all $\gamma \in \mathbb{R}$. Of course in our case, the bound on the average number of particles also follows from $f_0^N \le \nu_\rho^N$ and the monotonicity of $N^{-d}\sum_x \eta(x)$ in η.
(3) While the size of κ is certainly not optimal, it is qualitatively correct since has the expected polynomial dependence on N. As far as we are aware, it also constitutes the first example of an explicit rate of convergence of the zero range process to the hydrodynamic limit and the first example of a uniform-in-time rate of convergence. It has the added advantage that the exponents do not depend on the function g. Thus, for example, it should allow for perturbative arguments to be applied to prove the hydrodynamic limit of small perturbations of the zero range process as given in the assumptions.

Proof of Corollary 2.4.9. First of all we can choose $\mu_0^N := \nu_{f_0(\cdot)}^N$ which was defined in (2.11). Then in a rough first estimate it holds that

$$\langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^1}\rangle \le \langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^2}\rangle^{\frac{1}{2}} \le \frac{C}{\sqrt{\epsilon N}}.$$

We can deduce this as follows. First, it holds that

$$\big\langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^2}^2 \big\rangle = \int_{\mathbb{T}^d} \Big\langle \mu_0^N, \frac{1}{N^{2d}} \sum_{x,y} \eta(x)\eta(y)\delta^{(\epsilon)}_{\frac{x}{N}}(u)\delta^{(\epsilon)}_{\frac{y}{N}}(u) - \frac{2}{N^d}\sum_x \eta(x)\delta^{(\epsilon)}_{\frac{x}{N}} f_0(u) + f_0(u)^2 \Big\rangle \, du.$$

Since $\eta(x)$ and $\eta(y)$ are independently distributed under μ_0^N as long as $x \neq y$, this equals

$$\int_{\mathbb{T}^d} \bigg(\frac{1}{N^{2d}} \sum_{x\neq y} f_0(\tfrac{x}{N}) f_0(\tfrac{y}{N}) \delta^{(\epsilon)}_{\frac{x}{N}}(u)\delta^{(\epsilon)}_{\frac{y}{N}}(u) + \frac{1}{N^{2d}} \sum_{x\in\mathbb{T}_N^d} \langle \nu^N_{f_0(\frac{x}{N})}, \eta(0)^2\rangle \delta^{(\epsilon)}_{\frac{x}{N}}(u)^2 - \frac{2}{N^d}\sum_{x\in\mathbb{T}_N^d} f_0(\tfrac{x}{N})\delta^{(\epsilon)}_{\frac{x}{N}} f_0(u) + f_0(u)^2 \bigg) \, du.$$

Since $f_0 \in C^1(\mathbb{T}^d)$ is bounded, it follows that the second moment $\langle \nu^N_{f_0(\frac{x}{N})}, \eta(0)^2\rangle$ is bounded uniformly in x and N. Furthermore it holds that $\|\delta^{(\epsilon)}_{x/N}\|_{L^2}^2 \leq C\epsilon^{-d}$. Thus the above is bounded from above by

$$\bigg\| \frac{1}{N^d} \sum_{x\in\mathbb{T}_N^d} f_0(\tfrac{x}{N})\delta^{(\epsilon)}_{\frac{x}{N}} - f_0 \bigg\|_{L^2}^2 + \mathcal{O}\Big(\frac{1}{(\epsilon N)^d}\Big),$$

Note that $\int_{\mathbb{T}^d} \chi(u)\, du = 1$ and hence

$$\bigg| \frac{1}{(\epsilon N)^d} \sum_{x\in\mathbb{T}_N^d} \chi\Big(\frac{x}{\epsilon N}\Big) - 1 \bigg| \leq \|\nabla\chi\|_\infty \frac{C}{\epsilon N}. \tag{2.33}$$

Since $f_0 \in C^1(\mathbb{T}^d)$ is uniformly Lipschitz and the support of χ in (2.30) is compact, this shows that

$$\bigg| \frac{1}{N^d} \sum_{x\in\mathbb{T}_N^d} f_0(\tfrac{x}{N})\delta^{(\epsilon)}_{\frac{x}{N}}(u) - f_0(u) \bigg| \leq \frac{C}{\epsilon N}.$$

Thus we have shown that

$$\big\langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^2}^2 \big\rangle \leq \frac{C}{\epsilon N}.$$

In order to estimate a rate of convergence for the hydrodynamic limit, we make the Ansatz that $\epsilon = \epsilon(N), l = l(N), \varrho = \varrho(N)$, and $T = T(N)$ are all monomials in N. If we optimize over the set of possible powers, we find that indeed

$$\big\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle_{L^2}\big) - F\big(\langle f_t, \varphi\rangle_{L^2}\big) \big\rangle = \mathcal{O}(N^{-\kappa})$$

for some $\kappa > 0$. Since $d = 1$, we obtain that, for example, we can achieve any rate κ with $\kappa < 1/6700$. Note that this bound is much larger than one would expect in view of the law of large numbers and not optimal. On the other hand, it is independent of the rate function g, as long as g satisfies Assumption 1. $\square$

As in Section 2.3 we have a collection of semigroups S_t^N and T_t^N describing the dynamics of the particle process as well as S_t^∞ and T_t^∞ describing the evolution of the limit equation. The semigroup S_t^∞ is defined by

$$S_t^\infty f_0 := f_t,$$

for all $f_0 \in H$, where $f_t \in H$ is the solution (2.3) corresponding to the initial datum f_0. Uniqueness of the solutions shows that it is indeed a semigroup. Then T_t^∞ is again given by

$$T_t^\infty \Psi(f) = \Psi(S_t^\infty f)$$

for all $\Psi \in C_b(H)$ and $f \in H$. The relationships of the semigroups can be summarized as

$$S_t^N : P(X_N) \to P(X_N) \text{ with dual } T_t^N : C_b(X_N) \to C_b(X_N),$$
$$S_t^\infty : H \to H \text{ with pullback } T_t^\infty : C_b(H) \to C_b(H).$$

The semigroup T_t^N has generator G^N given in equation (2.2), whereas the time-derivative G^∞ of T_t^∞ will be given in Lemma 2.4.18 below. Using the empirical measures, we also define an embedding $\pi^{N,\epsilon} : C_b(H) \to C_b(X_N)$ via

$$\big(\pi^{N,\epsilon}\Psi\big)(\eta) = \Psi(\alpha_\eta^{N,\epsilon}),$$

where we shall usually drop the superscript ϵ for ease of notation. This embedding will allow us to compare the semigroups T_t^N and T_t^∞ directly.

Remark 2.4.11. The heat equation admits measure-valued solutions and hence we could give sense to $\Delta\alpha_\eta^N$. Even though there exist solutions to the nonlinear heat equation $\partial_t f = \Delta\sigma(f)$ started from a measure, this approach is not feasible here, since we cannot give sense to $G^\infty\Psi(f) = D\Psi(f)(\Delta\sigma(f))$ if f is just a measure. This is the main reason we need to use the mollified empirical measure

$$\alpha_\eta^{N,\epsilon} = \alpha_\eta^N * \delta^{(\epsilon)},$$

which can be seen as obtained through a convolution. The mollified empirical measure induces the following local averages: For any function $h : \mathbb{N} \to \mathbb{R}$, we set

$$(h \circ \eta)^{(\epsilon)}(u) := \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} h(\eta(x))\delta_{\frac{x}{N}}^{(\epsilon)}(u) \tag{2.34}$$

where we recall that $\delta^{(\epsilon)}(u)$ is given in (2.30). The mollification introduces another scale, which might be called *mesoscopic*. It has microscopic size ϵN and macroscopic size ϵ.

Such an intermediate scale appears in virtually all works on the hydrodynamic limit, see for example the replacement lemma. Here the intermediate scale is inherent in the (mollified) empirical measure.

2.4.2 Regularity of the limit equation

We have seen in Section 2.3, that our proof of the hydrodynamic limit relies on a stability and a consistency result. Since the limit equation in Section 2.3 is linear, its stability is reduced to some bounds on its solutions. Here the question of stability is much more difficult and relies on delicate estimates on the (uniform) propagation of higher regularity. These estimates are crucial to obtaining stability by interpolating with weak contractivity estimates. The weak contractivity estimates and some a-priori bounds on the solutions are the content of the following Lemma 2.4.12, whereas the preservation of higher regularity in $d = 1$ dimension will be proved in Lemma 2.4.13 below.
The filtration equation (2.3) satisfies the following basic estimates, which can all be shown by simple differentiation in time, c.f. Vazquez [83].

Lemma 2.4.12 (Basic estimates)**.** *Let $f_0 \in H^1(\mathbb{T}^d) \cap L^\infty(\mathbb{T}^d)$ and denote by f_t the corresponding solution to* (2.3) *with initial datum f_0. Then the following bounds hold for all $t \geq 0$. The L^p–norms do not grow, i.e.*

$$\|f_t\|_{L^p} \leq \|f_0\|_{L^p} \tag{2.35}$$

for all $1 \leq p \leq \infty$. The H^1–norm of f_t is bounded since

$$\int_{\mathbb{T}^d} |\nabla\sigma(f_t)|^2 \, du + 2\int_0^t \int_{\mathbb{T}^d} \sigma'(f_s)|\Delta\sigma(f_s)|^2 \, duds = \int_{\mathbb{T}^d} |\nabla\sigma(f_0)|^2 \, du. \tag{2.36}$$

In particular, it follows $\|\nabla f_t\|_{L^2} \leq C\|\nabla f_0\|_{L^2}$. If $\tilde{f}_t$ is another solution to (2.3) *with initial datum $\tilde{f}_0$, the following stability estimates hold:*

$$\int_{\mathbb{T}^d} |\tilde{f}_t(u) - f_t(u)| \, du \leq \int_{\mathbb{T}^d} |\tilde{f}_0(u) - f_0(u)| \, du \tag{2.37}$$

for all $\tilde{f}_0, f_0 \in H$, $t \geq 0$, as well as

$$\|\tilde{f}_t - f_t\|^2_{H^{-1}} + 2\int_0^t \int_{\mathbb{T}^d} \big(\tilde{f}_s - f_s\big)\big(\sigma(\tilde{f}_s) - \sigma(f_s)\big) \, duds = \|\tilde{f}_0 - f_0\|^2_{H^{-1}} \tag{2.38}$$

for all $\tilde{f}_0, f_0 \in H$ such that $\int_{\mathbb{T}^d} \tilde{f}_0(u) \, du = \int_{\mathbb{T}^d} f_0(u) \, du$ and $t \geq 0$.

The above bound in $H^1(\mathbb{T}^d)$ does not suffice to prove stability. We will also need an estimate on the conservation of higher regularity. This is harder for the nonlinear filtration equation (2.3) than it was for the heat equation. Given $f_0 \in H$, consider the solution f_t to the filtration equation (2.3) with initial datum f_0. It is a classical result that solutions to the nonlinear, uniformly parabolic equation (2.3) are smooth, i.e. $f_t \in C^\infty(\mathbb{T}^d)$ for all $t > 0$, if $f_0 \in H$. On the other hand, in order to prove the hydrodynamic limit with an explicit rate of convergence, we need to obtain *explicit* information on the size of $\|f_t\|_{H^k}$ for some large enough $k > 0$ in terms of f_0. In $d = 1$ dimensions, this can be achieved by elementary calculations. This is the reason why in the hydrodynamic limit, Theorem 2.4.6, we restricted ourselves to the case $d = 1$. Recall that in order to emphasize the generality of our approach, we still write out the parameter d, understanding $d = 1$ and that we shall illustrate in Section 2.7 how we plan to remove the assumption in future research.

For any integer $k > 0$ and $f \in H^k(\mathbb{T}^d)$, let $D^k f$ denote the k–th derivative of f, a tensor. Furthermore we denote multi-indices in $\mathbb{N}^d$ by $\mathfrak{s}, \mathfrak{r}$ and the corresponding scalar derivatives by $D^{\mathfrak{s}} f_t, D^{\mathfrak{r}} f_t$.

Lemma 2.4.13. *Assume that $d = 1$. Then for every $k > 0$, it holds that*

$$\|D^k f_t\|_{L^2} \leq C\big(1 + \|D^k f_0\|_{L^2} + \|f_0\|_{L^\infty}^{2k^2} \|\nabla f_0\|_{L^2}^{2k^2+k}\big)$$

for all $t \geq 0$ and $f_0 \in H^k(\mathbb{T}^d)$.

Proof. Let $\mathfrak{s} \in \mathbb{N}^d$ be any multi-index such that $|\mathfrak{s}| = k$. The filtration equation yields that

$$\frac{d}{dt} \int_{\mathbb{T}^d} |D^{\mathfrak{s}} f_t|^2 \, du = -2 \int_{\mathbb{T}^d} \nabla D^{\mathfrak{s}} f_t D^{\mathfrak{s}} \big(\sigma'(f_t) \nabla f_t\big) \, du$$

By Faà di Bruno's formula, this is bounded by

$$-2 \int_{\mathbb{T}^d} \sigma'(f_t) |\nabla D^{\mathfrak{s}} f_t|^2 \, du + \sum_{m;\mathfrak{r}_i} C(\mathfrak{r}) \int_{\mathbb{T}^d} \sigma^{(m+1)}(f_t) \; \nabla D^{\mathfrak{s}} f_t \cdot \nabla D^{\mathfrak{s} - \sum_i \mathfrak{r}_i} f_t \prod_{j=1}^m D^{\mathfrak{r}_j} f_t$$

where the sum is over all integers $m > 0$ and multi-indices $\mathfrak{r}_i \in \mathbb{N}^d$, $i = 1, \ldots, m$, such that $\sum_{i=1}^m \mathfrak{r}_i \leq \mathfrak{s}$ and $\mathfrak{r}_i \neq 0$ for all i. Here $C(\mathfrak{r})$ denotes a constant depending only on $\mathfrak{r}$ and we shall now bound each of the above summands of this sum. Thanks to Lemma 2.4.1, each summand is bounded by

$$C \big\|\nabla D^{\mathfrak{s}} f_t\big\|_{L^2} (1 + \|f_t\|_{L^\infty}^m) \big\|\nabla D^{\mathfrak{s} - \sum_i \mathfrak{r}_i} f_t \prod_{j=1}^m D^{\mathfrak{r}_j} f_t\big\|_{L^2}.$$

Now we choose any coefficients $p, (p_i)_{i=1}^m$ such that $1/2 = 1/p + \sum_i 1/p_i$ to obtain that

$$\big\|\nabla D^{\mathfrak{s} - \sum_i \mathfrak{r}_i} f_t \prod_{j=1}^m D^{\mathfrak{r}_j} f_t\big\|_{L^2} \leq \big\|\nabla D^{\mathfrak{s} - \sum_i \mathfrak{r}_i} f_t\big\|_{L^p} \prod_{j=1}^m \big\|D^{\mathfrak{r}_j} f_t\big\|_{L^{p_j}}.$$

Note that every order n of the derivatives appearing in this product satisfies $1 \leq n \leq k$. Recall that a generalized Gagliardo-Nirenberg-Sobolev inequality yields

$$\|D^{\mathfrak{r}} f\|_{L^p} \leq C \|D^{k+1} f\|_{L^2}^{\theta} \|\nabla f\|_{L^2}^{1-\theta},$$

if

$$|\mathfrak{r}| - \frac{d}{p} = \theta\Big(k + 1 - \frac{d}{2}\Big) + (1-\theta)\Big(1 - \frac{d}{2}\Big),$$

as well as $0 \leq \theta \leq 1$, $0 \leq |\mathfrak{r}| < k+1$, and $\theta \geq (|\mathfrak{r}| - 1)/k$, see [20]. Set

$$\theta_i = \frac{|\mathfrak{r}_i| - 1 + d(\frac{1}{2} - \frac{1}{p_i})}{k}, \qquad \theta = \frac{|\mathfrak{s} - \sum_i \mathfrak{r}_i| + d(\frac{1}{2} - \frac{1}{p})}{k}$$

and note that $\theta_i \geq (|\mathfrak{r}_i| - 1)/k$ since $p_i \geq 2$ (likewise for θ). Summing over all θ_i yields

$$\theta + \sum_{i=1}^{m} \theta_i = \frac{k - m + \frac{d}{2}(m+1) - \frac{d}{2}}{k} = \frac{k - \frac{m}{2}}{k} \leq 1 - \frac{1}{2k},$$

since $\sum_i 1/p_i + 1/p = 1/2$, $1 \leq m \leq k$, and $d = 1$. We also calculate

$$(1-\theta) + \sum_{i=1}^{m} (1 - \theta_i) = m + 1 - \frac{k - \frac{m}{2}}{k} = m + \frac{m}{2k} \leq k + \frac{1}{2}$$

Therefore the Gagliardo-Nirenberg-Sobolev inequality yields

$$\begin{aligned} \big\|\nabla D^{\mathfrak{s} - \sum_i \mathfrak{r}_i} f_t\big\|_{L^p} \prod_{i=1}^{m} \big\|D^{\mathfrak{r}_i} f_t\big\|_{L^{p_i}} &\leq C \|D^{k+1} f_t\|_{L^2}^{\frac{2k-m}{2k}} \|\nabla f_t\|_{L^2}^{m + \frac{m}{2k}} \\ &\leq C\big(\|D^{k+1} f_t\|_{L^2}^{\frac{2k-1}{2k}} \|\nabla f_t\|_{L^2}^{\frac{2k+1}{2}} + 1\big). \end{aligned}$$

By Lemma 2.4.12, it holds that $\|\nabla f_t\|_{L^2} \leq C \|\nabla f_0\|_{L^2}$ and $\|f_t\|_{L^\infty} \leq \|f_0\|_{L^\infty}$. Therefore we conclude that for any $k > 0$, there exist constants $0 < c$ and $C < \infty$ such that

$$\frac{d}{dt} \|D^k f_t\|_{L^2}^2 \leq -c \|D^{k+1} f_t\|_{L^2}^2 + C\big(\|D^{k+1} f_t\|_{L^2}^{2 - \frac{1}{2k}} \|f_0\|_{L^\infty}^k \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1\big). \tag{2.39}$$

Since the integral of the derivative $D^k f_t$ over the torus $\mathbb{T}^d$ vanishes, Poincaré's inequality yields

$$\|D^k f_t\|_{L^2}^2 \leq C \|D^{k+1} f_t\|_{L^2}^2.$$

Hence we can choose $C' > 0$ large enough, such that whenever $\|D^k f_t\|_{L^2} \geq C'$ holds, then the right hand side of estimate (2.39) is negative. Therefore we deduce that

$$\|D^k f_t\|_{L^2}^{\frac{1}{2k}} \leq C \max\big\{\|D^k f_0\|_{L^2}^{\frac{1}{2k}}, \|f_0\|_{L^\infty}^k \|\nabla f_0\|_{L^2}^{\frac{2k+1}{2}} + 1\big\},$$

which concludes the proof of the proposition. □

Remark. Lemma 2.4.12 yielded a-priori bounds in $H^1(\mathbb{T}^d)$, which is stronger in $d = 1$ dimension than the $L^\infty(\mathbb{T}^d)$–bound from the maximum principle. Furthermore $L^\infty(\mathbb{T}^d)$ is just the critical case, in which simple interpolation arguments do not yield a bound on $D^k f_t$ of the form of Lemma 2.4.13. Thus, without any stronger bounds, we needed to restrict ourselves to $d = 1$. This dichotomy in regularity between low and high dimensions is natural for quasilinear parabolic equations like the filtration equation (2.3). The regularity of the filtration equation in $d = 1, 2$ was known even before de Giorgi's and Nash's famous results on the Hölder-continuity of the solutions to parabolic equations. Indeed our proposed approach in Section 2.7 depends on the regularity result of de Giorgi and Nash.

2.4.3 Consistency and stability

Before we prove the hydrodynamic limit Theorem 2.4.6, we need to prove stability and consistency estimates similar to Section 2.3. Since the limit PDE is nonlinear, this is more involved and we shall mostly work with H^k–norms, not the C^k–norms of Section 2.3 (where the choice was convenient because of the use of Dirac distributions). Again, we first show stability estimates on the filtration equation. These estimates allow us to control the fluctuations around the hydrodynamic limit along the evolution of the filtration equation. The consistency result concerns the closeness of the generators generators G^N and G^∞.

Lemma 2.4.14 (Stability)**.** *Assume $d = 1$ and let $F \in C_b^2(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$, and define Ψ as in equation* (2.19)*.*
(i) *For any $t \geq 0$, the map $S_t^\infty : H \to H$ is differentiable with respect to the H^{-1}–norm in the sense given below. Its derivative $DS_t^\infty(f) : H \to H$ can be given as the weak solution $v_t := DS_t^\infty(f)(\tilde{f} - f) \in H$ to the linearized filtration equation*

$$\partial_t v_t = \Delta\left(\sigma'(S_t^\infty f) v_t\right), \tag{2.40}$$

such that $v_0 = \tilde{f} - f$ at time $t = 0$. Differentiability holds in the sense that for each integer $k > (d+2)/2$ and

$$\theta = \theta(k) = \frac{2k - d - 2}{2k + 2},$$

there exists a constant $C < +\infty$ such that

$$\begin{aligned} \|S_t^\infty \tilde{f} - S_t^\infty f\|_{H^{-1}} &\leq \|\tilde{f} - f\|_{H^{-1}}, \\ \|S_t^\infty \tilde{f} - S_t^\infty f - DS_t^\infty(f)(\tilde{f} - f)\|_{H^{-1}} &\leq C \max\{\Lambda(\tilde{f}), \Lambda(f)\} \|\tilde{f} - f\|_{H^{-1}}^{1+\theta}, \end{aligned}$$

for all $\tilde{f}, f \in H^k(\mathbb{T}^d)$ *such that* $\int_{\mathbb{T}^d} \tilde{f}(u)du = \int_{\mathbb{T}^d} f(u)du$. *The factor* $\Lambda(f)$ *is given by*

$$\Lambda(f) = 1 + \|f\|_{L^\infty}\left(1 + \|D^k f\|_{L^2} + \|f\|_{L^\infty}^{2k^2}\|\nabla f\|_{L^2}^{2k^2+k}\right)^{\frac{d+4}{2k+2}} \tag{2.41}$$

for all $f \in H^k(\mathbb{T}^d)$.
(ii) *Furthermore* $S_t^\infty : H \to H$ *satisfies the continuity estimates*

$$\|S_t^\infty f - f\|_{H^{-1}} \leq C\|f\|_{L^2}\sqrt{t} \qquad \text{and} \qquad \|S_t^\infty f - f\|_{H^{-1}} \leq C\|\nabla f\|_{L^2} t$$

for all $f \in H$ *and* $t \geq 0$.
(iii) *For any* $t \geq 0$, *the map* $T_t^\infty \Psi : H \to \mathbb{R}$ *is differentiable with respect to the* H^{-1}*–norm in the sense detailed below and it holds that*

$$D\left(T_t^\infty \Psi\right)(f) = F'\left(\langle S_t^\infty f, \varphi\rangle_{L^2}\right) DS_t^\infty(f)^*\varphi \in H^1(\mathbb{T}^d) \tag{2.42}$$

for all $f \in H$. *The function* $w_t := DS_t^\infty(f)^*\varphi \in H$ *is given as the weak solution of*

$$\partial_t w_t = \sigma'(S_t^\infty f)\Delta w_t, \tag{2.43}$$

such that $w_0 = \varphi$. *We have the estimates*

$$\begin{aligned}
&|T_t^\infty\Psi(\tilde{f}) - T_t^\infty\Psi(f)| \leq \|F'\|_{L^\infty}\|\varphi\|_{H^1}\|\tilde{f} - f\|_{H^{-1}} \text{ and} \\
&|T_t^\infty\Psi(\tilde{f}) - T_t^\infty\Psi(f) - DT_t^\infty\Psi(f)(\tilde{f} - f)| \\
&\leq \frac{1}{2}\|F'\|_{C^1}\|\varphi\|_{H^1}^2\|\tilde{f} - f\|_{H^{-1}}^2 + C\max\{\Lambda(\tilde{f}), \Lambda(f)\}\|F'\|_{L^\infty}\|\varphi\|_{H^1}\|\tilde{f} - f\|_{H^{-1}}^{1+\theta}
\end{aligned}$$

for all $\tilde{f}, f \in H^k(\mathbb{T}^d)$ *such that* $\int_{\mathbb{T}^d} \tilde{f}(u)du = \int_{\mathbb{T}^d} f(u)du$, *where* $\Lambda(\cdot)$ *denotes the same function as in (i).*
(iv) *Furthermore, it holds that* $DS_t^\infty(f)^*\varphi \in L^\infty(0,\infty; H^1(\mathbb{T}^d)) \cap L^2(0,\infty; H^2(\mathbb{T}^d))$ *with uniform bounds*

$$\|\nabla DS_t^\infty(f)^*\varphi\|_{L^2} \leq \|\nabla\varphi\|_{L^2}, \quad \text{and} \quad \int_0^t \|\Delta DS_s^\infty(f)^*\varphi\|_{L^2}^2\, ds \leq C\|\nabla\varphi\|_{L^2}^2$$

for all $\varphi \in H^1(\mathbb{T}^d)$, $f \in H$, *and* $t \geq 0$.

Proof. (i) The filtration equation (2.3) yields

$$\frac{d}{dt}\|\tilde{f}_t - f_t\|_{H^{-1}}^2 = -2\int (\sigma(\tilde{f}_t) - \sigma(f_t))(\tilde{f}_t - f_t)\, du \leq 0$$

because σ is monotonous. This contraction property in weak measure distance is key to most stability estimates.

Let now additionally v_t denote the solution to (2.40). The respective equations for f_t, $\tilde{f}_t$, and v_t yield

$$\frac{d}{dt}\|\tilde{f}_t - f_t - v_t\|_{H^{-1}}^2 = -2\int (\sigma(\tilde{f}_t) - \sigma(f_t) - \sigma'(f_t)v_t)(\tilde{f}_t - f_t - v_t)\, du.$$

The mean value theorem implies that the right hand side is bounded by

$$-2\int \left(\sigma'(f_t)(\tilde{f}_t - f_t - v_t)^2 + \frac{1}{2}\sigma''(\xi)(\tilde{f}_t - f_t)^2(\tilde{f}_t - f_t - v_t)\right)\, du$$

for some $\xi(u)$ (measurable in u) in the interval between $f_t(u)$ and $\tilde{f}_t(u)$. Therefore the bound (2.24) on σ' yields that

$$\frac{d}{dt}\|\tilde{f}_t - f_t - v_t\|_{H^{-1}}^2 \leq -c\|\tilde{f}_t - f_t - v_t\|_{L^2}^2 - \int \sigma''(\xi)(\tilde{f}_t - f_t)^2(\tilde{f}_t - f_t - v_t)\, du$$

for a positive constant $c > 0$. Now, Lemma 2.4.1 yields $|\sigma''(\rho)| \leq C(1+\rho)$. Hence Young's inequality yields a bound

$$\begin{aligned}(2.44)\quad &\frac{d}{dt}\|\tilde{f}_t - f_t - v_t\|_{H^{-1}}^2 \\ &\leq -\frac{c}{2}\|\tilde{f}_t - f_t - v_t\|_{L^2}^2 - C\big(1 + \|\tilde{f}_t\|_{L^\infty}^2 + \|f_t\|_{L^\infty}^2\big)\int_{\mathbb{T}^d}(\tilde{f}_t - f_t)^4\, du.\end{aligned}$$

Now the Cauchy-Schwarz inequality in Fourier space and the standard Gagliardo-Nirenberg-Sobolev inequality yield

$$\begin{aligned}\|f\|_{L^2} &\leq C\|f\|_{H^k}^{\frac{1}{1+k}}\|f\|_{H^{-1}}^{\frac{k}{k+1}}\\ \|f\|_{L^4} &\leq C\|f\|_{H^k}^{\frac{d}{4k}}\|f\|_{L^2}^{1-\frac{d}{4k}}\end{aligned}$$

for all $f \in H^k$. Taken together these inequalities yield

$$\|f\|_{L^4}^4 \leq C\|f\|_{H^k}^{\frac{d+4}{k+1}}\|f\|_{H^{-1}}^{\frac{4k-d}{1+k}}.$$

Since $d = 1$, Lemma 2.4.13 implies

$$\frac{d}{dt}\|\tilde{f}_t - f_t - v_t\|_{H^{-1}}^2 \leq C\max\{\Lambda(\tilde{f}), \Lambda(f)\}\|\tilde{f}_t - f_t\|_{H^{-1}}^{\frac{4k-d}{1+k}},$$

where $\Lambda(\cdot)$ is given in (2.41). Thus the H^{-1}–contractivity yields the desired result.
(ii) Recall that we set $f_t = S_t^\infty f$. Since $\int_{\mathbb{T}^d} f_t(u)du = \int_{\mathbb{T}^d} f(u)du$, it holds that

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}}^2 = -2\int_{\mathbb{T}^d}\sigma(f_t)(f_t - f)\, du.$$

Adding and subtracting $\sigma(f)$ from $\sigma(f_t)$ yields

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}}^2 = -2\int_{\mathbb{T}^d} (\sigma(f_t) - \sigma(f))(f_t - f)\, du - 2\int_{\mathbb{T}^d} \sigma(f)(f_t - f)\, du. \tag{2.45}$$

We apply ellipticity of σ on the first summand and the Cauchy-Schwarz inequality on the second summand to obtain that

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}}^2 \le -c\|f_t - f\|_{L^2}^2 + C\|f\|_{L^2}\|f_t - f\|_{L^2}.$$

for some finite constants $c, C > 0$. Young's inequality yields

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}}^2 \le C\|f\|_{L^2}^2$$

which yields

$$\|f_t - f\|_{H^{-1}}^2 \le C\|f\|_{L^2}^2 t.$$

On the other hand, estimate (2.45) yields

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}}^2 \le -c\|f_t - f\|_{L^2}^2 + C\|\nabla f\|_{L^2}\|f_t - f\|_{H^{-1}}.$$

by interpolation between H^1 and H^{-1}, see (2.27). Here we have used again that

$$\int_{\mathbb{T}^d} f_t(u)\, du = \int_{\mathbb{T}^d} f(u)\, du.$$

Hence it holds that

$$\frac{d}{dt}\|f_t - f\|_{H^{-1}} \le C\|\nabla f\|_{L^2},$$

which yields the desired estimate by integration over t.

(iii) First we want to show that $DS_t^\infty(f)^*$ is the adjoint in $L^2(\mathbb{T}^d)$ of the operator $DS_t^\infty(f)$. This is standard except for the time-dependence through f_t of the coefficients of the linearized equation (2.40). Let us denote for all $0 \le s < t$ the propagator from time s to time t of the evolution equation (2.40) with time-dependent coefficients by $S(t,s)$. Likewise the propagator from s to t of equation (2.43) is denoted by $S(t,s)^*$. To be precise, we denote by $S(\cdot,s)f$ the solution to equation (2.40) such that at time s the solution equals f and similarly for $S(t,s)^*$. We show that $S(t,0)^*$ is indeed the adjoint of $S(t,0)$. For all $0 \le s < t$, it holds that

$$\begin{aligned}
&\frac{d}{ds}\big\langle S(t,s)(\tilde f - f), S(s,0)^*\varphi\big\rangle_{L^2} \\
&= \big\langle S(t,s)(\tilde f - f), \sigma'(f_s)\Delta[S(s,0)^*\varphi]\big\rangle_{L^2} - \big\langle \Delta\big(\sigma'(f_s)[S(t,s)(\tilde f - f)]\big), S(s,0)^*\varphi\big\rangle_{L^2} \\
&= 0.
\end{aligned}$$

Integrating with respect to s yields

$$\big\langle DS_t^\infty(f)(\tilde f - f), \varphi \big\rangle_{L^2} = \big\langle \tilde f - f, DS_t^\infty(f)^* \varphi \big\rangle_{L^2}. \tag{2.46}$$

The differentiability estimates are a consequence of the chain rule and (i) as follows. Lipschitz continuity of F and (i) yield the first estimate. Using equation (2.46), the second term to be estimated can be rewritten as

$$\Big| F\big(\langle S_t^\infty \tilde f, \varphi\rangle\big) - F\big(\langle S_t^\infty f, \varphi\rangle\big) - F'\big(\langle S_t^\infty f, \varphi\rangle\big) \langle DS_t^\infty(f)(\tilde f - f), \varphi\rangle \Big|.$$

We bound this term by the sum of the following two terms:

$$\Big| F'\big(\langle S_t^\infty f, \varphi\rangle\big) \Big\langle S_t^\infty \tilde f - S_t^\infty f - DS_t^\infty(f)(\tilde f - f), \varphi \Big\rangle \Big|$$

and

$$\Big| F\big(\langle S_t^\infty \tilde f, \varphi\rangle\big) - F\big(\langle S_t^\infty f, \varphi\rangle\big) - F'\big(\langle S_t^\infty f, \varphi\rangle\big) \langle S_t^\infty \tilde f - S_t^\infty f, \varphi\rangle \Big|.$$

The results of part (i) yield a bound on the first term by

$$C \|F'\|_{L^\infty} \|\varphi\|_{H^1} \max\{\Lambda(\tilde f), \Lambda(f)\} \|\tilde f - f\|_{H^{-1}}^{1+\theta},$$

whereas the second term is bounded by

$$\frac{1}{2} \|F'\|_{C^1} \big| \langle S_t^\infty \tilde f - S_t^\infty f, \varphi\rangle \big|^2 \le \frac{1}{2} \|F'\|_{C^1} \|\varphi\|_{H^1}^2 \|\tilde f - f\|_{H^{-1}}^2.$$

(iv) Equation (2.43) yields

$$\frac{d}{dt} \int_{\mathbb{T}^d} |\nabla w_t(u)|^2 \, du = -2 \int_{\mathbb{T}^d} \sigma'(S_t^\infty f(u)) |\Delta w_t(u)|^2 \, du \le 0, \tag{2.47}$$

since $\sigma' > 0$. Since furthermore $\nabla w_0(u) = \nabla \varphi(u)$, integration of this equation yields

$$2 \int_0^\infty \int_{\mathbb{T}^d} \sigma'(S_t^\infty f(u)) |\Delta w_t(u)|^2 \, du dt \le \|\nabla \varphi\|_{L^2}^2,$$

uniformly and f and φ. Thus we obtain that

$$\int_0^\infty \int_{\mathbb{T}^d} |\Delta w_t(u)|^2 \, du dt \le C \|\nabla \varphi\|_{L^2}^2$$

using the uniform ellipticity of σ' again, see (2.24). □

Next provide some large–time decay estimates which will enable us to provide uniform in time bounds in the hydrodynamic limit.

Lemma 2.4.15 (Spectral gap). *Let $F \in C_b^2(\mathbb{R})$ and $\varphi \in C^3(\mathbb{T}^d)$ and define Ψ as in* (2.19). *Using the notation of the stability lemma 2.4.14, let $\tilde{f}, f \in H$. Furthermore let $f_\infty = \int f(u)du$ denote the spatial average of f and set*

$$\mathfrak{T}_1(\tilde{f}, f; \Psi) := \Psi(\tilde{f}) - \Psi(f) - D\Psi(f)(\tilde{f} - f). \tag{2.48}$$

(This is the difference of the function Ψ evaluated at $\tilde{f} \in H$ and its first Taylor polynomial around $f \in H$.) Then there exist finite, positive constants c, C such that

$$\begin{aligned}
\|S_t^\infty f - f_\infty\|_{L^p}^p &\le Ce^{-ct}\|f - f_\infty\|_{L^p}^p, \\
\|S_t^\infty f - f_\infty\|_{H^{-1}} &\le Ce^{-ct}\|f - f_\infty\|_{H^{-1}}, \\
\|\mathfrak{T}_1(\tilde{f}, f; S_t^\infty)\|_{H^{-1}}^2 &\le Ce^{-ct}\Big(\|f - f_\infty\|_{L^4}^4 + \|\tilde{f} - \tilde{f}_\infty\|_{L^4}^4\Big), \text{ and} \\
\|\nabla DS_t^\infty(f)^*\varphi\|_{L^2} &\le Ce^{-ct}\|\nabla\varphi\|_{L^2}
\end{aligned}$$

for all $2 \le p < +\infty$. Furthermore it holds that

$$|\mathfrak{T}_1(\tilde{f}, f; T_t^\infty\Psi)| \le Ce^{-ct}\Big(\|f - f_\infty\|_{L^4}^2 + \|\tilde{f} - \tilde{f}_\infty\|_{L^4}^2\Big)$$

where Ψ is defined in (2.19) *with $F \in C_b^2(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$.*

Proof. We will use the notation of the stability lemma 2.4.14, letting

$$f_t := S_t^\infty f \quad \text{and} \quad \tilde{f}_t := S_t^\infty \tilde{f}$$

denote two solutions of the filtration equation and

$$v_t := DS_t^\infty(f)(\tilde{f} - f) \quad \text{and} \quad w_t := DS_t^\infty(f)^*\varphi$$

the linearization around f_t as well as its L^2-dual.
First of all, conservation of mass yields $\int f_t(u)\,du = f_\infty$. Set $\bar{f}_t := f_t - f_\infty$, which solves the equation

$$\partial_t \bar{f}_t = \nabla \cdot \big(\sigma'(\bar{f}_t + f_\infty)\nabla \bar{f}_t\big).$$

Note that in contrast to f_t, the function $\bar{f}_t$ is no longer non-negative everywhere. The equation for $\bar{f}_t$ yields

$$\frac{d}{dt}\int_{\mathbb{T}^d} |\bar{f}_t|^p\,du = p\int_{\mathbb{T}^d} |\bar{f}_t|^{p-2}\bar{f}_t\nabla \cdot \big(\sigma'(\bar{f}_t + f_\infty)\nabla \bar{f}_t\big)\,du.$$

Now integration by parts yields

$$\frac{d}{dt}\int_{\mathbb{T}^d} |\bar{f}_t|^p\,du = -p(p-1)\int_{\mathbb{T}^d} \sigma'(\bar{f}_t + f_\infty)|\bar{f}_t|^{p-2}|\nabla \bar{f}_t|^2\,du.$$

Since

$$|\bar{f}_t|^{p-2}|\nabla \bar{f}_t|^2 = \big||\bar{f}_t|^{p/2-1}\nabla \bar{f}_t\big|^2 = \frac{4}{p^2}\big|\nabla|\bar{f}_t|^{p/2}\big|^2,$$

it holds that

$$\frac{d}{dt}\int_{\mathbb{T}^d}|\bar{f}_t|^p\,du = -\frac{4(p-1)}{p}\int_{\mathbb{T}^d}\sigma'(\bar{f}_t+f_\infty)\big|\nabla|\bar{f}_t|^{p/2}\big|^2\,du \le -c\int_{\mathbb{T}^d}\big|\nabla|\bar{f}_t|^{p/2}\big|^2\,du.$$

Now Poincaré's inequality in the L^2–norm applied to $|\bar{f}_t|^{p/2}$ yields

$$\frac{d}{dt}\int_{\mathbb{T}^d}|\bar{f}_t|^p\,du \le -c\int_{\mathbb{T}^d}|\bar{f}_t|^p\,du,$$

which yields the decay of the L^p–norms of $\bar{f}_t = f_t - f_\infty$. Note that c, C can be taken to be independent of the choice of $p \ge 2$.
The decay of the H^{-1}–norm follows from

$$\frac{d}{dt}\|f_t - f_\infty\|_{H^{-1}}^2 = -2\int_{\mathbb{T}^d}(\sigma(f_t(u)) - \sigma(f_\infty))(f_t(u) - f_\infty)\,du \le -c\|f_t - f_\infty\|_{H^{-1}}^2$$

by uniform ellipticity and (2.27).
The third statement follows directly from equation (2.44) and the exponential decay of the L^4–norm.
To prove the fourth statement, recall equation (2.47). The lower bound on σ' yields

$$\frac{d}{dt}\int_{\mathbb{T}^d}|\nabla w_t(u)|^2\,du \le -c\int_{\mathbb{T}^d}|\Delta w_t(u)|^2\,du.$$

Applying once again Poincaré's inequality yields

$$\frac{d}{dt}\int_{\mathbb{T}^d}|\nabla w_t(u)|^2\,du \le -c\int_{\mathbb{T}^d}|\nabla w_t(u)|^2\,du,$$

and hence exponential decay. Consequently, the proof of Lemma 2.4.14 yields

$$|\mathfrak{T}_1(\tilde{f}, f; T_t^\infty\Psi)| \le Ce^{-ct}\Big(\|f - f_\infty\|_{L^4}^2 + \|\tilde{f} - \tilde{f}_\infty\|_{L^4}^2 + \|f - f_\infty\|_{H^{-1}}^2 + \|\tilde{f} - \tilde{f}_\infty\|_{H^{-1}}^2\Big),$$

and the result follows since the $H^{-1}(\mathbb{T}^d)$–norm is bounded by the $L^4(\mathbb{T}^d)$–norm. □

Many of the differentiability properties we have just shown fit in the framework of differentiable functions on $C_b(H)$ whose derivative is bounded uniformly with respect to a weight function. The following definition formalizes this. It is an adaptation of Definition 2.10 in [67].

Definition 2.4.16. Let $\tilde{H}_1$ and $\tilde{H}_2$ be any two metric spaces and consider two Banach spaces $(H_1, \|\cdot\|_{H_1}), (H_2, \|\cdot\|_{H_2})$ such that $\tilde{H}_i - \tilde{H}_i \subset H_i$, $i = 1, 2$. In general the metric of the subspace $\tilde{H}_i$ is stronger than the norm of H_i. We can understand H_i to be a tangent space of $\tilde{H}_i$. Let

$$\Lambda : \tilde{H}_1 \to [0, +\infty)$$

be a weight function. Abusing notation, we also set

$$\Lambda(\tilde{f}, f) := \max\{\Lambda(\tilde{f}), \Lambda(f)\}.$$

Then we denote by $C^{1,\theta}_{\Lambda}(\tilde{H}_1, H_1; \tilde{H}_2, H_2)$, the space of continuously differentiable function from $\tilde{H}_1$ to $\tilde{H}_2$ whose derivative approximates the original function to the order $1+\theta$ and is uniformly bounded with respect to the weight function Λ. Specifically, a function

$$\Phi : \tilde{H}_1 \to \tilde{H}_2 \quad \text{is in} \quad C^{1,\theta}_{\Lambda}(\tilde{H}_1, H_1; \tilde{H}_2, H_2)$$

if and only if there exists a continuous function

$$D\Phi : \tilde{H}_1 \to \mathcal{L}(H_1, H_2)$$

and finite constants C_1, C_2, and C_3, such that it holds

$$\|\Phi(\tilde{f}) - \Phi(f)\|_{H_2} \leq C_1 \Lambda(\tilde{f}, f) \|\tilde{f} - f\|_{H_1} \tag{2.49}$$

$$\|D\Phi(f)(\tilde{f} - f)\|_{H_2} \leq C_2 \Lambda(\tilde{f}, f) \|\tilde{f} - f\|_{H_1} \text{ and} \tag{2.50}$$

$$\|\Phi(\tilde{f}) - \Phi(f) - D\Phi(f)(\tilde{f} - f)\|_{H_2} \leq C_3 \Lambda(\tilde{f}, f) \|\tilde{f} - f\|^{1+\theta}_{H_1} \tag{2.51}$$

for all $\tilde{f}, f \in \tilde{H}_1$. Let C^{opt}_i, $i = 1, 2, 3$, be the optimal constant in each of (2.49)-(2.51), i.e. the infimum over all C_i, $i = 1, 2, 3$, such that each of the inequalities holds. Then we set

$$[\Phi]_{C^{0,1}_{\Lambda}} := C^{\text{opt}}_1, \quad [\Phi]_{C^{1,0}_{\Lambda}} := C^{\text{opt}}_2, \quad \text{and} \quad [\Phi]_{C^{1,\theta}_{\Lambda}} := C^{\text{opt}}_3,$$

which are seminorms associated to $C^{1,\theta}_{\Lambda}(\tilde{H}_1, H_1; \tilde{H}_2, H_2)$.

Note that the proof of the hydrodynamic limit can be understood without using the above notation, since in principle all we need to do is keep track of various differences. We include it to provide context and simplify notation, especially in order to distinguish clearly between stability and consistency estimates. Let us translate the stability result (i) and (ii) of Lemma 2.4.14 to the language of Definition 2.4.16.

Corollary 2.4.17 (Stability in terms of differentiability)**.** *Let $R \geq 0$, $k \in \mathbb{N}$ and denote*

$$H_R := \left\{ f \in H^k(\mathbb{T}^d) | \textstyle\int_{\mathbb{T}^d} f(u)\, du = R \right\}.$$

Furthermore, let $F \in C^2_b(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$, and define Ψ as in equation (2.19)*. Then there exists a constant $C = C(F, \varphi)$ independent of t and R such that the following holds.*

(i) *For any $t \geq 0$ and $k > (d+2)/2$, it holds that*

$$S_t^\infty \in C_\Lambda^{1,\theta}(H_R, H^{-1}(\mathbb{T}^d); H_R, H^{-1}(\mathbb{T}^d)) \quad \textit{and} \quad [S_t^\infty]_{C_\Lambda^{1,\theta}} \leq C$$

in the sense of Definition 2.4.16, where

$$\theta = \frac{2k-d-2}{2k+2} \text{ and } \Lambda(f) = 1 + \|f\|_{L^\infty}\left(1 + \|D^k f\|_{L^2} + \|f\|_{L^\infty}^{2k^2}\|\nabla f\|_{L^2}^{2k^2+k}\right)^{\frac{d+4}{2k+2}}.$$

(ii) *For any $t \geq 0$, it holds that*

$$T_t^\infty \Psi \in C_\Lambda^{1,\theta}(H_R, H^{-1}(\mathbb{T}^d); \mathbb{R}, \mathbb{R}) \quad \textit{and} \quad [T_t^\infty \Psi]_{C_\Lambda^{1,\theta}} \leq C$$

where θ and Λ are given as above.

Proof. Again, part (ii) is a direct consequence of the corresponding estimates on part (i) and the regularity of $F \in C_b^2(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$. To show (i), just let $\tilde{H}_1 = \tilde{H}_2 = H_R$ and $H_1 = H_2 = H^{-1}(\mathbb{T}^d)$. Note that since all functions in H_R have the same integral over $\mathbb{T}^d$, it holds that indeed

$$H_R - H_R \subset H^{-1}(\mathbb{T}^d).$$

The function S_t^∞ maps H_R to H_R according to Lemma 2.4.13. Note that the (distributional) solution

$$v_t = DS_t^\infty(f)(\tilde{f} - f)$$

to (2.40) also exists for initial data $\tilde{f} - f \in H^{-1}(\mathbb{T}^d)$ and satisfies the bounds given in Lemma 2.4.14. Hence $[\Psi]_{C_\Lambda^{0,1}}$ and $[\Psi]_{C_\Lambda^{1,\theta}}$ of Definition 2.4.16 are indeed finite. We just need to estimate $[\Psi]_{C_\Lambda^{1,0}}$. Calculations similar to the proof of Lemma 2.4.14 yield

$$\frac{d}{dt}\|v_t\|_{H^{-1}}^2 = -2\int_{\mathbb{T}^d} v_t \sigma'(f_t) v_t \, du \leq 0,$$

if the initial datum satisfies $\tilde{f} - f \in L^2(\mathbb{T}^d)$. This shows

$$\|DS_t^\infty(f)(\tilde{f} - f)\|_{H^{-1}} \leq \|\tilde{f} - f\|_{H^{-1}},$$

if $\tilde{f} - f \in L^2(\mathbb{T}^d)$, and by approximation in general. In particular, it holds that

$$DS_t^\infty(f) \in \mathcal{L}(H^{-1}(\mathbb{T}^d), H^{-1}(\mathbb{T}^d)).$$

It remains to prove the continuity of $DS_t^\infty(f) \in \mathcal{L}(H^{-1}(\mathbb{T}^d), H^{-1}(\mathbb{T}^d))$ with respect to $f \in H_R$ (even though we shall not make use of this property in this thesis). This is easiest to see in the dual setting. Let $\tilde{f}, f \in H_R$. As in the stability result, Lemma 2.4.14, we set $w_t := DS_t^\infty(f)^*\varphi$ and we also set $\tilde{w}_t := DS_t^\infty(\tilde{f})^*\varphi$. Then the continuity estimate

$$\big\|DS_t^\infty(f) - DS_t^\infty(\tilde{f})\big\|_{\mathcal{L}(H^{-1},H^{-1})} \to 0 \text{ as } \|\tilde{f} - f\|_{H^k} \to 0$$

corresponds by duality to showing that

$$\|\nabla(\tilde{w}_t - w_t)\|_{L^2} \leq \omega(\|\tilde{f} - f\|_{H^k})\|\nabla\varphi\|_{L^2} \tag{2.52}$$

for some *modulus of continuity* ω, i.e. some function $\omega : [0,\infty) \to [0,\infty)$ such that $\omega(\tau) \to 0$ as $\tau \to 0$. Note that we may allow ω to depend on $\|\tilde{f}\|_{H^k}$, $\|f\|_{H^k}$, and t. The equations for $\tilde{w}_t$ and w_t yield

$$\frac{d}{dt}\int_{\mathbb{T}^d} |\nabla(\tilde{w}_t - w_t)|^2\, du = -2\int_{\mathbb{T}^d} \Delta(\tilde{w}_t - w_t)\big(\sigma'(\tilde{f}_t)\Delta\tilde{w}_t - \sigma'(f_t)\Delta w_t\big)\, du.$$

Hence it holds that

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{T}^d} |\nabla(\tilde{w}_t - w_t)|^2\, du = -2\int_{\mathbb{T}^d} &|\Delta(\tilde{w}_t - w_t)|^2\sigma'(\tilde{f}_t)\, du \\ &- 2\int_{\mathbb{T}^d} \Delta(\tilde{w}_t - w_t)\big(\sigma'(\tilde{f}_t) - \sigma'(f_t)\big)\Delta w_t\, du.\end{aligned}$$

Young's inequality yields a bound on the right hand side by

$$C\big\|(\sigma'(\tilde{f}_t) - \sigma'(f_t))\Delta w_t\big\|_{L^2}^2. \tag{2.53}$$

The mean value theorem and Lemma 2.4.1 yield

$$\big|\sigma'(\tilde{f}_t) - \sigma'(f_t)\big| \leq C\ (\|\tilde{f}_t\|_{L^\infty} + \|f_t\|_{L^\infty})\|\tilde{f}_t - f_t\|_{L^\infty}.$$

By the maximum principle and since $k > (d+2)/2$ yields an embedding $H^k(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$, we can therefore bound (2.53) by

$$C\big(\|\tilde{f}\|_{H^k}, \|f\|_{H^k}\big)\|\tilde{f}_t - f_t\|_{L^\infty}\|\Delta w_t\|_{L^2}^2,$$

where $C(\|\tilde{f}\|_{H^k}, \|f\|_{H^k})$ denotes some constant depending on its arguments, but not on t or w_t. Again since $k > (d+2)/2$, there exists a bounded embedding $H^{k-1}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ and therefore

$$\|\tilde{f}_t - f_t\|_{L^\infty} \leq C\|\tilde{f}_t - f_t\|_{H^{k-1}}.$$

Hence interpolation yields

$$\|\tilde{f}_t - f_t\|_{H^{k-1}} \leq \|\tilde{f}_t - f_t\|_{H^k}^{\frac{k}{k+1}}\|\tilde{f}_t - f_t\|_{H^{-1}}^{\frac{1}{k+1}}$$

Since Lemma 2.4.13 yields uniform-in-time bounds on the H^k–norms of $\tilde{f}$ and f, the contractivity of S_t^∞ with respect to the H^{-1}–norm yields

$$\|\tilde{f}_t - f_t\|_{H^k}^{\frac{k}{k+1}} \|\tilde{f}_t - f_t\|_{H^{-1}}^{\frac{1}{k+1}} \leq C\big(\|\tilde{f}\|_{H^k}, \|f\|_{H^k}\big)\|\tilde{f} - f\|_{H^{-1}}^{\frac{1}{k+1}},$$

for some (possibly different) constant $C(\|\tilde{f}\|_{H^k}, \|f\|_{H^k})$. In summary, we have proved that

$$\frac{d}{dt}\|\nabla(\tilde{w}_t - w_t)\|_{L^2}^2 \leq C\big(\|\tilde{f}\|_{H^k}, \|f\|_{H^k}\big)\|\tilde{f} - f\|_{H^{-1}}^{\frac{1}{k+1}} \|\Delta w_t\|_{L^2}^2.$$

Since $\tilde{w}_0 = \varphi = w_0$, integration with respect to time yields

$$\|\nabla(\tilde{w}_t - w_t)\|_{L^2}^2 \leq C\big(\|\tilde{f}\|_{H^k}, \|f\|_{H^k}\big)\|\tilde{f} - f\|_{H^{-1}}^{\frac{1}{k+1}} \int_0^t \|\Delta w_s\|_{L^2}^2 \, ds.$$

Lemma 2.4.14 (iv) yields

$$\|\nabla(\tilde{w}_t - w_t)\|_{L^2}^2 \leq C\big(\|\tilde{f}\|_{H^k}, \|f\|_{H^k}\big)\|\tilde{f} - f\|_{H^{-1}}^{\frac{1}{k+1}} \|\nabla\varphi\|_{L^2}^2,$$

which shows the desired estimate (2.52). □

Now let us identify an expression for the time-derivative $dT_t^\infty \Psi(f)/dt$.

Lemma 2.4.18. *Let $F \in C_b^1(\mathbb{R})$ and $\varphi \in C^2(\mathbb{T}^d)$, and define Ψ as in equation (2.19). Furthermore let $S_t^\infty f$ solve the filtration equation with initial datum $f \in H^k(\mathbb{T}^d)$ with $k > (d+2)/2$. Then we obtain the following characterizations of the derivative in t of the limit evolution.*
(i) It holds that

$$\frac{d}{dt} S_t^\infty f = DS_t^\infty(f)(\Delta\sigma(f)).$$

(ii) We can lift this result to the level of observables. Recalling the definition

$$G^\infty T_t^\infty \Psi(f) := \frac{d}{dt} T_t^\infty \Psi(f),$$

the result (i) translates to T_t^∞ as

$$G^\infty T_t^\infty \Psi(f) = F'\left(\langle S_t^\infty f, \varphi\rangle_{L^2}\right) \langle \Delta\sigma(f), DS_t^\infty(f)^* \varphi\rangle_{L^2} =: T_t^\infty G^\infty \Psi(f).$$

for all $f \in H^k(\mathbb{T}^d)$ and all $t \geq 0$, where Ψ is given in (2.19).

Proof. (i) Consider

$$I := \frac{1}{s}\Big(S_{t+s}^\infty f - S_t^\infty f\Big) - DS_t^\infty(f)(\Delta\sigma(f))$$

The semigroup property of S_t^∞ (a direct consequence of uniqueness of solutions to the filtration equation (2.3)) yields

$$I = \frac{1}{s}\Big(S_t^\infty S_s^\infty f - S_t^\infty f\Big) - DS_t^\infty(f)(\Delta\sigma(f)).$$

Therefore, the stability result of Lemma 2.4.14 yields

$$(2.54)\quad \|I\|_{H^{-1}} = \left\|\frac{1}{s}\Big(DS_t^\infty(f)(S_s^\infty f - f)\Big) - DS_t^\infty(f)(\Delta\sigma(f))\right\|_{H^{-1}} + \mathcal{O}\big(s^{-1}\Lambda(f, S_s^\infty f)\|S_s^\infty f - f\|_{H^{-1}}^{1+\theta}\big),$$

where $\theta = (2k-d-2)/(2k+2) > 0$. The maximum principle and the improved regularity of Lemma 2.4.13 yield that $\Lambda(f, S_s^\infty f) \le C(f)$ independent of s. Furthermore Lemma 2.4.14 (ii) yields

$$\|S_s^\infty f - f\|_{H^{-1}} \le C\|\nabla f\|_{L^2} s,$$

and hence

$$\mathcal{O}\Big(s^{-1}\Lambda(f, S_s^\infty f)\|S_s^\infty f - f\|_{H^{-1}}^{1+\theta}\big)\Big) = \mathcal{O}(s^\theta)$$

for fixed $f \in H^k(\mathbb{T}^d)$. Since $DS_t^\infty(f) \in \mathcal{L}(H^{-1}(\mathbb{T}^d), H^{-1}(\mathbb{T}^d))$ is a contraction, the other summand on the right hand side of (2.54) equals

$$\left\|DS_t^\infty(f)\left(\frac{S_s^\infty f - f}{s}\right) - DS_t^\infty(f)(\Delta\sigma(f))\right\|_{H^{-1}} \le \left\|\frac{S_s^\infty f - f}{s} - \Delta\sigma(f)\right\|_{H^{-1}},$$

where we have used that

$$\int_{\mathbb{T}^d} \big(S_s^\infty f(u) - f(u)\big)\, du = 0 = \int_{\mathbb{T}^d} \Delta\sigma(f(u))\, du.$$

The right hand side vanishes since f_t is a solution to equation (2.3).
(ii) This part is a direct consequence of (i) and the chain rule. □

For the statement of the consistency result, we will need a replacement lemma, which in the spirit of an ergodic theorem (or a law of large numbers) allows us to replace locally the spatial average of a function of the number of particles over a small box with its expectation value with respect to the local density in this box. Since we are interested in obtaining qualitative results, we will prove a quantitative L^2–version with an explicit upper bound on the rate of convergence. The proof is deferred until Section 2.6.

Lemma 2.4.19 (A quantitative replacement lemma)**.** *Assuming that the initial data possess bounded relative entropy and are bounded with respect to some Gibbs measure, i.e.*

$$H^N\big(\mu_0^N|\nu_\rho^N\big) \le CN^d, \quad \textit{and} \quad \mu_0^N \le \nu_\rho^N$$

for some $\rho > 0$. Then it holds that

$$\left(\frac{1}{T}\int_0^T \int_{\mathbb{T}^d} \left\langle \mu_t^N, \left|(g\circ\eta)^{(\epsilon)}(uN) - \sigma(\eta^{(\epsilon)}(uN))\right|^2\right\rangle \, dudt\right)^{1/2} \leq r_{\mathrm{RL}}(\varrho, l, \epsilon, N),$$

where we recall definition (2.34)*. The rate function r_{RL} satisfies*

$$r_{\mathrm{RL}}(\varrho, l, \epsilon, N) \leq C\Big((N^{-\frac{1}{2}} l^{\frac{1}{2}} + \epsilon^{\frac{1}{2}} l^{\frac{1}{4}})\varrho l^{\frac{d}{4}} + \varrho l^{-\frac{d}{4}} + \varrho^{-\frac{1}{4}} + \frac{l}{\epsilon N}\Big)$$

for all $N \in \mathbb{N}$, $1/N < \epsilon < 1$, $l < N$, and $\varrho > 0$.

Now we are ready to state the consistency result.

Lemma 2.4.20 (Consistency)**.** *Let $F \in C_b^2(\mathbb{R})$ and $\varphi \in C^3(\mathbb{T}^d)$, and define Ψ as in equation* (2.19)*. Furthermore assume that the initial data μ_0^N of the ZRP have bounded relative entropy and are bounded relative to some Gibbs measure*

$$H^N\big(\mu_0^N | \nu_\rho^N\big) \leq C N^d \quad \text{and} \quad \mu_0^N \leq \nu_\rho^N$$

for all $N \in \mathbb{N}$. Then it holds that

$$\left|\int_0^t \left\langle \mu_s^N, \left(G^N \pi^N - \pi^N G^\infty\right) T_{t-s}^\infty \Psi\right\rangle \, ds\right| \leq r_{\mathrm{C}}(T, \varrho, l, \epsilon, N)$$

for all $0 \leq t < +\infty$, $T > 0$, $N \in \mathbb{N}$, and $1/N < \epsilon < 1$. The consistency bound $r_{\mathrm{C}}(T, \varrho, l, \epsilon, N)$ is given explicitly by the function

$$\begin{aligned}(2.55)\quad C\Big(&\epsilon^{-\frac{d\theta}{2}} N^{1-\theta(d+1)} T \sup_{0\leq s\leq t}\sup_{x\sim y}\left\langle \mu_{t-s}^N, \left[T_s^\infty \Psi\right]_{C^{1+\theta}} \Lambda(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}) N^{-d} \textstyle\sum_z \eta(z)\right\rangle \\ &+ \epsilon^{-(3+\frac{d}{2})} \sup_{\eta \in X_N} \int_T^\infty \|\nabla(D S_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi)\|_{L^2(\mathbb{T}^d)} \, ds \\ &+ N^{2+d} \sup_{t\geq T} \int_T^t \left\langle \mu_{t-s}^N, \sup_{x\sim y} \left|\mathfrak{T}_1(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}; T_s^\infty \Psi)\right|\right\rangle ds \\ &+ \left\|\Delta(D S_t^\infty(\alpha_\eta^{N,\epsilon})^* \varphi)\right\|_{L_\eta^\infty L_{t,u}^2} \sqrt{T}\big(r_{\mathrm{RL}}(\varrho, l, \epsilon, N) + \epsilon^{-(2+\frac{d}{2})} N^{-2}\big)\Big).\end{aligned}$$

for any $\theta = \theta(k)$ and $k > 0$. Here θ, Λ, and $[T_s^\infty \Psi]_{C_\Lambda^{1+\theta}}$ are given in Corollary 2.4.17 and $r_{\mathrm{RL}}(\varrho, l, \epsilon, N)$ stems from Lemma 2.4.19. The notation $\mathfrak{T}_1$ is explained in Lemma 2.4.15 and the function $D S_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi$ is given in Lemma 2.4.14.

Note that in contrast to Section 2.3, the form (2.19) of Ψ is not conserved under the application T_t^∞, hence we need to keep track of T_{t-s}^∞. This also explains why we needed to derive the above fairly complex stability results.

Proof of Lemma 2.4.20. Let us first assume that $t \leq T$. Denote the quantity to be estimated by

$$I := \left| \int_0^t \left\langle \mu_{t-s}^N, \left(G^N \pi^N - \pi^N G^\infty\right) T_s^\infty \Psi \right\rangle ds \right|.$$

Inserting the expressions for the generators G^N and G^∞, cf. Lemma 2.4.18, we obtain that

$$I = \left| \int_0^t \left\langle \mu_{t-s}^N, N^2 \sum_{x \sim y} g(\eta(x)) \left[T_s^\infty \Psi(\alpha_{\eta^{x,y}}^{N,\epsilon}) - T_s^\infty \Psi(\alpha_\eta^{N,\epsilon}) \right] \right.\right.$$
$$\left.\left. - \langle DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon}), \Delta\sigma(\alpha_\eta^{N,\epsilon}) \rangle_{L^2} \right\rangle ds \right|,$$

where $DT_s^\infty \Psi$ is defined in equation (2.42). Linearizing $T_s^\infty \Psi$ around $\alpha_\eta^{N,\epsilon}$ yields

$$I \leq \mathcal{R}_1 + \left| \int_0^t \left\langle \mu_{t-s}^N, N^2 \sum_{x \sim y} g(\eta(x)) DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon})(\alpha_{\eta^{x,y}}^{N,\epsilon} - \alpha_\eta^{N,\epsilon}) \right.\right.$$
$$\left.\left. - \langle DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon}), \Delta\sigma(\alpha_\eta^{N,\epsilon}) \rangle_{L^2} \right\rangle ds \right|$$

with an error term

$$\mathcal{R}_1 = \int_0^t \left\langle \mu_{t-s}^N, N^2 \sum_{x \sim y} g(\eta(x)) \left| T_s^\infty \Psi(\alpha_{\eta^{x,y}}^{N,\epsilon}) - T_s^\infty \Psi(\alpha_\eta^{N,\epsilon}) \right.\right.$$
$$\left.\left. - DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon})(\alpha_{\eta^{x,y}}^{N,\epsilon} - \alpha_\eta^{N,\epsilon}) \right| \right\rangle ds. \tag{2.56}$$

Substituting the definition (2.29) of the empirical measure into the right hand side then yields

$$I \leq \mathcal{R}_1 + \left| \int_0^t \left\langle \mu_{t-s}^N, N^{2-d} \sum_{x \sim y} g(\eta(x)) DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon})(\delta_{\frac{y}{N}}^{(\epsilon)} - \delta_{\frac{x}{N}}^{(\epsilon)}) \right.\right.$$
$$\left.\left. - \langle DT_s^\infty \Psi(\alpha_\eta^{N,\epsilon}), \Delta\sigma(\alpha_\eta^{N,\epsilon}) \rangle_{L^2} \right\rangle ds \right|.$$

The explicit expression for $DT_s^\infty\Psi$, see (2.42), then yields

$$\begin{aligned}I \le \mathcal{R}_1 &\\ + \Bigg| \int_0^t \Bigg\langle \mu_{t-s}^N, F'\left(\left\langle S_s^\infty \alpha_\eta^{N,\epsilon}, \varphi\right\rangle_{L^2}\right) &\Bigg(N^{-d} \sum_x g(\eta(x)) \left\langle DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi, \Delta_N \delta^{(\epsilon)}_{\frac{x}{N}} \right\rangle_{L^2} \\ &- \left\langle DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi, \Delta \sigma(\alpha_\eta^{N,\epsilon}) \right\rangle_{L^2} \Bigg) \Bigg\rangle \, ds \Bigg|.\end{aligned}$$

Next, up to an error $\mathcal{R}_2$, we replace the discrete Laplacian Δ_N by its continuous version Δ and, after an integration by parts, obtain that

$$\begin{aligned}I \le \mathcal{R}_1 + \mathcal{R}_2 + \Bigg| \int_0^t \Bigg\langle \mu_{t-s}^N, F'\left(\langle S_s^\infty \alpha_\eta^{N,\epsilon}, \varphi\rangle_{L^2}\right) \int_{\mathbb{T}^d} &\Big(N^{-d} \sum_x g(\eta(x)) \delta^{(\epsilon)}_{\frac{x}{N}}(u) \\ &- \sigma(\alpha_\eta^{N,\epsilon}(u)) \Big) \Delta \left(DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi \right)(u) \, du \Bigg\rangle \, ds \Bigg|.\end{aligned}$$

The explicit expression for the error term is

$$\begin{aligned}\mathcal{R}_2 = \Bigg| \int_0^t \Bigg\langle \mu_{t-s}^N, &F'\left(\langle S_s^\infty \alpha_\eta^{N,\epsilon}, \varphi\rangle_{L^2}\right) \\ &\Bigg[N^{-d} \sum_x g(\eta(x)) \langle DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi, \Delta_N \delta^{(\epsilon)}_{\frac{x}{N}} - \Delta \delta^{(\epsilon)}_{\frac{x}{N}} \rangle_{L^2} \Bigg] \Bigg\rangle \, ds \Bigg|\end{aligned} \tag{2.57}$$

Recall that $DS_s^\infty(\alpha_\eta^{N,\epsilon})^*\varphi \in L^2(0,\infty; H^2(\mathbb{T}^d))$. Thus we apply Hölder's inequality to obtain

$$\begin{aligned}I \le \mathcal{R}_1 + \mathcal{R}_2 + \|F'\|_{L^\infty} \times &\\ \left(\int_0^t \int_{\mathbb{T}^d} \left\langle \mu_{t-s}^N, \left(\frac{1}{N^d} \sum_x g(\eta(x)) \delta^{(\epsilon)}_{\frac{x}{N}}(u) - \sigma(\alpha_\eta^{N,\epsilon}(u)) \right)^2 \right\rangle \, du ds \right)^{1/2} &\\ \times \left\| \Delta_u (DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi) \right\|_{L_\eta^\infty L_{s,u}^2}&.\end{aligned}$$

Since $t \le T$, Lemma 2.4.19 yields

$$I \le \mathcal{R}_1 + \mathcal{R}_2 + \sqrt{T} \left\| \Delta_u (DS_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi) \right\|_{L_\eta^\infty L_{s,u}^2} r_{\mathrm{RL}}(\varrho, l, \epsilon, N).$$

It remains to find a bound on $\mathcal{R}_1$ and $\mathcal{R}_2$ to finish the proof of the consistency result. Since

$$\int_{\mathbb{T}^d} \alpha_\eta^{N,\epsilon}(u) \, du = \int_{\mathbb{T}^d} \alpha_{\eta^{x,y}}^{N,\epsilon}(u) \, du,$$

the first error term (2.56) is bounded from above by

$$\mathcal{R}_1 \leq N^{2+d} T \sup_{t\in[0,T]} \sup_{s\in[0,t]} \langle \mu^N_{t-s}, \left[T^\infty_s \Psi\right]_{C^{1,\theta}_\Lambda} \Lambda(\alpha^{N,\epsilon}_{\eta^{x,y}}, \alpha^{N,\epsilon}_\eta) \|\alpha^{N,\epsilon}_{\eta^{x,y}} - \alpha^{N,\epsilon}_\eta\|^{1+\theta}_{H^{-1}} \rangle,$$

where we have used the notation of Definition 2.4.16. To calculate the difference $\|\alpha^{N,\epsilon}_{\eta^{x,y}} - \alpha^{N,\epsilon}_\eta\|^{1+\theta}_{H^{-1}}$, we test with a function $\omega \in H^1(\mathbb{T}^d)$. Thus we obtain that

$$\begin{aligned}\langle \omega, \alpha^{N,\epsilon}_{\eta^{x,y}} - \alpha^{N,\epsilon}_\eta \rangle_{L^2} &= \int \omega(u) \frac{1}{N^d} \left(\delta^{(\epsilon)}_{\frac{y}{N}} - \delta^{(\epsilon)}_{\frac{x}{N}} \right) du \\ &= \int \frac{1}{N^d} \left(\omega(u + \frac{y}{N}) - \omega(u + \frac{x}{N}) \right) \delta^{(\epsilon)}_0 \, du \\ &\leq \frac{C}{N^{d+1}} \|\nabla \omega\|_{L^2} \|\delta^{(\epsilon)}_0\|_{L^2},\end{aligned}$$

and hence

$$\|\alpha^{N,\epsilon}_{\eta^{x,y}} - \alpha^{N,\epsilon}_\eta\|_{H^{-1}} \leq C \epsilon^{-d/2} N^{-(d+1)}.$$

The second error term (2.57) is bounded from above by

$$\begin{aligned}\mathcal{R}_2 \leq g^* \|F'\|_{L^\infty} &\left(\int_0^t \left\langle \mu^N_{t-s}, \sum_{x\in\mathbb{T}^d_N} \frac{\eta(x)}{N^d} \right\rangle^2 ds \right)^{\frac{1}{2}} \\ &\times \|\Delta D S^\infty_s (\alpha^{N,\epsilon}_\eta)^* \varphi\|_{L^\infty_\eta L^2_{s,u}} \|(-\Delta)^{-1}(\Delta_N - \Delta)\delta^{(\epsilon)}_0\|_{L^2_u}.\end{aligned}$$

Now it holds that

$$\|(-\Delta)^{-1}(\Delta_N - \Delta)\delta^{(\epsilon)}_0\|_{L^2} \leq C N^{-2} \|D^2 \delta^{(\epsilon)}_0\|_{L^2} \leq \frac{C}{N^2 \epsilon^{2+d/2}}. \tag{2.58}$$

Hence we obtain that

$$\mathcal{R}_2 \leq C\sqrt{T} \|\Delta D S^\infty_s (\alpha^{N,\epsilon}_\eta)^* \varphi\|_{L^\infty_\eta L^2_{s,u}} N^{-2} \epsilon^{-(2+d/2)},$$

which completes the proof of Lemma 2.4.20 if $t \leq T$. If $t > T$, all bounds remain valid for

$$\left| \int_0^T \left\langle \mu^N_{t-s}, (G^N \pi^N - \pi^N G^\infty) T^\infty_s \Psi \right\rangle ds \right|,$$

and it remains to estimate

$$II := \left| \int_T^t \left\langle \mu^N_{t-s}, (G^N \pi^N - \pi^N G^\infty) T^\infty_s \Psi \right\rangle ds \right|.$$

Again we will have three contributions to this quantity. The first one equals

$$\widetilde{\mathfrak{R}}_1 = \int_T^t \Big\langle \mu_{t-s}^N, N^2 \sum_{x\sim y} g(\eta(x)) \Big| T_t^\infty \Psi(\alpha_{\eta^{x,y}}^{N,\epsilon}) - T_t^\infty \Psi(\alpha_\eta^{N,\epsilon}) - DT_t^\infty \Psi(\alpha_\eta^{N,\epsilon})(\alpha_{\eta^{x,y}}^{N,\epsilon} - \alpha_\eta^{N,\epsilon}) \Big| \Big\rangle ds.$$

It holds that

$$\widetilde{\mathfrak{R}}_1 \leq CN^{2+d} \sup_{t\geq T} \int_T^t \Big\langle \mu_{t-s}^N, \sup_{x\sim y} \big| \mathfrak{T}_1(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}; T_s^\infty \Psi) \big| N^{-d} \sum_z \eta(z) \Big\rangle \, ds,$$

where the second supremum is taken over all neighbours x and y in $\mathbb{T}_N^d$. The second contribution to II is given by

$$\widetilde{\mathfrak{R}}_2 \leq \Bigg| \int_T^t \Big\langle \mu_{t-s}^N, F'(\langle S_s^\infty \alpha_\eta^{N,\epsilon}, \varphi\rangle_{L^2}) \Big(N^{-d} \sum_x g(\eta(x)) \langle DS_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi, \Delta_N \delta_{\frac{x}{N}}^{(\epsilon)} - \Delta \delta_{\frac{x}{N}}^{(\epsilon)} \rangle_{L^2} \Big) \Big\rangle \, ds \Bigg|.$$

Since the mass is conserved and bounded, it follows that

$$\widetilde{\mathfrak{R}}_2 \leq C\|F'\|_{L^\infty} \|(\Delta - \Delta_N)\delta_0^{(\epsilon)}\|_{H^{-1}} \sup_{\eta\in X_N} \int_T^\infty \|\nabla DS_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi\|_{L^2} \, ds$$

Similarly to (2.58), we obtain

$$\|(\Delta - \Delta_N)\delta_0^{(\epsilon)}\|_{H^{-1}} \leq CN^{-2} \|D^3 \delta_0^{(\epsilon)}\|_{L^2} \leq C\epsilon^{-(3+d/2)} N^{-2}.$$

Thus we have shown

$$\widetilde{\mathfrak{R}}_2 \leq C\epsilon^{-(3+d/2)} N^{-2} \sup_{\eta\in X_N} \int_T^\infty \|\nabla DS_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi\|_{L^2} \, ds$$

Finally, the remaining term is bounded by

$$\Bigg| \int_T^t \Big\langle \mu_{t-s}^N, F'(\langle S_s^\infty \alpha_\eta^{N,\epsilon}, \varphi\rangle_{L^2}) \int_{\mathbb{T}^d} \nabla \Big(N^{-d} \sum_x g(\eta(x)) \delta_{\frac{x}{N}}^{(\epsilon)}(u) - \sigma(\alpha_\eta^{N,\epsilon}(u)) \Big) \nabla \big(DS_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi \big)(u) \, du \Big\rangle \, ds \Bigg|.$$

Hölder's inequality yields a bound by

$$\|F'\|_{L^\infty}\int_T^t \Big\langle \mu_{t-s}^N, \Big\|\nabla\big(N^{-d}\sum_x g(\eta(x))\delta_{\frac{x}{N}}^{(\epsilon)}(u)-\sigma(\alpha_\eta^{N,\epsilon}(u))\big)\Big\|_{L^2}\times \\ \Big\|\nabla\big(DS_s^\infty(\alpha_\eta^{N,\epsilon})^*\varphi\big)\Big\|_{L^2}\Big\rangle\, ds.$$

Since g and σ are uniformly Lipschitz-continuous, the first term is bounded by

$$\Big\|\nabla\big(N^{-d}\sum_x g(\eta(x))\delta_{\frac{x}{N}}^{(\epsilon)}-\sigma(\alpha_\eta^{N,\epsilon})\big)\Big\|_{L^2}\le CN^{-d}\sum_x \eta(x)\|\nabla\delta_{\frac{x}{N}}^{(\epsilon)}\|_{L^2}.$$

By the conservation of particles, this term is uniformly bounded by $C\epsilon^{-(1+d/2)}$, which completes the proof. □

Remark 2.4.21. Similarly to the proof of Lemma 2.4.18, where we needed to take the time-derivative at $t=0$ and which can be understood as proving

$$\pi^N G^\infty T_t^\infty\Psi=\pi^N T_t^\infty G^\infty\Psi = DT_t^\infty\Psi(\Delta\sigma(\alpha^{N,\epsilon})),$$

the term $\mathcal{R}_1$ can be seen as capturing the "commutation relation"

$$G^N\pi^N T_t^\infty\Psi(\eta)\approx DT_t^\infty\Psi(G^N\alpha_\eta^{N,\epsilon}).$$

Closer inspection of the proof shows that in order to prove the former relationship between G^∞ and T_t^∞, we just need $\theta>0$ in the stability result, Lemma 2.4.14. On the other hand, we need $\theta>1/(d+1)$ in order to guarantee that the error term $\mathcal{R}_1$ coming from the latter relationship between G^N and T_t^∞ vanishes in the limit.

2.4.4 Proof of the hydrodynamic limit

Using the stability and consistency results, we can prove the hydrodynamic limit.

Proof of Theorem 2.4.6. Let us split the left hand side of (2.31) into three separate contributions which we shall call $\mathcal{T}_1$ to $\mathcal{T}_3$. It holds that

$$\Big|\big\langle\mu_t^N, F\big(\langle\alpha_\eta^N,\varphi\rangle\big)\big\rangle - F\big(\langle f_t,\varphi\rangle_{L^2}\big)\Big| \\ \le \Big|\big\langle\mu_t^N, F\big(\langle\alpha_\eta^N,\varphi\rangle\big)\big\rangle - F\big(\langle\alpha_\eta^{N,\epsilon},\varphi\rangle_{L^2}\big)\Big| + \Big|\big\langle\mu_t^N, F\big(\langle\alpha_\eta^{N,\epsilon},\varphi\rangle_{L^2}\big)\big\rangle - F\big(\langle f_t,\varphi\rangle_{L^2}\big)\Big|.$$

As before, the definitions of Ψ, see (2.19), and the generators T_t^N and T_t^∞ yield

$$\Big|\big\langle\mu_t^N, F\big(\langle\alpha_\eta^{N,\epsilon},\varphi\rangle_{L^2}\big)\big\rangle - F\big(\langle f_t,\varphi\rangle_{L^2}\big)\Big| = \Big|\big\langle\mu_0^N, T_t^N\pi^N\Psi - T_t^\infty\Psi(f_0)\big\rangle\Big|.$$

If we add and subtract $\langle \mu_0^N, \pi^N T_t^\infty \Psi \rangle = \langle \mu_0^N, T_t^\infty \Psi(\alpha_\eta^{N,\epsilon}) \rangle$, we obtain that the right hand side is bounded by

$$\begin{aligned} &\Big|\big\langle \mu_0^N, T_t^N \pi^N \Psi - \pi^N T_t^\infty \Psi \big\rangle\Big| + \Big|\big\langle \mu_0^N, T_t^\infty \Psi(\alpha_\eta^{N,\epsilon}) - T_t^\infty \Psi\big(f_0\big)\big\rangle\Big| \\ &\qquad\qquad\qquad\qquad + \Big|\big\langle \mu_t^N, \Psi\big(\alpha_\eta^N\big) - \Psi\big(\alpha_\eta^{N,\epsilon}\big)\big\rangle\Big| \\ &=: \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3, \end{aligned}$$

where we have written $\Psi(\alpha_\eta^N) = F(\langle \alpha_\eta^N, \varphi \rangle)$ in analogy with (2.19), even though α_η^N is not in H. As in Section 2.3 it holds that

$$\frac{d}{ds}\big(T_s^N \pi^N T_{t-s}^\infty(\eta)\big) = T_s^N G^N \pi^N T_{t-s}^\infty \Psi(\eta) - T_s^N \pi^N G^\infty T_{t-s}^\infty \Psi(\eta).$$

Hence Lemma 2.4.20 yields

$$\mathcal{T}_1 \leq \int_0^t \big|\langle S_s^N \mu_0^N, (G^N \pi^N - \pi^N G^\infty)(T_{t-s}^\infty \Psi)(\eta) \rangle\big| \; ds \leq r_{\mathrm{C}}(T, \varrho, l, \epsilon, N),$$

where $r_{\mathrm{C}}(T, \varrho, l, \epsilon, N)$ is given in the consistency lemma 2.4.20 as

$$\begin{aligned} C\Big(&\epsilon^{-\frac{d\theta}{2}} N^{1-\theta(d+1)} T \sup_{0 \leq s \leq t} \sup_{x \sim y} \big\langle \mu_{t-s}^N, \big[T_s^\infty \Psi\big]_{C^{1+\theta}} \Lambda(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}) N^{-d} \textstyle\sum_z \eta(z) \big\rangle \\ &\quad + \epsilon^{-(3+\frac{d}{2})} \sup_{\eta \in X_N} \int_T^\infty \|\nabla (D S_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi)\|_{L^2(\mathbb{T}^d)} \; ds \\ &\quad + N^{2+d} \sup_{t \geq T} \int_T^t \Big\langle \mu_{t-s}^N, \sup_{x \sim y} \big|\mathfrak{T}_1(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}; T_s^\infty \Psi)\big| \Big\rangle \; ds \\ &\quad + \big\|\Delta (D S_t^\infty(\alpha_\eta^{N,\epsilon})^* \varphi)\big\|_{L_\eta^\infty L_{t,u}^2} \sqrt{T}\big(r_{\mathrm{RL}}(\varrho, l, \epsilon, N) + \epsilon^{-(2+\frac{d}{2})} N^{-2}\big)\Big). \end{aligned}$$

Next, using the stability result, we need to make the expression for $r_{\mathrm{C}}(T, \varrho, l, \epsilon, N)$ explicit in terms of l, ϵ, and N. Let us consider first the two middle terms, which describe the large–time behaviour $t \geq T$. Lemma 2.4.15 yields

$$\int_T^\infty \|\nabla D S_s^\infty(\alpha_\eta^{N,\epsilon})^* \varphi\|_{L^2} \; ds \leq C e^{-cT} \|\nabla \varphi\|_{L^2}$$

as well as

$$\begin{aligned} \int_T^\infty \big|\mathfrak{T}_1(\alpha_{\eta^{x,y}}^{N,\epsilon}, \alpha_\eta^{N,\epsilon}; T_s^\infty \Psi)\big| \; ds \leq C e^{-cT} \Big(&\|\alpha_{\eta^{x,y}}^{N,\epsilon} - N^{-d} \textstyle\sum_z \eta(z)\|_{L^4}^2 \\ &+ \|\alpha_\eta^{N,\epsilon} - N^{-d} \textstyle\sum_z \eta(z)\|_{L^4}^2\Big), \end{aligned}$$

since

$$\int_{\mathbb{T}^d} \alpha^{N,\epsilon}_{\eta^{x,y}}(u)\, du = \int_{\mathbb{T}^d} \alpha^{N,\epsilon}_{\eta}(u)\, du = \frac{1}{N^d} \sum_{z \in \mathbb{T}^d_N} \eta(z).$$

The bound $\delta^{(\epsilon)}_0(u) \leq C\epsilon^{-d}$ yields

$$\|\alpha^{N,\epsilon}_\eta\|^4_{L^4_u} = \int_{\mathbb{T}^d} \Big| \frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \delta^{(\epsilon)}_{\frac{x}{N}}(u) \Big|^4 du \leq C\epsilon^{-4d} \Big(\frac{1}{N^d} \sum_{z \in \mathbb{T}^d_N} \eta(z) \Big)^4.$$

Collecting the three previous equations, we have shown that

$$\sup_{t \geq T} \big| \mathfrak{T}_1(\alpha^{N,\epsilon}_{\eta^{x,y}}, \alpha^{N,\epsilon}_\eta; T^\infty_t \Psi) \big| \leq Ce^{-cT} \epsilon^{-2d} \Big(\frac{1}{N^d} \sum_{z \in \mathbb{T}^d_N} \eta(z) \Big)^2$$

uniformly in x, y, and η. Conservation of the number of particles and the assumption $\mu^N_0 \leq \nu^N_\rho$ now yield uniform bounds

$$\begin{aligned} \Big\langle \mu^N_t, \Big(\frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \Big)^m \Big\rangle &= \Big\langle \mu^N_0, \Big(\frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \Big)^m \Big\rangle \\ &\leq \Big\langle \nu^N_\rho, \Big(\frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \Big)^m \Big\rangle \leq C_m \end{aligned} \tag{2.59}$$

for each $m > 0$.
The stability results of Lemma 2.4.14 yield

$$\sup_{s \geq 0} \big[T^\infty_s \Psi \big]_{C^{1,\theta}_\Lambda} \leq C.$$

Furthermore, it holds that

$$\|\alpha^{N,\epsilon}_\eta\|_{L^\infty} \leq C \frac{1}{\epsilon^d N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x)$$

as well as

$$\|\alpha^{N,\epsilon}_\eta\|_{H^k} \leq N^{-d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \|\delta^{(\epsilon)}\|_{H^k} \leq C\epsilon^{-(k+\frac{d}{2})} N^{-d} \sum_{x \in \mathbb{T}^d_N} \eta(x).$$

Corollary 2.4.17 yields

$$\begin{aligned} \Lambda(\alpha^{N,\epsilon}_\eta) \leq C \Bigg(1 &+ \epsilon^{-(k+\frac{d}{2})\frac{d+4}{2k+2} - d} \Big(\frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \Big)^{\frac{d+4}{2k+2}+1} \\ &+ \epsilon^{-(1+\frac{d}{2})(d+4)\frac{2k^2+k}{2k+2} - kd(d+4) - d} \Big(\frac{1}{N^d} \sum_{x \in \mathbb{T}^d_N} \eta(x) \Big)^{(\frac{2k^2+k}{2k+2}+k)(d+4)+1} \Bigg) \end{aligned}$$

Since $k > (d+2)/2$ and $\epsilon < 1$ is small, conservation of the number of particles yields

$$\left\langle \mu_t^N, \Lambda(\alpha_\eta^{N,\epsilon}) N^{-d} \textstyle\sum_z \eta(z) \right\rangle \le C\epsilon^{-(1+\frac{d}{2})(d+4)\frac{2k^2+k}{2k+2} - kd(d+4) - d}.$$

for some constant C depending on the quantities k, d, and ρ appearing in the statement of the hydrodynamic limit. Replacing above η by $\eta^{x,y}$ yields the identical bound

$$\left\langle \mu_t^N, \Lambda(\alpha_\eta^{N,\epsilon}, \alpha_{\eta^{x,y}}^{N,\epsilon}) N^{-d} \textstyle\sum_z \eta(z) \right\rangle \le C\epsilon^{-(1+\frac{d}{2})(d+4)\frac{2k^2+k}{2k+2} - kd(d+4) - d}.$$

Finally we just have to recall that Lemma (2.4.14) (iv) yields the uniform bound

$$\|\Delta_u D S_s^\infty (\alpha_\eta^{N,\epsilon})^* \varphi\|_{L^\infty_\eta L^2_{s,u}} \le C,$$

in order to obtain that

$$\begin{aligned} \mathcal{T}_1 \le C_k \Big(&\epsilon^{-(1+\frac{d}{2})(d+4)\frac{2k^2+k}{2k+2} - kd(d+4) - d} \epsilon^{-\theta\frac{d}{2}} N^{-\theta(d+1)} + \epsilon^{-(2+\frac{d}{2})} N^{-2} \\ &+ e^{-cT} N^{2+d} \epsilon^{-2d} + T^{\frac{1}{2}} r_{\mathrm{RL}}(\varrho, l, \epsilon, N) \Big). \end{aligned}$$

The stability estimate (2.37) yields

$$\mathcal{T}_2 = \left| \left\langle \mu_0^N, T_t^\infty \Psi\left(\alpha_\eta^{N,\epsilon}\right) - T_t^\infty \Psi(f_0) \right\rangle \right| \le \|F'\|_{L^\infty} \|\varphi\|_{L^\infty} \langle \mu_0^N, \|\alpha_\eta^{N,\epsilon} - f_0\|_{L^1} \rangle.$$

The stability estimate (2.38) yields the validity of Remark 2.4.8, once we have substracted $\int_{\mathbb{T}^d} \varphi(y)\, du$ from φ. Finally, the last term equals

$$\mathcal{T}_3 = \left| \left\langle \mu_t^N, F(\langle \alpha_\eta^N, \varphi \rangle) - F(\langle \alpha_\eta^{N,\epsilon}, \varphi \rangle_{L^2}) \right\rangle \right| \le \|F'\|_{L^\infty} \left| \left\langle \mu_t^N, \langle \alpha_\eta^N - \alpha_\eta^{N,\epsilon}, \varphi \rangle_{L^2} \right\rangle \right|.$$

Note that

$$\begin{aligned} \langle \alpha_\eta^N - \alpha_\eta^{N,\epsilon}, \varphi \rangle &= \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \int_{\mathbb{T}^d} \frac{1}{\epsilon^d} \chi(\tfrac{u}{\epsilon}) (\varphi(\tfrac{x}{N}) - \varphi(u + \tfrac{x}{N}))\, du \\ &= \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \int_{\mathbb{T}^d} \chi(u) (\varphi(\tfrac{x}{N}) - \varphi(\epsilon u + \tfrac{x}{N})))\, du, \end{aligned}$$

and hence

$$\left| \langle \alpha_\eta^N - \alpha_\eta^{N,\epsilon}, \varphi \rangle \right| \le C\epsilon \|\nabla \varphi\|_{L^2} \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)$$

Since the total mass is conserved and $F \in C_b^2(\mathbb{T}^d)$ is Lipschitz-continuous, it follows that

$$\mathcal{T}_3 \le C\epsilon \|F'\|_{L^\infty} \|\nabla \varphi\|_{L^2} \Big\langle \mu_t^N, \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x) \Big\rangle \le C\epsilon,$$

since the average number of particles is bounded. Collecting all available bounds, this completes the proof of the hydrodynamic limit. □

Remark. As in the proof of the hydrodynamic limit for independent random walks, Theorem 2.3.1, the term $\mathcal{T}_1$ is a measure for the difference of the particle semigroup and the limit semigroup on the level of observables and is (for fixed Ψ) bounded by a consistency result on the two generators. Furthermore we have seen that this consistency estimate is transported along the flow of the limit equation by the stability result. The second term $\mathcal{T}_2$ measures the propagation of the difference between the initial data of the particle system and the limit partial differential equation along the flow of the limit equation. Hence it is bounded by a stability result on the limit equation. The last term $\mathcal{T}_3$ did not appear in the proof of Theorem 2.3.1 and measures the error due to the mollification of the empirical measure.

2.5 Convergence of the entropy

One important question in the field of statistical mechanics is the convergence of the microscopic entropy $N^{-d}H^N(\mu_t^N|\nu_\rho^N)$ towards the macroscopic entropy. In this section we investigate this problem and its relation to entropic chaos. The problem can be thought of independently from the results of the previous sections, once a hydrodynamic limit has been established. In order to make this explicit, let us consider a zero range process with generator (2.2) and with the filtration equation (2.3) as the limit equation. Suppose that the function space for the limit equation is $H \subseteq L^\infty(\mathbb{T}^d)$. The hydrodynamic limit will be codified in Assumption 2. Throughout this section we suppose that any rate functions $r(N)$, which is only a function of N, vanishes in the limit as $N \to \infty$ and we absorb any constants in the rate function, i.e. without loss of generality $Cr(N) = r(N)$. Furthermore suppose that all rate functions are polynomial in N.

Assumption 2. *Let us fix solutions $(f_t)_{t\geq 0}$ and $(\mu_t^N)_{t\geq 0}$ to the limit equation and the zero range process, respectively, and assume that they satisfy a hydrodynamic limit, i.e. for all $F \in C_b^2(\mathbb{R})$, $\varphi \in C^3(\mathbb{T}^d)$, and $N \in \mathbb{N}$, it holds that*

$$\left\langle \mu_t^N, F\big(\langle \alpha_\eta^N, \varphi\rangle_{L^2}\big) - F\big(\langle f_t, \varphi\rangle_{L^2}\big)\right\rangle \leq \|F\|_{C^2}(1 + \|\varphi\|_{H^1}^2 + \|\varphi\|_{C^3}) r_{\mathrm{HL}}(N)$$

for a rate function $r_{\mathrm{HL}}(N)$ which vanishes as $N \to \infty$, cf. Corollary 2.4.9.
Furthermore assume that the limit solution $f_t \in H$ satisfies $f_t \in C^3(\mathbb{T}^d)$ and that there exists a constant $c > 0$ such that $f_t \geq c$ for all $t \geq 0$. Finally assume a replacement

lemma with a rate $r_{\mathrm{RL}}(\epsilon, N)$, *i.e.*

$$\frac{1}{TN^d}\int_0^T \sum_{x\in\mathbb{T}_N^d} \left\langle \mu_t^N, \left|(g\circ\eta)^{(\epsilon)}(x) - \sigma(\eta^{(\epsilon)}(x))\right|\right\rangle \, dt \le r_{\mathrm{RL}}(\epsilon, N)$$

for $\epsilon > 0$, $N \in \mathbb{N}$ *such that* $\epsilon N < 1$ *and all* $T > 0$, *where we suppose that*

$$\limsup_{\epsilon\to 0}\limsup_{N\to\infty} r_{\mathrm{RL}}(\epsilon, N) = 0.$$

To keep notation simple, we allow all constants in this section (in contrast to the last) to depend on $(f_t)_{t\in[0,\infty)} \subset C^3(\mathbb{T}^d)$, although it is possible in principle to keep track of this dependence as well. We set

$$f_\infty = \int_{\mathbb{T}^d} f_t(u)\, du,$$

which is independent of t since f_t solves the limit equation (2.3). The notation is furthermore justified on noting that we expect $f_t \to f_\infty$ as $t \to \infty$, cf. Lemma 2.4.15. Furthermore we denote the pressure by

$$p(\lambda) = \log Z(e^\lambda), \tag{2.60}$$

where Z is the partition function given in equation (2.7). Then we define the macroscopic entropy as

$$H^\infty(f_t) := \int_{\mathbb{T}^d} h(f_t(u))\, du - h(f_\infty), \tag{2.61}$$

where the function h is given by

$$h(\rho) = \rho\log\sigma(\rho) - p\big(\log\sigma(\rho)\big).$$

Let us find the corresponding macroscopic Fisher information by differentiating in time. It holds that

$$\frac{d}{dt}H^\infty(f_t) = \int_{\mathbb{T}^d}\Big(\partial_t f_t \log\sigma(f_t) + f_t\frac{\sigma'(f_t)}{\sigma(f_t)}\partial_t f_t - p'(\log\sigma(f_t))\frac{\sigma'(f_t)}{\sigma(f_t)}\partial_t f_t\Big)\, du.$$

Since σ is the inverse function of $\rho\partial_\rho \log Z(\rho)$, we find that $p'(\lambda) = \sigma^{-1}(e^\lambda)$ and hence

$$\frac{d}{dt}H^\infty(f_t) = -\int_{\mathbb{T}^d}\frac{|\nabla\sigma(f_t(u))|^2}{\sigma(f_t(u))}\, du =: -\mathcal{D}^\infty(f_t), \tag{2.62}$$

where $\mathcal{D}^\infty(f_t)$ is called the *macroscopic Fisher information.* Next we establish a microscopic analogue of equation (2.62), relating the microscopic entropy $H^N(\mu_t^N|\nu_\rho^N)$ and its

Fisher information $\mathcal{D}^N(\mu_t^N|\nu_\rho^N)$, to be defined presently. Let $f_t^N \in C_b(X_N)$ denote the density of $\mu_t^N \in P(X_N)$ with respect to the grand-canonical measure $\nu_{f_\infty}^N \in P(X_N)$, i.e. set

$$f_t^N(\eta) := \frac{d\mu_t^N}{d\nu_{f_\infty}^N}(\eta). \tag{2.63}$$

The microscopic Fisher information is then defined as

$$\begin{aligned} \mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N) &:= \int_{X_N} \sqrt{f_t^N} N^{-2} G^N \sqrt{f_t^N}\, d\nu_{f_\infty}^N \\ &= \left\langle \sqrt{f_t^N}, N^{-2} G^N \sqrt{f_t^N} \right\rangle_{L^2(\nu_{f_\infty}^N)}. \end{aligned} \tag{2.64}$$

Remark 2.5.1. Abusing notation, we shall sometimes refer to $\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N)$ by $\mathcal{D}^N(f_t^N|\nu_{f_\infty}^N)$, where f_t^N is the density defined in (2.63). Also note that we have left out a factor of N^2 as opposed to the natural (macroscopic) time-scaling, i.e. the time scale of the microscopic Fisher information is the microscopic time scale.

As a first result we show the equivalence of the convergence of the entropy and *entropic chaos*, by which we mean

$$\lim_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_t(\cdot)}^N) = 0.$$

.

Lemma 2.5.2. *Under assumption 2, it holds that*

$$\frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) = H^\infty(f_t) + \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_t(\cdot)}^N) + \mathcal{O}\Big(\frac{1}{N} + r_{\mathrm{HL}}(N)\Big).$$

In particular, the microscopic entropy $N^{-d} H^N(\mu_t^N|\nu_{f_\infty}^N)$ converges to the macroscopic entropy $H^\infty(f_t)$ if and only if there is entropic chaos.

Proof. It holds that

$$\begin{aligned} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) &= \frac{1}{N^d} \int_{X_N} \log\left(\frac{d\mu_t^N}{d\nu_{f_\infty}^N}\right) d\mu_t^N \\ &= \frac{1}{N^d} \int_{X_N} \log\left(\frac{d\mu_t^N}{d\nu_{f_t(\cdot)}^N}\right) d\mu_t^N + \int_{X_N} \log\left(\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}\right) d\mu_t^N. \end{aligned}$$

By definition, it also holds that

$$\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}(\eta) = \prod_{x\in\mathbb{T}_N^d} \frac{Z(\sigma(f_\infty))}{Z(\sigma(f_t(\frac{x}{N})))} \left(\frac{\sigma(f_t(\frac{x}{N}))}{\sigma(f_\infty)}\right)^{\eta(x)}. \tag{2.65}$$

Consequently, the second term equals

$$\begin{aligned}
&\frac{1}{N^d}\int_{X_N}\log\left(\frac{d\nu^N_{f_t(\cdot)}}{d\nu^N_{f_\infty}}\right)\,d\mu^N_t\\
&=\frac{1}{N^d}\sum_{x\in\mathbb{T}^d_N}\int_{X_N}\left(\log\frac{Z(\sigma(f_\infty))}{Z(\sigma(f_t(\frac{x}{N})))}+\eta(x)\log\frac{\sigma(f_t(\frac{x}{N}))}{\sigma(f_\infty)}\right)d\mu^N_t(\eta).
\end{aligned}$$

By Assumption 2, the macroscopic solution f_t is differentiable, and the hydrodynamic limit yields that the right hand side converges to

$$\int_{\mathbb{T}^d} f_t(u)\log\sigma(f_t(u))\,du-\int_{\mathbb{T}^d} p\big(\log\sigma(f_t(u))\big)\,du-f_\infty\log\sigma(f_\infty)+p\big(\log\sigma(f_\infty)\big)$$

as $N\to\infty$. Thus, in view of (2.61), we have shown that

$$\frac{1}{N^d}H^N(\mu^N_t|\nu^N_{f_\infty})=\frac{1}{N^d}H^N(\mu^N_t|\nu^N_{f_t(\cdot)})+H^\infty(f_t)+\mathcal{O}\Big(\frac{1}{N}+r_{\mathrm{HL}}(N)\Big).$$

which concludes the proof. $\square$

The main result of this section is the following theorem.

Theorem 2.5.3. *Under Assumption 2, let the initial microscopic entropy converge, i.e. let*

$$\Big|\frac{1}{N^d}H^N(\mu^N_0|\nu^N_{f_\infty})-H^\infty(f_0)\Big|\le r_{H,0}(N) \tag{2.66}$$

for some rate function $r_{H,0}(N)$. Then both the microscopic entropy and the time average of the Fisher information converge towards the corresponding macroscopic quantities. Specifically, it holds that

$$\Big|\frac{1}{N^d}H^N(\mu^N_t|\nu^N_{f_\infty})-H^\infty(f_t)\Big|\le r_{H,0}(N)+C\Big(\epsilon+\frac{1}{N}+\frac{1}{\epsilon^{3+d}}r_{\mathrm{HL}}(N)+t\ r_{\mathrm{RL}}(\epsilon,N)\Big),$$

and

$$\begin{aligned}
&\Big|\int_0^t 4N^{2-d}\mathcal{D}^N(\mu^N_s|\nu^N_{f_\infty})\,ds-\int_0^t\mathcal{D}^\infty(f_s)\,ds\Big|\\
&\qquad\le r_{H,0}(N)+C\Big(\epsilon+\frac{1}{N}+\frac{1}{\epsilon^{3+d}}r_{\mathrm{HL}}(N)+t\ r_{\mathrm{RL}}(\epsilon,N)\Big)
\end{aligned}$$

for all $\epsilon>0$, $N\in\mathbb{N}$, and $t\ge 0$ (note that this bound is not uniform in time). In *particular, it holds that*

$$\lim_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) = H^\infty(f_t) \quad \textit{and}$$
$$\lim_{N\to\infty} \int_0^t 4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\,ds = \int_0^t \mathcal{D}^\infty(f_s)\,ds$$

for all $t \geq 0$.

The key to the proof of Theorem 2.5.3 is the following lemma.

Lemma 2.5.4. *Under the assumptions of Theorem 2.4.6, it holds that*

$$\frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) \geq H^\infty(f_t) - C\Big(\frac{1}{N} + r_{\mathrm{HL}}(N)\Big),$$

as well as

$$\int_0^t 4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\,ds \geq \int_0^t \mathcal{D}^\infty(f_t)\,ds - C\Big(\frac{1}{N} + \epsilon + \frac{1}{\epsilon^{3+d}} r_{\mathrm{HL}}(N) + t r_{\mathrm{RL}}(\epsilon, N)\Big).$$

In particular, it holds that

$$\liminf_{N\to\infty} \frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) \geq H^\infty(f_t) \textit{ and } \liminf_{N\to\infty} \int_0^t 4\frac{N^2}{N^d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\,ds \geq \mathcal{D}^\infty(f_t)$$

for all $t \geq 0$.

Proof. The bound on the relative entropy is a direct consequence of Lemma 2.5.2 and the fact that all entropies H^N are non-negative. As a warm-up for the bound on the Fisher-information, let us give an alternative proof. The well-known variational formula for the relative entropy, see [47], yields

$$H^N(\mu_t^N|\nu_{f_\infty}^N) = \sup_{f\in C_b(X_N)} \Big\{\langle \mu_t^N, f\rangle - \log\langle \nu_{f_\infty}^N, e^f\rangle\Big\},$$

where the supremum is (formally) obtained by taking $f = \log d\mu_t^N/d\nu_{f_\infty}^N$. In view of the hydrodynamic limit and Yau's results using the relative entropy method, we expect that μ_t^N is close to the local Gibbs state $\nu_{f_t(\cdot)}^N$. Thus we choose

$$f(\eta) = \log \frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}(\eta).$$

Then we obtain a lower bound

$$\frac{1}{N^d} H^N(\mu_t^N|\nu_{f_\infty}^N) \geq \frac{1}{N^d}\int_{X_N} \log \frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}(\eta)\,d\mu_t^N(\eta).$$

Equation (2.65) thus yields a lower bound on the entropy of the form

$$\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\int_{X_N}\left(\eta(x)\log\frac{\sigma\big(f_t(\frac{x}{N})\big)}{\sigma(f_\infty)}+\log\frac{Z(\sigma(f_\infty))}{Z\big(\sigma\big(f_t(\frac{x}{N})\big)\big)}\right)d\mu_t^N(\eta).$$

As in the proof of Lemma 2.5.2, since the macroscopic solution f_t is differentiable, the hydrodynamic limit yields a bound from below by

$$H^\infty(f_t)-C\Big(\frac{1}{N}+r_{\mathrm{HL}}(N)\Big).$$

To prove a similar estimate for the Fisher information, we need the following variational formula, cf. [47]. It holds that

$$\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N)=\sup_f\Big\{-\int_{X_N}\frac{N^{-2}G^Nf(\eta)}{f(\eta)}\,d\mu_t^N(\eta)\Big\},$$

where the supremum is taken over all positive $f\in C_b(X_N)$ such that f is strictly bounded away from zero. The supremum is (formally) obtained at the function $f=\sqrt{d\mu_t^N/d\nu_{f_\infty}^N}$, so here we choose

$$f(\eta)=\sqrt{\frac{d\nu_{f_t(\cdot)}^N}{d\nu_{f_\infty}^N}(\eta)}.$$

After cancelling factors, this corresponds to taking

$$f(\eta)=\prod_{x\in\mathbb{T}_N^d}\sqrt{\sigma\Big(f_t(\frac{x}{N})\Big)}^{\eta(x)}.$$

We obtain that

$$N^{-2}G^Nf(\eta)=\sum_{x\in\mathbb{T}_N^d}\sum_{|e|=1}g(\eta(x))\Bigg(\sqrt{\frac{\sigma\big(f_t(\frac{x+e}{N})\big)}{\sigma\big(f_t(\frac{x}{N})\big)}}-1\Bigg)f(\eta),$$

and hence

$$\frac{G^Nf(\eta)}{N^2f(\eta)}=\sum_{x\in\mathbb{T}_N^d}\sum_{|e|=1}\frac{g(\eta(x))}{\sqrt{\sigma\big(f_t(\frac{x}{N})\big)}}\Bigg(\sqrt{\sigma\big(f_t(\frac{x+e}{N})\big)}-\sqrt{\sigma\big(f_t(\frac{x}{N})\big)}\Bigg).$$

Hence it holds that

$$4N^{2-d}\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N)\geq-4\int_{X_N}\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\frac{g(\eta(x))}{\sqrt{\sigma\big(f_t(\frac{x}{N})\big)}}\Delta_N\sqrt{\sigma\big(f_t(\frac{x}{N})\big)}d\mu_t^N(\eta),$$

where we recall that Δ_N denotes the discrete Laplacian (2.22). Even though f as chosen above is not strictly bounded away from zero (uniformly in η), this can be made rigorous by a standard approximation argument. Since $f_t \in C^3(\mathbb{T}^d)$ is bounded away from zero, we replace $g(\eta(x))$ by $(g\circ\eta)^{(\epsilon)}(x)$, up to an error of $\mathcal{O}(\epsilon)$. Now the replacement lemma yields

$$\int_0^t 4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\,ds \geq -4\int_0^t\int_{X_N}\Bigg(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\frac{\sigma(\eta^{(\epsilon)}(x))}{\sqrt{\sigma\big(f_s(\frac{x}{N})\big)}} \times \Delta_N\sqrt{\sigma\big(f_s(\frac{x}{N})\big)}\Bigg)\,d\mu_s^N(\eta)ds - C(\epsilon + tr_{\mathrm{RL}}(\epsilon,N)).$$

It holds that $\eta^{(\epsilon)}(x) = \langle \alpha_\eta^N, \delta^{(\epsilon)}_{\frac{x}{N}}\rangle$ and the following bounds are satisfied:

$$\|\delta^{(\epsilon)}_{\frac{x}{N}}\|_{C^3} \leq \epsilon^{-3-d} \quad\text{as well as}\quad \|\delta^{(\epsilon)}_{\frac{x}{N}}\|^2_{H^1} \leq \epsilon^{-2-d}.$$

Hence the hydrodynamic limit yields

$$4N^{2-d}\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N) \geq -4\int_{\mathbb{T}^d}\sqrt{\sigma(f_t(u))}\Delta_N\sqrt{\sigma(f_t(u))}\,du - C(\epsilon + tr_{\mathrm{RL}}(\epsilon,N) + \epsilon^{-3-d}r_{\mathrm{HL}}(N)).$$

Finally we replace, up to an error $\mathcal{O}(N^{-1})$, the discrete Laplacian Δ_N by its continuous version Δ and note that

$$-4\int_{\mathbb{T}^d}\sqrt{\sigma(f_t(u))}\Delta\sqrt{\sigma(f_t(u))}\,du = \int_{\mathbb{T}^d}\frac{|\nabla\sigma(f_t(u))|^2}{\sigma(f_t(u))}\,du.$$

This completes the proof of Lemma 2.5.4. □

Proof of Theorem 2.5.3. Equation (2.62) yields

$$H^\infty(f_t) + \int_0^t \mathcal{D}^\infty(f_s)\,ds = H^\infty(f_0). \tag{2.67}$$

Next, we establish a corresponding microscopic relation. First we note that f_t^N defined in (2.63) satisfies the forward Kolmogorov equation

$$\partial_t f_t^N(\eta) = G^N f_t^N(\eta).$$

Since G^N is self-adjoint in $L^2(\nu_{f_\infty}^N)$ and in particular $\langle G^N f_t^N, 1\rangle_{L^2(\nu_{f_\infty}^N)} = 0$, it holds that

$$\frac{d}{dt}H^N(\mu_t^N|\nu_{f_\infty}^N) = \frac{d}{dt}\int_{X_N} f_t^N\log f_t^N d\nu_{f_\infty}^N = \int_{X_N}\left(G^N f_t^N\right)\log f_t^N d\nu_{f_\infty}^N. \tag{2.68}$$

Now we note that

$$\begin{aligned}\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N) &= \langle \sqrt{f_t^N}, N^{-2}G^N\sqrt{f_t^N}\rangle_{L^2(\nu_{f_\infty}^N)} \\ &= \frac{1}{2}\int_{X_N}\sum_{x\in\mathbb{T}_N^d}\sum_{|e|=1} g(\eta(x))\Big(\sqrt{f_t^N(\eta^{x,x+e})}-\sqrt{f_t^N(\eta)}\Big)^2\, d\nu_{f_\infty}^N,\end{aligned}$$

see for example [47, Appendix 1]. Polarization yields

$$\begin{aligned}&\int_{X_N}\big(N^{-2}G^N f_t^N\big)\log f_t^N d\nu_{f_\infty}^N = \langle N^{-2}G^N f_t^N, \log f_t^N\rangle_{L^2(\nu_{f_\infty}^N)} \\ &= \frac{1}{2}\int_{X_N}\sum_{\substack{x\in\mathbb{T}_N^d\\|e|=1}} g(\eta(x))\big(f_t^N(\eta^{x,x+e})-f_t^N(\eta)\big)\big(\log f_t^N(\eta^{x,x+e})-\log f_t^N(\eta)\big)\, d\nu_{f_\infty}^N.\end{aligned}$$

Therefore the elementary inequality $(\sqrt{a}-\sqrt{b})^2 \le (a-b)(\log a - \log b)/4$, which holds for all $a, b > 0$, yields

$$\int_{X_N}\big(N^{-2}G^N f_t^N\big)\log f_t^N d\nu_{f_\infty}^N \ge 4\int_{X_N}\sqrt{f_t^N}N^{-2}G^N\sqrt{f_t^N}d\nu_{f_\infty}^N = 4\mathcal{D}^N(\mu_t^N|\nu_{f_\infty}^N).$$

Therefore time-integration of equation (2.68) yields

$$H^N(\mu_t^N|\nu_{f_\infty}^N) + 4N^2\int_0^t \mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N)\, ds \le H^N(\mu_0^N|\nu_{f_\infty}^N). \tag{2.69}$$

Note that this inequality holds for any $\rho > 0$ replacing $f_\infty > 0$. Since the microscopic entropy converges initially and Lemma 2.5.4 yields lower bounds on each term on the left hand side, a simple technical lemma completes the proof, i.e. we set

$$a = \frac{1}{N^d}H^N(\mu_t^N|\nu_{f_\infty}^N) - H^\infty(f_t) \text{ and } b = \int_0^t \big(4N^{2-d}\mathcal{D}^N(\mu_s^N|\nu_{f_\infty}^N) - \mathcal{D}^\infty(f_s)\big)\, ds$$

in Lemma 2.5.5. □

Lemma 2.5.5. *Let $a, b \in \mathbb{R}$, and $r_i > 0$, $i = 1, 2, 3$ be any reals such that*

$$|a+b| \le r_1,\ a \ge -r_2, \quad \textit{and} \quad b \ge -r_3.$$

Then it holds that

$$|a| \le r_1 + r_2 + r_3 \quad \textit{and} \quad |b| \le r_1 + r_2 + r_3.$$

Proof. For any $\lambda \in \mathbb{R}$, we set

$$\lambda_+ = \max\{0, \lambda\} \quad \text{and} \quad \lambda_- = \max\{0, -\lambda\},$$

i.e. $\lambda = \lambda_+ - \lambda_-$, $|\lambda| = \lambda_+ + \lambda_-$. The first inequality of the assumptions yields

$$a + b = a_+ - a_- + b_+ - b_- \leq |a + b| \leq r_1.$$

On the other hand, the other two assumptions yield

$$a_- \leq r_2 \quad \text{and} \quad b_- \leq r_3$$

and hence

$$a_+ + b_+ \leq r_1 + r_2 + r_3.$$

Since both terms on the left hand side are positive and we already established bounds on a_- and b_-, this shows the hypothesis. □

As a consequence of Lemma 2.5.2 and Theorem 2.5.3, we recover Yau's result on entropic chaos. Of course, our proof is very different in spirit, since we assumed the hydrodynamic limit in order to arrive at entropic chaos. In other words, we conclude the conservation of the hydrodynamic limit in the strong form of Theorem 2.2.3 from the conservation of the hydrodynamic limit in the weak form of Theorem 2.2.2.

Corollary 2.5.6. *Under Assumption 2, suppose that entropic chaos holds initially, i.e.*

$$\lim_{N\to\infty} \frac{1}{N^d} H^N\left(\mu_0^N | \nu_{f_0(\cdot)}^N\right) = 0.$$

Then this property is conserved along the evolution of the process, i.e.

$$\lim_{N\to\infty} \frac{1}{N^d} H^N\left(\mu_t^N | \nu_{f_t(\cdot)}^N\right) = 0 \qquad \textit{for all } t \geq 0.$$

Note that so far we have not proved that the rate of convergence of the microscopic entropy is uniform in time. This should be done in future work.

2.6 The replacement lemma

In this section we want to prove the replacement lemma, Lemma 2.4.19. This is a quantitative L^2–version of the usual replacement lemma found in the literature, e.g. [47],with an explicit estimate on its rate of convergence. The biggest difference from the classical proof of Guo, Papanicolaou, and Varadhan [36] lies in the use of a logarithmic Sobolev inequality (LSI) to obtain a rate of convergence. The classical reference for LSI is [33]; for the zero range process, the LSI has been proven in [27] using only that the rate function satisfies Assumption 1 (i)-(iii). The plan of this section is as follows. In Subsection 2.6.1, we use Assumption 1 (iv) to deduce uniform (in N) bounds on all moments. We state the block estimates and use them to deduce the replacement lemma in Subsection 2.6.2. Subsection 2.6.3 deals with the equivalence of ensembles, a statement concerning the closeness of grand-canonical and canonical measures and which appears in the proof of the block estimates. In Subsection 2.6.4 we show how to restrict ourselves to bounded particle configurations and consequently introduce the density bound ϱ, which can be understood as introducing a density scale. Finally, we prove the block estimates in Subsections 2.6.5 and 2.6.6.

The aim of this section is to prove Lemma 2.4.19, which we restate here for the reader's convenience.

Lemma (A quantitative replacement lemma)**.** Assuming that the initial data possess bounded relative entropy and are bounded with respect to some Gibbs measure, i.e.

$$H^N\big(\mu_0^N|\nu_\rho^N\big) \le CN^d, \quad \text{and} \quad \mu_0^N \le \nu_\rho^N$$

for some $\rho > 0$. Then it holds that

$$\left(\frac{1}{T}\int_0^T \int_{\mathbb{T}^d} \left\langle \mu_t^N, \left|(g\circ\eta)^{(\epsilon)}(uN) - \sigma(\eta^{(\epsilon)}(uN))\right|^2\right\rangle \, dudt\right)^{\frac{1}{2}} \le r_{\mathrm{RL}}(\varrho, l, \epsilon, N),$$

where we recall definition (2.34). The rate function r_{RL} satisfies

$$r_{\mathrm{RL}}(\varrho, l\epsilon, N) \le C\Big((N^{-\frac{1}{2}}l^{\frac{1}{2}} + \epsilon^{\frac{1}{2}}l^{\frac{1}{4}})\varrho l^{\frac{d}{4}} + \varrho l^{-\frac{d}{4}} + \varrho^{-\frac{1}{4}} + \frac{l}{\epsilon N}\Big)$$

for all $N \in \mathbb{N}$, $1/N < \epsilon < 1$, $l < N$, and $\varrho > 0$.

The proof will take up the rest of this section. First we note the following consequence of the bound on the initial microscopic entropy. Equation (2.69) yields

$$H^N\big(\mu_t^N|\nu_\rho^N\big) \le CN^d \quad \text{and} \quad \frac{1}{t}\int_0^t \mathcal{D}^N(\mu_t^N|\nu_\rho^N)\,dt \le CN^{d-2} \tag{2.70}$$

for all $t \ge 0$ and $N \in \mathbb{N}$.

2.6.1 Attractivity and moment bounds

This section is the only place where we need to take advantage of attractivity, i.e. Assumption 1 (iv). This assumption is useful when combined with a *coupling* of two processes and allows us to provide uniform estimates on the particle moments. Since we do not make use of attractivity anywhere else and the theory of attractivity is well-developed,

see [47, 54], we simply sketch the results here.
Consider two copies of the zero range process with initial configurations $\eta, \zeta \in X_N$, which satisfy

$$\eta \leq \zeta, \quad \text{i.e.} \quad \eta(x) \leq \zeta(x) \quad \text{for all } x \in \mathbb{T}_N^d.$$

Assumption 1 (iv) simply states $g(n+1) \geq g(n)$ for all $n \in \mathbb{N}$ and hence we can always let particles of the process with more particles jump at a higher rate. Specifically, at an arbitrary site $x \in \mathbb{T}_N^d$, at time $t = 0$ where we have $\eta(x) \leq \zeta(x)$, we let one particle at $x \in \mathbb{T}_N^d$ of both processes η and ζ jump at the same time at a rate $g(\eta(x))$ and additionally let just one particles of ζ jump at a rate $g(\zeta(x)) - g(\eta(x)) \geq 0$. This coupling almost surely preserves the property $\eta(x) \leq \zeta(x)$ for all $x \in \mathbb{T}_N^d$. Thus we have arrived at a random particle process $(\eta_t, \zeta_t)_{t \geq 0}$ (understood as random variables) with state space $X_N \times X_N$ and whose marginals η_t and ζ_t each are zero range processes with jump rate g, such that the property $\eta_t(x) \leq \zeta_t(x)$ for all $x \in \mathbb{T}_N^d$ is almost surely preserved by the evolution of the process.
A consequence of this coupling is the preservation of stochastic ordering. Recall that in Section 2.4, we defined a function $f^N \in C_b(X_N)$ to be monotonous if $f^N(\eta) \leq f^N(\zeta)$ for all $\eta \leq \zeta$. Two probability measures $\mu, \nu \in P(X_N)$ were said to be ordered, $\mu \leq \nu$, if

$$\langle \mu, f^N \rangle \leq \langle \nu, f^N \rangle \quad \text{for all monotonous } f^N \in C_b(X_N).$$

Suppose now $\mu_0^N, \tilde{\mu}_0^N \in P(X_N)$ are two initial measures of the zero range process such that

$$\tilde{\mu}_0^N \leq \mu_0^N.$$

It can be shown [54, Theorem II.2.4] that this property is equivalent to the existence of a coupling measure on $X_N \times X_N$ with marginals $\tilde{\mu}_0^N$ and μ_0^N that concentrates on $\{\eta \leq \zeta\}$. As shown above, under the evolution of the coupled process, the support of the coupled probability measure remains within $\{\eta \leq \zeta\}$ and it follows, again by [54, Theorem II.2.4], that $\tilde{\mu}_t^N \leq \mu_t^N$.
Let us now turn to the problem of bounding moments of the particle system. We define the k-th order moment as

$$M_k\left[\mu_t^N\right] := \left\langle \mu_t^N, \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^k \right\rangle.$$

Recall that in Remark 2.4.10 we have already obtained a bound on the average number of particles $M_1[\mu_t^N]$ (which is conserved by the evolution).

Lemma 2.6.1. *Assume that the initial measure is bounded from above by ν_ρ^N for some*

$\rho > 0$, i.e. $\mu_0^N \le \nu_\rho^N$. Then for any $k > 0$, it holds that

$$M_k\left[\mu_t^N\right] \le M_k\left[\nu_\rho^N\right] = C_k < +\infty$$

for all $N > 0$ and $t \ge 0$.

Proof. Attractivity yields

$$\mu_t^N \le \nu_\rho^N,$$

and hence

$$M_k\left[\mu_t^N\right] \le M_k\left[\nu_\rho^N\right]$$

by monotonicity of $\eta(x)^k$. All moments of ν_ρ^N are finite and translation-invariance yields

$$M_k\left[\nu_\rho^N\right] = \langle \nu_\rho^N, \eta(0)^k \rangle = C_k$$

uniformly in N. □

2.6.2 Proof of the replacement lemma from the block estimates

In order to prove the replacement lemma with the correct rates, we shall separate scales and introduce another scaling parameter l. Thus we shall first prove a one block estimate, which corresponds to the replacement lemma on blocks of size l instead of ϵN. Then we will prove a two blocks estimate which allows us to estimate the difference in the scales l and ϵN and conclude the replacement lemma with an explicit rate of convergence. Here we shall also use that the one block estimate is proved on boxes where $\delta^{(\epsilon)}$ is approximately constant and hence there is no added difficulty compared to the classical replacement lemma in [36] by introducing χ different from a characteristic function. Similarly to the definition (2.34), where we defined weighted averages $(h \circ \eta)^{(\epsilon)}(u)$, we define the average number of a function $h : \mathbb{N} \to \mathbb{R}$ of the number of particles over the translation of a box Λ_l by $x \in \mathbb{T}_N^d$ to be

$$\overline{h \circ \eta}^l(x) = \frac{1}{(2l+1)^d} \sum_{|y| \le l} h(\eta(x+y)).$$

Furthermore, we set $\overline{\eta}^l = \overline{\mathrm{id} \circ \eta}^l$.

Lemma 2.6.2 (A quantitative one block estimate)**.** *Under the assumptions of the Lemma 2.4.19, it holds that*

$$\left(\frac{1}{TN^d} \int_0^T \sum_{x \in \mathbb{T}_N^d} \left\langle \mu_t^N, \left| \overline{g \circ \eta}^l(x) - \sigma(\overline{\eta}^l(x)) \right|^2 \right\rangle dt \right)^{\frac{1}{2}} \le r_{\mathrm{OBE}}(\varrho, l, N)$$

for some rate function satisfying

$$r_{\mathrm{OBE}}(\varrho, l, N) = C\left(N^{-\frac{1}{2}} l^{\frac{2+d}{4}} \varrho + \varrho l^{-\frac{d}{4}} + \varrho^{-\frac{1}{4}}\right)$$

for all $l, N \in \mathbb{N}$, $T > 0$, $0 < l < N$, *and* $\varrho > 0$.

The two blocks estimate estimates the error made when averaging over the smaller box of size l instead of the box of size ϵN (with a weighted average given by χ).

Lemma 2.6.3 (A quantitative two blocks estimate)**.** *Under the assumptions of Lemma 2.4.19, it holds that*

$$\left(\sup_{|y| \le \epsilon N} \frac{1}{TN^d} \int_0^T \sum_{x \in \mathbb{T}_N^d} \left\langle \mu_t^N, \left|\overline{\eta}^l(x+y) - \eta^{(\epsilon)}(x)\right|^2 \right\rangle dt\right)^{\frac{1}{2}} \le r_{\mathrm{TBE}}(\varrho, l, \epsilon, N)$$

for some rate function satisfying

$$r_{\mathrm{TBE}}(\varrho, l, \epsilon, N) = C\Big(\big(N^{-\frac{1}{2}} l^{\frac{1}{2}} + \epsilon^{\frac{1}{2}} l^{\frac{1}{4}}\big) l^{\frac{d}{4}} \varrho + \varrho l^{-\frac{d}{4}} + \varrho^{-\frac{1}{4}} + \frac{l}{\epsilon N}\Big)$$

for all $l, N \in \mathbb{N}$, $T > 0$, $1/N < \epsilon < 1$, $0 < l < N$, *and* $\varrho > 0$.

From these two estimate we shall presently deduce the Lemma 2.4.19.

Proof of Lemma 2.4.19. First we replace the integral over $u \in \mathbb{T}^d$ by am discrete sum over $x \in \mathbb{T}_N^d$, thus allowing us to only bound the quantity

$$\left(\frac{1}{TN^d} \int_0^T \sum_{x \in \mathbb{T}_N^d} \left\langle \mu_t^N, \left|(g \circ \eta)^{(\epsilon)}(\tfrac{x}{N}) - \sigma(\eta^{(\epsilon)}(\tfrac{x}{N}))\right|^2 \right\rangle dt\right)^{\frac{1}{2}}. \tag{2.71}$$

This will be done as follows. Let us define

$$\tilde{V}_{\epsilon N, x}(\eta) := (g \circ \eta)^{(\epsilon)}(\tfrac{x}{N}) - \sigma(\eta^{(\epsilon)}(\tfrac{x}{N})).$$

For notational convenience we leave out the integration over t and η in comparison to (2.71) from now on. It holds that

$$\left|\int_{\mathbb{T}^d} \tilde{V}_{\epsilon N, uN}^2 \, du - \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \tilde{V}_{\epsilon N, x}^2\right|^{\frac{1}{2}} \le \left(\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \sup_{|e| \le \sqrt{d}} \left|\tilde{V}_{\epsilon N, x+e}^2 - \tilde{V}_{\epsilon N, x}^2\right|\right)^{\frac{1}{2}},$$

where the supremum is taken over all $e \in \mathbb{R}^d$ such that $|e| \le \sqrt{d}$. It holds that

$$\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \sup_{|e| \le \sqrt{d}} \left|\tilde{V}^2_{\epsilon N, x+e} - \tilde{V}^2_{\epsilon N, x}\right|$$
$$\le \left(\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \sup_{|e| \le \sqrt{d}} \left|\tilde{V}_{\epsilon N, x+e} - \tilde{V}_{\epsilon N, x}\right|^2\right)^{\frac{1}{2}} \left(\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \sup_{|e| \le \sqrt{d}} \left|\tilde{V}_{\epsilon N, x+e} + \tilde{V}_{\epsilon N, x}\right|^2\right)^{\frac{1}{2}}$$

by Cauchy-Schwarz. Next note that Lipschitz-continuity g^* yields that

$$\left|(g \circ \eta)^{(\epsilon)}(\tfrac{x+e}{N}) - (g \circ \eta)^{(\epsilon)}(\tfrac{x}{N})\right| \le \frac{C}{\epsilon N} \|\nabla \chi\|_{L^\infty} \frac{1}{\epsilon^d N^d} \sum_{|y| \le C\epsilon N} \eta(y+x),$$

since $x \mapsto \delta_0^{(\epsilon)}(x/N)$ vanishes outside of a box of size $C\epsilon N$, cf. the definition of the smoothed empirical measure (2.29). Jensen's inequality (convexity) yields

$$\left(\frac{1}{(2\epsilon N+1)^d} \sum_{|y| \le \epsilon N} \eta(x+y)\right)^2 \le \frac{1}{(2\epsilon N+1)^d} \sum_{|y| \le \epsilon N} \eta(x+y)^2. \tag{2.72}$$

Therefore we obtain a bound

$$\frac{1}{N^d} \sum_{x \in \mathbb{T}^d} \sup_{|e| \le \sqrt{d}} \left|(g \circ \eta)^{(\epsilon)}(\tfrac{x+e}{N}) - (g \circ \eta)^{(\epsilon)}(\tfrac{x}{N})\right|^2 \le C(\epsilon N)^{-2} \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^2.$$

Thus Lemma 2.6.1 allows us to replace, up to an error of $\mathcal{O}(1/\epsilon N)$, the integral over $u \in \mathbb{T}^d$ by a discrete sum and we just need to estimate the term (2.71). Let us add and subtract the expression

$$\frac{1}{(\epsilon N)^d} \sum_{y \in \mathbb{T}_N^d} \chi\left(\frac{y}{\epsilon N}\right)\left(\overline{g \circ \eta}^l(x+y) - \sigma(\overline{\eta}^l(x+y))\right)$$

inside the absolute value appearing in (2.71). Then we obtain

$$\begin{aligned}
&\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\big|(g\circ\eta)^{(\epsilon)}(x)-\sigma(\eta^{(\epsilon)}(x))\big|^2\Big)^{\frac12}\\
&\qquad\le\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|(g\circ\eta)^{(\epsilon)}(x)-\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi\big(\frac{y}{\epsilon N}\big)\overline{g\circ\eta}^{\,l}(x+y)\Big|^2\Big)^{\frac12}\\
&\qquad+\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi\big(\frac{y}{\epsilon N}\big)\Big(\overline{g\circ\eta}^{\,l}(x+y)-\sigma(\overline{\eta}^{l}(x+y))\Big)\Big|^2\Big)^{\frac12}\\
&\qquad\qquad+\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi\big(\frac{y}{\epsilon N}\big)\sigma(\overline{\eta}^{l}(x+y))-\sigma(\eta^{(\epsilon)}(x))\Big|^2\Big)^{\frac12}.
\end{aligned}$$

We estimate the three terms separately. The first one equals

$$\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi\big(\frac{y}{\epsilon N}\big)\Big(g(\eta(x+y))-\overline{g\circ\eta}^{\,l}(x+y)\Big)\Big|^2\Big)^{\frac12}.$$

Since

$$|\chi(\tfrac{y}{\epsilon N})-\chi(\tfrac{z}{\epsilon N})|\le\frac{l}{\epsilon N}\|\nabla\chi\|_{L^\infty}\quad\text{if}\quad|z-y|\le l$$

and $g(\eta(x))\le g^*\eta(x)$, this term is bounded by

$$C\frac{l}{\epsilon N}\Big(\sum_{x\in\mathbb{T}_N^d}\frac{\eta(x)^2}{N^d}\Big)^{\frac12},$$

and hence by $\mathcal{O}(l/\epsilon N)$ in view of the moment bound of Lemma 2.6.1. Recall that similarly to the previous replacement of the integral over $u\in\mathbb{T}^d$ by a discrete sum, the identity $\int_{\mathbb{T}^d}\chi(u)\,du=1$ yields (2.33). A change of variables $x\to x+y$ yields a bound on the second term by

$$C\|\chi\|_{L^\infty}\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|\overline{g\circ\eta}^{\,l}(x+y)-\sigma(\overline{\eta}^{l}(x+y))\Big|^2\Big)^{\frac12}.$$

This in turn is bounded by the one block estimate. The third term is bounded from above as follows. It holds that

$$(2.73)\quad \Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\Big|\sigma(\eta^{(\epsilon)}(x))-\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi(\frac{y}{\epsilon N})\sigma(\overline{\eta}^l(x+y))\Big|^2\Big)^{\frac{1}{2}}$$
$$\leq\Big(\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\frac{1}{(\epsilon N)^d}\sum_{y\in\mathbb{T}_N^d}\chi(\frac{y}{\epsilon N})\Big|\sigma(\eta^{(\epsilon)}(x))-\sigma(\overline{\eta}^l(x+y))\Big|^2\Big)^{\frac{1}{2}}+\mathcal{O}(\frac{1}{\epsilon N}),$$

where we employed (2.33) and the moment bounds again. Recall that $\chi(y/(\epsilon N))=0$ if $|y|>\epsilon N$. Hence, up to a term $\mathcal{O}(\frac{1}{\epsilon N})$, it holds that (2.73) is bounded from above by

$$C\|\chi\|_\infty\Big(\sup_{|y|\leq\epsilon N}\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\big|\eta^{(\epsilon)}(x)-\overline{\eta}^l(x+y)\big|^2\Big)^{\frac{1}{2}}$$

which is bounded by the two blocks estimate. Note in view of the statement of the two blocks estimate that if we include the the integration over t and η, we take the supremum *outside* the integration. □

Thus it remains to prove the one and two block estimates in order to deduce the replacement lemma.
However, we are still missing one important ingredient in order to be able to present the proof of the block estimates. This is the *equivalence of ensembles* which concerns the closeness of the grand-canonical measures ν_ρ^L and the canonical measures $\nu^{L,K}$ for large L under the condition that the densities are identical. Here L denotes the size of an arbitrary lattice, not necessarily $\mathbb{T}_N^d$.

2.6.3 Equivalence of ensembles

Equivalence of ensembles concerns the closeness of the canonical and the grand-canonical measures in the limit of infinitely many sites. Consider a lattice Λ_L of size $|\Lambda_L|=(2L+1)^d$. For now, we shall not assume anything except Assumption 1 (i), (ii), (iii). These assumptions guarantee the existence of the grand-canonical measures ν_ρ^L, defined in (2.6), with finite exponential moments for all $\rho\in\mathbb{R}$. Let us fix some notation: From now on, for any integer l, we set $l_*:=2l+1$. Let Λ_l be a box of size $|\Lambda_l|=l_*^d$ with $l<L$ and assume that $\Lambda_l\subset\Lambda_L$.
We denote the standard deviation of the grand-canonical (product) measure ν_ρ^L by

$$s(\rho)^2=\mathbb{E}_{\nu_\rho^L}\left[\eta(0)^2\right]-\mathbb{E}_{\nu_\rho^L}\left[\eta(0)\right]^2.$$

Recall that, with σ given as the inverse function (2.23), the measure ν_ρ^L is the invariant measure with particle density ρ, i.e.

$$\mathbb{E}_{\nu_\rho^L}[\eta(0)] = \rho.$$

Let H_m denote the m-th Hermite polyomial

$$H_m(\lambda) = (-1)^m e^{\frac{\lambda^2}{2}} \frac{d^m}{d\lambda^m} e^{-\frac{\lambda^2}{2}}$$

for all $\lambda \in \mathbb{R}$. Define two polynomials

$$\begin{aligned} q_0(\lambda) &= \frac{1}{\sqrt{2\pi}} e^{-\frac{\lambda^2}{2}} \qquad \text{and} \\ q_1(\lambda) &= \frac{1}{\sqrt{2\pi}} e^{-\frac{\lambda^2}{2}} H_3(\lambda) \frac{\gamma_3(\rho)}{6s(\rho)^3} = \frac{\gamma_3(\rho)}{6\sqrt{2\pi}s(\rho)^3} e^{-\frac{\lambda^2}{2}} (\lambda^3 - 3\lambda), \end{aligned}$$

where

$$\gamma_3(\rho) = \mathbb{E}_{\nu_\rho^L}\left[\left(\eta(0) - \rho\right)^3\right].$$

The case of bounded densities

The contents of this section are mostly contained in [47, Appendix 2] and [52]. We include them here for the reader's convenience. Let us state, without proof, the following uniform central limit theorem. The theorem, including higher order expansions, can be found in [47], see also [73]. The results of this subsection are essentially valid without Assumption 1 (iii).

Lemma 2.6.4. *For all $0 < \rho_0 < +\infty$, there exist finite constants $E_1 = E_1(\rho_0)$ and $E_2 = E_2(\rho_0)$ such that*

$$\sup_{K \geq 0} \left| \sqrt{L_*^d} s(\rho) \mathbb{P}_{\nu_\rho^L}\left(\textstyle\sum_{x \in \Lambda_L} \eta(x) = K \right) - q_0(\lambda) - \frac{q_1(\lambda)}{\sqrt{L_*^d}} \right| \leq \frac{E_1}{L_*^d s(\rho)^2}$$

for all $\rho \leq \rho_0$, such that $s(\rho)^2 L_*^d \geq E_2$. Here we set $\lambda = (K - L_*^d \rho)/(L_*^{d/2} s(\rho))$.

The following result is Corollary 1.6 in Appendix 2 of Kipnis and Landim [47].

Lemma 2.6.5. *Fix $0 < \rho_0 < \infty$, a positive integer l and a cylinder function $f : \mathbb{N}^{\Lambda_l} \to \mathbb{R}$ with finite second moment with respect to ν_ρ^L for all $\rho \leq \rho_0$. Then there exist finite* *constants $E_3 = E_3(\rho_0)$ and $E_4 = E_4(\rho_0)$, independent of the choice of f, such that*

$$\begin{aligned}(2.74) \qquad & \left|\mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_{K/L_*^d}}[f]\right| \\ & \le E_3 \frac{l_*^d}{L_*^d}\left(\frac{1}{s(\rho)^2}\mathbb{E}_{\nu^L_\rho}\left[\left|f - \mathbb{E}_{\nu^L_\rho}[f]\right|\right] + \frac{1}{s(\rho)}\sqrt{\mathbb{E}_{\nu^L_\rho}\left[\left(f - \mathbb{E}_{\nu^L_\rho}[f]\right)^2\right]}\right)\end{aligned}$$

for all $L \ge 2l$ and all K such that $K/L_*^d \le \rho_0$ and $s(K/L_*^d)^2 L_*^d \ge E_4$. On the right hand side of the inequality, we have set $\rho = K/L_*^d$.

Proof. First, we note that there exist constants $0 < c_1(\rho_0)$ and $c_2(\rho_0) < \infty$ such that

$$c_1 \le \frac{\rho}{s(\rho)^2} \le c_2 \text{ and } c_1 \le \frac{\gamma_3(\rho)}{s(\rho)^2} \le c_2.$$

For ρ bounded away from zero, this is an obvious consequence of continuity in ρ, whereas for small ρ, all moments of η grow linearly in ρ to first order, see equation (2.80) below. It holds that

$$\frac{q_1(\lambda)}{\sqrt{L_*^d}} \le C\frac{|\lambda|}{\sqrt{L_*^d s(\rho)^2}} \le C\Big(\frac{1}{L_*^d s(\rho)^2} + |\lambda|^2\Big)$$

uniformly in ρ, λ, and L. Consequently, Lemma 2.6.4 yields

$$\begin{aligned}(2.75) \quad \sup_{K\ge 0}\left|\sqrt{L_*^d - l_*^d}\, s(\rho)\mathbb{P}_{\nu^L_\rho}\Big(\textstyle\sum_{x\in\Lambda_L\setminus\Lambda_l}\eta(x) = K\Big) - \frac{1}{\sqrt{2\pi}}e^{-\frac{\lambda^2}{2}}\right| \\ \le C\Big(\frac{1}{L_*^d s(\rho)^2} + |\lambda|^2\Big),\end{aligned}$$

where

$$\lambda = \frac{M(\xi) - l_*^d\rho}{\sqrt{(L_*^d - l_*^d)s(\rho)^2}}$$

and $M(\xi) = \sum_{x\in\Lambda_l}\xi(x)$. The difference $|\mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_\rho}[f]|$ equals

$$(2.76) \qquad \left|\sum_{\xi\in\mathbb{N}^{\Lambda_l}} \nu^l_\rho(\xi)\Big(f(\xi) - \mathbb{E}_{\nu^l_\rho}[f]\Big)\left\{\frac{\nu^L_\rho(\sum_{x\in\Lambda_L\setminus\Lambda_l}\eta(x) = K - M(\xi))}{\nu^L_\rho(\sum_{x\in\Lambda_L}\eta(x) = K)} - 1\right\}\right|.$$

Thus the central limit theorem, see Lemma 2.6.4, yields a bound on the term in braces by

$$(2.77) \qquad \left|\frac{\sqrt{L_*^d s(\rho)^2}}{\sqrt{(L_*^d - l_*^d)s(\rho)^2}}e^{-\frac{\lambda^2}{2}} - 1\right| + C\Big(\frac{1}{L_*^d s(\rho)^2} + |\lambda|^2\Big),$$

where in the denominator, we have used that $s(\rho)^2 L_*^d \geq E_2$. We now bound

$$|\lambda|^2 = \frac{1}{L_*^d - l_*^d} \frac{(M(\xi) - l_*^d \rho)^2}{s(\rho)^2} \leq C \frac{l_*^d}{L_*^d} \frac{(\sqrt{l_*^{-d}} M(\xi) - \sqrt{l_*^d} \rho)^2}{s(\rho)^2}$$

and plug this into (2.77). Since $s(\rho)^2 \leq C_1(\rho_0)\rho_0$, it follows that (2.77) is bounded by

$$E_3'(\rho_0) \frac{l_*^d}{L_*^d s(\rho)^2} \Big(1 + \Big(\sqrt{l_*^{-d}} M(\xi) - \sqrt{l_*^d} \rho\Big)^2\Big).$$

By a law of large numbers (a straightforward direct computation) together with bounds similar to the bounds at the beginning of this proof, it holds that

$$\mathbb{E}_{\nu_\rho^l}\Big[\sum_{x \in \Lambda_l} (\eta(x) - \rho)^4\Big] \leq C\big(l_*^{2d} s(\rho)^4 + l_*^d \mathbb{E}_{\nu_\rho^l}[(\eta(x) - \rho)^4]\big) \leq E_3'(\rho_0) l_*^{2d} s(\rho)^2$$

after possibly changing the value of $E_3'(\rho_0)$. Therefore it holds that

$$\mathbb{E}_{\nu_\rho^l}\Big[\big(\sqrt{l_*^{-d}} M(\xi) - \sqrt{l_*^d} \rho\big)^4\Big] \leq E_3'(\rho_0) s(\rho)^2,$$

and therefore the Cauchy-Schwarz inequality yields a bound on (2.76) by

$$E_3 \frac{l_*^d}{L_*^d} \left(\frac{1}{s(\rho)^2} \mathbb{E}_{\nu_\rho^L}\Big[\big|f - \mathbb{E}_{\nu_\rho^L}[f]\big|\Big] + \frac{1}{s(\rho)} \sqrt{\mathbb{E}_{\nu_\rho^L}\Big[\big(f - \mathbb{E}_{\nu_\rho^L}[f]\big)^2\Big]} \right)$$

for some constant $E_3 = E_3(\rho_0)$. □

This lemma is used in [47] to prove the equivalence of ensembles without the lower bound $s(\rho)^2 L_*^d \geq E_4$. Since we are interested in obtaining explicit bounds on the rate of convergence to the hydrodynamic limit, we need to be a bit more careful in our analysis to identify the dependence on the size l and not just L. The good news so far is that E_1 and E_2 do not depend on l and f, and that in our proof of the replacement lemma we shall not need to consider any cylinder function f, but only the function

$$f(\xi) := \frac{1}{l_*^d} \sum_{x \in \Lambda_l} g(\xi(x))^2 \leq \frac{(g^*)^2}{l_*^d} \sum_{x \in \Lambda_l} \xi(x)^2. \tag{2.78}$$

Carefully keeping track of the dependence on the integer l, we now prove equivalence of ensembles.

Lemma 2.6.6 (Equivalence of ensembles for bounded densities)**.** *Fix $0 < \rho_0 < \infty$ and let f as in (2.78). Then there exists a constant $E_5 = E_5(\rho_0)$ such that*

$$\Big|\mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_{K/L_*^d}}[f]\Big| \leq E_5 \frac{l_*^d}{L_*^d}$$

for all L large enough, all $L \geq 2l$ and all K such that $0 \leq K/L_*^d \leq \rho_0$.

Proof. The proof follows Corollary 1.7 in Appendix II of [47]. Let E_3, E_4 as in Lemma 2.6.5 and consider first the case $s(K/L_*^d)^2 L_*^d \geq E_4$. In this case, if $\rho = K/L_*^d$ is bounded strictly away from zero, the bracket on the right hand side of the inequality in Lemma 2.6.5 is bounded by a constant since the variance $s(\rho)^2$ and all the expectations on the right hand side are continuous with respect to $\rho \leq \rho_0$. Hence let us consider ρ close to zero and $s(\rho)^2 L_*^d \geq E_4$. It holds

$$\mathbb{E}_{\nu_\rho^L}[f] = \sum_{M=0}^{\infty} \mathbb{E}_{\nu_{l,M}}[f] \cdot \nu_\rho^l\big(\textstyle\sum_{x\in\Lambda_l} \xi(x) = M\big).$$

Since g grows at most linearly, the explicit form (2.78) yields that $f(\xi) \leq CM^2$ for particle configurations ξ with M particles. For $M \geq 2$ particles it holds that

$$\mathbb{E}_{\nu_{l,M}}[f] \cdot \nu_\rho^l\big(\textstyle\sum_{x\in\Lambda_l} \xi(x) = M\big) \leq CM^2\rho^M, \tag{2.79}$$

where we have used that $\nu_\rho^l(\xi(x) = n) = \sigma(\rho)^n/(Z(\sigma(\rho))g(n)!) \leq C\rho^k$ since $g \geq \tilde{\delta}k$ and $\rho \leq \rho_0$. Furthermore, for $M = 0, 1$ we obtain

$$\nu_\rho^l\big(\textstyle\sum_{x\in\Lambda_l} \xi(x) = M\big) \leq \begin{cases} \frac{1}{Z(\rho)^l} \text{ if } M = 0, \\ l\frac{\rho}{g(1)Z(\rho)^l} \text{ if } M = 1. \end{cases}$$

Hence we can expand

$$\mathbb{E}_{\nu_\rho^l}[f] = f(\mathfrak{o}) + \sum_{x\in\Lambda_l}\{f(\mathfrak{d}_x) - f(\mathfrak{o})\}\frac{\rho}{g(1)} + \mathcal{O}(\rho^2)$$

for ρ small enough, where $\mathfrak{o}$ denotes the particle configuration in $\mathbb{N}^{\Lambda_l}$ without any particles and $\mathfrak{d}_x$ denotes the configuration containing only a single particle situated at the site $x \in \Lambda_l$. Note that (2.79) yields that the term $\mathcal{O}(\rho^2)$ is bounded independently of l and K for small enough ρ. Likewise we obtain

$$\mathbb{E}_{\nu_\rho^l}\left[\Big(f - \mathbb{E}_{\nu_\rho^l}[f]\Big)^2\right] = \sum_{x\in\Lambda_l}\{f(\mathfrak{d}_x) - f(\mathfrak{o})\}^2\frac{\rho}{g(1)} + \mathcal{O}(\rho^2) \text{ and}$$
$$\mathbb{E}_{\nu_\rho^l}[f] = \left[\Big|\sum_{x\in\Lambda_l}\{f(\mathfrak{d}_x) - f(\mathfrak{o})\}\Big| + \sum_{x\in\Lambda_l}|f(\mathfrak{d}_x) - f(\mathfrak{o})|\right]\frac{\rho}{g(1)} + \mathcal{O}(\rho^2).$$

Of course, in our case these expressions simplify due to $f(\mathfrak{o}) = 0$ but we shall not take advantage of this just yet. Replacing f by $\xi(0)$ we also see that

$$s(\rho)^2 = \frac{\rho}{g(1)} + \mathcal{O}(\rho^2). \tag{2.80}$$

Putting all together we can bound the right hand side of inequality (2.74) by $E_3 l_*^d / L_*^d$. Hence it remains only to consider the case of densities K/L_*^d such that $0 \le s(K/L_*^d)^2 L_*^d \le E_4$. Note that as before equation (2.80) implies that

$$0 < c_1 \le \frac{s(\rho)^2}{\rho} \le c_2 < +\infty$$

near $\rho = 0$ and hence for all $0 \le \rho \le \rho_0$. Hence the particle numbers $K = \rho L_*^d$ under consideration are bounded by $K \le c_2 E_4$. In the following we shall use the explicit form of f. Translation invariance of the canonical measures yields that

$$\mathbb{E}_{\nu^{L,K}}[f] = \mathbb{E}_{\nu^{L,K}}\left[\frac{1}{l_*^d}\sum_{x\in\Lambda_l} g(\xi(x))^2\right] \le \frac{(g^*)^2}{L_*^d}\mathbb{E}_{\nu^{L,K}}\left[\sum_{x\in\Lambda_L}\xi(x)^2\right] \le \frac{(g^* K)^2}{L_*^d}$$

as well as

$$\mathbb{E}_{\nu^L_{\sigma(K/L_*^d)}}[f] \le (g^*)^2 \mathbb{E}_{\nu^L_{K/L_*^d}}[\eta(0)^2]$$
$$= (g^*)^2\Big(s(\tfrac{K}{L_*^d})^2 + (\tfrac{K}{L_*^d})^2\Big) \le \frac{(g^*)^2 E_2}{L_*^d} + \frac{(g^* K)^2}{L_*^{2d}}.$$

Similar computations hold for the expectations of f^2. Again, this shows that the right hand side of (2.74) is bounded by $E_5 l_*^d / L_*^d$. This concludes the proof of the equivalence of ensembles in the case of bounded densities. □

The case of large densities

Using Assumption 1 (i)-(iii), the following result has been shown in [52]. The proof is similar to the proof of the equivalence of ensembles in the case of bounded densities, but relies on Assumption 1 (iii) in order to obtain estimates on the growth of moments of $\eta(x)$ under ν^L_ρ.

Lemma 2.6.7. *There exist $0 < \rho_1 < \infty$ and constants E_6, L_0 such that*

$$\left|\mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_{K/L_*^d}}[f]\right| \le E_6 \frac{l_*^d}{L_*^d}\sqrt{\mathbb{E}_{\nu^L_\rho}\left[\Big(f - \mathbb{E}_{\nu^L_\rho}[f]\Big)^2\right]}$$

for all $l > 0$, cylinder functions $f : \mathbb{N}^{\Lambda_l} \to \mathbb{R}$ with finite second moment with respect to ν^L_ρ, $L \ge \max\{L_0, 2l\}$, and K such that $\rho = K/L_*^d \ge \rho_1$.

Choosing f as in (2.78), we obtain that

$$\mathbb{E}_{\nu^L_\rho}\left[\Big(f - \mathbb{E}_{\nu^L_\rho}[f]\Big)^2\right] \le C\rho^4$$

for all $\rho \geq \rho_1$. Consequently Lemma (2.6.7) yields the equivalence of ensembles for large densities.

Lemma 2.6.8 (Equivalence of ensembles for large densities)**.** *Let f as in* (2.78)*. There exist* $0 < \rho_1 < \infty$ *and constants* E_7*,* L_0 *such that*

$$\left| \mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_{K/L_*^d}}[f] \right| \leq E_7 \frac{l_*^d}{L_*^d} \rho^2$$

for all $L \geq L_0$ large enough, $l < L/2$, and K such that $\rho = K/L_*^d \geq \rho_1$.

Equivalence of ensembles for arbitrary densities

Combining Lemmas 2.6.6 and 2.6.8, we arrive at the main result of this section.

Theorem 2.6.9. *Let f as in* (2.78)*. Then there exist constants E_8 and L_0 such that*

$$\left| \mathbb{E}_{\nu^{L,K}}[f] - \mathbb{E}_{\nu^L_{K/L_*^d}}[f] \right| \leq E_8 \frac{l_*^d}{L_*^d} \left(1 + \frac{K^2}{L_*^{2d}} \right)$$

for all $L \geq L_0$ large enough, $l < L/2$ and $K > 0$.

2.6.4 Restriction to bounded particle configurations

As a first step we prove that it suffices to take bounded configurations.

Lemma 2.6.10. *Under the assumptions of Lemma 2.4.19, there exists a constant $C < +\infty$ such that*

$$\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \mathbb{E}_{\mu_t^N} \left[\overline{\eta}^l(x)^2 \chi_{\{\overline{\eta}^l(x) \geq \varrho\}} \right] \leq \frac{C}{\sqrt{\varrho}}$$

for all $l > 0$ and $\varrho > 0$.

Proof. The proof follows Kipnis and Landim [47], Lemma V.4.2. A few modifications are necessary in order to obtain an explicit, sufficiently fast rate of convergence.
First, by convexity it suffices to prove Lemma 2.6.10 with $\overline{\eta}^l(x)^2$ replaced by $\eta(x)^2$ in the hypothesis. Then Hölder's inequality yields

$$\begin{aligned} (2.81) \qquad & \frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \mathbb{E}_{\mu_t^N} \left[\eta(x)^2 \chi_{\{\overline{\eta}^l(x) \geq \varrho\}} \right] \\ & \leq \mathbb{E}_{\mu_t^N} \left[\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \eta(x)^4 \right]^{1/2} \left(\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \mathbb{P}_{\mu_t^N} \left(\overline{\eta}^l(x) \geq \varrho \right) \right)^{1/2}. \end{aligned}$$

Lemma 2.6.1 yields a uniform bound on the fourth moment and we shall presently deduce a vanishing bound on the probability $\mathbb{P}(\overline{\eta}^l(x) \geq \varrho)$. The second term on the right hand side of (2.81) can be estimated by the entropy inequality (2.32), which yields

$$\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\mathbb{P}_{\mu_t^N}\left(\overline{\eta}^l(x)\geq\varrho\right) \leq \frac{1}{\gamma N^d}\left(H^N(\mu_t^N|\nu_\rho^N)+\log\int_{X_N}\exp\left(\gamma\sum_{x\in\mathbb{T}_N^d}\chi_{\{\overline{\eta}^l(x)\geq\varrho\}}\right)d\nu_\rho^N(\eta)\right)$$

for any $\gamma > 0$. Since the relative entropy is bounded by assumption, we have that

$$\frac{1}{\gamma N^d}H^N\left(\mu_t^N|\nu_\rho^N\right)\leq\frac{C_0}{\gamma}.$$

The second term on the right hand side can be split up as follows. Let the set $\Gamma_x := \{z\in\mathbb{T}_N^d | z-x\in(2l+1)\mathbb{Z}^d\}$ denote the sites in $\mathbb{T}_N^d$ equal to x modulo $2l+1$. With this notation, we can write

$$\sum_{x\in\mathbb{T}_N^d}\chi_{\{\overline{\eta}^l(x)\geq\varrho\}}=\sum_{|x|\leq l}\sum_{y\in\Gamma_x}\chi_{\{\overline{\eta}^l(y)\geq\varrho\}}.$$

Together with the independence of $\overline{\eta}^l(x)$ and $\overline{\eta}^l(y)$ for $|x-y|>2l$, Hölder's inequality yields

$$\frac{C_0}{\gamma}+\frac{1}{\gamma N^d}\log\int_{X_N}\exp\left[\gamma\sum_x\chi_{\{\overline{\eta}^l(x)\geq\varrho\}}\right]d\nu_\rho^N(\eta) \leq\frac{C_0}{\gamma}+\frac{1}{\gamma(2l+1)^d}\log\int_{X_N}\exp\left[\gamma(2l+1)^d\chi_{\{\overline{\eta}^l(0)\geq\varrho\}}\right]\,d\nu_\rho^l(\eta).$$

The presence of the indicator function means that the integral of the exponential on the right hand side can be estimated by

$$1+\mathbb{E}_{\nu_\rho^l}\left[\chi_{\{\overline{\eta}^l(0)\geq\varrho\}}e^{\gamma(2l+1)^d}\right].$$

Then Chebyshev's inequality yields a bound on the last expectation by

$$e^{(2l+1)^d(\gamma-\varrho)}\mathbb{E}_{\nu_\rho^l}\left[e^{\sum_{|x|\leq l}\eta(x)}\right]\leq\exp\left(-(2l+1)^d(\varrho-\gamma-\log E_\rho(1))\right),$$

where

$$E_\rho(\theta):=\mathbb{E}_{\nu_\rho^N}\left[e^{\theta\eta(x)}\right]=\frac{Z(e^\theta\rho)}{Z(\rho)}$$

can be thought of as the Laplace transform of ν_ρ^1. Under Assumption 1, all exponential moments are finite. Now the elementary inequality $\log(1+x) \leq x$ yields a bound

$$\frac{1}{N^d} \sum_{x \in \mathbb{T}_N^d} \mathbb{P}_{\mu_t^N} \left(\overline{\eta}^l(x) \geq \varrho \right) \leq \frac{C_0}{\gamma} + \frac{1}{\gamma(2l+1)^d} \exp\left[-(2l+1)^d(\varrho - \gamma - \log E_\rho(1)) \right]$$

Hence we can choose $\gamma = \varrho - \log E_\rho(1)$ and use that the second term vanishes at least as fast as the first term if $l > 0$. □

2.6.5 Proof of the one block estimate

The aim of this section is to prove Lemma 2.6.2. Up to an error of $C/\sqrt{\varrho}$, Lemma 2.6.10 allows us to consider only configurations with bounded particle numbers. Therefore we will assume that the support of the density function f_t^N, defined in equation (2.63), is contained in

$$\left\{ \eta \in X_N \mid \overline{\eta}^l(x) \leq \varrho \text{ for all } x \in \mathbb{T}_N^d \right\}.$$

Specifically, recall that

$$f_t^N(\eta) = \frac{d\mu_t^N}{d\nu_{f_\infty}^N}(\eta).$$

Setting

$$V_{l,x}(\eta) := \left| \overline{g \circ \eta}^l(x) - \sigma(\overline{\eta}^l(x)) \right|^2 \tag{2.82}$$

and $V_l := V_{l,0}$, we need to control the term

$$\frac{1}{TN^d} \int_0^T \sum_{x \in \mathbb{T}_N^d} \int_{X_N} V_{l,x}(\eta) f_t^N(\eta) d\nu_\rho^N(\eta).$$

Next we reduce the problem to only a box of size l. Let us introduce the short-hand

$$\overline{f}^N = \frac{1}{TN^d} \int_0^T \sum_x \tau_x f_t^N \, dt, \tag{2.83}$$

were τ_x is the translation operator $\tau_x f(\eta) \equiv f(\tau_x \eta)$ and $(\tau_x \eta)(y) = \eta(y - x)$. Then it holds that

$$\frac{1}{TN^d} \int_0^T \sum_{x \in \mathbb{T}_N^d} \int_{X_N} V_{l,x}(\eta) f_t^N(\eta) d\nu_\rho^N(\eta) = \int_{X_N} V_l(\eta) \overline{f}^N(\eta) d\nu_\rho^N(\eta). \tag{2.84}$$

Due to convexity and translation invariance of the Fisher information, it also holds that

$$\mathcal{D}^N\big(\overline{f}^N|\nu_\rho^N\big) \le \frac{1}{T}\int_0^T \mathcal{D}^N\big(f_t^N|\nu_\rho^N\big)\,dt \le CN^{d-2}, \tag{2.85}$$

where the last bound follows from (2.70). Now let $\overline{f}_l(\xi)$ be the density with respect to ν_ρ^l of the marginal of $\overline{f}^N(\eta)d\nu_\rho^N(\eta)$ on Λ_l, i.e. let

$$\overline{f}_l(\xi) = \frac{1}{\nu_\rho^l(\xi)}\int_{\{\eta:\eta|_{\Lambda_l}=\xi\}} \overline{f}^N(\eta)d\nu_\rho^N(\eta)$$

where

$$\Lambda_l = \{-l,\dots,l\}^d, \tag{2.86}$$

is a box of size l and where ν_ρ^l is the Λ_l-marginal of the translation invariant measure ν_ρ^N. Then it holds

$$\int_{X_N} V_l(\eta)\overline{f}^N(\eta)d\nu_\rho^N(\eta) = \int_{\mathbb{N}^{\Lambda_l}} V_l(\xi)\overline{f}_l(\xi)d\nu_\rho^l(\xi). \tag{2.87}$$

The Fisher information on the box Λ_l is given by

$$\mathcal{D}_l\big(f|\nu_\rho^l\big) = \sum_{x,y\in\Lambda_l,x\sim y} I_{x,y}(f|\nu_\rho^l), \tag{2.88}$$

where

$$I_{x,y}(f|\nu_\rho^l) = \frac{1}{2}\int g(\xi(x))\left(\sqrt{f(\xi^{x,y})}-\sqrt{f(\xi)}\right)^2 d\nu_\rho^l(\xi). \tag{2.89}$$

Thus we can formally write

$$\mathcal{D}_l\big(f|\nu_\rho^l\big) = -\int_{\mathbb{N}^{\Lambda_l}} \sqrt{f}G^N\sqrt{f}\;d\nu_\rho^l(\xi),$$

if we neglect jumps that would take particles outside the box Λ_l. By convexity of the "bond-Fisher-information" $I_{x,y}$ we obtain

$$I_{x,y}(\overline{f}_l|\nu_\rho^l) \le I_{x,y}(\overline{f}^N|\nu_\rho^N). \tag{2.90}$$

The Fisher information and the density $\overline{f}^N$ are translation invariant. Hence it holds

$$I_{x,y}(\overline{f}^N|\nu_\rho^l) \le \frac{C}{N^d}\mathcal{D}^N\big(\overline{f}^N|\nu_\rho^l\big).$$

Summing (2.90) over all neighbours $x \sim y \in z + \Lambda_l$ yields

$$N^d \mathcal{D}_l\big(\overline{f}_l|\nu_\rho^l\big) \leq (2l+1)^d \mathcal{D}^N\big(\overline{f}^N|\nu_\rho^N\big) \overset{(2.85)}{\leq} C(2l+1)^d N^{d-2}. \tag{2.91}$$

Now we would like to apply the logarithmic Sobolev inequality. This means we have to decompose along the canonical measures. Thus we shall only consider the problem on hyperplanes of given particle numbers

$$\Omega_K := \Big\{\xi \in \mathbb{N}^{\Lambda_l} \;\Big|\; \sum_{x\in\Lambda_l} \xi(x) = K\Big\}.$$

The canonical measures on Λ_l are given by

$$\nu^{l,K}(\xi) = \nu_\rho^l\Big(\xi\big|\sum_{x\in\Lambda_l}\xi(x) = K\Big),$$

for all $\xi \in \Omega_K$, cf. (2.8). We decompose this problem along the canonical measures on noting

$$\nu_\rho^l = \sum_{K=0}^{\infty} \nu_\rho^l(\Omega_K)\nu^{l,K}.$$

Thus we define

$$\begin{aligned} \overline{f}_{l,K} &:= Z_K^{-1}\nu_\rho^l(\Omega_K)\overline{f}_l\big|_{\Omega_K}, \qquad \text{where} \\ Z_K &:= \int_{\Omega_K} \overline{f}_l\big|_{\Omega_K}(\xi)d\nu_\rho^l(\xi). \end{aligned}$$

This definition yields

$$\int_{\mathbb{N}^{\Lambda_l}} \overline{f}_{l,K}(\xi)\; d\nu^{l,K}(\xi) = 1, \quad Z_K \geq 0 \quad \text{and} \quad \sum_K Z_K = 1$$

Let us now consider the canonical Fisher information on Λ_l given by

$$\mathcal{D}_l\big(\overline{f}_{l,K}|\nu^{l,K}\big) := -\int_{\Omega_K} \sqrt{\overline{f}_{l,K}}G^N\sqrt{\overline{f}_{l,K}}d\nu^{l,K},$$

where again we neglect possible jumps given by G^N outside of Λ_L, cf. (2.88). Denote the relative entropy of measures on the smaller box by

$$H_l(\mu|\nu^{l,K}) := \int_{\mathbb{N}^{\Lambda_l}} \log\frac{d\mu}{d\nu^{l,K}}d\mu$$

for all $\mu \in P(\Omega_K)$. Under Assumption 1 (i)-(iii), the canonical Fisher information satisfies the logarithmic Sobolev inequality

$$H_l(\mu|\nu^{l,K}) \le Cl^2 \mathcal{D}_l(\mu|\nu^{l,K}) \tag{2.92}$$

for all square boxes Λ_l, all $K > 0$, and all $\mu \in P(\Omega_K)$, cf. (2.13) and [27]. The definitions yield that

$$\begin{aligned} \mathcal{D}_l(\overline{f}_l|\nu^l_\rho) &= -\int_{\mathbb{N}^{\Lambda_l}} \sqrt{\overline{f}_l} G^N \sqrt{\overline{f}_l} d\nu^l_\rho \\ &= -\sum_{K=0}^{\infty} \nu^l_\rho(\Omega_K) \int_{\Omega_K} \sqrt{\overline{f}_l|_{\Omega_K}} G^N \sqrt{\overline{f}_l|_{\Omega_K}} d\nu^{l,K} \\ &= -\sum_{K=0}^{\infty} Z_K \int_{\Omega_K} \sqrt{\overline{f}_{l,K}} G^N \sqrt{\overline{f}_{l,K}} d\nu^{l,K} \\ &= \sum_{K=0}^{\infty} Z_K \mathcal{D}_l(\overline{f}_{l,K}|\nu^{l,K}). \end{aligned} \tag{2.93}$$

Equation (2.93) and the logarithmic Sobolev inequality (2.92) then yield

$$\begin{aligned} \sum_K Z_K H^l(\overline{f}_{l,K}|\nu^{l,K}) &\overset{(2.92)}{\le} \sum_K Z_K Cl^2 \mathcal{D}_l(\overline{f}_{l,K}|\nu^{l,K}) \overset{(2.93)}{=} Cl^2 \mathcal{D}_l(\overline{f}_l|\nu^l_\rho) \\ &\overset{(2.91)}{\le} Cl^2(2l+1)^d N^{-d} \mathcal{D}^N(\overline{f}^N|\nu^N_\rho) \le C\frac{l^2}{N^2}(2l+1)^d. \end{aligned}$$

Hence the Csiszár-Kullback-Pinsker inequality, cf. [47], yields

$$\sum_{K=0}^{\infty} Z_K \left\| \overline{f}^{l,K} - 1 \right\|_{L^1(d\nu^{l,K})} \le C(2l+1)^{d/2} \frac{l}{N}. \tag{2.94}$$

Remark 2.6.11. The two functional inequalities, the logarithmic Sobolev inequality and the Csiszár-Kullback-Pinsker inequality, were thus instrumental in replacing locally in the infinitesimal volume element Λ_l the particle distribution by its local thermodynamic equilibrium with an explicit error estimate.

Now we decompose the right hand side of (2.87) to obtain that

$$\int_{\mathbb{N}^{\Lambda_l}} V_l(\xi) \overline{f}_l(\xi) d\nu^l_\rho(\xi) = \sum_{K=0}^{\infty} Z_K \int_{\Omega_K} V_l(\xi) \overline{f}_{l,K}(\xi) d\nu^{l,K}(\xi). \tag{2.95}$$

Recall that Lemma 2.6.10 allowed us to restrict ourselves to density functions with support contained in $\{\overline{\eta}^l(x) \le \varrho\}$. This implies that $Z_K = 0$ for all $K > \varrho(2l+1)^d$. On Ω_K, the function $V_l(\xi)$ is bounded by a multiple of ϱ^2. Thus estimate (2.94) implies that we can bound (2.95) by

$$C(2l+1)^{\frac{d}{2}}\frac{l}{N}\varrho^2+\sum_K Z_K\int_{\Omega_K}V_l(\xi)d\nu^{l,K}(\xi). \tag{2.96}$$

Let us show that the equivalence of ensembles yields a bound on the latter term. To this end, we introduce another parameter $k<l$, to be chosen later in terms of l, such that $(2k+1)^d$ divides $(2l+1)^d$, i.e. $(2l+1)^d/(2k+1)^d=m\in\mathbb{N}$. Then split up the box Λ_l into m disjoint smaller boxes B_i, such that for each $i=1,\dots,m$, the box B_i is a translation of Λ_k, defined in (2.86). Furthermore we note that

$$\sigma\Big(\frac{1}{(2l+1)^d}\sum_{|x|\le l}\xi(x)\Big)=\mathbb{E}_{\nu^l_{K/(2l+1)^d}}\big[g(\xi(0))\big]$$

under the law $\nu^{l,K}$. Thus we split

$$\begin{aligned}&\int_{\Omega_K}V_l(\xi)d\nu^{l,K}(\xi)\\ &=\int_{\Omega_K}\left|\frac{1}{(2l+1)^d}\sum_{|x|\le l}g(\xi(x))-\sigma\Big(\frac{1}{(2l+1)^d}\sum_{|x|\le l}\xi(x)\Big)\right|^2d\nu^{l,K}(\xi)\\ &\le\sum_{i=1}^m\frac{|B_i|}{|\Lambda_l|}\int_{\Omega_K}\left|\frac{1}{|B_i|}\sum_{x\in B_i}g(\xi(x))-\mathbb{E}_{\nu^l_{K/(2l+1)^d}}[g(\xi(0))]\right|^2d\nu^{l,K}(\xi),\end{aligned}$$

by convexity of the function $x\mapsto x^2$. By translation invariance, the above sum can be rewritten as

$$\frac{|\Lambda_k|}{|\Lambda_l|}\sum_{i=1}^m\int_{\Omega_K}\left|\frac{1}{(2k+1)^d}\sum_{|x|\le k}g(\xi(x))-\mathbb{E}_{\nu^l_{K/(2l+1)^d}}[g(\xi(0))]\right|^2d\nu^{l,K}(\xi).$$

Since by construction $m(2k+1)^d/(2l+1)^d=1$, this in turn is bounded by

$$\int_{\Omega_K}\left|\frac{1}{(2k+1)^d}\sum_{|x|\le k}g(\xi(x))-\mathbb{E}_{\nu^l_{K/(2l+1)^d}}[g(\xi(0))]\right|^2d\nu^{l,K}(\xi)$$

Since $K(2l+1)^{-d}\le\varrho$, the equivalence of ensembles, Lemma 2.6.9, yields a bound of

$$\int_{\mathbb{N}^{\Lambda_l}}\left|\frac{1}{(2k+1)^d}\sum_{|x|\le k}g(\xi(x))-\mathbb{E}_{\nu^l_{K/(2l+1)^d}}[g(\xi(0))]\right|^2d\nu^l_{K/(2l+1)^d}(\xi)+C\frac{|\Lambda_k|}{|\Lambda_l|}\varrho^2.$$

Finally due to the law of large numbers, this is bounded by

$$C\Big(\frac{1}{(2k+1)^d}+\frac{(2k+1)^d}{(2l+1)^d}\Big)\varrho^2. \tag{2.97}$$

We can still choose k as a function of l. The asymptotically optimal choice is $k = \sqrt{l}$, and in this case the last bound (2.97) vanishes as $l^{-d/2}\varrho^2$. This error term together with Lemma 2.6.10 and the error term appearing in (2.96) yield the one block estimate.

Remark 2.6.12. Note that the hydrodynamic limit is an asymptotic statement, in which we choose l arbitrarily large. Therefore it was justified that k can be chosen in such a way that $(2k+1)^d$ divides $(2l+1)^d$ and still $k \sim \sqrt{l}$.

2.6.6 Proof of the two blocks estimate

The aim of this section is to prove Lemma 2.6.3. First let us simplify the term under investigation. Recall that

$$\eta^{(\epsilon)}(\tfrac{x}{N}) = \frac{1}{(\epsilon N)^d} \sum_{z\in\mathbb{T}_N^d} \chi(\frac{z}{\epsilon N})\eta(x+z), \quad \text{and} \quad \overline{\eta}^l(x) = \frac{1}{(2l+1)^d}\sum_{|z|\le l}\eta(x+z).$$

Furthermore recall that the term to be estimated is

$$\left(\sup_{|y|\le\epsilon N}\frac{1}{TN^d}\int_0^T\sum_{x\in\mathbb{T}_N^d}\left\langle \mu_t^N, \left|\overline{\eta}^l(x+y)-\eta^{(\epsilon)}(x)\right|^2\right\rangle\,dt\right)^{\frac{1}{2}}.$$

For ease of notation, let us temporarily drop the integral over t and η in the next line. Since χ is differentiable, we can replace each $\eta(x+z)$ appearing in the definition of $\eta^{(\epsilon)}(x)$ by $\overline{\eta}^l(x+z)$ to obtain

$$\left(\sup_{|y|\le\epsilon N}\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\left|\overline{\eta}^l(x+y)-\eta^{(\epsilon)}(\tfrac{x}{N})\right|^2\right)^{\frac{1}{2}} \le \left(\frac{Cl^2}{(\epsilon N)^2}\sum_{x\in\mathbb{T}_N^d}\frac{\eta(x)^2}{N^d}\right)^{\frac{1}{2}} + $$
$$+\left(\sup_{|y|\le\epsilon N}\frac{1}{N^d}\sum_{x\in\mathbb{T}_N^d}\left|\overline{\eta}^l(x+y)-\frac{1}{(\epsilon N)^d}\sum_{z\in\mathbb{T}_N^d}\chi(\tfrac{z}{\epsilon N})\overline{\eta}^l(x+z)\right|^2\right)^{\frac{1}{2}}.$$

Hence upon inserting estimate (2.33) we deduce that, up to an error term $\mathcal{O}(\frac{l}{\epsilon N})$, the term to be estimated in the two blocks estimate is bounded by

$$\left(\sup_{cl<|y|\le 2\epsilon N}\frac{1}{TN^d}\int_0^T\sum_{x\in\mathbb{T}_N^d}\mathbb{E}_{\mu_t^N}\left[\left|\overline{\eta}^l(x)-\overline{\eta}^l(x+y)\right|^2\right]\,dt\right)^{\frac{1}{2}}$$

for a suitable $c>0$. Hence it suffices to estimate the rate of convergence of

$$\sup_{cl<|y|\le 2\epsilon N}\frac{1}{TN^d}\int_0^T\sum_{x\in\mathbb{T}_N^d}\mathbb{E}_{\mu_t^N}\left[\left|\overline{\eta}^l(x)-\overline{\eta}^l(x+y)\right|^2\right]\,dt.$$

As before, let f_t^N denote the Radon-Nikodym density

$$f_t^N = \frac{d\mu_t^N}{d\nu_\rho^N}.$$

Recalling definition (2.83) for the average $\overline{f}^N$ over time T and lattice $\mathbb{T}_N^d$ of the density f_t^N, the above expression is equal to

$$\sup_{cl<|y|\leq 2\epsilon N} \int_{X_N} \overline{f}^N(\eta) \left|\overline{\eta}^l(0) - \overline{\eta}^l(y)\right|^2 d\nu_\rho^N(\eta).$$

Furthermore, we can bound the number of particles on the disjoint boxes $x + \Lambda_l$ and $x + y + \Lambda_l$ as in Lemma 2.6.10. Again the resulting error is bounded by $C/\sqrt{\varrho}$ for some constant $C < +\infty$. Hence it is enough to consider

$$\sup_{cl<|y|\leq 2\epsilon N} \int_{X_N} \overline{f}^N(\eta) V_{2,l}(\eta) d\nu_\rho^N(\eta)$$

where

$$V_{2,l}(\eta) := \chi_{\{\overline{\eta}^l(0)\vee\overline{\eta}^l(y)\leq\varrho\}} \left|\overline{\eta}^l(0) - \overline{\eta}^l(y)\right|^2 \tag{2.98}$$

with the notation $a \vee b = \max\{a, b\}$. From here the proof of the two blocks estimate is similar to the proof of the one block estimate and we will only highlight the differences. It would now suffice to restrict the problem to a union of boxes $\Lambda_l \cup (y + \Lambda_l)$, but, put together, these do not form a square (hypercubic) box of equal side length and hence they do not guarantee the validity of an LSI. Hence we take into account a larger hypercube of side length $4l + 2$, which contains (translations of) both boxes Λ_l and $(y + \Lambda_l)$ glued together. Since the number of sites in this larger box still scales as l^d, this choice does not change the scaling of the rate of convergence. Specifically, consider a square (hypercubic) box in $\mathbb{Z}^d$ with each side length being exactly equal to $4l + 2$. Now we split up this box along a plane into two equal halfs Λ_l^1 and Λ_l^2 and translate each part such that $\Lambda_l \subset \Lambda_l^1$, $y + \Lambda_l \subset \Lambda_l^2$. Since $|y| > cl$, we can choose $c > 0$ (depending only on the dimension d) such that $\Lambda_l^1 \cap \Lambda_l^2 = \emptyset$. Then we set

$$\Lambda_{y,l} := \Lambda_l^1 \cup \Lambda_l^2$$

and we shall presently consider the process only on $\Lambda_{y,l}$. First we introduce some new notation. Let $X_{2,l} := \mathbb{N}^{\Lambda_l^1} \times \mathbb{N}^{\Lambda_l^2}$ be the configuration space on the two boxes, $\nu_\rho^{2,l}$ be the product measure ν_ρ^N restricted to $X_{2,l}$, and $\xi = (\xi_1, \xi_2)$ be a configuration in $X_{2,l}$. Let $\overline{f}_{y,l}$

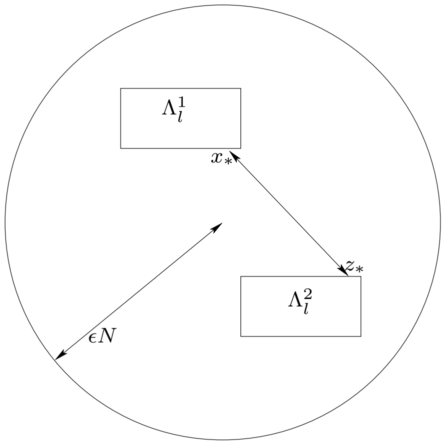

Figure 2.1: The two boxes Λ_l^1 and Λ_l^2. Opposite faces have been chosen for Γ, defined below, and it holds $(x_*, z_*) \in \Gamma$.

to be the density conditional on configurations $\xi \in X_{2,l}$, i.e.

$$\overline{f}_{y,l}(\xi) = \frac{1}{\nu_\rho^{2,l}(\xi)} \int_{X_{2,l}} \chi_{\{\eta \in X_N : \eta|_{\Lambda_{y,l}} = \xi\}} \overline{f}^N(\eta) d\nu_\rho^{2,l}(\eta).$$

In a next step, we need to obtain bounds on the Fisher information of $\overline{f}_{y,l}$. Since $\overline{f}_{y,l}$ is a density over two disjoint boxes, this is technically more involved than the corresponding calculations in the proof of the one block estimate. First we recall that convexity yields

$$\mathcal{D}^N\left(\overline{f}^N | \nu_\rho^N\right) \leq \frac{1}{T} \int_0^T \mathcal{D}^N\left(f_t^N | \nu_\rho^N\right) dt \leq C N^{d-2}.$$

Now we compare with an appropriate Fisher information on $X_{2,l}$. For all $f \in C_b(X_{2,l})$, we set

$$I_{x,z}^{1,l}(f|\nu_\rho^{2,l}) = \frac{1}{2} \int_{X_{2,l}} g(\xi(x)) \left(\sqrt{f(\xi_1^{x,z}, \xi_2)} - \sqrt{f(\xi)}\right)^2 d\nu_\rho^{2,l}(\xi)$$

for all neighbours $x, z \in \Lambda_l^1$,

$$I_{x,z}^{2,l}(f|\nu_\rho^{2,l}) = \frac{1}{2} \int_{X_{2,l}} g(\xi(x)) \left(\sqrt{f(\xi_1, \xi_2^{x,z})} - \sqrt{f(\xi)}\right)^2 d\nu_\rho^{2,l}(\xi)$$

for all neighbours $x, z \in \Lambda_l^2$, and

$$I_{x_*,z_*}^{l,+}(f|\nu_\rho^{2,l}) = \frac{1}{2} \int_{X_{2,l}} g(\xi_1(x_*)) \left(\sqrt{f(\xi_1^{x_*,-}, \xi_2^{z_*,+})} - \sqrt{f(\xi)}\right)^2 d\nu_\rho^{2,l}(\xi)$$

for all $x_* \in \partial\Lambda_l^1, z_* \in \partial\Lambda_l^2$ on the boundaries of the boxes. Here $\xi^{x,z}$ is the configuration ξ after a particle jumped from site x to site z, cf. (2.2), and $(\xi_1^{x_*,-}, \xi_2^{z_*,+})$ is the configuration $\xi = (\xi_1, \xi_2)$ after a particle jumped from the boundary point x_* of the first box to the boundary point z_* of the second box, i.e. we set

$$\xi_j^{x,\pm}(z) = \begin{cases} \xi_j(x) \pm 1 & \text{if } z = x \in \Lambda_l^j, \\ \xi_j(z) & \text{otherwise} \end{cases}$$

for all $z \in \Lambda_l^j$. Now consider one face each of the two rectangular boxes Λ_l^1, Λ_l^2, which are facing each other and along which we have split up the original box. Then we say that $(x_*, z_*) \in \Gamma$ if and only if x_* is on the face belonging to one face of $\partial\Lambda_l^1$, and z_* is the corresponding site directly opposite x_* on the face of $\partial\Lambda_l^2$ belonging to the other box, see Figure 2.1. In this fashion we join two faces of $\Lambda_{y,l}$ back together. Note that it holds that $|\Gamma| = (4l+2)^{d-1}$. Using the above "bond-Fisher-information", we define a corresponding Fisher information on $\Lambda_{y,l}$ as

$$\mathcal{D}_{2,l}\big(f|\nu_\rho^{2,l}\big) := \sum_{(x_*,z_*)\in\Gamma} I_{x_*,z_*}^{l,+}(f|\nu_\rho^{2,l}) + \sum_{|x-z|=1} \big(I_{x,z}^{1,l}(f|\nu_\rho^{2,l}) + I_{x,z}^{2,l}(f|\nu_\rho^{2,l})\big) \tag{2.99}$$

for all $f \in C_b(X_{2,l})$. This Fisher information corresponds to a particle process where particles move according to a zero range process on each box and where they can jump from the boundary of one box to the other. As in inequality (2.90), convexity yields

$$I_{x,z}^{1,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big) \le I_{x,z}\big(\overline{f}^N\big) \quad \text{and} \quad I_{x,z}^{2,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big) \le I_{x+y,z+y}\big(\overline{f}^N\big),$$

where $I_{x,z}$ was defined in (2.89). Summing over all $x, z \in \mathbb{T}_N^d$ such that $|x-z| = 1$ we obtain by translation invariance that

$$\sum_{|x-z|=1} \Big(I_{x,z}^{1,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big) + I_{x,z}^{2,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big)\Big) \le 2C(2l+1)^d N^{-2}. \tag{2.100}$$

since $\mathcal{D}^N(\overline{f}^N|\nu_\rho^N) \le CN^{d-2}$. Recall from Subsection 2.6.3 that $\mathfrak{d}_x$ denotes the configuration with a single particle at $x \in \mathbb{T}_N^d$. Since

$$\mathbb{P}_{\nu_\rho^N}\big(\eta(x) = n\big) = \frac{\sigma(\rho)^n}{g(n)!Z(\sigma(\rho))},$$

a change of variables $\xi' = \xi + \mathfrak{d}_{x_*}$ resp. $\eta' = \eta + \mathfrak{d}_x$ yields

$$I_{x_*,z_*}^{l,+}(f|\nu_\rho^{2,l}) = \frac{\sigma(\rho)}{2} \int_{X_{2,l}} \left(\sqrt{f(\xi_1^{x_*,+}, \xi_2)} - \sqrt{f(\xi_1, \xi_2^{z_*,+})}\right)^2 d\nu_\rho^{2,l}(\xi), \text{ and}$$
$$I_{x,z}(f^N) = \frac{\sigma(\rho)}{2} \int_{X_N} \left(\sqrt{f^N(\eta^{x,+})} - \sqrt{f^N(\eta^{z,+})}\right)^2 d\nu_\rho^N(\eta),$$

where $f \in C_b(X_{2,l})$ and $f^N \in C_b(X_N)$, and where $I_{x,z}(f)$ is the ordinary bond-Fisher information defined in (2.89). Again we take advantage of convexity to see that

$$I^{l,+}_{x_*,z_*}\big(\overline{f}_{y,l}|\nu^{2,l}_\rho\big) \le \frac{\sigma(\rho)}{2}\int \left(\sqrt{\overline{f}^N(\eta^{x_*,+})} - \sqrt{\overline{f}^N(\eta^{z_*,+})}\right)^2 d\nu^N_\rho(\eta) \tag{2.101}$$

for the average $\overline{f}^N$ defined in (2.83). Of course the right hand side is not a summand of $\mathcal{D}^N(\overline{f}^N|\nu^N_\rho)$. Therefore we consider a path $(x_k)_{0\le k\le R}$ from $x_* \in \partial\Lambda^1_l$ to $z_* \in \partial\Lambda^2_l$. Here

$$R := \|z_* - x_*\|_{\ell^1} = \sum_{1\le j\le d} |z_{*j} - x_{*j}|$$

represents the ℓ^1–norm on $\mathbb{T}^d_N$, and the path satisfies

$$x_0 = x_*, \quad x_R = z_*, \quad \text{and} \quad |x_{k+1} - x_k| = 1 \text{ for every } 0 \le k \le R-1.$$

The telescope identity

$$\sqrt{\overline{f}^N(\eta^{x_*,+})} - \sqrt{\overline{f}^N(\eta^{z_*,+})} = \sum_{k=0}^{R-1}\left(\sqrt{\overline{f}^N(\eta^{x_{k+1},+})} - \sqrt{\overline{f}^N(\eta^{x_k,+})}\right)$$

together with Cauchy–Schwarz inequality

$$\left(\sum_{k=0}^{R-1} a_k\right)^2 \le R\sum_{k=0}^{R-1} a_k^2$$

yields a bound on the right hand side of (2.101) by

$$\frac{R\sigma(\rho)}{2}\sum_{k=0}^{R-1}\int_{X_N}\left(\sqrt{\overline{f}^N(\eta^{x_k,+})} - \sqrt{\overline{f}^N(\eta^{x_{k+1},+})}\right)^2 d\nu^N_\rho(\eta) = R\sum_{k=0}^{R-1} I_{x_k,x_{k+1}}(\overline{f}^N).$$

Since $\overline{f}^N$ is translation-invariant and x_k, x_{k+1} are neighbours, we obtain

$$I_{x_k,x_{k+1}}(\overline{f}^N) \le N^{-d}\mathcal{D}^N(\overline{f}^N|\nu^N_\rho)$$

and hence

$$I^{l,+}_{x_*,z_*}\big(\overline{f}_{y,l}|\nu^{2,l}_\rho\big) \le R^2 N^{-d}\mathcal{D}^N\big(\overline{f}^N|\nu^N_\rho\big).$$

Without loss of generality we can assume that we joined the two boxes such that $|x_* - z_*| \le |y| \le 2\epsilon N$ and hence

$$R = \|z_* - x_*\|_{\ell^1} \le \sqrt{d}|y| \le 2\sqrt{d}\epsilon N.$$

The bound on the Fisher information $\mathcal{D}^N(\overline{f}^N|\nu_\rho^N) \leq CN^{d-2}$ thus yields

$$I^{l,+}_{x_*,z_*}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big) \leq C\epsilon^2.$$

Summing over all pairs $(x_*, z_*) \in \Gamma$, yields another factor of Cl^{d-1}. In conjunction with (2.100), we have shown that the Fisher information defined in (2.99) satisfies

$$\mathcal{D}_{2,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big) \leq C\big(\frac{l^d}{N^2} + \epsilon^2 l^{d-1}\big). \tag{2.102}$$

As before, we decompose the problem along hyperplanes of configurations on $X_{2,l}$ with constant number of particles K and corresponding canonical measure

$$\nu^{2,l,K}(\xi) = \nu_\rho^{2,l}\Big(\xi\big|\sum_{x\in\Lambda_l^1}\xi^1(x) + \sum_{x\in\Lambda_l^2}\xi^2(x) = K\Big).$$

Similarly to the proof of the one block estimate we denote

$$\Omega_K^2 = \Big\{\xi \in \Lambda_{y,l}\big|\sum_{x\in\Lambda_l^1}\xi^1(x) + \sum_{x\in\Lambda_l^2}\xi^2(x) = K\Big\},$$

see Subsection 2.6.5. On Ω_K^2, we introduce the density

$$\begin{aligned}\overline{f}_{2,l,K} &:= Z_K^{-1}\nu_\rho^{2,l}(\Omega_K^2)\overline{f}_{y,l}\big|_{\Omega_K^2},\\ Z_K &:= \int_{\Omega_K^2}\overline{f}_{y,l}\big|_{\Omega_K^2}\,d\nu_\rho^{2,l}(\eta).\end{aligned}$$

Then it holds that

$$\int_{\mathbb{N}^{\Lambda_l}} V_{2,l}(\xi)\overline{f}_{y,l}(\xi)d\nu_\rho^{2,l}(\xi) = \sum_{K=0}^{\infty} Z_K\int_{\Omega_K^2} V_{2,l}(\xi)\overline{f}_{2,l,K}(\xi)d\nu^{2,l,K}(\xi). \tag{2.103}$$

By construction, the Fisher information (2.99) is equivalent to the Fisher information of a ZRP on a box of side length $4l+2$. Thus it satisfies an LSI, if we replace $\nu_\rho^{2,l}$ by its canonical version $\nu^{2,l,K}$. The measure $\nu^{2,l,K}$ is invariant with respect to this zero range process and again we define a canonical Fisher information by

$$\mathcal{D}_{2,l}\big(\overline{f}_{2,l,K}|\nu^{2,l,K}\big) = \sum_{(x_*,z_*)\in\Gamma} I^{l,+}_{x_*,z_*}(f|\nu^{2,l,K}) + \sum_{|x-z|=1}\big(I^{1,l}_{x,z}(f|\nu^{2,l,K}) + I^{2,l}_{x,z}(f|\nu^{2,l,K}\big)\,.$$

We can formally write

$$\mathcal{D}_{2,l}\big(\overline{f}_{2,l,K}|\nu^{2,l,K}\big) = \int_{\mathbb{N}^{\Lambda_{y,l}}}\sqrt{\overline{f}_{2,l,K}}G^N\sqrt{\overline{f}_{2,l,K}}\;d\nu^{2,l,K}$$

if we neglect jumps outside of $\Lambda_{y,l}$. Of course, equation (2.93) holds for the equivalent quantities on $\Lambda_{y,l}$ as well. Also denote the relative entropy on $X_{2,l}$ by

$$H^{2,l}(\mu|\nu^{2,l,K}) := \int_{X_{2,l}} \log \frac{d\mu}{d\nu^{2,l,K}} d\mu$$

for all $\mu \in P(\Omega_K^2)$. Furthermore, we constructed our canonical Fisher information in such a way that it is the canonical Fisher information of a zero range process on the square lattice $\Lambda_{y,l}$ with the two faces glued together. Hence [27] yields the logarithmic Sobolev inequality

$$H^{2,l}(\mu|\nu^{2,l,K}) \leq Cl^2 \mathcal{D}_{2,l}(\mu|\nu^{2,l,K})$$

uniformly in $l > 0$, $K > 0$, and $\mu \in P(\Omega_K^2)$, cf. (2.92). This logarithmic Sobolev inequality yields

$$\sum_K Z_K H\big(\overline{f}_{2,l,K}|\nu^{2,l,K}\big) \leq \sum_K Z_K Cl^2 \mathcal{D}_{2,l}\big(\overline{f}_{2,l,K}|\nu^{2,l,K}\big) \overset{(2.93)}{=} Cl^2 \mathcal{D}_{2,l}\big(\overline{f}_{y,l}|\nu_\rho^{2,l}\big)$$

as in Subsection 2.6.5. Now the Csiszár-Kullback-Pinsker inequality and estimate (2.99) yield

$$\sum_{K=0}^{\infty} Z_K \left\|\overline{f}_{2,l,K} - 1\right\|_{L^1(d\nu^{2,l,K})} \leq C\big(lN^{-1} + \epsilon\sqrt{l}\big)l^{d/2}.$$

Therefore we can replace $\overline{f}_{2,l,K}$ by 1 in (2.103), up to an error bounded by

$$C\big(lN^{-1} + \epsilon\sqrt{l}\big)l^{d/2}\varrho^2,$$

where ϱ is the bound on the number of particles introduced in Lemma 2.6.10, see also (2.98). Thus we are left to consider

$$\sum_{K=0}^{\infty} Z_K \int_{\Omega_K^2} V_{2,l}(\xi) d\nu^{2,l,K}(\xi),$$

which is bounded by $C\varrho^2 l^{-d/2}$ analogously to Subsection 2.6.5 by the equivalence of ensembles and the law of large numbers.

2.7 Perspective: the case of $d \geq 2$ dimensions

Disclaimer: This section is included for its mathematical interest, but does not constitute a proof of any of its statements - all results are still work in progress.

So far in our proof of the hydrodynamic limit, we have assumed $d = 1$. Let us now give an exposition of work in progress on how to remove this restriction. Regularity results for uniformly parabolic equations in higher dimensions usually rely on the famous results of Nash, de Giorgi, and Moser. We shall see that this is the case here, too. First make the following conjecture on the propagation of higher regularity in $H^k(\mathbb{T}^d)$ for general dimensions.

Conjecture 1 (Improved regularity)**.** *We conjecture that for each $k > 0$, there exist constants $C < +\infty$ and $\alpha, \beta > 0$ such that*

$$\|f_t\|_{H^k} \leq C\big(1 + \|f_0\|_{H^k} + \|f_0\|_{L^\infty}^\alpha \|f_0\|_{H^k}^\beta\big)$$

for all $f_0 \in H^k(\mathbb{T}^d)$ and $t \geq 0$.

Let us derive the consequences for the hydrodynamic limit if we assume this conjecture to be true.
Stability estimates: Lemma 2.4.14 remains true if we change Λ to be

$$\Lambda(f) = \|f_0\|_{L^\infty}\big(1 + \|f_0\|_{H^k} + \|f_0\|_{L^\infty}^\alpha \|f_0\|_{H^k}^\beta\big)^{\frac{d+4}{2k+2}}.$$

Abstract differential calculus of the semigroup: Lemma 2.4.17 remains true with Λ given as in the previous equation.
Rate of convergence on the hydrodynamic limit: Theorem 2.4.6 remains true if we change r_{HL} to be

$$\begin{aligned} r_{\mathrm{HL}}(T, \varrho, l, \epsilon, N) \leq C\Big(&\epsilon + \epsilon^{-d-(d\alpha+(k+\frac{d}{2})\beta)\frac{d+4}{2k+2}} N^{1-\theta(d+1)} + \epsilon^{-\frac{4+d}{2}} N^{-2} \\ &+ e^{-cT} N^{2+d} \epsilon^{-2d} + T^{\frac{1}{2}}\big(N^{-\frac{1}{2}} l^{\frac{1}{2}} + \epsilon^{\frac{1}{2}} l^{\frac{1}{4}}\big)\varrho l^{\frac{d}{4}} + \varrho^2 l^{-\frac{d}{4}} + \varrho^{-\frac{1}{4}} + \frac{l}{\epsilon N}\Big). \end{aligned}$$

Optimal rate of convergence: Corollary 2.4.9 remains true with a different optimal rate $N^{-\kappa}$, with κ depending on the exact values of α and β.

The strategy for the proof is the following: We know that solutions to equation (2.3) are smooth due to the ellipticity of σ. The difficulty lies in obtaining explicit bounds on the propagation of the Sobolev norms in $H^k(\mathbb{T}^d)$. First of all, let us go back to the proof of the regularity estimate, Lemma 2.4.13. Instead of interpolating $D^{\mathfrak{r}_i} f_t$ between $\|D^{k+1} f_t\|_{L^2}$ and $\|\nabla f_t\|_{L^2}$, we can interpolate between $\|D^{k+1} f_t\|_{L^2}$ and $\|f_t\|_{L^\infty}$. The generalized Gagliardo-Nirenberg-inequality, see [20], yields

$$\|D^{\mathfrak{r}} f\|_{L^p} \leq C\|D^{k+1} f\|_{L^2}^\theta \|f\|_{L^\infty}^{1-\theta},$$

if

$$|\mathfrak{r}| - \frac{d}{p} = \theta\Big(k + 1 - \frac{d}{2}\Big)$$

and $1 \geq \theta \geq |\mathfrak{r}|/(k+1)$. Interpolating between, say, $\|D^k f_t\|_{L^2}$, $\|D^{k+1} f_t\|_{L^2}$, and $\|f_t\|_{L^\infty}$, we should be able to obtain a local in time bound of the form

$$\|D^k f_t\|_{L^2} \leq C\|D^k f_0\|_{L^2} \quad \text{for all} \quad t \leq T(\|D^k f_0\|_{L^2}, \|f_0\|_{L^\infty})$$

with polynomial dependence of $T(\cdot,\cdot)$ in each argument. (Otherwise there are analytic norms available to perform a similar job.) Thus we have reduced the problem to obtaining "large" time bounds only. In the terms that appear in the proof of Lemma 2.4.13, we choose $p_i = |\mathfrak{r}_i|/(2(k+1))$, which corresponds to the critical case $\theta_i = |\mathfrak{r}_i|/(k+1)$. This choice yields

$$\frac{d}{dt}\|D^{\mathfrak{s}} f_t\|_{L^2}^2 \leq -c\|\nabla D^{\mathfrak{s}} f_t\|_{L^2}^2 + C(1 + \|f_0\|_{L^\infty}^{k+1})\|\nabla D^{\mathfrak{s}} f_t\|_{L^2}^2,$$

which is exactly the critical case. Therefore we need a slightly better space than $L^\infty(\mathbb{T}^d)$ to interpolate. A suitable function space is the space $C^{0,s}(\mathbb{T}^d)$ of s–Hölder-continuous functions. There are several ways to obtain an interpolation inequality between $W^{|\mathfrak{r}|,p}(\mathbb{T}^d)$, $H^{k+1}(\mathbb{T}^d)$ and $C^{0,s}(\mathbb{T}^d)$. A suitable approach could be Littlewood-Paley theory (microlocal analysis). Assuming the correctness of this approach, we simply need to find a (polynomial) bound on the $C^{0,s}$–norm of the solutions for some $s > 0$. Now by Nash's result [68] on the Hölder-continuity of solutions to uniformly parabolic equations there indeed exists some $s > 0$ such that

$$[f_t]_{C^{0,s}} \leq C\|f_0\|_{L^\infty} t^{\frac{s}{2}}$$

for all $t > 0$. Applying this bound for $t \geq T(\|D^k f_t\|_{L^2}, \|f_t\|_{L^\infty})$ completes the proof.

Part II

Analysis of nonlinear Schrödinger equations

Chapter 3

On the Cauchy-problem of nonlinear Schrödinger equations with angular momentum rotation term

The work in this chapter has been carried out in collaboration with Paolo Antonelli and Christof Sparber, most of which has been published in [2].

3.1 Introduction

Ever since the realization of Bose-Einstein condensation (BEC) in dilute atomic gases, much attention has been given to dynamical phenomena associated to its superfluid nature. One remarkable feature of a superfluid is the appearance of quantized vortices, cf. [1] for a broad introduction to these kind of phenomena. In physical experiments, the BEC is thereby set into rotation by a stirring potential, which is usually induced by a laser [61, 62, 64, 79] (see also [6] for numerical simulations). The corresponding mathematical model is a nonlinear Schrödinger equation (NLS) of Gross-Pitaevskii type with angular momentum rotation term, i.e.

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2}\Delta\psi + \lambda|\psi|^2\psi + U(x)\psi - \Omega\cdot L\psi, \quad (t,x)\in\mathbb{R}\times\mathbb{R}^3, \tag{3.1}$$

where $\psi = \psi(t,x)$ is the complex-valued wave function of the condensate and $\hbar$ is Planck's constant. In the physics literature, (3.1) is known as the *Gross-Pitaevskii equation* for rotating Bose gases. The coupling constant $\lambda \in \mathbb{R}$ can be experimentally tuned to account for both *defocusing* ($\lambda > 0$) and *focusing* ($\lambda < 0$) nonlinearities. The potential

$U(x)$ describes the magnetic trap and is usually assumed to be of the form

$$U(x) = \frac{1}{2} \sum_{j=1}^{3} \gamma_j^2 x_j^2, \quad \gamma_j \in \mathbb{R}. \tag{3.2}$$

Finally, $\Omega \cdot L$ denotes rotation term, where

$$L := -ix \wedge \nabla \tag{3.3}$$

is the quantum mechanical *angular momentum operator* and $\Omega \in \mathbb{R}^3$ is a given *angular velocity vector*. For a rigorous derivation of (3.1) in the stationary case, we refer to [53]. Furthermore, we remark that the appearance of quantized vortices has been rigorously proved in [77], by means of a spontaneous symmetry breaking for the ground state of the stationary equations (provided $\lambda > 0$ is sufficiently big). For further mathematical results in this direction we refer to [1] and the references given therein.

The aforementioned works illustrate the fact that there is a considerable amount of mathematical studies devoted the stationary equation. On the other hand, the time-dependent equation (3.1), has not been given as much attention, even though it is considered to provide the basis for a dynamical description of vortex creation. Indeed, except for numerical simulations [6], we are only aware of [37, 38] providing rigorous results for (3.1). In [37] global well-posedness of the Cauchy problem (in the energy space) is proved in the case where $\lambda > 0$, $U(x) = \frac{\gamma^2}{2}|x|^2$, i.e. an isotropic confinement, and $|\Omega| = \gamma$. The analogous result in $d = 2$ spatial dimensions is given in [38].

Remark 3.1.1. Let us mention that in [56, 57], the NLS model (3.1) is also rigorously studied. The results, however, mainly concern an asymptotic regime, the so-called *semi-classical limit*, and are thus very different from the present work.

In view of these results the main goal of our work is twofold: First, we shall prove global well-posedness of (3.1) in the defocusing case, without any restriction on $|\Omega|$ or $\{\gamma_j\}_{j=1}^3$. The latter is needed to describe actual physical experiments, which often require $|\Omega| \neq \gamma$. To this end, we shall show that by a suitable time-dependent change of coordinates, we can transform equation (3.1) into a nonlinear Schrödinger equation *without* rotation term but with a *time-dependent trapping potential*. In a second step, we shall analyze the possibility of finite time blow-up of solutions, in the case of a focusing nonlinearity. Recall that finite time blow-up means, that there is a $T^* < +\infty$, such that

$$\lim_{t \to T^*} \|\nabla \psi(t)\|_{L^2} = +\infty.$$

As we shall see, the usual proof of finite time blow-up, based on the classical virial argument of Glassey [32] (see also [19]), in general does not go through in a straightforward way, due to the influence of the rotation term. Instead, it has to be slightly modified, yielding blow-up conditions which depend on $|\Omega|$, and which coincide with the usual conditions in the limit $|\Omega| \to 0$.

3.2 Mathematical setting and main result

In the following we shall consider the Cauchy problem for the following, slightly more general NLS type model

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + \lambda|\psi|^{2\sigma}\psi + U(x)\psi - \Omega \cdot L\psi, \quad \psi(0) = \psi_0(x), \tag{3.4}$$

where $x \in \mathbb{R}^d$, for $d = 2$ or $d = 3$, respectively, and $\sigma < \frac{2}{d-2}$, i.e. the nonlinearity is assumed to be *energy-subcritical.* In $d = 2$ the rotation term simply reads

$$\Omega \cdot L = -i\omega(x_1\partial_{x_2} - x_2\partial_{x_1}) \tag{3.5}$$

for some $\omega \in \mathbb{R}$.

Remark 3.2.1. In $d = 3$ we could, without restriction of generality, choose a reference frame such that $\Omega = (0, 0, \omega)^\top$, $\omega \in \mathbb{R}$, yielding the same formula as in (3.5). For the sake of generality we shall not do so but consider the term $\Omega \cdot L \equiv -i\Omega \cdot (x \wedge \nabla)$ in full generality.

A potential $U(x) \in \mathbb{R}^d$, satisfying $(\Omega \cdot L)U(x) = 0, \quad \forall x \in \mathbb{R}^d$, is said to be *axially symmetric* (with respect to the rotation axis $\Omega \in \mathbb{R}^3$). In particular, this holds in the case of an isotropic trap potential, i.e. a potential of the form (3.2) with $\gamma_1 = \gamma_2 = \gamma_3$.

Formally, (3.4) preserves the total mass

$$M := \int_{\mathbb{R}^d} |\psi(t, x)|^2 \, dx,$$

and the energy

$$E_\Omega := \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\psi|^2 + U(x)|\psi|^2 + \frac{\lambda}{\sigma + 1}|\psi|^{2\sigma+2} - \overline{\psi}(\Omega \cdot L)\psi \, dx. \tag{3.6}$$

Note that, the last term is indeed real valued (as can be seen by a partial integration). In order for these two quantities to be well defined, we shall study the Cauchy problem corresponding to (3.4) in the space

$$\Sigma := \{f \in H^1(\mathbb{R}^d) \ : \ |x|f \in L^2(\mathbb{R}^d)\},$$

equipped with the norm

$$\|f\|_{\Sigma}^2 := \|f\|_{L^2}^2 + \|\nabla f\|_{L^2}^2 + \|xf\|_{L^2}^2.$$

We remark that even if the potential $U(x)$ is chosen to be identically zero, it would not be enough to consider the Cauchy problem for $\psi \in H^1(\mathbb{R}^d)$, since in this case we can no longer guarantee that

$$L_{\Omega}(t) := \int_{\mathbb{R}^d} \overline{\psi}(t)(\Omega \cdot L)\psi(t)\, dx < +\infty. \tag{3.7}$$

Physically speaking, this means that ψ has finite angular momentum. The choice of Σ is therefore natural in our situation and not necessarily linked to the presence of a harmonic trapping potential, in contrast to [16, 17, 18]. The usual definition of a solution ψ to the nonlinear Schrödinger equation (3.4) is the following.

Definition 3.2.2. We say that ψ is a (mild) solution to (3.4) if $\psi \in C([0,T];\Sigma)$ and it holds that

$$\psi(t) = S(t)\psi_0 - i\int_0^t S(t-s)|\psi(s)|^{2\sigma}\psi(s)\, ds, \tag{3.8}$$

where $S(t) = e^{iHt}$ denotes the unitary semigroup generated by the Hamiltonian

$$H = -\frac{1}{2}\Delta + U(x) - \Omega \cdot L, \tag{3.9}$$

which corresponds to solving the linear Schrödinger equation.

Equation (3.8) is usually called *Duhamel's formula*. Existence of $S(t)$ is established in Yajima [85], cf. Section 3.3. We can now state the main result of this work.

Theorem 3.2.3. *Let* $0 < \sigma < 2/(d-2)$, $\lambda \in \mathbb{R}$, $\Omega \in \mathbb{R}^d$, *for* $d = 2, 3$ *and denote the smallest trap frequency by* $\underline{\gamma} := \min\{\gamma_j\}_{j=1}^d$.
(1) *Then, for any given initial data* $\psi_0 \in \Sigma$, *there exists a unique global in-time solution* $\psi \in C([0,\infty);\Sigma)$ *to* (3.4), *provided one of the following conditions is satisfied:*

(i) the nonlinearity is L^2*-subcritical* $\sigma < 2/d$, *or*

(ii) $\sigma \geq 2/d$ *and* $\lambda \geq 0$, *i.e. the nonlinearity is defocusing.*

(2) *On the other hand, if* $\lambda < 0$, *and if either:*

(i) $(\Omega \cdot L)U = 0$, *i.e.* U *is axially symmetric, and* $\sigma \geq 2/d$,

(ii) $(\Omega \cdot L)U \neq 0$, $|\Omega| \leq \underline{\gamma}$, *and* $\sigma \geq \kappa_\Omega/d$, *where*

$$\kappa_\Omega := \sqrt{\frac{4\underline{\gamma}^2}{\underline{\gamma}^2 - |\Omega|^2}}, \text{ or} \tag{3.10}$$

(iii) $\sigma \geq 2/d$, *without loss of generality* $\Omega = (0,0,\omega)^\top$, *and there exists a* $T > 0$ *such that*

$$T < \frac{2\underline{\gamma}}{|(\gamma_1^2 - \gamma_2^2)\omega|} \text{ and } (E_\Omega - L_\Omega(0))T^2 + \dot{I}(0)T + I(0) \leq 0. \tag{3.11}$$

Then there exist initial data $\psi_0 \in \Sigma$ *such that finite time blow-up of the corresponding solution* $\psi(t)$ *occurs.*

Note that assertions (2)(ii) coincides with (2)(i) in the limit $\Omega \to 0$ and that (2)(iii) coincides with (2)(i) in the limit as $\gamma_1 - \gamma_2 \to 0$.

In fact, we shall prove Assertions (1)(i) and (ii) under the more general assumptions on $U(x)$, see Assumption 3 below. This, together with the fact that no condition on the size of $|\Omega|$ or $\{\gamma_j\}_{j=1}^d$ is required, generalizes the earlier results given in [37, 38].

Remark 3.2.4. The exact conditions on the initial data for Assertion (2) of the Theorem 3.2.3 can be found in Lemma 3.4.1.

Concerning the possibility of finite time blow-up, we see that one has to distinguish between the case of axially symmetric potential and the case where this symmetry is broken. The reason will become clear in the proof given below. In the case of a non-axially symmetric potential we can rigorously prove the occurrence of blow-up only under the additional restrictions $|\Omega| \leq \underline{\gamma}$, and $\sigma \geq \kappa_\Omega/d$, i.e. only for a limited range of nonlinearities. It is easily seen that in $d = 3$, the set of σ's satisfying our conditions is non-empty, provided $|\Omega|^2 < \frac{8}{9}\underline{\gamma}^2$. Also note that in the case of vanishing rotation $\lim_{|\Omega|\to 0} \kappa_\Omega = 2$, yielding the usual range of L^2-supercritical nonlinearities. At this point it is not clear if these additional restrictions are only due to the strategy of our proof, or if they indicate an actual difference in the behavior of solutions to (3.4). In particular, the question whether or not finite time blow-up occurs in situations where $\Omega > \underline{\gamma}$ is completely open so far. In terms of physics, the latter would correspond to the case where the rotation is stronger than the trap and thus one would expect a behavior which is similar (at least qualitatively) to the "free" case, i.e. without any potential. We finally remark that the question whether or not rotation can stabilize an attractive BEC is also debated from the physics point of view, see [44] and [81].

This Chapter is now organized as follows: Section 3.3 is devoted to the proof of Assertion (1) of Theorem 3.2.3. To this end, we shall first prove local in-time existence for solutions to (3.4). Also, we shall see that a naive use of the conservation laws for mass and energy in general leads to restrictions on $|\Omega|$ or $\{\gamma_j\}_{j=1}^d$. We shall show in a second step how to overcome this problems using a coordinate-change. Assertion (2) of our main Theorem is then proved in Section 3.4 and we finally collect some concluding remarks in Chapter 5.

3.3 Local and global existence

In this section we shall allow for more general class of potentials $U(x)$ satisfying the following assumption.

Assumption 3. *The potential $U : \mathbb{R}^d \to \mathbb{R}$ is assumed to be smooth and* sub-quadratic*, i.e. for all multi-indices $k \in \mathbb{N}^d$, with $|k| \geq 2$, there exists a constant $C = C(k) > 0$ such that*

$$|\partial^k U(x)| \leq C \qquad \text{for all } x \in \mathbb{R}^d. \tag{3.12}$$

Remark 3.3.1. Clearly, a harmonic trapping potential of the form (3.2) is sub-quadratic. Assumption 3 allows us to take into account more general situations of physical interest, such as a combined harmonic trap plus optical lattice potential, see e.g. [22]. Note however, that under Assumption 3, the potential is not necessarily bounded below (or confining). In particular we can also allow for repulsive potentials such as $U(x) = -\gamma^2|x|^2$, see [16].

As a first, preliminary step, we shall prove the following local well-posedness result.

Lemma 3.3.2. *Let $\psi_0 \in \Sigma$, $\omega \in \mathbb{R}$, and $0 < \sigma < 2/(d-2)$. Moreover, assume that U satisfies Assumption 3. Then there exists a time $T = T(\|\psi_0\|_\Sigma) > 0$ and a unique solution $\psi \in C([0,T];\Sigma)$ of equation (3.1) with $\psi(0) = \psi_0$.*
Thus we can construct a maximal solution $\psi \in C([0,T_{\max});\Sigma)$. The solution is maximal in the sense that, if $T_{\max} < +\infty$, then

$$\lim_{t\to T_{\max}} \|\nabla\psi(t)\|_{L^2} = +\infty.$$

Moreover, the following conservation laws hold:

$$M(t) = M(0), \quad \text{and} \quad E_\Omega(t) = E_\Omega(0), \tag{3.13}$$

whereas for the angular momentum we have

$$L_\Omega(t) + \int_0^t \int_{\mathbb{R}^d} i|\psi|^2(\Omega \cdot L)U(x)dx = L_\Omega(0). \tag{3.14}$$

The proof is an adaptation of classical arguments, based on a contraction mapping (via Duhamel's formula (3.8)) and Strichartz estimates for the linear (unitary) group $S(t) = e^{itH}$ generated by the Hamiltonian (3.9). In our case, Strichartz estimates can be obtained by following the approach of Yajima [85]. As defined, the Hamiltonian is not of the form necessary for the results in [85] to hold. However, the Hamiltonian can be rewritten as

$$H = \frac{1}{2}(i\nabla + A(x))^2 + U(x) - \frac{1}{2}A(x)^2, \qquad \text{where} \quad A(x) = \Omega \wedge x.$$

Indeed it holds that

$$\begin{aligned}(i\nabla + \Omega \wedge x)^2 &= -\Delta + (\Omega \wedge x)^2 + 2i(\Omega \wedge x) \cdot \nabla + i(\nabla \cdot A) \\ &= -\Delta + (\Omega \wedge x)^2 + 2i\Omega \cdot (x \wedge \nabla).\end{aligned}$$

Since the rotation $B(x) = \nabla \wedge A(x) = 2\Omega$ is constant and the potential $U(x) - A(x)^2/2$ is subquadratic, the results in [85] imply that there exist finite, positive, constants C and δ such that

$$\|S(t)\varphi\|_{L^\infty} \leq \frac{C}{|t|^{d/2}}\|\varphi\|_{L^1}, \quad \text{for } |t| < \delta.$$

In particular it follows that the Strichartz estimates for H are analogous to those found in the well-known case of NLS with quadratic potentials [17], i.e. the rotation term does not influence the dispersive behavior (locally in time). These Strichartz estimates have been proven under general circumstances in [46]. Recall that p' denotes the conjugate Hölder coefficient of p, i.e. $1/p + 1/p' = 1$.

Lemma 3.3.3 (Strichartz estimates)**.** *The unitary group $S(t) = e^{itH}$ with Hamiltonian H defined in* (3.9) *satisfies a local in time Strichartz estimate. There exist $T_S > 0$ and constants $C_q, C_{q,\tilde{q}}$ such that*

$$\|S(t)\varphi\|_{L^p(0,T_S;L^q(\mathbb{R}^d))} \leq C_q\|\varphi\|_{L^2(\mathbb{R}^d)}$$

for all $\varphi \in L^2(\mathbb{R}^d)$ and

$$\Big\| \int_0^t S(t-s)F(s)\, ds \Big\|_{L^p(0,T_S;L^q(\mathbb{R}^d))} \leq C_{q,\tilde{q}}\|F\|_{L^{\tilde{p}'}(0,T_S;L^{\tilde{q}'}(\mathbb{R}^d))}$$

if (p,q) and $(\tilde{p},\tilde{q})$ are admissible *coefficients, i.e. $2 \leq q < 2d/(d-2)$ and $2/p = \delta(q) := d(1/2 - 1/q)$ and likewise for $(\tilde{p},\tilde{q})$.*

Since the semigroup $(S(t))_{t\in\mathbb{R}} \subset \mathcal{L}(L^2(\mathbb{R}^d))$ is continuous in time, the Strichartz estimates also yield the following continuity property.

Remark 3.3.4. Under the conditions of Lemma 3.3.3, it holds that

$$S(t)\varphi \in C([0,T_S];L^2(\mathbb{R}^d)) \quad \text{and} \quad \int_0^t S(t-s)F(s)\,ds \in C([0,T_S];L^2(\mathbb{R}^d)),$$

which will later allow us to prove continuity of time of fixed points of Duhamel's formula (3.8).

The existence of a local in-time solution is then standard and we repeat it here for the reader's convenience.

Proof of Lemma 3.3.2. The idea is to write the nonlinear Schrödinger equation as the solution of a fixed point equation, using Duhamel's formula:

$$\begin{aligned}\psi(t) &= S(t)\psi_0 - i\lambda\int_0^t S(t-s)\left(|\psi|^{2\sigma}(s)\psi(s)\right)\,ds\\ &=: \Phi(\psi)(t).\end{aligned}$$

Let us define parameters

$$q = 2\sigma+2, \qquad p = \frac{4\sigma+4}{d\sigma}, \qquad k = \frac{2\sigma(2\sigma+2)}{2-(d-2)\sigma}.$$

We will presently show that Φ as a maps the space

$$X_T := \left\{\psi \in L^\infty(0,T;\Sigma) : \psi, x\psi, \nabla\psi \in L^p(0,T;L^q(\mathbb{R}^d))\right\}$$

onto itself. Indeed, setting $R := \|\psi_0\|_\Sigma$, we shall establish that Φ is a contraction mapping in

$$\begin{aligned}X_{T,R} := \big\{\psi \in X_T : \|\psi\|_{L^\infty(0,T;\Sigma)} \le 2R,&\\ \|x\psi\|_{L^p(0,T;L^q)}, \|\nabla\psi\|_{L^p(0,T;L^q)} \le 2C_qR\big\},&\end{aligned}$$

for all T small enough. We equip the space $X_{T,R}$ with a metric

$$d(\psi,\widetilde{\psi}) = \|\psi-\widetilde{\psi}\|_{L^\infty_t L^2_x} + \|\psi-\widetilde{\psi}\|_{L^p_t L^q_x}.$$

Then $(X_{T,R}, d)$ forms a complete metric space, cf. [19].

In order to proceed, we calculate the commutators $[\nabla, S(t)]$ and $[x, S(t)]$. We find that

$$\begin{aligned}[\nabla, H] =& -\frac{1}{2}[\nabla, \Delta] + [\nabla, U] + i[\nabla, \Omega \cdot (x \wedge \nabla)] \\ =& \nabla U + i[\nabla, x \cdot (\nabla \wedge \Omega)] \\ =& \nabla U + i\nabla \wedge \Omega\end{aligned}$$

by the well-known formula $a \cdot (b \wedge c) = \det(a, b, c) = (a \wedge b) \cdot c$ for three-dimensional vectors a, b, c. Similar calculations yield

$$[x, H] = \nabla - i\Omega \wedge x.$$

Since

$$i\partial_t[\nabla, S(t)] = [\nabla, HS(t)] = H[\nabla, S(t)] + [\nabla, H]S(t),$$

we deduce that

$$\begin{aligned}\nabla\Phi(\psi)(t) = S(t)\nabla\psi_0 - i\lambda \int_0^t S(t-\tau)\nabla\left(|\psi(\tau)|^{2\sigma}\psi(\tau)\right)\, d\tau \\ - i\int_0^t S(t-\tau)\left(\nabla U - i\Omega \wedge \nabla\right)\Phi(\psi)(\tau)\, d\tau,\end{aligned} \tag{3.15}$$

and

$$\begin{aligned}x\Phi(\psi)(t) = S(t)\nabla\psi_0 - i\lambda \int_0^t S(t-\tau)\nabla\left(|\psi(\tau)|^{2\sigma}\psi(\tau)\right)\, d\tau \\ - i\int_0^t S(t-\tau)\left(\nabla - i\Omega \wedge x\right)\Phi(\psi)(\tau)\, d\tau.\end{aligned}$$

Since $T < T_S$, the Strichartz estimates of Lemma 3.3.3 yield

$$\begin{aligned}\|\nabla\Phi(\psi)\|_{L_t^p L_x^q} \leq C_q\|\psi_0\|_\Sigma + |\lambda| C_{q,q}\big\|\nabla\left(|\psi(\tau)|^{2\sigma}\psi(\tau)\right)\big\|_{L_t^{p'} L_x^{q'}} \\ + C_{q,2}\big\|\nabla U\Phi(\psi)\big\|_{L_t^1 L_x^2} + C_{q,2}\big\|\Omega \wedge \nabla\Phi(\psi)\big\|_{L_t^1 L_x^2}.\end{aligned} \tag{3.16}$$

Since

$$\frac{1}{q'} = \frac{2\sigma}{q} + \frac{1}{q} \qquad \text{and} \qquad \frac{1}{p'} = \frac{2\sigma}{k} + \frac{1}{p},$$

Hölder's inequality yields

$$\begin{aligned}\big\|\nabla\big(|\psi|^{2\sigma}\psi\big)\big\|_{L_t^{p'} L_x^{q'}} &\leq (2\sigma+1)\big\||\psi|^{2\sigma}\nabla\psi\big\|_{L_t^{p'} L_x^{q'}} \\ &\leq (2\sigma+1)\big\|\psi\big\|_{L_t^k L_x^q}^{2\sigma}\big\|\nabla\psi\big\|_{L_t^p L_x^q}.\end{aligned}$$

Furthermore, it holds that

$$\|\psi\|_{L_t^k L_x^q}^{2\sigma} \leq T^{\frac{2\sigma}{k}} \|\psi\|_{L_t^\infty L_x^q}^{\frac{2\sigma}{k}} \leq T^{\frac{2\sigma}{k}} \|\psi\|_{L_t^\infty H_x^1}^{2\sigma}$$

where we used the Gagliardo-Nirenberg inequality in the last estimate. Recall that the Gagliardo-Nirenberg inequality implies

$$\|\varphi\|_{L_x^q} \leq C \|\varphi\|_{L_x^2}^{1-\delta(q)} \|\nabla \varphi\|_{L_x^2}^{\delta(q)}$$

for all $\varphi \in H^1(\mathbb{R}^d)$, where $\delta(q)$ is defined in the statement of Lemma 3.3.3. Furthermore we can bound $|\nabla U| \leq Cx$. Thus estimate (3.16) yields

$$\begin{aligned}\|\nabla \Phi(\psi)\|_{L_t^p L_x^q} \leq C_q \|\psi_0\|_\Sigma + C T^{\frac{2\sigma}{k}} \|\psi\|_{L_t^\infty \Sigma_x}^{2\sigma} \|\nabla \psi\|_{L_t^p L_x^q} \\ + CT \big\| x \Phi(\psi) \big\|_{L_t^\infty L_x^2} + CT \big\| \nabla \Phi(\psi) \big\|_{L_t^\infty L_x^2}.\end{aligned}$$

Similarly we obtain that

$$\|\Phi(\psi)\|_{L_t^p L_x^q} \leq C_q \|\psi_0\|_\Sigma + C T^{\frac{2\sigma}{k}} \|\psi\|_{L_t^\infty \Sigma_x}^{2\sigma} \|\psi\|_{L_t^p L_x^q}$$

and

$$\begin{aligned}\|x \Phi(\psi)\|_{L_t^p L_x^q} \leq C_q \|\psi_0\|_\Sigma + C T^{\frac{2\sigma}{k}} \|\psi\|_{L_t^\infty \Sigma_x}^{2\sigma} \|x \psi\|_{L_t^p L_x^q} \\ + CT \big\| \nabla U \Phi(\psi) \big\|_{L_t^\infty L_x^2} + CT \big\| \nabla \Phi(\psi) \big\|_{L_t^\infty L_x^2}.\end{aligned}$$

Since $(\infty, 2)$ is an admissible pair, the same estimates hold for the $L_t^\infty L_x^2$-norm, with C_q replaced by 1. If we choose T sufficiently small, this shows that Φ indeed constitutes a mapping $\Phi : X_{T,R} \to X_{T,R}$. In order to show that $\Phi : X_{T,R} \to X_{T,R}$ is also a contraction, we take two functions $\psi, \widetilde{\psi} \in X_{T,R}$ and estimate the difference $\Phi(\psi) - \Phi(\widetilde{\psi})$. In the same way as above, we obtain that

$$\begin{aligned}\big\| \Phi(\psi) - \Phi(\widetilde{\psi}) \big\|_{L_t^p L_x^q} &= \left\| \int_0^t S(t-s) \big(|\psi(s)|^{2\sigma} \psi(s) - |\widetilde{\psi}(s)|^{2\sigma} \widetilde{\psi}(s) \big) \, ds \right\|_{L_t^p L_x^q} \\ &\leq \big\| |\psi|^{2\sigma} \psi - |\widetilde{\psi}|^{2\sigma} \widetilde{\psi} \big\|_{L_t^{p'} L_x^{q'}},\end{aligned}$$

The point-wise inequality

$$\big| |\psi|^{2\sigma} \psi - |\widetilde{\psi}|^{2\sigma} \widetilde{\psi} \big| \leq 2\sigma \big(|\psi|^{2\sigma} + |\widetilde{\psi})|^{2\sigma} \big) |\psi - \widetilde{\psi}|$$

and the same Hölder and Gagliardo-Nirenberg estimates used before then yield

$$\begin{aligned}
&\big\|\Phi(\psi)-\Phi(\widetilde{\psi})\big\|_{L^p_tL^q_x}+\big\|\Phi(\psi)-\Phi(\widetilde{\psi})\big\|_{L^\infty_tL^2_x}\\
&\leq C\Big(\|\psi\|^{2\sigma}_{L^k_tL^q_x}+\|\widetilde{\psi}\|^{2\sigma}_{L^k_tL^q_x}\Big)\|\psi-\widetilde{\psi}\|_{L^p_tL^q_x}\\
&\leq CT^{\frac{2\sigma}{k}}\Big(\|\psi\|^{2\sigma}_{L^\infty_tH^1_x}+\|\widetilde{\psi}\|^{2\sigma}_{L^\infty_tH^1_x}\Big)\|\psi-\widetilde{\psi}\|_{L^p_tL^q_x}.
\end{aligned}$$

Thus, choosing $T \leq T_S$ small enough, there exists a fixed point $\psi \in X_{T,R}$ satisfying $\Phi(\psi) = \psi$. Remark 3.3.4 applied to the fixed point equations, e.g. (3.15), yields $\psi \in C([0,T];\Sigma)$. Hence ψ is indeed a mild solution to the Schrödinger equation (3.4). The conservation laws (3.13) follow from straightforward calculations in combination with a standard density argument and reversibility (see e.g. [19]). Finally, in order to prove the blow-up alternative we first notice that the above local existence argument can be iterated as long as $\|\psi(t)\|_\Sigma$ stays bounded. Thus we obtain a maximal solution $\psi \in C([0,T_{\max});\Sigma)$ with $T_{\max} > 0$. Assume that $T_{\max} < +\infty$. In view of mass conservation, it follows that

$$\lim_{t\to T_{\max}}\big(\|x\psi(t)\|_{L^2}+\|\nabla\psi(t)\|_{L^2}\big)=+\infty.$$

Furthermore we compute

$$\frac{d}{dt}\|x\psi(t)\|^2_{L^2}=2\mathrm{Im}\int_{\mathbb{R}^d}x\overline{\psi}(t)\nabla\psi(t)\,dx\leq\|x\psi(t)\|^2_{L^2}+\|\nabla\psi(t)\|^2_{L^2}. \tag{3.17}$$

Thus, as long as $\|\nabla\psi(t)\|_{L^2}$ is bounded, Gronwall's inequality yields a bound on $\|x\psi(t)\|_{L^2}$ as well. The only obstruction to global existence is therefore given by the possible unboundedness of $\|\nabla\psi(t)\|_{L^2}$ in $[0,T]$. □

Remark 3.3.5. For quadratic potentials of the form (3.2), Strichartz estimates can be obtained explicitly by invoking a generalization of Mehler's formula for the kernel of $S(t)$, c.f. [18]. Indeed, by making the following ansatz

$$S(t)\psi_0(x)=\prod_{j=1}^d\big(2\pi i\mu_j(t)\big)^{-1/2}\int_{\mathbb{R}}^d e^{\frac{i}{2}F(t,x,y)}\psi_0(y)\,dy,$$

where $\mu_j(t) \in \mathbb{R}_+$ and $F(t,x,y)$ is a general quadratic form in x and y with (yet to be determined) time-dependent coefficients. Substituting this into the linear Schrödinger equation yields a coupled system of differential equations for these coefficients. Solving this system, however, is in general rather tedious. This approach is therefore only feasible under some simplifying assumptions, such as $\Omega = 0$ [16, 17], or $U(x) = \frac{\gamma^2}{2}|x|^2$ with $|\Omega| = \gamma$ as it is done in [37, 38].

In view, of (3.14), we immediately conclude the following important corollary.

Corollary 3.3.6. *If $U(x)$ is such that $(\Omega \cdot L)U = 0$, then we also have conservation of angular momentum, i.e. $L_\Omega(t) = L_\Omega(0)$, and in addition it holds*

$$E_0(t) \equiv \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\psi|^2 + U(x)|\psi|^2 + \frac{\lambda}{\sigma+1}|\psi|^{2\sigma+2}dx = E_0(0). \tag{3.18}$$

Thus, in the case of axially symmetric potentials $U(x)$, there are in fact two conserved energy functionals corresponding to (3.4).

With a local existence result in hand, we can ask about global existence. In order to infer $T = +\infty$, one usually invokes the conservation of mass and energy (3.13). The problem is, that due to the appearance of the angular momentum rotation term, the energy $E_\Omega(t)$ has no definite sign even if $U \geq 0$ and $\lambda \geq 0$ (defocusing nonlinearity). A possible strategy to overcome this problem is to rewrite the linear Hamiltonian as

$$H = -\frac{1}{2}\Delta - \Omega \cdot L + U(x) = \frac{1}{2}(-i\nabla - A(x))^2 + U(x) - \frac{|\Omega|^2}{2}r^2, \tag{3.19}$$

where $A(x) = \Omega \wedge x$ and $r = |x \wedge \Omega|/|\Omega|$ denotes the radial distance perpenticular to Ω. Note that $A(x)$ can be considered as the vector potential corresponding to a constant magnetic field $B = \nabla \wedge A = 2\Omega$. The corresponding "magnetic derivative" $D_A := -i(\nabla + A(x))$ is known to satisfy, cf. [19, Chapter 7]:

$$\|\nabla|\psi|\|_{L^2} \leq \|D_A\psi\|_{L^2} \leq \|\nabla\psi\|_{L^2} + \|x\psi\|_{L^2}.$$

It can therefore be used to control the nonlinear potential energy $\propto \|\psi\|_{L^{2\sigma+2}}$ via Gagliardo-Nirenberg type inequalities. If in addition, $U(x)$ is given by (3.2) with $|\Omega| \leq \underline{\gamma}$ we infer that $U(x) - \frac{|\Omega|^2}{2}r^2 \geq 0$. In this case, the linear part of the energy is seen to be a sum of non-negative terms, and global existence can be concluded as in the case of NLS with quadratic confinement [17]. However, it seems impossible to extend this approach to situations in which $|\Omega| > \gamma$, even if $\lambda > 0$. In order to do so, we shall follow a different idea, which invokes a time-dependent change of coordinates.

Proof of Assertion (1) of Theorem 3.2.3. We start with the L^2-subcritical case, i.e. $0 < \sigma < 2/d$ which follows by standard arguments. Recall that in the proof of Lemma 3.3.2 we showed that

$$\|\psi\|_{L^p(0,T;L^q)\cap L^\infty(0,T;L^2)} \leq C\|\psi_0\|_{L^2} + C\|\psi\|^{2\sigma}_{L^k(0,T;L^q)},$$

where

$$q = 2\sigma + 2, \quad p = \frac{4\sigma+4}{d\sigma}, \quad k = \frac{2\sigma(2\sigma+2)}{2-(d-2)\sigma}.$$

Moreover, we showed that

$$\begin{aligned}
&\|x\psi\|_{L^p(0,T;L^q)\cap L^\infty(0,T;L^2)} + \|\nabla\psi\|_{L^p(0,T;L^q)\cap L^\infty(0,T;L^2)} \\
&\le C\|\psi_0\|_\Sigma + C\|\psi\|^{2\sigma}_{L^k(0,T;L^q)}\left(\|x\psi\|_{L^p(0,T;L^q)} + \|\nabla\psi\|_{L^p(0,T;L^q)}\right) + \\
&+ CT\left(\|x\psi\|_{L^\infty(0,T;L^2)} + \|\nabla\psi\|_{L^\infty(0,T;L^2)}\right).
\end{aligned}$$

If $\sigma < 2/d$, it holds that $1/p < 1/k$ and thus

$$\|\psi\|_{L^k(0,T;L^q)} \le T^{1/k-1/p}\|\psi\|_{L^p(0,T;L^q)}.$$

If we choose $T = T^* > 0$ small enough, we can absorb all terms on the right hand side except the term involving ψ_0 and obtain a bound on $\|\psi\|_{L^\infty(0,T^*;\Sigma)}$. Since we can shift the time interval $[0,T^*]$ by an arbitrary amount of time, in the same way we can get a uniform bound on $\|\psi\|_{L^\infty(0,T^*;\Sigma)}$ for every interval of length $|I| \le T^*$. Thus, by splitting any arbitrarily large time interval $[0,T]$ into sufficiently small sub-intervals $\{I_n\}_{n=1}^N$ such that $|I_n| \le T^*$ and iterating the bound $\|\psi\|_{L^p(I_n;L^q)\cap L^\infty(I;L^2)} \le C^*$, we infer $\|\psi\|_{L^p(0,T;L^q)\cap L^\infty(0,T;L^2)} \le C$ where $C < +\infty$ depends on the value of T. From here, we proceed as before to obtain a uniform bound for the left hand side for small T^* and thus by iteration for arbitrary time intervals $[0,T]$.

Next we consider the case of an L^2-supercritical nonlinearity $\sigma > 2/d$. In this case, the iterative argument given above breaks down. The basic idea is to use a change of coordinates in order to bring equation (3.4) into a more suitable form. For the sake of notation we shall only consider the case $d = 3$ in the following. We first note that by using the skew-symmetric matrix

$$\Theta := \begin{pmatrix} 0 & \Omega_3 & -\Omega_2 \\ -\Omega_3 & 0 & \Omega_1 \\ \Omega_2 & -\Omega_1 & 0 \end{pmatrix},$$

the wedge product with the angular momentum can be written as

$$\Omega \wedge x = -\Theta \cdot x.$$

Then the matrix-exponential

$$X(t,x) := \mathrm{e}^{\Theta t} \cdot x$$

defines a rotation of the vector $x \in \mathbb{R}^3$ around the axis Ω by an angle of $-|\Omega|t$. Its time-derivative can be calculated as

$$\partial_t X(t,x) = \Theta \cdot X(t,x) = -\Omega \wedge X(t,x). \tag{3.20}$$

Denoting the wave function in rotated coordinates via

$$\widetilde{\psi}(t,x) = \psi(t, X(t,x)), \tag{3.21}$$

we conclude from (3.20) that

$$i\partial_t\widetilde{\psi}(t,x) = i\partial_t\psi(t, X(t,x)) - i\,(\Omega \wedge X(t,x)) \cdot \nabla\psi(t, X(t,x)).$$

Rewriting $-i(\Omega \wedge X) \cdot \nabla = -i\Omega \cdot (X \wedge \nabla) = \Omega \cdot L$, we arrive at

$$i\partial_t\widetilde{\psi} = -\frac{1}{2}\Delta\widetilde{\psi} + \lambda|\widetilde{\psi}|^{2\sigma}\widetilde{\psi} + U(X(t,x))\widetilde{\psi},$$

where we have also used the fact that the Laplace operator is invariant with respect to rotations, i.e.

$$\Delta_X\psi(t, X(t,x)) = \Delta_x\psi(t, X(t,x)).$$

Dropping all the tildes and denoting $W(t,x) = U(X(t,x))$, we conclude that up to a change of coordinates, equation (3.4) is equivalent to the following NLS with time-dependent potential

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + \lambda|\psi|^{2\sigma}\psi + W(t,x)\psi. \tag{3.22}$$

Note that $W(t,x)$ is smooth w.r.t. $t \in \mathbb{R}$ and sub-quadratic w.r.t. $x \in \mathbb{R}^3$ with the same (uniform) constants $C(k)$ as given in Assumption 3 for $U(x)$. Moreover, if $U(x)$ is axially symmetric, i.e. $(\Omega \cdot L)U(x) = 0$, equation (3.20) implies that

$$\partial_t W(t,x) = -\Omega \wedge X(t,x) \cdot \nabla U(X(t,x)) = -i(\Omega \cdot L)U(X(t,x)) = 0,$$

and hence $W(t,x) = W(0,x) \equiv U(x)$. The energy corresponding to the transformed NLS (3.22) is given by

$$E_W(t) := \int \frac{1}{2}|\nabla\psi(t,x)|^2 + \lambda|\psi(t,x)|^{2\sigma+2} + W(t,x)|\psi(t,x)|^2\,dx.$$

However, since the potential $W(t,x)$ in general is time-dependent, the $E_W(t)$ is no longer a conserved quantity. Rather, we obtain that

$$\frac{d}{dt}E_W(t) = \int \partial_t W(t,x)|\psi(t,x)|^2\,dx. \tag{3.23}$$

Nevertheless it is not hard to prove Assertion (1)(ii) of Theorem 3.2.3: In view of the blow-up alternative, stated in Lemma 3.3.2, it suffices to show $\|\nabla\psi(t)\|_{L^2} < +\infty$, for all

$T > 0$. To this end, we first estimate

$$\frac{1}{2}\|\nabla\psi(t)\|_{L^2}^2 \leq E_W(t) + \left|\int W(t,x)|\psi(t,x)|^2\,dx\right| \leq E_W(t) + C\|x\psi(t)\|_{L^2}^2,$$

under the assumption that $\lambda > 0$. Integrating equation (3.23) and having in mind that $W(t,x)$ is sub-quadratic in x, we obtain that

$$\begin{aligned}\|\nabla\psi(t)\|_{L^2}^2 &\leq E_W(0) + \int_0^t \frac{d}{ds}E_W(s)\,ds + C\|x\psi(t)\|_{L^2}^2 \\ &\leq C_0\left(1 + \|x\psi(t)\|_{L^2}^2 + \int_0^t \|x\psi(s)\|_{L^2}^2\,ds\right).\end{aligned} \tag{3.24}$$

Recalling inequality (3.17), we infer

$$\frac{d}{dt}\|x\psi(t)\|_{L^2}^2 + \|x\psi(t)\|_{L^2}^2 \leq C_0\left(1 + \|x\psi(t)\|_{L^2}^2 + \int_0^t \|x\psi(s)\|_{L^2}^2\,ds\right),$$

which by Gronwall's inequality yields an uniform bound on $\|x\psi(t)\|_{L^2}$ for every time interval $[0,T]$. With this in hand, we can bound $\|\nabla\psi(t)\|_{L^2}$ by simply using inequality (3.24) once more. □

Remark 3.3.7. In particular, for $\Omega = (0,0,\omega)^\top$ and $U(x)$ given by (3.2), we explicitly find

$$\begin{aligned}W(t,x) = \frac{1}{2}\Big(&\left(\gamma_1^2\cos^2(\omega t) + \gamma_2^2\sin^2(\omega t)\right)x_1^2 \\ &+ \left(\gamma_1^2\sin^2(\omega t) + \gamma_2^2\cos^2(\omega t)\right)x_2^2 + \sin(2\omega t)\left(\gamma_1^2 - \gamma_2^2\right)x_1x_2 + \gamma_3^2x_3^2\Big).\end{aligned}$$

Clearly, $W = \frac{1}{2}(\gamma_1^2x_1^2 + \gamma_2^2x_2^2 + \gamma_3^2x_3^2)$ in the axially symmetric case $\gamma_1^2 = \gamma_2^2$.

3.4 Finite time blow-up

This section is devoted to the proof of assertion (2) of Theorem 3.2.3. The statements (2)(i) and (ii) follow from the following lemma.

Lemma 3.4.1. *Let $\lambda < 0$, $\sigma < 2/(d-2)$, $\Omega \in \mathbb{R}^d$, for $d = 2,3$, and $U(x)$ be a quadratic potential of the form* (3.2)*. Denote $\underline{\gamma} = \min\{\gamma_j\}_{j=1}^d$ and let κ_Ω be as in* (3.10)*. If either*

(i) $(\Omega\cdot L)U = 0$, $\sigma \geq 2/d$, *and* $E_0(0) < 0$, *or*

(ii) $(\Omega\cdot L)U \neq 0$, $|\Omega| \leq \underline{\gamma}$, $\sigma \geq \kappa_\Omega/d$, *and* $E_\Omega(0) < 0$,

then the corresponding solution to equation (3.4) *necessarily blows up in finite time.*

Note that the condition for the energy of the initial data ψ_0 are not identical in both cases. The reason will become clear in the proof given below.

Proof. To simplify the arguments later on, let us first compute the conservation laws for the mass and momentum densities, i.e. $\rho := |\psi|^2$ and $J := \mathrm{Im}(\overline{\psi}\nabla\psi)$. Indeed a straightforward calculation yields

$$\partial_t \rho + \operatorname{div} J = i\Omega \cdot L\rho. \tag{3.25}$$

On the other hand, for the current density J we find

$$\begin{aligned}\partial_t \left(\mathrm{Im}(\overline{\psi}\nabla\psi)\right) = \mathrm{Im}&\left(\left(-\frac{i}{2}\Delta\overline{\psi} + iU(x)\overline{\psi} + i\lambda|\psi|^{2\sigma}\psi + i\Omega\cdot L\overline{\psi}\right)\nabla\psi\right)\\ &+ \mathrm{Im}\left(\overline{\psi}\nabla\left(\frac{i}{2}\Delta\psi - iU(x)\psi - i\lambda|\psi|^{2\sigma}\psi + i(\Omega\cdot L\psi)\right)\right).\end{aligned} \tag{3.26}$$

Next, we calculate

$$\mathrm{Im}\left(\overline{\psi}\nabla(i\Omega\cdot L\psi)\right) = \mathrm{Im}\left(\overline{\psi}(i\Omega\cdot L)\nabla\psi\right) - \Omega\wedge J.$$

Thus we can combine the two terms in (3.26) which stem from the rotation via

$$\mathrm{Im}\left((i\Omega\cdot L)\overline{\psi}\nabla\psi\right) + \mathrm{Im}\left(\overline{\psi}(i\Omega\cdot L)\nabla\psi\right) - \Omega\wedge J = (i\Omega\cdot L)J - \Omega\wedge J$$

where we have used that $i\Omega\cdot L$ is real-valued. The other terms in (3.26) are usual in quantum hydrodynamics, see e.g. [3], yielding the following equation for J:

$$\partial_t J + \operatorname{div}\left(\mathrm{Re}(\nabla\overline{\psi}\otimes\nabla\psi)\right) + \frac{\lambda\sigma}{\sigma+1}\nabla|\psi|^{2\sigma+2} + \rho\nabla U = \frac{1}{4}\Delta\nabla\rho + (i\Omega\cdot L)J - \Omega\wedge J. \tag{3.27}$$

The proof of finite time blow-up now follows by the classical argument of Glassey [32]. To this end, we consider the time evolution of

$$I(t) := \frac{1}{2}\int_{\mathbb{R}^d} |x|^2|\psi(t,x)|^2\,dx.$$

Differentiating with respect to time and using (3.25), we obtain

$$\frac{d}{dt}I(t) = \int_{\mathbb{R}^d} x\cdot J(t,x)\,dx + \int_{\mathbb{R}^d}\frac{|x|^2}{2}(i\Omega\cdot L)\rho(t,x)\,dx.$$

Integrating by parts and using $(\Omega\cdot L)|x|^2 = 0$ shows that the second integral in fact vanishes, i.e. we have

$$\frac{d}{dt}I(t) = \int_{\mathbb{R}^d} x\cdot J\,dx.$$

Differentiating in time once more and using (3.27), we obtain

$$\frac{d}{dt}\int x\cdot J\,dx = \int x\cdot\Big(-\operatorname{div}\big(\mathrm{Re}(\nabla\overline{\psi}\otimes\nabla\psi)\big) - \lambda\frac{\sigma}{\sigma+1}\nabla|\psi|^{2\sigma+2} - \rho\nabla U + \frac{1}{4}\Delta\nabla\rho + (i\Omega\cdot L)J - \Omega\wedge J\Big)dx,$$

which we rewrite as

$$\frac{d}{dt}\int x\cdot J\,dx = \int\Big(|\nabla\psi|^2 + \lambda\frac{d\sigma}{\sigma+1}|\psi|^{2\sigma+2} - \rho x\cdot\nabla U + x\cdot(i\Omega\cdot L)J - x\cdot\Omega\wedge J\Big)\;dx. \tag{3.28}$$

Now we first note that for any potential $U(x)$ of the form (3.2) we have $x\cdot\nabla U = 2U$. Moreover, we compute

$$\begin{aligned}\int_{\mathbb{R}^d} x\cdot(i\Omega\cdot LJ)\;dx &= -\int_{\mathbb{R}^d}(\Omega\cdot Lx)\cdot J\;dx = -\int_{\mathbb{R}^d}(\Omega\cdot(x\wedge\nabla)x)\cdot J\;dx\\ &= -\int_{\mathbb{R}^d}((\Omega\wedge x)\cdot\nabla)\,x\cdot J\;dx = -\int_{\mathbb{R}^d}(\Omega\wedge x)\cdot J\;dx,\end{aligned}$$

which shows that the last two terms in (3.28) cancel each other. In summary we arrive at the following identity

$$\frac{d^2}{dt^2}I(t) = \int\Big(|\nabla\psi|^2 + \lambda\frac{d\sigma}{\sigma+1}|\psi|^{2\sigma+2} - 2U|\psi|^2\Big)\;dx, \tag{3.29}$$

which is in fact exactly the same as in the case of NLS without rotation, c.f. [19].

We can now prove assertion (i): Recall from Corollary 3.3.6 that if the potential $U(x)$ is axially symmetric, then $E_0(t) = E_0(0)$, with E_0 defined in (3.18). Hence from (3.29) and $U \geq 0$ we can write

$$\frac{d^2}{dt^2}I(t) \leq 2E_0 + \lambda\frac{d\sigma-2}{\sigma+1}\int_{\mathbb{R}^d}|\psi|^{2\sigma+2}dx.$$

Assuming $E_0 < 0$, $\lambda < 0$, and $\sigma \geq 2/d$, we consequently obtain

$$\frac{d^2}{dt^2}I(t) < -C,$$

for some constant $C > 0$. Integrating this relation twice, we obtain

$$I(t) < -\frac{C}{2}t^2 + c_1 t + c_2$$

with some integration constants c_1 and c_2. Thus, if the solution $\psi(t) \in \Sigma$ were to exist for all times, there would be a time $T^* < +\infty$, such that $I(T^*) < 0$. This however is in contradiction with the fact that, by definition, $I(t) \geq 0$ for all $t \in \mathbb{R}$ and hence the assertion is proved.

In order to prove assertion (ii) we again consider (3.29): The problem is that in the case of a non-axially symmetric potential ($\Omega \cdot LU(x) \neq 0$), the energy E_0 is no longer conserved. Rather we only have the conservation law for $E_\Omega(t) = E_\Omega(0)$. In order to use this piece of information, we first add and subtract to (3.29) a multiple of the angular momentum $L_\Omega(t)$, i.e.

$$\frac{d^2}{dt^2}I(t) = \int_{\mathbb{R}^d} \left(|\nabla\psi|^2 + \frac{\lambda\sigma d}{\sigma+1}|\psi|^{2\sigma+2} - 2U|\psi|^2 + \kappa\overline{\psi}\Omega \cdot L\psi \right) dx - \int \kappa\overline{\psi}\Omega \cdot L\psi \, dx,$$

where $\kappa > 0$ is a parameter to be chosen later on. Using Cauchy-Schwarz and Young's inequality, the last term on the right hand side can be bounded by

$$\kappa \int_{\mathbb{R}^d} \overline{\psi}\Omega \cdot L\psi dx \leq \kappa|\Omega| \|\nabla\psi\|_{L^2}\|x\psi\|_{L^2} \leq \frac{\kappa\theta}{2}\|\nabla\psi\|^2_{L^2} + \frac{\kappa|\Omega|^2}{2\theta}\|x\psi\|^2_{L^2},$$

where $\theta > 0$ is another free parameter to be chosen later on. We consequently estimate

$$\begin{aligned}\frac{d^2}{dt^2}I(t) \leq \int_{\mathbb{R}^d} \left(1 + \frac{\kappa\theta}{2}\right)|\nabla\psi|^2 + \frac{\lambda\sigma d}{\sigma+1}|\psi|^{2\sigma+2} + \left(-2U + \frac{\kappa|\Omega|^2}{2\theta}|x|^2\right)|\psi|^2 \, dx \\ - \int_{\mathbb{R}^d} \kappa\overline{\psi}\Omega \cdot L\psi \, dx.\end{aligned}$$

Now, we choose θ such that $2(1 + \frac{\kappa\theta}{2}) = \kappa$, that is $\theta = \frac{\kappa-2}{\kappa}$. In this way we have

$$\begin{aligned}\frac{d^2}{dt^2}I(t) \leq \int_{\mathbb{R}^d} \kappa \left(\frac{1}{2}|\nabla\psi|^2 + \lambda\frac{1}{\sigma+1}|\psi|^{2\sigma+2} + U|\psi|^2 - \overline{\psi}\Omega \cdot L\psi\right) dx \\ + \int_{\mathbb{R}^d} \lambda\frac{\sigma d - \kappa}{\sigma+1}|\psi|^{2\sigma+2}dx + \int_{\mathbb{R}^d} \left(-(\kappa+2)U + \frac{\kappa^2|\Omega|^2}{2(\kappa-2)}|x|^2\right)|\psi|^2 dx.\end{aligned}$$

Let $\underline{\gamma} := \min(\gamma_1, \gamma_2, \gamma_3)$, and choose κ such that

$$\frac{(\kappa+2)}{2}\underline{\gamma}^2 = \kappa^2\frac{|\Omega|^2}{2(\kappa-2)}.$$

This yields $\kappa = \kappa_\Omega$ with

$$\kappa_\Omega = \sqrt{\frac{4\underline{\gamma}^2}{\underline{\gamma}^2 - |\Omega|^2}}.$$

By doing so, the last term in the previous inequality is seen to be non-positive and furthermore we conclude that, for $\lambda < 0$ and $\sigma \geq \frac{\kappa_\Omega}{d}$, it holds:

$$\frac{d^2}{dt^2}I(t) \leq \kappa_\Omega E_\Omega(t) \equiv \kappa_\Omega E_\Omega(0). \tag{3.30}$$

Thus, if the initial energy $E_\Omega(0) < 0$ the second derivative of $I(t)$ is again negative and we can argue (by contradiction) as before. □

The next lemma gives a proof of assertion (2)(ii) in Theorem 3.2.3.

Lemma 3.4.2. *Let $\lambda < 0$, $\sigma < 2/(d-2)$, $d = 2, 3$, and $U(x)$ be a quadratic potential of the form* (3.2). *Denote $\underline{\gamma} = \min\{\gamma_j\}_{j=1}^d$ and suppose that $\Omega = (0,0,\omega)^\top$ if $d = 3$ or $\Omega \cdot L$ is of the form* (3.5) *if $d = 2$. If there exists a $T > 0$ such that*

$$T < \frac{2\underline{\gamma}^2}{|(\gamma_1^2 - \gamma_2^2)\omega|}$$

as well as

$$E_0(0)T^2 + \dot{I}(0)T + I(0) < 0,$$

then the corresponding solution to equation (3.4) *necessarily blows up in finite time.*

Note that if one does not care about the orientation of the rotation, one can always change the sign of Ω such that $L_\Omega(0) \leq 0$ in which case $E_\Omega < 0$ implies $E_0(0) < 0$.

Proof. Again, we let

$$I(t) = \int x^2 |\psi(t,x)|^2 \, dx$$

denote the second moment of $|\psi|^2$. In equation (3.29), we already showed that

$$\frac{d^2}{dt^2} I(t) = \int_{\mathbb{R}^d} \left(|\nabla \psi|^2 + \frac{\lambda d \sigma}{\sigma + 1} |\psi|^{2\sigma+2} - 2U|\psi|^2 \right) dx.$$

In the special case where $\Omega = (0,0,\omega)^\top$, equation (3.14) yields

$$\frac{d}{dt} L_\Omega(t) = (\gamma_1^2 - \gamma_2^2)\omega \int_{\mathbb{R}^d} x_1 x_2 |\psi|^2 \, dx.$$

Integrating twice and applying Hölder's inequality yields

$$\begin{aligned}
\int_0^t L_\Omega(s) \, ds &= t L_\Omega(0) + \int_0^t \int_0^s (\gamma_1^2 - \gamma_2^2)\omega \int_{\mathbb{R}^d} x_1 x_2 |\psi(\tau)|^2 \, dx \, d\tau ds \\
&\leq t L_\Omega(0) + \int_0^t \int_0^s |(\gamma_1^2 - \gamma_2^2)\omega| \int_{\mathbb{R}^d} \frac{1}{2}(x_1^2 + x_2^2)|\psi(\tau)|^2 \, dx \, d\tau ds.
\end{aligned}$$

The integrand on the right hand side is positive and we can estimate the integral over $\{0 \leq \tau \leq s\}$ by the integral over the larger set $\{0 \leq \tau \leq t\}$. Hence it holds that

$$\begin{aligned}
\int_0^t L_\Omega(s) \, ds &\leq t L_\Omega(0) + t \int_0^t |(\gamma_1^2 - \gamma_2^2)\omega| \int_{\mathbb{R}^d} \frac{1}{2}(x_1^2 + x_2^2)|\psi(s)|^2 \, dx \, ds \\
&\leq t L_\Omega(0) + t \int_0^t \frac{|(\gamma_1^2 - \gamma_2^2)\omega|}{\underline{\gamma}^2} \int_{\mathbb{R}^d} U|\psi(s)|^2 \, dx \, ds
\end{aligned} \tag{3.31}$$

by the definition of $\underline{\gamma}$. Integrating (3.29) yields

$$\dot{I}(t) = \dot{I}(0) + \int_0^t \int_{\mathbb{R}^d} \left(|\nabla\psi|^2 + \frac{\lambda d\sigma}{\sigma+1} |\psi|^{2\sigma+2} - 2U|\psi|^2 \right) dx\, ds$$

Adding and substracting the integral over $2L_\Omega$ yields

$$\dot{I}(t) = \dot{I}(0) + \int_0^t \int_{\mathbb{R}^d} \left(|\nabla\psi|^2 + \frac{\lambda d\sigma}{\sigma+1} |\psi|^{2\sigma+2} - 2U|\psi|^2 \right) dx\, ds \\ + 2\int_0^t L_\Omega(s)\, ds - 2\int_0^t L_\Omega(s)\, ds.$$

The definition of the energy (3.6) thus yields

$$\dot{I}(t) = \dot{I}(0) + \int_0^t E_\Omega\, ds + \frac{\lambda(d\sigma - 2)}{\sigma+1} \int_0^t \int_{\mathbb{R}^d} |\psi|^{2\sigma+2}\, dx\, ds \\ - 4\int_0^t \int_{\mathbb{R}^d} U|\psi|^2\, dx\, ds - 2\int_0^t L_\Omega(s)\, ds.$$

The energy E_Ω is constant, the term involving the nonlinearity is non-positive, and hence estimate (3.31) yields

$$\dot{I}(t) \leq \dot{I}(0) + 2t(E_\Omega - L_\Omega(0)) + \int_0^t \left(2\left(t\frac{|(\gamma_1^2 - \gamma_2^2)\omega|}{\underline{\gamma}^2} - 2 \right) \int_{\mathbb{R}^d} U|\psi(s)|^2\, dx \right) ds$$

Of course, $E_0(0) = E_\Omega - L_\Omega(0)$. Under the conditions of the theorem, we obtain $I(T) \leq 0$ upon another integration with respect to time, thus yielding a contradiction! □

3.5 Numerical simulations of a rotating Bose-Einstein condensate

In this section, we will present some numerical results regarding the numerical simulation of equation (3.4). Numerical simulations of the nonlinear Schrödinger equations will also be necessary in Chapter 4, so that this section can be seen as a preparation for the next chapter. It is well-known that the nonlinear Schrödinger equation without rotation term, i.e. (3.4) with $\Omega = 0$, can be efficiently simulated using operator splitting combined with pseudo–spectral methods. For example, let us suppose we want to solve the rotation-less NLS

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + U(x)\psi + \lambda|\psi|^{2\sigma}\psi, \quad \psi(t=0) = \psi_0(x), \tag{3.32}$$

with $(t,x) \in [0,T] \times \mathbb{R}^d$. In order to perform numerical simulations, we restrict ourselves to a bounded set, say, $[-L,L]^d$ for some $L \in [0,\infty)$ and periodic solutions ψ. This can be justified by choosing a trapping potential U or a focusing nonlinearity $\lambda < 0$ which is strong enough to ensure that the support of the solution effectively remains within the box $[-L,L]^d$. In practice, we stop simulations if the numerical support of the wave function ψ reaches the boundary of our domain $[-L,L]^d$. We discretize time and space into the equidistant grid

$$\begin{aligned} t_n &= n\Delta t, n = 0,\dots,N \text{ such that } t_N = T \text{ and} \\ x_m &= -L + m\Delta x, m = 0,\dots,M \text{ such that } \Delta x = \frac{2L}{M}. \end{aligned}$$

Our goal is to calculate approximations $\Psi_{n,m}$ to the correct solution $\psi(t_n, x_m)$ for all $n = 0,\dots,N$ and $m = 0,\dots,M$. Let us first consider only the discretization in time. We perform an *operator-splitting method*, i.e. at each time-step we split equation (3.32) into two equations

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta\psi(t,x), \qquad t \in [t_n, t_{n+1}] \tag{3.33}$$

and

$$i\partial_t \psi(t,x) = U(x)\psi(t,x) + \lambda|\psi(t,x)|^{2\sigma}\psi(t,x), \qquad t \in [t_n, t_{n+1}]. \tag{3.34}$$

Thus, at each time step, given initial datum $\psi_n(x)$ (which we take to be an approximation of $\psi(t_n,x)$), we solve the first equation to obtain a solution $\widetilde{\psi}_{n+1}(x)$ at $t = t_{n+1}$. Then we use $\widetilde{\psi}_{n+1}$ as initial datum in the second equation to obtain $\psi_{n+1}(x)$.
The first equation (3.33) is solved exactly in Fourier space

$$i\partial_t \mathcal{F}\psi(t,k) = \frac{k^2}{2}\mathcal{F}\psi(t,k), \quad t \in [t_n, t_{n+1}], x \in \mathbb{R}^d$$

where $\mathcal{F} : L^2(\mathbb{T}^d) \to L^2(\mathbb{R}^d)$ is the Fourier transform. Thus we obtain that

$$\widetilde{\psi}_{n+1} = \mathcal{F}^{-1}\Big[e^{-i\frac{k^2}{2}\Delta t}\mathcal{F}\psi(t_n,\cdot)\Big], \quad t \in [t_n, t_{n+1}], x \in \mathbb{R}^d, \tag{3.35}$$

where $\mathcal{F}^{-1}$ denotes the inverse Fourier transform. Since the probability density $|\psi(t,x)|$ is constant under the evolution of equation (3.34), the (exact) solution of equation (3.34) is given by

$$\psi_{n+1}(x) = e^{-i(U(x)+\lambda|\psi(t,x)|^2)\Delta t}\widetilde{\psi}_{n+1}(x).$$

By iterating this procedure, we obtain an approximate solution $\psi(t_n,\cdot), n = 0,\dots,N$. When introducing the time-discretization equation, we just need to replace the Fourier transform in (3.35) by the discrete Fourier transform on the spatial lattice. Thus we obtain an approximate function $(\psi(t_n, x_m))$, $n = 0, \ldots, N$, $m = 0, \ldots, M$. The numerical mass

$$\sum_{x_m \in \Lambda_M} |\psi(t_n, x_m)|^2 (\Delta x)^d$$

is conserved up to rounding errors.
In the linear case, convergence of the time-splitting scheme as $\Delta t \to 0$ is a direct consequence of Trotter's product formula

$$e^{(A+B)t} = \lim_{N \to \infty} \left(e^{A\frac{t}{N}} e^{B\frac{t}{N}} \right)^N$$

where A and B are generators of C_0-continuous semigroups. Here we take $A = i\Delta/2$ to be the free Schrödinger operator and $B = U$ to be the multiplaction operator with the potential U. For examples of explicit error estimates, see the works [43, 80]. In the nonlinear case, convergence has been investigated in, for example, [30, 60]. In practice we use Fast Fourier Transform (FFT) and Strang-splitting which is second-order in time and of spectral order in space. A Strang-splitting time-step consists of performing half a time-step $\Delta t/2$ solving (3.34), then a full time-step Δt solving (3.33), followed by another half-step $\Delta t/2$ solving (3.34).
In the presence of the angular momentum rotation term $-\Omega \cdot L$ with L given in (3.3), we would need to include the rotation term in equation (3.33) or (3.34). Then it is in general no longer possible to solve the separate equations exactly. In the literature several discretizations for the nonlinear Schrödinger equations (3.4) have been suggested, see [6, 8, 9, 88]. Here we point out a simple alternative approach based on the change of coordinates (3.21) and present some numerical experiments. As detailed in section 3.3, after the change of coordinates, the wave function ψ solves the NLS with a time-dependent potential (3.22). Again we restrict ourselves to the finite box $[-L, L]^d$ for L large enough. Then the time-splitting procedure given by (3.33) and (3.34) remains valid with $U(x)$ replaced by $W(t, x)$.
This well-known pseudo-spectral time-splitting method is an efficient and easy-to-implement alternative to numerical methods for equation (3.4) proposed in the literature [6, 8, 9, 88]. Note that many of the proposed methods are also valid for more general equations, e.g. the NLS with a dissipation term. On the other hand, the pseudo-spectral method does not introduce highly undesirable numerical dissipation to the solution of (3.4). Let us compare the pseudo-spectral method based on the change of coordinates with an example taken from the work [6]. We take $d = 2$, $\lambda = 1000$, and $\Omega = 0.9$ in (3.4). We replace $U(x)$ by a time-dependent potential

$$W(t, x) = \frac{1}{2}\big((1+\epsilon)\tilde{x}^2 + (1-\epsilon)\tilde{y}^2\big),$$

where $\tilde{x} = x\cos(\tilde{\omega}t) + y\sin(\tilde{\omega}t)$, $\tilde{y} = y\cos(\tilde{\omega}t) - x\sin(\tilde{\omega}t)$ and we take $\epsilon = 0.35$. This a rotating potential with frequency $\tilde{\omega}$, which in rotating coordinates rotates with frequency $\omega + \tilde{\omega}$. Note that our results also hold for time-dependent potentials, cf. [18]. The problem is solved (in rotating coordinates) on the numerical domain $[-14, 14]$ with $N = 358$ steps and $\Delta t = 0.0001$. The initial datum is taken to be a groundstate of (3.4) with $\epsilon = 0$ and $\tilde{\omega} = 0$ which has been obtained by the normalized gradient flow for (3.4) with the backward Euler finite difference method proposed in [10]. Our results are shown in Figure 3.1 and, for comparison, the results of [6] are shown in Figure 3.2. Our results are transformed back into the original (non-rotating) coordinates so that both figures show the wave functions in the same coordinates. Note that the back-transformation from the rotated lattice to the lattice in the original coordinates introduces small errors into some of the plots in Figure 3.1, which are not present in Figure 3.2 and which could in principle be reduced by using a more suitable (numerical) back-transformation. Comparison of the results shows that the gradient-flow method produces slightly different vortex lattices as a ground state. The lattice seems to be slightly less stable, but the results agree both in the number of vortices as well as the orientation of the condensate, down to the position of the four outer-most vortices (at $t = 0$, these are the two on the north-facing side of the condensate and the two on the south-facing side).

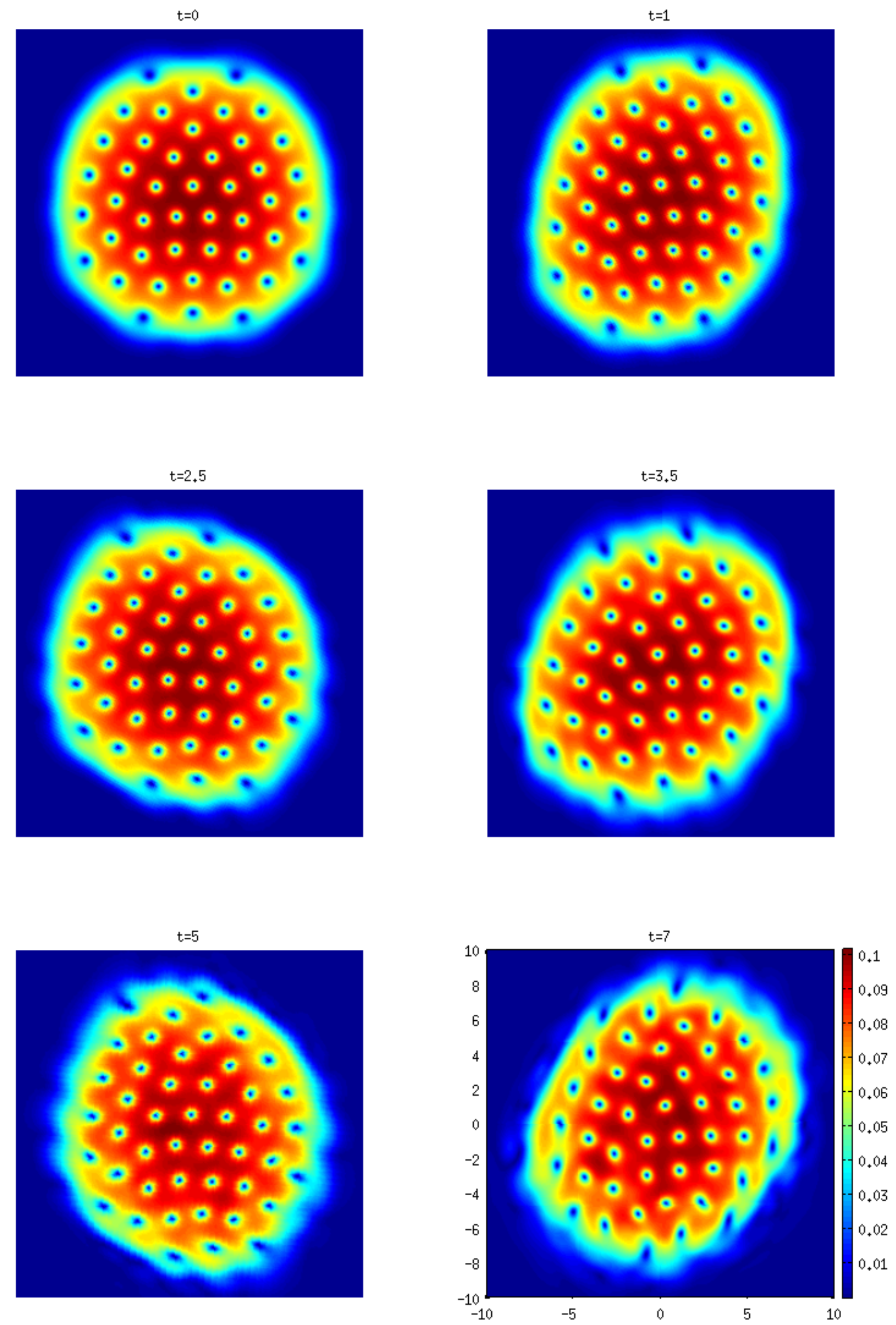

Figure 3.1: Contour plots of the density function $|\psi(t,x)|^2$ for dynamics of a vortex lattice at different times

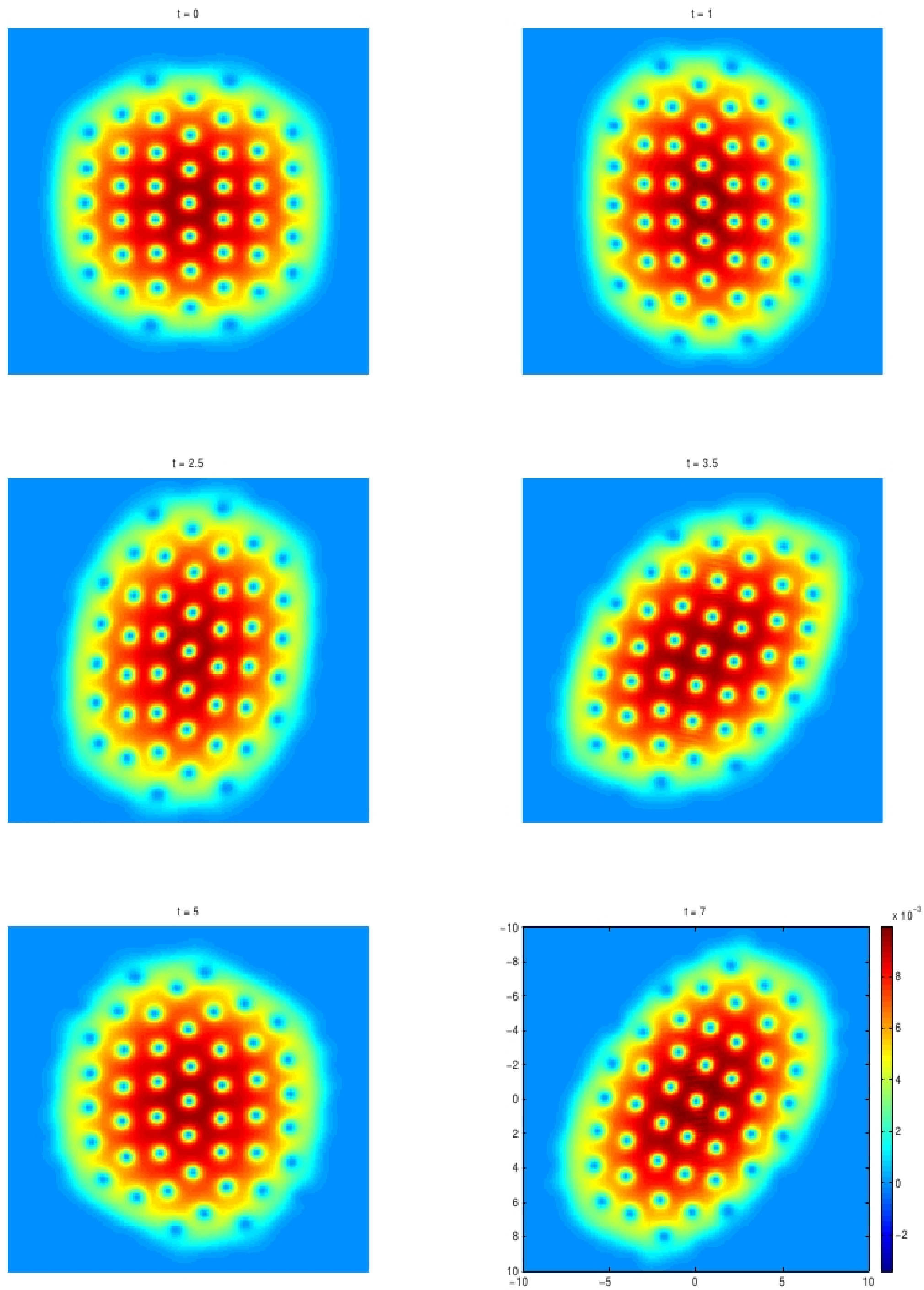

Figure 3.2: Contour plots of the density function $|\psi(t,x)|^2$ for dynamics of a vortex lattice as found in [6]

Chapter 4

Optimal bilinear control of Gross–Pitaevskii equations

The work in this chapter has been carried out in collaboration with Michael Hintermüller, Peter A. Markowich, and Christof Sparber and is a slightly extended version of the published work [39].

4.1 Introduction

4.1.1 Physics background

Ever since the first experimental realization of *Bose–Einstein condensates* (BECs) in 1995, the possibility to store, manipulate, and measure a single quantum system with extremely high precision has provided great stimulus in many fields of physical and mathematical research, among them *quantum control theory.* In the regime of dilute gases, a BEC, consisting of N particles, can be modeled by the *Gross–Pitaevskii equation* [74], i.e. a cubically nonlinear Schrödinger equation (NLS) of the form

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + U(x)\psi + Ng|\psi|^2\psi + W(t,x)\psi, \quad x \in \mathbb{R}^3, t \in \mathbb{R},$$

with m denoting the mass of the particles, $\hbar$ Planck's constant, $g = 4\pi\hbar^2 a_{\text{sc}}/m$, and $a_{\text{sc}} \in \mathbb{R}$ their characteristic scattering length, describing the inter-particle collisions. The function $U(x)$ describes an external trapping potential which is necessary for the experimental realization of a BEC. Typically, $U(x)$ is assumed to be a *harmonic confinement.* In situations where $U(x)$ is strongly anisotropic, one experimentally obtains a quasi one-dimensional ("cigar-shaped"), or quasi two-dimensional ("pancake shaped") BEC, see for instance [49]. In the following, we shall assume $U(x)$ to be *fixed.* The condensate is consequently manipulated via a time-dependent *control potential* $W(t,x)$, which we shall assume to be of the following form:

$$W(t,x) = \alpha(t)V(x),$$

Here, $\alpha(t)$ denotes the *control parameter* (typically, a switching function acting within a certain time-interval $[0,T]$) and $V(x)$ is a given potential. In our context, the potential $V(x)$ models the spatial profile of a laser field used to manipulate the BEC and $\alpha(t)$ its intensity.

The problem of quantum control, i.e. the coherent manipulation of quantum systems (in particular Bose–Einstein condensates) via external potentials $W(t,x)$, has attracted considerable interest in the physics literature, cf. [15, 23, 40, 41, 72, 75, 89]. From the mathematical point of view, quantum control problems are a specific example of *bilinear control systems* [24]. It is known that linear or nonlinear Schrödinger–type equations are in general *not exactly controllable* in, say, $L^2(\mathbb{R}^3)$, cf. [82]. Similarly, approximate controllability is known to hold for only some specific systems, such as [65]. More recently, however, sufficient conditions for approximate controllability of linear Schrödinger equations with purely discrete spectrum have been derived in [21]. In [63] these conditions have been shown to be generically satisfied, but, to the best of our knowledge, a generalization to the case of nonlinear Schrödinger equations is still lacking.

The goal of the current paper is to consider quantum control systems within the framework of *optimal control*, cf. [84] for a general introduction, from a partial differential equation constrained point of view. The objective of the control process is thereby quantified through an objective functional $J = J(\psi, \alpha)$, which is minimized subject to the condition that the time-evolution of the quantum state is governed by the Gross–Pitaevskii equation (GPE). Such objective functionals $J(\psi, \alpha)$ usually consist of two parts, one being the desired physical quantity (observable) to be minimized, the other one describing the cost it takes to obtain the desired outcome through the control process. In quantum mechanics, the wave function $\psi(t,\cdot)$ itself is not a physical observable. Rather, one considers self-adjoint linear operators A acting on $\psi(t,\cdot)$ and aims for a prescribed *expectation value* of A at time $t = T > 0$, the final time of the control process. Such expectation values are computed by taking the L^2–inner product $\langle \psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2(\mathbb{R}^d)}$. Note that this implies that the corresponding $\psi(t,\cdot)$ is only determined up to a constant phase. This fact makes quantum control less "rigid" when compared to classical control problems in which one usually aims to optimize for a prescribed target state.

There are many possible ways of modeling the cost it takes to reach a certain prescribed expectation value. The corresponding cost terms within $J(\psi, \alpha)$ are often given by the norm of the control $\alpha(t)$ in some function space. Typical choices are $L^2(0,T)$ or $H^1(0,T)$. However, these choices of function spaces for $\alpha(t)$ often lack a clear physical interpretation.

In addition, cost terms based on, say, the L^2–norm of α tend to yield highly oscillatory optimal controls due to the oscillatory nature of the underlying (nonlinear) Schrödinger equation. The same is true for quantum control via so-called Lyapunov tracking methods, see, e.g., [25]. In the present work we shall present a novel choice for the cost term, which is based on the corresponding physical work performed throughout the control process.

We continue this introductory section by describing the mathematical setting in more detail.

4.1.2 Mathematical setting

We consider a quantum mechanical system described by a wave function $\psi(t,\cdot) \in L^2(\mathbb{R}^d)$ within $d = 1, 2, 3$ spatial dimensions. The case $d = 1, 2$ models the effective dynamics within strongly anisotropic potentials (resulting in a quasi one or two-dimensional BEC). The time-evolution of $\psi(t,\cdot)$ is governed by the following generalized Gross–Pitaevskii equation (rescaled into dimensionless form):

$$i\partial_t\psi = -\frac{1}{2}\Delta\psi + U(x)\psi + \lambda|\psi|^{2\sigma}\psi + \alpha(t)V(x)\psi, \quad x \in \mathbb{R}^d, t \in \mathbb{R}, \tag{4.1}$$

with $\lambda \geq 0$, $\sigma < 2/(d-2)$, and subject to initial data

$$\psi(0,\cdot) = \psi_0 \in L^2(\mathbb{R}^d), \quad \alpha(0) = \alpha_0 \in \mathbb{R}.$$

For physical reasons we normalize $\|\psi_0\|_{L^2(\mathbb{R}^d)} = 1$, which is henceforth preserved by the time-evolution of (4.1). In addition, the control potential is assumed to be $V \in W^{1,\infty}(\mathbb{R}^d)$, whereas for $U(x)$ we require

$$U \in C^\infty(\mathbb{R}^d) \text{ such that } \partial^k U \in L^\infty(\mathbb{R}^d) \text{ for all multi-indices } k \text{ with } |k| \geq 2.$$

In other words, the external potential is assumed to be smooth and *subquadratic*. One of the most important examples is the harmonic oscillator $U(x) = \frac{1}{2}|x|^2$. Due to the presence of a subquadratic potential, we restrict ourselves to initial data ψ_0 in the *energy space*

$$\Sigma := \left\{\psi \in H^1(\mathbb{R}^d) \ : \ x\psi \in L^2(\mathbb{R}^d)\right\}. \tag{4.2}$$

In particular, this definition guarantees that the quantum mechanical energy functional

$$E(t) = \int_{\mathbb{R}^d} \frac{1}{2}|\nabla\psi(t,x)|^2 + \frac{\lambda}{\sigma+1}|\psi(t,x)|^{2\sigma+2} + (\alpha(t)V(x) + U(x))|\psi(t,x)|^2 dx \tag{4.3}$$

associated to (4.1) is well defined.

Remark 4.1.1. Note that $\sigma < 2/(d-2)$ allows for general power law nonlinearities in dimensions $d = 1, 2$, whereas in $d = 3$ the nonlinearity is assumed to be less than quintic. From the physics point of view a cubic nonlinearity $\sigma = 1$ is the most natural choice, but higher order nonlinearities also arise in systems with more complicated inter-particle interactions, in particular in lower dimensions; compare [49]. From the mathematical point of view, it is well known that the restriction $\sigma < 2/(d-2)$ guarantees well-posedness of the initial value problem in the energy space Σ; see [18, 19]. In addition, the condition $\lambda \geq 0$ (defocusing nonlinearity) guarantees the existence of global in-time solutions to (4.1); see [18]. Hence, we do not encounter the problem of finite-time blow-up in our work.

Although (4.1) conserves mass, i.e. $\|\psi(t,\cdot)\|_{L^2(\mathbb{R}^d)} = \|\psi_0\|_{L^2(\mathbb{R}^d)}$ for all $t \in \mathbb{R}$, the energy $E(t)$ is not conserved. This is in contrast to the case of time-independent potentials. In our case, rather one finds that

$$\frac{d}{dt}E(t) = \dot{\alpha}(t)\int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2 dx. \tag{4.4}$$

The *physical work* performed by the system within a given time-interval $[0,T]$ is therefore equal to

$$E(T) - E(0) = \int_0^T \dot{\alpha}(t)\int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2 dx\, dt. \tag{4.5}$$

Thus a control $\alpha(t)$ acting for $t \in [0,T]$ upon a system described by (4.1) requires a certain amount of energy, which is given by (4.5). It, thus, seems natural to include such a term in the cost functional of our problem in order to quantify the control action.

Indeed, for any given final control time $T > 0$, and parameters $\gamma_1 \geq 0, \gamma_2 > 0$, we define the following *objective functional*:

$$J(\psi,\alpha) := \langle \psi(T,\cdot), A\psi(T,\cdot)\rangle^2_{L^2(\mathbb{R}^d)} + \gamma_1 \int_0^T (\dot{E}(t))^2\, dt + \gamma_2 \int_0^T (\dot{\alpha}(t))^2\, dt, \tag{4.6}$$

where $A : \Sigma \to L^2(\mathbb{R}^d)$ is a bounded linear operator which is assumed to be essentially self-adjoint on $L^2(\mathbb{R}^d)$. In other words, A represents a physical observable with spectrum $\operatorname{spec}(A) \subseteq \mathbb{R}$. A typical choice for A would be $A = A' - a$ where $a \in \mathbb{R}$ is some prescribed expectation value for the observable A' in the state $\psi(T,x)$. For example, if $a \in \operatorname{spec}(A')$ is chosen to be an eigenvalue of A', the first term in $J(\psi,\alpha)$ is zero as soon as the target state $\psi(T,\cdot)$ is, up to a phase factor, given by an associated eigenfunction of A'. However, one may consider choosing $a \in \mathbb{R}$ such that it "forces" the functional to equidistribute between, say, two eigenfunctions.

Remark 4.1.2. We also remark that in the case $A = P_\varphi - 1$, where P_φ denotes the orthogonal projection onto a given *target state* $\varphi \in L^2(\mathbb{R}^d)$, the first term on the right hand side of (4.6) reads

$$\langle \psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2(\mathbb{R}^d)} = \left|\langle \psi(T,\cdot), \varphi(\cdot)\rangle_{L^2(\mathbb{R}^d)}\right|^2 - 1, \tag{4.7}$$

using the fact that $\|\psi(T,\cdot)\|_{L^2(\mathbb{R}^d)} = 1$. Expression (4.7) is the same as used in recent works in the physics literature; see [40].

Using (4.4), we find that the objective functional $J(\psi,\alpha)$ explicitly reads

$$\begin{aligned} J(\psi,\alpha) := {} & \langle \psi(T,\cdot), A\psi(T,\cdot)\rangle^2_{L^2(\mathbb{R}^d)} \\ & + \gamma_1 \int_0^T (\dot\alpha(t))^2 \left(\int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2\, dx\right)^2 dt + \gamma_2 \int_0^T (\dot\alpha(t))^2\, dt. \end{aligned} \tag{4.8}$$

Here, the second line on the right hand side displays two cost (or penalization) terms for the control: The first one, involving $\gamma_1 \geq 0$, is given by the square of the physical work, i.e. the right hand side of (4.4). The second is a classical cost term as used in [40]. In our case, the second term is required as a mathematical *regularization* of the optimal control problem, since for general (sign changing) potentials $V \in L^\infty(\mathbb{R}^d)$ the weight factor

$$\omega(t) := \int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2 dx \tag{4.9}$$

might vanish for some $t \in \mathbb{R}$. In such a situation, the boundedness of variations of $\alpha(t)$ is in jeopardy and the optimal control problem lacks well-posedness. Hence, we require $\gamma_2 > 0$ for our mathematical analysis, but typically take $\gamma_2 \ll \gamma_1$ in our numerics in Section 4.5 to keep its influence small. Note, however, that in the case where the control potential satisfies the positivity condition

$$V(x) \geq \delta > 0 \ \ \forall x \in \mathbb{R}^d,$$

we may choose $\gamma_2 = 0$ and all of our results remain valid.

Remark 4.1.3. In situations where the above positivity condition on $V(x)$ does not hold, one might think of performing a time-dependent *gauge transform* of ψ, i.e.

$$\tilde\psi(t,x) = \exp\left(-i\kappa \int_0^t \alpha(s)\, ds\right)\psi(t,x),$$

with a constant $\kappa > \min_{x\in\mathbb{R}^d} V(x)$, assuming that the minimum exists. This yields a Gross–Pitaevskii equation for the wave function $\tilde\psi$ with modified control potential $\tilde V(x) = (\kappa + V(x)) > 0$ for all $x \in \mathbb{R}^d$. Note, however, that this gauge transform leaves the expression (4.8) unchanged and hence does not improve the stuation. Only if one also changes the potential $V(x)$ within $J(\psi, \alpha)$ into $\tilde{V}(x)$, the problem does not require any regularization term (proportional to γ_2). Note, however, that such a modification yields a control system which is no longer (mathematically) equivalent to the original problem. In fact, replacing $V(x)$ by $\tilde{V}(x)$ in the objective functional $J(\psi, \alpha)$ corresponds to increasing the parameter γ_2 by κ.

4.1.3 Relation to other works and organization of the chapter

The mathematical research field of optimal bilinear control of systems governed by partial differential equations is by now classical, cf. [31, 55] for a general overview. Surprisingly, rigorous mathematical work on optimal (bilinear) control of quantum systems appears very limited, despite the physical significance of the involved applications (cf. the references given above). Results on simplified situations, as, e.g., for finite dimensional quantum systems, can be found in [14] (see also the references therein). More recently, optimal control problems for linear Schrödinger equations have been studied in [11, 13, 42]. In addition, numerical questions related to quantum control are studied in [12, 87]. Among these papers, the work in [42] appears closest to our effort. Indeed, in [42], the authors provide a framework for bilinear optimal control of abstract (linear) Schrödinger equations. The considered objective functional involves a cost term proportional to the L^2–norm of the control parameter $\alpha(t)$. The present work goes beyond the results obtained in [42] in several repects: First, we generalize the cost functional to account for oscillations in $\alpha(t)$ and in particular for the physical work load performed throughout the control process. In addition, we allow for observables A which are unbounded operators on L^2. Second, we consider nonlinear Schrödinger equations of Gross–Pitaevskii type, including unbounded (subquadratic) potentials, which are highly significant in the quantum control of BECs. This type of equation makes the study of the associated control problem considerably more involved from a mathematical point of view.

The rest of this work is organized as follows. In section 4.2 we clarify existence of a minimizer for our control problem. In particular, we prove that the corresponding optimal solution $\psi_*(t, x)$ is indeed a mild (and not only a weak) solution of (4.1), depending continuously on the initial data ψ_0. Then, in section 4.3 the adjoint equation is derived and analyzed with respect to existence and uniqueness of a solution. It is our primary tool for the description of the derivative of the objective function reduced onto the control space through considering the solution of the Gross-Pitaevskii equation as a function of the control variable α. The results of section 4.3 are paramount for the derivation of the first order optimality system in section 4.4. In section 4.5 a gradient- and a Newton-type descent method are defined, respectively, and then used for computing numerical solutions for several illustrative quantum control problems. In particular, we consider the optimal shifting of a linear wave package, splitting of a linear wave package and splitting of a BEC. The paper ends with conclusions on our findings in Chapter 5.

Throughout this chapter we shall denote strong convergence of a sequence $(x_n)_{n\in\mathbb{N}}$ by $x_n \to x$ and weak convergence by $x_n \rightharpoonup x$. For simplicity, we shall often write $\psi(t) \equiv \psi(t,\cdot)$ and also use the shorthand notation $L^p_t L^q_x$ instead of $L^p(0,T;L^q(\mathbb{R}^d))$. Similarly, H^1_t stands for $H^1(0,T)$, with dual $(H^1_t)^* = (H^1(0,T))^*$.

4.2 Existence of minimizers

We start by specifying the basic functional analytic framework. For any given $T > 0$, we consider $H^1(0,T)$ as the real vector space of control parameters $\alpha(t) \in \mathbb{R}$. It is known [19] that for every $\alpha \in H^1(0,T)$, there exists a unique *mild solution* $\psi \in C([0,T];\Sigma)$ of the Gross-Pitaevskii equation, also see Chapter 3. More precisely, ψ solves

$$\psi(t,x) = S(t)\psi_0(x) - i\int_0^t S(t-s)\left(\lambda|\psi(s,\cdot)|^{2\sigma}\psi(s,\cdot) + \alpha(s)V\psi(s,\cdot)\right)(x)ds,$$

where from now on we denote by

$$S(t) = e^{-itH}, \quad H = -\frac{1}{2}\Delta + U(x), \tag{4.10}$$

the group of unitary operators $\{S(t)\}_{t\in\mathbb{R}}$ generated by the Hamiltonian H. In other words, $S(t)$ describes the time-evolution of the linear, uncontrolled system. Next, we define

$$\Upsilon(0,T) := L^2(0,T;\Sigma) \cap H^1(0,T;\Sigma^*), \tag{4.11}$$

where Σ^* is the dual of the energy space Σ. Then the appropriate space for our minimization problem is

$$\Lambda(0,T) := \{(\psi,\alpha) \in \Upsilon(0,T) \times H^1(0,T) : \psi \text{ is a mild solution of (4.1) }\}.$$

Since the control α is real-valued, it is natural to consider $\Lambda(0,T)$ as a *real vector space* and we shall henceforth equip $L^2(\mathbb{R}^d)$ with the scalar product

$$\langle \xi, \psi\rangle_{L^2(\mathbb{R}^d)} = \mathrm{Re}\int_{\mathbb{R}^d} \xi(x)\overline{\psi(x)}\,dx, \tag{4.12}$$

which is subsequently inherited by all L^2-based Sobolev spaces. (Note that this choice is also used in [19].) From what is said above, we infer that the space $\Lambda(0,T)$ is indeed nonempty.

With these definitions at hand, the optimal control problem under investigation is to find

$$J_* = \inf_{(\psi,\alpha)\in\Lambda(0,T)} J(\psi,\alpha). \tag{4.13}$$

We are now in the position to state the first main result of this work.

Theorem 4.2.1. *Let $\lambda \geq 0$, $0 < \sigma < 2/(d-2)$, $V \in W^{1,\infty}(\mathbb{R}^d)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. Then, for any $T > 0$, any initial data $\psi_0 \in \Sigma$, $\alpha_0 \in \mathbb{R}$ and any choice of parameters $\gamma_1 \geq 0$, $\gamma_2 > 0$ the optimal control problem (4.13) has a minimizer $(\psi_*, \alpha_*) \in \Lambda(0,T)$.*

The proof of this theorem will be split into three steps: In subsection 4.2.1 we shall first prove a convergence result for minimizing, or more precisely, infimizing sequences. We consequently deduce in subsection 4.2.2 that the obtained limit ψ_* is indeed a mild solution of (4.1). Finally, we shall prove lower semicontinuity of $J(\psi,\alpha)$ with respect to the convergence obtained before.

4.2.1 Convergence of infimizing sequences

First note that there exists at least one infimizing sequence with an infimum $-\infty \leq J_* < +\infty$, since $\Lambda(0,T) \neq \emptyset$ and $J : \Lambda(0,T) \to \mathbb{R}$. Then we have the following result for any infimizing sequence.

Proposition 4.2.2. *Let $(\psi_n, \alpha_n)_{n\in\mathbb{N}}$ be an infimizing sequence of the optimal control problem given by (4.6). Then under the assumptions of Theorem 4.2.1 there exist a subsequence, still denoted by $(\psi_n, \alpha_n)_{n\in\mathbb{N}}$, and functions $\alpha_* \in H^1(0,T)$, $\psi_* \in L^\infty(0,T;\Sigma)$, such that*

$$\begin{aligned}
&\alpha_n \rightharpoonup \alpha_* \ \textit{in } H^1(0,T), \text{ and } \alpha_n \to \alpha_* \ \textit{in } L^2(0,T),\\
&\psi_n \rightharpoonup \psi_* \ \textit{in } L^2(0,T;\Sigma),\\
&\psi_n \to \psi_* \ \textit{in } L^2(0,T;L^2(\mathbb{R}^d)) \cap L^2(0,T;L^{2\sigma+2}(\mathbb{R}^d)),
\end{aligned}$$

as $n \to +\infty$. Furthermore it holds that

$$\psi_n(t) \to \psi_*(t) \ \textit{in } L^2(\mathbb{R}^d), \ \textit{and } \psi_n(t) \rightharpoonup \psi_*(t) \ \textit{in } \Sigma \tag{4.14}$$

for almost all $t \in [0,T]$.

Proof. By definition, $J \geq 0$ and thus it is bounded from below. For an infimizing sequence $(\psi_n, \alpha_n)_{n\in\mathbb{N}}$ the sequence of objective functional values $(J(\psi_n, \alpha_n))_{n\in\mathbb{N}}$ converges and is

bounded on $\mathbb{R}$. Hence, it holds that $J(\psi_n, \alpha_n) \le C < +\infty$ for all $n \in \mathbb{N}$. Since $\gamma_2 > 0$ it follows that
$$\int_0^T (\dot\alpha_n(t))^2 \, dt \le C < +\infty.$$
For smooth $\alpha_n : [0,T] \to \mathbb{R}$ we compute

$$\alpha_n(t) = \alpha_n(0) + \int_0^t \dot\alpha_n(s) \, ds \le \alpha_n(0) + \left(T \int_0^T (\dot\alpha_n(s))^2 \, ds \right)^{1/2} < +\infty,$$

and thus α_n is bounded in $L^\infty(0,T)$. By approximation (using the fact that $\alpha_n(0) = \alpha_0$ is fixed), the sequence $(\alpha_n)_{n\in\mathbb{N}}$ is uniformly bounded in $L^\infty(0,T)$, which in turn implies a uniform bound in $L^2(0,T)$ and thus in $H^1(0,T)$. Hence, there exists a subsequence, still denoted $(\alpha_n)_{n\in\mathbb{N}}$, and $\alpha_* \in H^1(0,T)$, such that

$$\alpha_n \rightharpoonup \alpha_* \in H^1(0,T).$$

Moreover, since $H^1(0,T)$ is compactly embedded into $L^2(0,T)$, we deduce that $\alpha_n \to \alpha_*$ in $L^2(0,T)$. Next, we recall that

$$\frac{d}{dt} E_n(t) = \dot\alpha_n(t) \int_{\mathbb{R}^d} V(x) |\psi_n(t,x)|^2 \, dx$$

and hence
$$\|\dot E_n\|_{L^2_t} \le \|\dot\alpha_n\|_{L^2_t} \|V\|_{L^\infty_x} \|\psi_0\|^2_{L^2_x},$$
in view of mass conservation $\|\psi_n(t)\|_{L^2_x} = \|\psi_0\|_{L^2_x}$. Since $E_n(0) = E_0$ depends only on ψ_0 and α_0 (and is thus independent of $n \in \mathbb{N}$), the same argument as before yields $\|E_n\|_{L^\infty_t} \le C$. Recalling the definition of the energy (4.3) and the fact that $\lambda \ge 0$, we obtain

$$\frac{1}{2} \|\nabla \psi_n(t)\|^2_{L^2_x} \le \|E_n\|_{L^\infty_t} + c \|\alpha_n\|_{L^\infty_t} \|\psi_0\|^2_{L^2_x} + C \|x \psi_n(t)\|^2_{L^2_x}, \tag{4.15}$$

again using conservation of mass $\|\psi_n(t)\|_{L^2_x} = \|\psi_0\|_{L^2_x}$. Furthermore, it holds that

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} |x|^2 |\psi|^2 \, dx &= 2 \operatorname{Re} \int_{\mathbb{R}^d} i |x|^2 \overline{\psi} \left(\frac{1}{2} \Delta \psi - \lambda |\psi|^{2\sigma} \psi - \lambda \alpha V \psi - U \psi \right) dx \\ &= 2 \operatorname{Im} \int_{\mathbb{R}^d} x \overline{\psi} \nabla \psi \, dx \le \|x \psi(t)\|^2_{L^2_x} + \|\nabla \psi(t)\|^2_{L^2_x}, \end{aligned}$$

which, in view of the bound (4.15) and Gronwall's inequality, yields

$$\|x \psi(t)\|^2_{L^2_x} \le C \left(\|E_n\|_{L^\infty_t} + \|\alpha_n\|_{L^\infty_t} \|\psi_0\|^2_{L^2_x} \right),$$

for all $t \in [0,T]$. In summary we have shown

$$\|\psi_n(t)\|_{\Sigma}^2 = \|\psi_n(t)\|_{H_x^1}^2 + \|x\psi_n(t)\|_{L_x^2}^2 \leq C, \tag{4.16}$$

where $C > 0$ is independent of $n \in \mathbb{N}$ and $t \in [0,T]$. Hence, ψ_n is uniformly bounded in $L^\infty(0,T;\Sigma)$ and in particular in $L^2(0,T;\Sigma)$. By reflexivity of $L^2(0,T;\Sigma)$, we consequently infer the existence of a subsequence (denoted by the same symbol) such that

$$\psi_n \rightharpoonup \psi_* \text{ in } L^2(0,T;\Sigma) \quad \text{as } n \to +\infty.$$

To obtain the strong convergence announced above, we first note that (4.1) implies $\partial_t \psi_n \in L^\infty(0,T;\Sigma^*)$. Now we notice the following Lemma.

Lemma 4.2.3. *The energy space Σ is compactly embedded in $L^2(\mathbb{R}^d)$.*

The proof of this statement can be found, for instance, in [26, Proposition 2.1]. We repeat it here for the reader's convenience. Due to the reflexivity of Σ it suffices to show that $\omega_n \to \omega$ in $L^2(\mathbb{R}^d)$ whenever a sequence $(\omega_n)_{n\in\mathbb{N}} \subset \Sigma$ satisfies $\omega_n \rightharpoonup \omega$ in Σ as $n \to \infty$. Take any ball $B_R \subset \mathbb{R}^d$ of radius $R > 0$ around the origin. Restricting to test functions with support in B_R, we see that $\omega_n|_{B_R} \rightharpoonup \omega|_{B_R}$ in $H^1(B_R)$ as $n \to \infty$. Since $H^1(B_R)$ is compactly embedded in $L^2(B_R)$, it follows $\omega_n|_{B_R} \to \omega|_{B_R}$ in $L^2(B_R)$. In order to show convergence on the whole $L^2(\mathbb{R}^d)$, we split up the L^2–norm as follows. It holds that

$$\int_{\mathbb{R}^d} |\omega(x) - \omega_n(x)|^2 \, dx = \int_{B_R} |\omega(x) - \omega_n(x)|^2 \, dx + \int_{\mathbb{R}^d \setminus B_R} |\omega(x) - \omega_n(x)|^2 \, dx$$

For fixed $R > 0$, the second term on the right hand side vanishes in the limit as $n \to \infty$. On the other hand, the first term on the right hand side is bounded by C/R^2, since $(\omega_n)_{n\in\mathbb{N}}$ is bounded in Σ by assumption. Given any $\epsilon > 0$, we thus choose first $R > 0$ large enough such that the first term is bounded by ϵ and then n large enough such that the second term is bounded by ϵ in order to show that $\omega_n \to \omega$ in $L^2(\mathbb{R}^d)$ as $n \to \infty$. Hence Σ is indeed compactly embedded in $L^2(\mathbb{R}^d)$.

Thus, we can apply the Aubin–Lions Lemma [78] to deduce

$$\psi_n \xrightarrow{n\to\infty} \psi_* \text{ in } L^2((0,T) \times \mathbb{R}^d).$$

In particular, there exists yet another subsequence (still denoted by the same symbol), such that

$$\psi_n(t) \xrightarrow{n\to\infty} \psi_*(t) \text{ in } L^2(\mathbb{R}^d), \text{ for almost all } t \in [0,T].$$

In order to obtain weak convergence in the energy space, i.e. $\psi_n(t) \rightharpoonup \psi_*(t)$ in Σ, we fix $t \in [0,T]$ such that $\psi_n(t) \to \psi_*(t)$ in $L^2(\mathbb{R}^d)$. In view of (4.16), every subsequence of $\psi_n(t)$ has yet another subsequence such that $\psi_n(t)$ converges weakly in Σ to some limit.

On the other hand, this limit is necessarily given by $\psi_*(t)$, since $\psi_n(t) \to \psi_*(t)$ in $L^2(\mathbb{R}^d)$. Hence the whole sequence converges weakly in Σ to $\psi_*(t)$. By lower-semicontinuity of the Σ–norm we can deduce $\|\psi_n(t)\|_\Sigma \leq C$ and thus $\psi_* \in L^\infty(0,T;\Sigma)$.

Finally, the announced convergence in $L^2(0,T;L^{2\sigma+2}(\mathbb{R}^d))$ is obtained by invoking the Gagliardo–Nirenberg inequality, i.e.

$$\|\xi\|_{L^r_x} \leq C\|\xi\|_{L^2_x}^{1-\delta(r)}\|\nabla\xi\|_{L^2_x}^{\delta(r)}, \tag{4.17}$$

where $2 \leq r < \frac{2d}{d-2}$ and $\delta(r) = d(\frac{1}{2} - \frac{1}{r})$. This concludes the proof of Proposition 4.2.2. □

4.2.2 Minimizers as mild solutions

Next we prove that the limit ψ_* obtained in the previous subsection is indeed a mild solution of (4.1) with corresponding control α_*. From the physical point of view, this is important since it implies continuous (in time) dependence of ψ_* upon a given initial data ψ_0. To this end, one should also note that $H^1(0,T) \hookrightarrow C(0,T)$ (using Sobolev imbeddings), and hence the obtained optimal control parameter $\alpha_*(t)$ is indeed a continuous function on $[0,T]$.

Proposition 4.2.4. *Let* $(\psi_*, \alpha_*) \in \Upsilon(0,T) \times H^1(0,T)$ *be the limit obtained in Proposition 4.2.2. Then* ψ_* *is a mild solution of* (4.1) *with control* α_* *and*

$$\psi_* \in C([0,T];\Sigma) \cap C^1([0,T];\Sigma^*).$$

In particular, this implies that the convergence result (4.14) *holds for all* $t \in [0,T]$.

Proof. First we note that, by construction, each ψ_n satisfies

$$\psi_n(t) = S(t)\psi_0 - i\int_0^t S(t-s)\left(\lambda|\psi_n(s)|^{2\sigma}\psi_n(s) + \alpha_n(s)V\psi_n(s)\right)ds \tag{4.18}$$

for all $t \in [0,T]$. Here and in the following we shall suppress the x–dependence of ψ for notational convenience. In order to prove that ψ_* is a mild solution corresponding to the control α_*, we take the L^2–scalar product of the above equation with a test function $\chi \in C_0^\infty(\mathbb{R}^d)$. This yields

$$\begin{aligned}\langle\psi_n(t),\chi\rangle_{L^2_x} = \langle S(t)\psi_0,\chi\rangle_{L^2_x} - i\lambda\int_0^t \left\langle S(t-s)|\psi_n(s)|^{2\sigma}\psi_n(s),\chi\right\rangle_{L^2_x} ds \\ - i\int_0^t \left\langle S(t-s)\alpha_n(s)V\psi_n(s),\chi\right\rangle_{L^2_x} ds.\end{aligned} \tag{4.19}$$

In view of Proposition 4.2.2, the term on the left hand side of this identity converges to the desired expression for almost all $t \in [0,T]$, i.e.

$$\lim_{n\to\infty} \langle \psi_n(t), \chi\rangle_{L^2_x} = \langle \psi_*(t), \chi\rangle_{L^2_x}.$$

In order to proceed further, we note that for any $f \in \mathcal{D}'(\mathbb{R}^d)$ it holds that

$$\langle S(t-s)f(s), \chi\rangle_{L^2_x} = \langle f(s), S(s-t)\chi\rangle_{L^2_x}, \tag{4.20}$$

and we therefore define

$$\tilde{\chi} : [0,t]\times\mathbb{R}^d \to \mathbb{C}, \quad \chi \mapsto \tilde{\chi}(\cdot, x) := S(\cdot - t)\chi(x), \tag{4.21}$$

for which we can prove the following regularity properties.

Lemma 4.2.5. *There exists a constant $C = C(T) > 0$ such that for all $t \in [0,T]$ it holds that*

$$\sup_{s\in[0,t]} \left(\|x\tilde{\chi}(s)\|_{L^2_x} + \|\nabla\tilde{\chi}(s)\|_{L^2_x}\right) \le C(T) < +\infty,$$

where the function $\tilde{\chi}$ is defined in (4.21). In particular, the function $\tilde{\chi}$ is bounded in $L^\infty(0,t;L^{2\sigma+2}(\mathbb{R}^d))$.

Proof of Lemma 4.2.5. The norm $\|\tilde{\chi}(s)\|_{L^2_x} = \|S(s-t)\chi\|_{L^2_x}$ is conserved since $S(t)$ is a unitary operator on $L^2(\mathbb{R}^d)$. Furthermore, it holds that

$$i\partial_t[\nabla, S(t)] = H[\nabla, S(t)] + [\nabla, H]S(t) = H[\nabla, S(t)] + \nabla U S(t),$$

and hence

$$[\nabla, S(t)] = -i\int_0^t S(t-s)\nabla U\ S(s)\,ds.$$

We can thus estimate

$$\begin{aligned} \|\nabla\tilde{\chi}(s)\|_{L^2_x} &= \|\nabla S(t-s)\chi\|_{L^2_x} \\ &\le \|S(t-s)\nabla\chi\|_{L^2_x} + \left\|\int_0^{t-s} S(t-s-\tau)\nabla U\tilde{\chi}(\tau)\,d\tau\right\|_{L^2_x} \\ &\le \|\nabla\chi\|_{L^2_x} + C\int_0^{t-s}\|x\tilde{\chi}(\tau)\|_{L^2_x}\,d\tau, \end{aligned} \tag{4.22}$$

since U is subquadratic, i.e. $|\nabla U(x)| \le C|x|$. Likewise, we deduce

$$[x, S(t)] = -i\int_0^t S(t-s)\nabla S(s)\,ds$$

and hence

$$\|x\tilde{\chi}(s)\|_{L^2_x} \le \|x\chi\|_{L^2_x} + \int_0^{t-s} \|\nabla\tilde{\chi}(\tau)\|_{L^2_x}\, d\tau. \tag{4.23}$$

Combining the estimates (4.22) and (4.23) and applying Gronwall's inequality yields

$$\|x\tilde{\chi}(s)\|_{L^2_x} + \|\nabla\tilde{\chi}(s)\|_{L^2_x} \le C\left(\|x\chi\|_{L^2_x} + \|\nabla\chi\|_{L^2_x}\right) < +\infty,$$

where $C > 0$. The bound in $L^\infty(0,t;L^{2\sigma+2}(\mathbb{R}^d))$ then follows from the uniform-in-time bound in $H^1(\mathbb{R}^d)$ and the Gagliardo–Nirenberg inequality (4.17). □

With the result of Lemma 4.2.5 at hand, we consider the second term on the right hand side of (4.19). Rewriting it using (4.20), we estimate

$$\begin{aligned}
&\left|\int_0^t \left\langle |\psi_n(s)|^{2\sigma}\psi_n(s) - |\psi_*(s)|^{2\sigma}\psi_*(s), \tilde{\chi}(s)\right\rangle_{L^2_x} ds\right| \\
&\le \int_0^t \int_{\mathbb{R}^d} \left||\psi_n(s,x)|^{2\sigma}\psi_n(s,x) - |\psi_*(s,x)|^{2\sigma}\psi_*(s,x)\right| |\tilde{\chi}(s,x)|\, dx\, ds \\
&\le\ C\int_0^t \int_{\mathbb{R}^d} \left(|\psi_n(s,x)|^{2\sigma} + |\psi_*(s,x)|^{2\sigma}\right) |\psi_n(s,x) - \psi_*(s,x)||\tilde{\chi}(s,x)|\, dx\, ds.
\end{aligned}$$

By Hölder's inequality, it holds that

$$\begin{aligned}
&\int_0^t \int_{\mathbb{R}^d} \left||\psi_n(s,x)|^{2\sigma} + |\psi_*(s,x)|^{2\sigma}\right| |\psi_n(s,x) - \psi_*(s,x)||\tilde{\chi}(s)|\, dx\, ds \\
&\le\ \sqrt{T}\left(\|\psi_n\|^{2\sigma}_{L^\infty_t L^{2\sigma+2}_x} + \|\psi_*\|^{2\sigma}_{L^\infty_t L^{2\sigma+2}_x}\right) \|\psi_n - \psi_*\|_{L^2_t L^{2\sigma+2}_x} \|\tilde{\chi}\|_{L^\infty_t L^{2\sigma+2}_x},
\end{aligned}$$

where, in view of Lemma 4.2.5, we have $\|\tilde{\chi}\|_{L^\infty_t L^{2\sigma+2}_x} < +\infty$. In addition, Proposition 4.2.2 implies that the factor inside the parentheses is bounded and that

$$\lim_{n\to\infty} \|\psi_n - \psi_*\|_{L^2_t L^{2\sigma+2}_x} = 0.$$

Thus, we have shown that the second term on the right hand side of (4.19) vanishes in the limit $n \to \infty$.

It remains to treat the last term on the right hand side of (4.19), rewritten via (4.20). We first estimate

$$\begin{aligned}
&\left|\int_0^t \left\langle \alpha_n(s)V\psi_n(s) - \alpha_*(s)V\psi_*(s), \tilde{\chi}(s)\right\rangle_{L^2_x} ds\right| \\
&\le \int_0^t \int_{\mathbb{R}^d} |\alpha_n(s)|\,|V(x)|\,|\psi_n(s,x) - \psi_*(s,x)|\,|\tilde{\chi}(s,x)|\, dx\, ds \\
&\quad + \int_0^t \int_{\mathbb{R}^d} |\alpha_n(s) - \alpha_*(s)|\,|V(x)|\,|\psi_*(s,x)||\tilde{\chi}(s,x)|\, dx\, ds.
\end{aligned}$$

Here, the last term on the right hand side can be bounded by

$$\int_0^t \int_{\mathbb{R}^d} |\alpha_n(s) - \alpha_*(s)||V(x)||\psi_*(s,x)||\tilde{\chi}(s,x)|\, dx\, ds \\ \leq \|\alpha_n - \alpha_*\|_{L^2_t} \|V\|_{L^\infty_x} \|\psi\|_{L^2_t L^2_x} \|\tilde{\chi}\|_{L^\infty_t L^2_x} \xrightarrow{n\to\infty} 0,$$

in view of the convergence of $\alpha_n \to \alpha_*$ in $L^2(0,T)$. For the remaining term we use the fact that $V \in L^\infty(\mathbb{R}^d)$ and Hölder's inequality to obtain that

$$\int_0^t \int_{\mathbb{R}^d} |\alpha_n(s)|\,|V(x)|\,|\psi_n(s,x) - \psi_*(s,x)||\tilde{\chi}(s,x)|\, dx\, ds \\ \leq \ \|\alpha_n\|_{L^2_t} \|V\|_{L^\infty_x} \|\psi_n - \psi_*\|_{L^2_t L^2_x} \|\tilde{\chi}\|_{L^\infty_t L^2_x} \xrightarrow{n\to\infty} 0,$$

due to the results of Proposition 4.2.2 and Lemma 4.2.5.

In summary this proves that $\psi_* \in \Upsilon(0,T)$ satisfies, for *almost all* $t \in [0,T]$,

$$\psi_*(t) = S(t)\psi_0 - i \int_0^t S(t-s) \left(\lambda |\psi_*(s)|^{2\sigma} \psi_*(s) + \alpha_*(s) V \psi_*(s)\right) ds,$$

i.e. ψ_* is a *weak* Σ*–solution* in the terminology of [19, Definition 3.1.1] (where the analogous notion of weak H^1–solutions is introduced). In order to obtain that ψ_* is indeed a mild solution we note that

$$\psi_* \in \Upsilon(0,T) \hookrightarrow C([0,T]; L^2(\mathbb{R}^d)) \cap C([0,T]; L^{2\sigma+2}(\mathbb{R}^d))$$

by interpolation and the Gagliardo–Nirenberg inequality (4.17). Classical arguments based on Strichartz estimates then yield uniqueness of the weak Σ–solution ψ_*. Arguing as in the proof of [19, Theorem 3.3.9], we infer that ψ_* is indeed a mild solution to (4.1), satisfying $\psi_* \in C([0,T];\Sigma) \cap C^1([0,T];\Sigma^*)$. □

4.2.3 Lower semicontinuity of objective functional

In order to conclude that the pair $(\psi_*, \alpha_*) \in \Lambda(0,T)$ is indeed a minimizer of our optimal control problem, it remains to show lower semicontinuity of the functional $J(\psi,\alpha)$ with respect to the convergence results established in Proposition 4.2.2.

Lemma 4.2.6. *For the sequence constructed in Proposition 4.2.2, it holds that*

$$J_* = \liminf_{n\to\infty} J(\psi_n, \alpha_n) \geq J(\psi_*, \alpha_*).$$

Proof. Since $A \in \mathcal{L}(\Sigma, L^2(\mathbb{R}^d))$ by assumption, the sequence $(A\psi_n(T))_{n\in\mathbb{N}}$ converges weakly to $A\psi(T)$ in $L^2(\mathbb{R}^d)$. In addition $\psi_n(T) \to \psi_*(T)$ in $L^2(\mathbb{R}^d)$ as $n \to \infty$ by

Proposition 4.2.4, and hence the estimate

$$\begin{aligned}&\left|\langle\psi_n(T), A\psi_n(T)\rangle_{L^2_x} - \langle\psi_*(T), A\psi_*(T)\rangle_{L^2_x}\right| \\ &\quad \leq \left|\langle\psi_n(T) - \psi_*(T), A\psi_n(T)\rangle_{L^2_x}\right| + \left|\langle\psi_*(T), A(\psi_n(T) - \psi_*(T))\rangle_{L^2_x}\right|.\end{aligned}$$

yields convergence of the corresponding term in the objective functional (4.8). Next, we consider the cost term involving γ_1. In view of (4.9), we define

$$\omega_n(t) := \int_{\mathbb{R}^d} V(x)|\psi_n(t,x)|^2 dx, \qquad \omega_*(t) := \int_{\mathbb{R}^d} V(x)|\psi_*(t,x)|^2 dx,$$

and estimate

$$\begin{aligned}&\liminf_{n\to\infty} \int_0^T (\dot\alpha_n(t))^2 \omega_n^2(t) dt \geq \\ &\liminf_{n\to\infty} \int_0^T (\dot\alpha_n(t))^2 \omega_*^2(t)\, dt + \liminf_{n\to\infty} \int_0^T (\dot\alpha_n(t))^2 \left(\omega_n^2(t) - \omega_*^2(t)\right) dt.\end{aligned} \tag{4.24}$$

Note that $0 \leq \omega_n(t) \leq \|V\|_{L^\infty_x} \|\psi_0\|^2_{L^2_x}$ independently of $n \in \mathbb{N}$ and $t \in [0,T]$ and that the same holds for $\omega_*(t)$. The first term on the right hand side of (4.24) is convex in α_n and thus satisfies

$$\liminf_{n\to\infty} \int_0^T (\dot\alpha_n(t))^2 \omega_*^2(t)\, dt \geq \int_0^T (\dot\alpha_*(t))^2 \omega_*^2(t)\, dt, \tag{4.25}$$

since any convex and lower semicontinuous functional is weakly lower semicontinuous. On the other hand, Proposition 4.2.2 implies

$$\liminf_{n\to\infty} \omega_n(t) \geq \omega_*(t) \geq 0 \quad \text{for all } t \in [0,T]. \tag{4.26}$$

Thus, using (4.25) and (4.26) together with Fatou's Lemma yields

$$\begin{aligned}&\liminf_{n\to\infty} \int_0^T (\dot\alpha_n(t))^2 \omega_n^2(t)\, dt \\ &\geq \int_0^T (\dot\alpha_*(t))^2 \omega_*^2(t)\, dt + \int_0^T \liminf_{n\to\infty} (\dot\alpha_n(t))^2 \liminf_{n\to\infty} \left(\omega_n^2(t) - \omega_*^2(t)\right) dt \\ &\geq \int_0^T (\dot\alpha_*(t))^2 \omega_*^2(t)\, dt.\end{aligned}$$

Finally the cost term involving γ_2 is lower semicontinuous by convexity and weak convergence of α_n in $H^1(0,T)$. □

In summary, we have shown that $J_* = \liminf_{n\to\infty} J(\psi_n, \alpha_n) \geq J(\psi_*, \alpha_*)$ and thus indeed $J_* = J(\psi_*, \alpha_*)$. In other words, $(\psi_*, \alpha_*) \in \Lambda(0,T)$ solves the optimization problem.

Remark 4.2.7. Note that the bound on $x\psi_n(t,\cdot)$ in $L^2(\mathbb{R}^d)$, obtained in Proposition 4.2.2, is indeed crucial for proving the weak lower-semicontinuity of $J(\psi,\alpha)$. Without such a bound on the second moment, we would only have

$$\psi_n(t) \xrightarrow{n\to\infty} \psi(t) \quad \text{in } L^2_{\text{loc}}(\mathbb{R}^d),$$

due to the lack of compactness of $H^1(\mathbb{R}^d) \hookrightarrow L^2(\mathbb{R}^d)$. In this case, the lower semi-continuity of the term $\langle\psi(T), A\psi(T)\rangle_{L^2_x}$ is not guaranteed. A possible way to circumvent this problem would be to assume that A is *positive definite*, which, however, is not true for general observables of the form $A = A' - a$, with $a \in \mathbb{R}$. A second possibility would be to assume that A is *localizing*, i.e. for all $\psi \in H^1(\mathbb{R}^d)$: $\text{supp}_{x\in\mathbb{R}^d}(A\psi(x)) \subseteq B(R)$, for some $R < +\infty$.

4.3 Derivation and analysis of the adjoint equation

In order to give a characterization of a minimizer $(\psi_*, \alpha_*) \in \Lambda(0,T)$, we need to derive the first order optimality conditions for our optimal control problem (4.13). For this purpose, we shall first formally compute the derivative of the objective functional $J(\psi,\alpha)$ in the next subsection and consequently analyze the resulting adjoint problem. A rigorous justification for the derivative will be given in Section 4.4.

4.3.1 Identification of the derivative of $J(\psi,\alpha)$

The mild solution of the nonlinear Schrödinger equation (4.1), corresponding to the control $\alpha \in H^1(0,T)$, induces a map

$$\psi : H^1(0,T) \to \Upsilon(0,T) : \quad \alpha \mapsto \psi(\alpha).$$

Using this map we introduce the unconstrained or *reduced functional*

$$\mathfrak{J} : H^1(0,T) \to \mathbb{R}, \quad \alpha \mapsto \mathfrak{J}(\alpha) := J(\psi(\alpha),\alpha).$$

For the characterization of critical points, we need to compute the derivative of $\mathfrak{J}$. For this calculation let $\delta_\alpha \in H^1(0,T)$ with $\delta_\alpha(0) = 0$ be a feasible control perturbation. (Recall that $H^1(0,T) \hookrightarrow C(0,T)$ and hence it makes sense to evaluate $\delta_\alpha(t)$ at $t = 0$.) Then the chain rule yields

$$\begin{aligned} \langle \mathfrak{J}'(\alpha), \delta_\alpha\rangle_{(H^1_t)^*,H^1_t} = {} & \langle \partial_\psi J(\psi(\alpha),\alpha), \psi'(\alpha)\delta_\alpha\rangle_{\Upsilon^*,\Upsilon} \\ & + \langle \partial_\alpha J(\psi(\alpha),\alpha), \delta_\alpha\rangle_{(H^1_t)^*,H^1_t} \end{aligned} \tag{4.27}$$

where Υ^* denotes the dual space of $\Upsilon \equiv \Upsilon(0,T)$ for any given $T > 0$. The main difficulty lies in computing $\psi'(\alpha)$ since ψ is given only implicitly through the nonlinear Schrödinger equation (4.1).

In the following, we shall write the (nonlinear) partial differential equation (4.1) in a more abstract form, i.e.

$$P(\psi, \alpha) := i\partial_t \psi - H\psi - \alpha(t)V(x)\psi - \lambda|\psi|^{2\sigma}\psi = 0, \tag{4.28}$$

where $H = -\frac{1}{2}\Delta + U(x)$ denotes the linear, uncontrolled Hamiltonian operator. Setting $\psi = \psi(\alpha)$ and differentiating with respect to α formally yields

$$\frac{d}{d\alpha}P(\psi(\alpha), \alpha) = \partial_\psi P(\psi(\alpha), \alpha)\psi'(\alpha) + \partial_\alpha P(\psi(\alpha), \alpha) = 0.$$

Next, assuming that $\partial_\psi P$ is invertible, we solve for $\psi'(\alpha)$ via

$$\psi'(\alpha) = -\partial_\psi P(\psi, \alpha)^{-1}\partial_\alpha P(\psi(\alpha), \alpha).$$

Thus it holds that

$$\begin{aligned}&\langle \partial_\psi J(\psi(\alpha), \alpha), \psi'(\alpha)\delta_\alpha\rangle_{\Upsilon^*,\Upsilon}\\ &= \left\langle -\partial_\psi J(\psi(\alpha), \alpha), \partial_\psi P(\psi(\alpha), \alpha)^{-1}\partial_\alpha P(\psi(\alpha), \alpha)\delta_\alpha\right\rangle_{\Upsilon^*,\Upsilon},\end{aligned}$$

which can be rewritten as

$$\begin{aligned}&\langle \partial_\psi J(\psi(\alpha), \alpha), \psi'(\alpha)\delta_\alpha\rangle_{\Upsilon^*,\Upsilon}\\ &= \left\langle -\partial_\alpha P(\psi(\alpha), \alpha)^*\partial_\psi P(\psi(\alpha), \alpha)^{-*}\partial_\psi J(\psi(\alpha), \alpha), \delta_\alpha\right\rangle_{(H_t^1)^*,H_t^1}.\end{aligned} \tag{4.29}$$

Here we abbreviate

$$\partial_\psi P(\psi(\alpha), \alpha)^{-*} := (\partial_\psi P(\psi(\alpha), \alpha)^*)^{-1} = (\partial_\psi P(\psi(\alpha), \alpha)^{-1})^*.$$

Substituting (4.29) into equation (4.27), we see that critical points of (4.13) satisfy

$$\begin{aligned}0 = \langle \mathcal{J}'(\alpha), \delta_\alpha\rangle_{(H_t^1)^*,H_t^1} &= \langle \partial_\alpha J(\psi(\alpha), \alpha), \delta_\alpha\rangle_{(H_t^1)^*,H_t^1} +\\ &\langle -\partial_\alpha P(\psi(\alpha), \alpha)^*\partial_\psi P(\psi(\alpha), \alpha)^{-*}\partial_\psi J(\psi(\alpha), \alpha), \delta_\alpha\rangle_{(H_t^1)^*,H_t^1}\end{aligned} \tag{4.30}$$

for all $\delta_\alpha \in H^1(0,T)$ such that $\delta_\alpha(0) = 0$. In order to obtain (4.30) in a more explicit form, we (formally) compute the derivative

$$\partial_\psi P(\psi, \alpha)\xi = i\partial_t\xi - H\xi - \alpha(t)V(x)\xi - \lambda(\sigma+1)|\psi|^{2\sigma}\xi - \lambda\sigma|\psi|^{2\sigma-2}\psi^2\overline{\xi}, \tag{4.31}$$

acting on $\xi \in L^2(\mathbb{R}^d) \subset \Sigma^*$. Analogously, we find

$$\partial_\alpha P(\psi, \alpha) = -V(x)\psi.$$

Next, we define

$$\varphi := \partial_\psi P(\psi(\alpha), \alpha)^{-*} \partial_\psi J(\psi(\alpha), \alpha), \tag{4.32}$$

which, in view of (4.30), allows us to express $\mathcal{J}'(\alpha) \in (H^1(0,T))^*$ in the following form:

$$\mathcal{J}'(\alpha) = \partial_\alpha J(\psi(\alpha), \alpha) - \partial_\alpha P(\psi(\alpha), \alpha)^* \varphi. \tag{4.33}$$

We consequently obtain $\mathcal{J}'(\alpha)$ by explicitly calculating the right hand side of this equation (given in (4.47) below), provided we can determine φ.

In order to perform this calculation, we recall that the duality pairing between $\xi \in L^2(\mathbb{R}^d) \subset \Sigma^*$ and $\psi \in \Sigma$ can be expressed by the inner product defined in (4.12). Thus, (4.32) implies

$$\langle \varphi, \partial_\psi P(\psi(\alpha), \alpha)\delta_\psi \rangle_{L^2_t L^2_x} = \langle \partial_\psi J(\psi(\alpha), \alpha), \delta_\psi \rangle_{L^2_t L^2_x}, \tag{4.34}$$

for all test functions $\delta_\psi \in \Upsilon(0,T)$ such that $\delta_\psi(0) = 0$. This is the correct "tangent space" for ψ in view of the Cauchy data

$$\psi(0) + \delta_\psi(0) = \psi_0 \text{ and } \psi(0) = \psi_0.$$

By virtue of the symmetry of the *linearized operator* $\partial_\psi P(\psi(\alpha), \alpha)$, equation (4.34) corresponds to the weak formulation of the following *adjoint equation*:

$$\begin{cases} i\partial_t \varphi - H\varphi - \alpha(t)V(x)\varphi - \lambda(\sigma+1)|\psi|^{2\sigma}\varphi - \lambda\sigma|\psi|^{2\sigma-2}\psi^2\overline{\varphi} = \dfrac{\delta J(\psi,\alpha)}{\delta\psi(t)}, \\ \text{for all } t \in [0,T] \text{ and with data: } \varphi(T) = i\dfrac{\delta J(\psi,\alpha)}{\delta\psi(T)}. \end{cases} \tag{4.35}$$

Here, $\frac{\delta J(\psi,\alpha)}{\delta\psi(t)}$ denotes the first variation of $J(\psi,\alpha)$ with respect to the value of $\psi(t) \in H^1(\mathbb{R}^d)$, where ψ is the solution of (4.1) with control α. Likewise, $\frac{\delta J(\psi,\alpha)}{\delta\psi(T)}$ denotes the first variation with respect to solutions of (4.1) evaluated at the final time $t = T$. Explicitly, these derivatives are given by

$$\begin{aligned} \frac{\delta J(\psi,\alpha)}{\delta\psi(t)} &= 4(\dot\alpha(t))^2 \left(\int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2 dx \right) V(x)\psi(t,x) \\ &\equiv 4(\dot\alpha(t))^2 \omega(t) V(x)\psi(t,x), \end{aligned} \tag{4.36}$$

in view of the definition (4.9), and

$$\frac{\delta J(\psi,\alpha)}{\delta\psi(T)} = 4\langle\psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2_x} A\psi(T,x). \tag{4.37}$$

The system (4.35) consequently defines a Cauchy problem for φ with data given at $t = T$, the final time. Thus, one needs to solve (4.35) backwards in time, a common feature of adjoint systems for time-dependent phenomena.

Remark 4.3.1. In fact, φ can also be seen as a *Lagrange multiplier* within the Lagrangian formulation of the optimal control problem. In oder to see this, one defines the Lagrangian

$$L(\psi,\alpha,\varphi) = J(\psi,\alpha) - \langle\varphi, P(\psi,\alpha)\rangle_{L^2_t L^2_x},$$

where $P(\psi,\alpha)$ is the nonlinear Schrödinger equation given in (4.28). Formally, the Euler–Lagrange equations associated to $L(\psi,\alpha,p)$ yield (4.33) and (4.35). In Section 4.5 we shall use the Lagrangian formulation to formally compute the Hessian of the reduced objective functional $\mathcal{J}(\alpha)$.

4.3.2 Local and global existence theory for solutions of higher regularity

In order to obtain existence of solutions to (4.35), we need sufficiently high regularity of ψ, the solution of the Gross–Pitaevskii equation (4.1). For this purpose, for every $m \in \mathbb{N}$ we define

$$\Sigma^m := \big\{\psi \in L^2(\mathbb{R}^d) \ : \ x^j\partial^k\psi \in L^2(\mathbb{R}^d) \text{ for all multi-indices } j \text{ and } k \text{ with } |j| + |k| \le m\big\},$$

equipped with the norm (note that $\Sigma^1 \equiv \Sigma$):

$$\|\psi\|_{\Sigma^m} := \sum_{|j|+|k|\le m} \left\|x^j\partial^k\psi\right\|_{L^2_x}.$$

Remark 4.3.2. If the external potential $U(x)$ were in $L^\infty(\mathbb{R}^d)$, it would be enough to work in the space $H^m(\mathbb{R}^d)$ instead of Σ^m. In the presence of an external subquadratic potential, however, we also require control of higher moments of the wave function ψ with respect to x.

The goal of this section is to show the following regularity result for solutions to (4.1).

Lemma 4.3.3. *Let $\lambda \geq 0$, $\sigma \in \mathbb{N}$ with $\sigma < 2/(d-2)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. For $m > d/2$, let $\psi_0 \in \Sigma^m$, and $V \in W^{m,\infty}(\mathbb{R}^d)$. Then the mild solution of* (4.1) *satisfies $\psi \in L^\infty(0,T;\Sigma^m)$.*

The proof of this lemma will require a local existence theory in Σ^m. This is the content of Lemma 4.3.7. The proof of Lemma 4.3.3 then consists of showing that the local solutions in Σ^m coincide with the (global) mild solutions in Σ. To proceed further, we need two technical results. The first concerns estimates on the nonlinearity in Σ^m.

Lemma 4.3.4. *Let $\sigma \in \mathbb{N}$, and $m > d/2$. Then there exists a constant $C > 0$, such that for all $\psi, \tilde{\psi} \in \Sigma^m$ it holds that*

$$\big\||\psi|^{2\sigma}\psi\|_{\Sigma^m} \leq C\|\psi\|_{L^\infty}^{2\sigma}\|\psi\|_{\Sigma^m}$$
$$\big\||\psi|^{2\sigma}\psi - |\tilde{\psi}|^{2\sigma}\tilde{\psi}\big\|_{\Sigma^m} \leq C\big(\|\psi\|_{L^\infty}^{2\sigma} + \|\tilde{\psi}\|_{L^\infty}^{2\sigma}\big)\|\psi - \tilde{\psi}\|_{\Sigma^m}.$$

In other words, $\psi \mapsto |\psi|^{2\sigma}\psi$ is locally Lipschitz in Σ^m.

Proof. Consider two multi-indices $j, k \in \mathbb{N}^d$ such that $n := |j| + |k| \leq m$ and any $\psi \in \Sigma^m$. Then it holds that $|x^j \partial^k \psi|$ is a sum of terms of the form

$$|x^j||\psi|^{2\sigma+1-r}\prod_{l=1}^{r}\big|\partial^{k^{(l)}}\psi\big| \tag{4.38}$$

for some $1 \leq r \leq 2\sigma+1$, and some multi-indices $k^{(l)}, l = 1, \ldots, r$ such that $\sum_{l=1}^r k^{(l)} = k$. Using Hölder's inequality, we bound the L^2–norm of each summand as follows:

$$\big\|x^j|\psi|^{2\sigma+1-r}\prod_{l=1}^{r}\partial^{k^{(l)}}\psi\big\|_{L^2} \leq \|x^j|\psi|^{2\sigma+1-r}\|_{L^{p_{r+1}}}\prod_{l=1}^{r}\big\|\partial^{k^{(l)}}\psi\big\|_{L^{p_l}},$$

where

$$p_l = \frac{2n}{|k^{(l)}|},\ l = 1, \ldots, r, \quad \text{and} \qquad p_{r+1} = \frac{2n}{|j|}.$$

It holds that

$$\begin{aligned}\big\|x^j|\psi|^{2\sigma+1-r}\big\|_{L^{p_{r+1}}} &= \Big\||x|^{\frac{|j|}{2}p_{r+1}}|\psi|^{\frac{2\sigma+1-r}{2}p_{r+1}}\Big\|_{L^2}^{\frac{2}{p_{r+1}}} \\ &\leq \|\psi\|_{L^\infty}^{2\sigma+1-r-\frac{2}{p_{r+1}}}\|x^n\psi\|_{L^2}^{\frac{2}{p_{r+1}}} \leq \|\psi\|_{L^\infty}^{2\sigma+1-r-\frac{|j|}{n}}\|\psi\|_{\Sigma^m}^{\frac{|j|}{n}}.\end{aligned}$$

Furthermore the Gagliardo–Nirenberg inequality yields

$$\big\|\partial^{k^{(l)}}\psi\big\|_{L^{p_l}} \leq C\|\psi\|_{L^\infty}^{1-\frac{|k^{(l)}|}{n}}\|\psi\|_{H^n}^{\frac{|k^{(l)}|}{n}}.$$

Since $|j| + \sum_l |k^{(l)}| = n \le m$, it follows that

$$\big\| x^j |\psi|^{2\sigma+1-r} \prod_{l=1}^{r} \partial^{k^{(l)}} \psi \big\|_{L^2} \le C \|\psi\|_{L^\infty}^{2\sigma} \|\psi\|_{\Sigma^m},$$

and hence

$$\big\| x^j \partial^k (|\psi|^{2\sigma}\psi) \big\|_{L^2} \le C \|\psi\|_{L^\infty}^{2\sigma} \|\psi\|_{\Sigma^m}.$$

Thus we conclude the proof of the first estimate of Lemma 4.3.4 by summing over all multi-indices k and j such that $|k| + |j| \le m$. The second estimate follows similarly once we apply the expansion

$$\prod_{l=1}^{r} a_l - \prod_{l=1}^{r} b_l = \sum_{l=1}^{r} \prod_{\tilde{l}<l} a_{\tilde{l}} \prod_{\tilde{l}>l} b_{\tilde{l}} (a_l - b_l)$$

to obtain

$$\begin{aligned}
& x^j |\psi|^{2\sigma+1-r} \prod_{l=1}^{r} \partial^{k^{(l)}} \psi - x^j |\tilde{\psi}|^{2\sigma+1-r} \prod_{l=1}^{r} \partial^{k^{(l)}} \tilde{\psi} \\
&= x^j \left(|\psi|^{2\sigma+1-r} - |\tilde{\psi}|^{2\sigma+1-r} \right) \prod_{l=1}^{r} \partial^{k^{(l)}} \psi \\
&\quad + x^j |\tilde{\psi}|^{2\sigma+1-r} \sum_{l=1}^{r} \prod_{\tilde{l}<l} \partial^{k^{(\tilde{l})}} \psi \prod_{\tilde{l}>l} \partial^{k^{(\tilde{l})}} \tilde{\psi} (\partial^{k^{(l)}} \psi - \partial^{k^{(l)}} \tilde{\psi}).
\end{aligned}$$

Then we can estimate each term separately using the estimates above. □

Remark 4.3.5. This technical lemma is ultimately the reason why we need to restrict ourselves to $\sigma \in \mathbb{N}$. If $\sigma \notin \mathbb{N}$, we cannot guarantee that $r \le 2\sigma + 1$ in (4.38) and hence $\|x^j |\psi|^{2\sigma+1-r}\|_{L^{p_{r+1}}}$ will not, in general, be bounded.

The second technical result yields a bound on the linear Schrödinger equation in Σ^m.

Lemma 4.3.6. *Let $S(t)$ be given by* (4.10) *with $U \in C^\infty(\mathbb{R}^d; \mathbb{R})$ and subquadratic. Then, there exists a constant $c > 0$ such that*

$$\|S(t)\psi_0\|_{\Sigma^m} \le e^{ct} \|\psi_0\|_{\Sigma^m},$$

for all $t \in [0, \infty)$ and $\psi_0 \in \Sigma^m$.

The proof can be found in Kitada [48, Theorem 6.3]. Next we use this technical lemma to prove local existence of mild solutions to equation (4.1) which lie in Σ^m.

Lemma 4.3.7. *Let $\lambda \ge 0$, $\sigma \in \mathbb{N}$ with $\sigma < 2/(d-2)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. For $m > d/2$, let $\psi_0 \in \Sigma^m$, and $V \in W^{m,\infty}(\mathbb{R}^d)$. Then there exists a $\tau > 0$ and a unique* *mild solution of* (4.1) *in* $\tilde{\psi} \in L^\infty(0,\tau;\Sigma^m)$. *If* $T_{\max}$ *is the finite time of existence and* $T_{\max}$ *happens to be finite, it holds that*

$$\limsup_{t\to T_{\max}} \|\psi(t)\|_{L^\infty} = +\infty,$$

which is the blow-up alternative for solutions in $L^\infty(0,\tau;\Sigma^m)$.

Proof. The proof is similar to the local existence proof of Lemma 3.3.2 and we only sketch it here. The proof in $H^m(\mathbb{R}^d)$ in the absence of a subquadratic potential can be found in [19, Theorem 4.10.1]. The idea is to find a mild solution as a fixed point of the map $\Phi : X_{\tau,R} \to X_{\tau,R}$ given by

$$\Phi(\psi)(t) = S(t)\psi_0 - i\int_0^t S(t-s)\left(\lambda|\psi(s)|^{2\sigma}\psi(s) + \alpha(s)V\psi(s)\right) ds,$$

in a suitable space $X_{\tau,R}$. Here we let

$$X_{\tau,R} := \left\{\psi \in L^\infty(0,\tau;\Sigma^m) : \|\psi\|_{L^\infty(0,\tau;\Sigma^m)} \le 2R\right\},$$

and set $R := \|\psi_0\|_{\Sigma^m}$. Lemma 4.3.4 and 4.3.6 immediately yield

$$\begin{aligned}(4.39)\quad \|\Phi(\psi)\|_{L^\infty(0,\tau;\Sigma^m)} &\le e^{c\tau}\|\psi_0\|_{\Sigma^m} \\ &\quad + C\int_0^\tau e^{\tau-s}\|\psi\|^{2\sigma}_{L^\infty(0,\tau;L^\infty)}\|\psi(s)\|_{L^\infty(0,\tau;\Sigma^m)}\, ds \le 2R,\end{aligned}$$

for all $\psi \in X_{\tau,R}$, if $\tau > 0$ is small enough. Furthermore, choosing τ possibly even smaller, it holds that

$$\begin{aligned}&\|\Phi(\psi) - \Phi(\tilde{\psi})\|_{L^\infty(0,\tau;\Sigma^m)} \\ &\qquad \le C\tau\Big(\|\psi\|^{2\sigma}_{L^\infty(0,\tau;\Sigma^m)} + \|\tilde{\psi}\|^{2\sigma}_{L^\infty(0,\tau;\Sigma^m)}\Big)\|\psi - \tilde{\psi}\|_{L^\infty(0,\tau;\Sigma^m)} < 1.\end{aligned}$$

Thus $\Phi : X_{\tau,R} \to X_{\tau,R}$ is indeed a contraction mapping and has a unique fixed point. This local solution can be extended as long as $\|\psi(t)\|_{\Sigma^m}$ stays bounded. The blow-up alternative follows from the fact that estimate (4.39) and Gronwall's inequality yield a bound on $\|\psi(t)\|_{\Sigma^m}$ as long as $\|\psi(t)\|_{L^\infty}$ remains bounded. □

Equipped with a local existence theory we now prove that the local solution $\tilde{\psi} \in L^\infty(0,\tau;\Sigma^m)$ coincides with the solution $\psi \in C([0,T];\Sigma)$, and hence the regularity in Σ^m propagates for all times $t \in [0,T]$.

Proof of Lemma 4.3.3. The proof now closely follows the proof of [19, Theorem 5.5.1]. For the sake of the reader's convenience, we state the proof in a self-contained form.

The Σ^m–solution is global on $[0,T]$ and indeed coincides with the Σ–solution if we can show that $\psi \in L^\infty(0,T;\Sigma^m)$. Let us first assume that $\psi \in L^{2\sigma}(0,T;L^\infty(\mathbb{R}^d))$. Then Lemma 4.3.4, Lemma 4.3.6, and the mild form of the NLS, cf. 4.18, yield

$$\|\psi(t)\|_{\Sigma^m} \leq C\|\psi_0\|_{\Sigma^m} + C\int_0^t \|\psi(s)\|_{L^\infty}^{2\sigma}\|\psi(s)\|_{\Sigma^m}\, ds$$

for all $t \in [0,T]$. Thus Gronwall's lemma yields

$$\|\psi(t)\|_{\Sigma^m} \leq C\exp\Big(C\int_0^t \|\psi(s)\|_{L^\infty}^{2\sigma}\, ds\Big),$$

which is bounded since $\psi \in L^{2\sigma}(0,T;L^\infty(\mathbb{R}^d))$. Therefore the solution indeed exists in $L^\infty(0,T;\Sigma^m)$.

It remains to prove $\psi \in L^{2\sigma}(0,T;L^\infty(\mathbb{R}^d))$. If $d = 1$, this follows directly from the embedding $H^1(\mathbb{R}) \hookrightarrow L^\infty(\mathbb{R})$, since $\psi \in L^\infty(0,T;H^1(\mathbb{R}^d))$. If $d \geq 2$, the local existence theory in Σ, which we will not repeat here (instead we refer to the proof of Lemma 3.3.2), yields that

$$\psi, x\psi, \nabla\psi \in L^{\frac{4\sigma+4}{d\sigma}}(0,T;L^{2\sigma+2}(\mathbb{R}^d)).$$

Now the same calculations, using Strichartz estimates, that yielded the existence of a solution via a fixed point argument, yield

$$\psi, x\psi, \nabla\psi \in L^p(0,T;L^q(\mathbb{R}^d))$$

for any admissible pair (p,q), cf. Lemma 3.3.3. Finally we choose some $d < q < 2d\sigma/(d\sigma - 2)$ and let p such that (p,q) is an admissible pair. This is indeed possible since $\sigma < 2/(d-2)$ ($\sigma < +\infty$, if $d = 2$), whence $d < 2d\sigma/(d\sigma - 2)$. It follows $p > 2\sigma$ and the embedding $W^{1,r}(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$ yields the desired property $\psi\ in L^{2\sigma}(0,T;L^\infty(\mathbb{R}^d))$. □

In the next subsection, we shall set up an existence theory for (4.35), which in turn will be used to rigorously justify the above derivation in Section 4.4 below.

4.3.3 Existence of solutions to the adjoint equation

Having obtained $\psi \in L^\infty(0,T;\Sigma^m)$, we infer $\psi \in L^\infty((0,T)\times\mathbb{R}^d)$ by the Sobolev embedding $H^m(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$ whenever $m > d/2$. Thus, all the ψ–dependent coefficients appearing in adjoint equation (4.35) are indeed in L^∞.

Remark 4.3.8. Note that Lemma 4.3.3 requires us to impose $\sigma \in \mathbb{N}$, which together with the condition $\sigma < 2/(d-2)$ necessarily implies $d \leq 3$. The reason is that for general $\sigma > 0$ (not necessarily an integer) the nonlinearity $|\psi|^{2\sigma}\psi$ is not locally Lipschitz in Σ^m

(cf. Lemma 4.3.4) and the life-span of solution $\psi(t,\cdot) \in \Sigma^m$ is in general not known, see [19] for more details.

From now on, we shall always assume that $V \in W^{m,\infty}(\mathbb{R}^d)$ for $m > d/2$ and $U \in C^\infty(\mathbb{R}^d)$ subquadratic. With the above regularity result at hand, classical semigroup theory [71] allows us to construct a solution to the adjoint problem.

Proposition 4.3.9. *Let $\lambda \geq 0$, $\sigma \in \mathbb{N}$ with $\sigma < 2/(d-2)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. For $m > d/2$, let $\psi_0 \in \Sigma^m$, $V \in W^{m,\infty}(\mathbb{R}^d)$. Then,* (4.35) *admits a unique mild solution*

$$\varphi \in C([0,T]; L^2(\mathbb{R}^d)).$$

Proof. First, we study the homogenous equation $\partial_\psi P(\psi(\alpha),\alpha)\xi = 0$, associated to (4.35). It can be written as

$$\partial_t \xi = -iH\xi + B(t)\xi,$$

where

$$B(t)\xi := -i\left(\lambda(\sigma+1)|\psi|^{2\sigma}\xi + \lambda\sigma|\psi|^{2\sigma-2}\psi^2\overline{\xi} + \alpha(t)V(x)\xi\right).$$

The operator $-iH : \Sigma^2 \to L^2(\mathbb{R}^d)$ is simply the generator of the Schrödinger group $S(t) = e^{-iHt}$. On the other hand, for any $t \in [0,T]$, $B(t)$ is a linear operator on the real vector space $L^2(\mathbb{R}^d)$, equipped with the inner product (4.12) (the same would not be true if we would consider $L^2(\mathbb{R}^d)$ as a complex vector space). In addition, $B(t)^* = B(t)$ is symmetric with respect to this inner product and the same is true for $iB(t)$. Since $V \in W^{m,\infty}(\mathbb{R}^d)$, $\alpha \in L^\infty(0,T)$ by assumption and $\psi \in L^\infty((0,T)\times\mathbb{R}^d)$ in view of Lemma 4.3.3, we infer $B \in L^\infty(0,T;\mathcal{L}(L^2(\mathbb{R}^d)))$. The operator $B(t)$ may therefore be considered as a (time-dependent) perturbation of the generator $-iH$. Following the construction given in Proposition 1.2, Chapter 3 of [71], we obtain the existence of a propagator $F(t,s)$, i.e. a family of bounded operators

$$\{F(t,s) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)\}_{s,t\in[0,T]}$$

which are strongly continuous in time and satisfy $F(t,s) = F(t,r)F(r,s)$. This propagator $F(t,s)$ is implicitly given by

$$F(t,s) = e^{-iH(t-s)} + \int_s^t e^{-iH(t-\tau)}B(\tau)F(\tau,s)\,d\tau. \tag{4.40}$$

It solves the homogeneous linearized equation in the sense that

$$\frac{d}{dt}F(t,s)\xi = \left(-iH + B(t)\right)F(t,s)\xi \tag{4.41}$$

weakly in $(\Sigma^2)^*$ for every $\xi \in L^2(\mathbb{R}^d)$ and almost every $t \in [0,T]$. Clearly, it provides a unique mild solution $\xi(t) = F(t,s)\varphi(s)$ of the homogenous equation. For the reader's convenience, we give here a detailed construction of $F(t,s)$. We iteratively set

$$F_0(t,s) := e^{-iH(t-s)}, \qquad F_{n+1}(t,s) := \int_s^t e^{-iH(t-\tau)} B(\tau) F_n(\tau,s)\, d\tau \tag{4.42}$$

for all $s,t \in [0,T]$. As a first step, we show that

$$\|F_n(s,t)\|_{\mathcal{L}(L^2)} \le \frac{\|B\|^n_{L^\infty(0,T;\mathcal{L}(L^2))}(t-s)^n}{n!}.$$

This is obviously true for $n = 0$. Assuming it is true for $n \in \mathbb{N}$, it follows from the definition of F_{n+1} that

$$\|F_{n+1}(s,t)\|_{\mathcal{L}(L^2)} \le \frac{\|B\|^{n+1}_{L^\infty(0,T;\mathcal{L}(L^2))}}{n!} \int_s^t (\tau - s)^n d\tau = \frac{\|B\|^{n+1}_{L^\infty(0,T;\mathcal{L}(L^2))}(t-s)^{n+1}}{(n+1)!}.$$

Hence the series

$$F(t,s) := \sum_{n=0}^{\infty} F_n(t,s) \tag{4.43}$$

converges absolutely in the operator topology of $\mathcal{L}(L^2(\mathbb{R}^d))$ with uniform convergence with respect to s and t on the (bounded) interval $[0,T]$. Hence the definitions (4.43) and (4.42) of F and F_n respectively, yield

$$\begin{aligned} F(t,s) &= \sum_{n=0}^{\infty} F_n(t,s) = e^{-iH(t-s)} + \sum_{n=0}^{\infty} F_{n+1}(t,s) \\ &= e^{-iH(t-s)} + \int_s^t e^{-iH(t-\tau)} B(\tau) \sum_{n=0}^{\infty} F_n(\tau,s)\, d\tau, \end{aligned}$$

due to the uniform in time convergence. Substituting the definition (4.43) of F, we obtain the desired expression (4.40). Differentiation of equation (4.40) indeed yields (4.41). Duhamel's formula applied to the adjoint problem (4.35) consequently yields

$$\varphi(t) = iF(t,T)\frac{\delta J(\psi,\alpha)}{\delta\psi(T)} + i\int_t^T F(t,s)\frac{\delta J(\psi,\alpha)}{\delta\psi(s)}\, ds. \tag{4.44}$$

Under our assumptions on ψ and A we have that

$$\frac{\delta J(\psi,\alpha)}{\delta\psi(t)} \in L^1(0,T;L^2(\mathbb{R}^d)), \quad \frac{\delta J(\psi,\alpha)}{\delta\psi(T)} \in L^2(\mathbb{R}^d),$$

which in view of Duhamel's formula (4.44) implies the existence of a mild solution

$\varphi \in C([0,T]; L^2(\mathbb{R}^d))$. Uniqueness follows from linearity and the uniqueness of the homogeneous equation. □

4.4 Rigorous characterization of critical points

A classical approach for making the derivation of the adjoint system rigorous is based on the implicit function theorem. The latter is used to show that $\partial_\psi P(\psi(\alpha),\alpha)$ is indeed invertible, but it requires the identification of a linear function space X such that

$$P : \Upsilon(0,T) \times H^1(0,T) \to X \ ; (\psi,\alpha) \mapsto P(\psi,\alpha),$$

and

$$\partial_\psi P(\psi,\alpha)^{-1} : X \to \Upsilon(0,T).$$

In other words, we require the solution of (4.35) with a right hand side in X to be in $\Upsilon(0,T)$. It seems, however, that the linearized operator $\partial_\psi P(\psi,\alpha)^{-1}$ is not sufficiently regularizing to allow for an easy identification of X. Therefore we shall not invoke the implicit function theorem but rather calculate the Gâteaux-derivative $\mathcal{J}'(\alpha)$ directly. (We do not prove Fréchet-differentiability; see Remark 4.4.3 below.) To this end, we shall first show that the solution $\psi = \psi(\alpha)$ to (4.1) depends Lipschitz-continuously on the control parameter α. This will henceforth be used to estimate the error terms appearing in the derivative of $\mathcal{J}(\alpha)$.

4.4.1 Lipschitz continuity with respect to the control

As a first step towards full Lipschitz continuity, we prove local-in-time Lipschitz continuity of $\psi = \psi(\alpha)$ with respect to the control parameter α.

Proposition 4.4.1. *Let $\lambda \geq 0$, $\sigma \in \mathbb{N}$ with $\sigma < 2/(d-2)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. For $m > d/2$, let $V \in W^{m,\infty}(\mathbb{R}^d)$ and $\tilde{\psi}, \psi \in L^\infty(0,T;\Sigma^m)$ be two mild solutions to* (4.1)*, corresponding to initial data $\tilde{\psi}_0, \psi_0 \in \Sigma^m$ and control parameters $\tilde{\alpha}, \alpha \in H^1(0,T)$, respectively. Assume that*

$$\|\tilde{\alpha}\|_{H^1_t}, \|\alpha\|_{H^1_t}, \|\tilde{\psi}(t,\cdot)\|_{\Sigma^m}, \|\psi(t,\cdot)\|_{\Sigma^m} \leq M$$

for some given $M \geq 0$. Then there exist $\tau = \tau(M) > 0$ and a constant $C = C(M) < +\infty$, such that

$$\|\tilde{\psi} - \psi\|_{L^\infty(I_t;\Sigma^m)} \leq C \left(\|\tilde{\psi}(t) - \psi(t)\|_{\Sigma^m} + \|\tilde{\alpha} - \alpha\|_{H^1_t} \right), \tag{4.45}$$

where $I_t := [t, t+\tau] \cap [0,T]$. *In particular, the mapping* $\alpha \mapsto \psi(\alpha) \in \Upsilon(0,T)$ *is continuous with respect to* $\alpha \in H^1(0,T)$.

Proof. To simplify notation, let us assume $t + \tau \leq T$. By construction, there exists a $\tau > 0$ depending only on M, such that $\psi|_{I_t}$ is a fixed point of the mapping

$$\psi \mapsto S(\,\cdot\,)\psi_0 - i \int_t^{\cdot} S(\cdot - s) \left(\lambda|\psi(s)|^{2\sigma}\psi(s) + \alpha(s)V\psi(s)\right)\, ds,$$

which maps the set

$$Y = \{\psi \in L^\infty(I_t; \Sigma^m) : \|\psi\|_{L^\infty(I_t;\Sigma^m)} \leq 2M\}$$

into itself. Of course, the same holds true for $\tilde{\psi}$ and $\tilde{\alpha}$ in place of ψ and α, respectively. In particular, the embedding $\Sigma^m(R^d) \hookrightarrow L^\infty(\mathbb{R}^d)$, $m > d/2$, yields

$$\|\psi\|_{L^\infty(I_t\times\mathbb{R}^d)} \leq 2CM.$$

Subtracting the two fixed point expressions for $\tilde{\psi}$ and ψ gives

$$\begin{aligned}\tilde{\psi}(s) - \psi(s) = {}& S(s-t)(\tilde{\psi}(t) - \psi(t)) \\ & - i \int_0^{s-t} S(s-r)\Big(\lambda(|\tilde{\psi}|^{2\sigma}\tilde{\psi} - |\psi|^{2\sigma}\psi) + V(x)(\tilde{\alpha}\,\tilde{\psi} - \alpha\,\psi)\Big)(\tau)\, d\tau\end{aligned}$$

for all $s \in [t, t+\tau]$. Taking the $L^\infty(I_t;\Sigma^m)$-norm and recalling Lemma 4.3.6, together with $\|\psi(s)\|_{\Sigma^m}, \|\tilde{\psi}(s)\|_{\Sigma^m} \leq 2M$, for $s \leq t+\tau$, yields

$$\begin{aligned}\|\tilde{\psi} - \psi\|_{L^\infty(I_t;\Sigma^m)} \leq {}& C\|\tilde{\psi}(t) - \psi(t)\|_{\Sigma^m} + 2M\|\tilde{\alpha} - \alpha\|_{H^1_t}\|V\|_{W^{m,\infty}_x} \\ & + C\tau\left(C(2M) + \|\tilde{\alpha}\|_{H^1_t}\|V\|_{W^{m,\infty}_x}\right)\|\tilde{\psi} - \psi\|_{L^\infty(t,t+\tau;\Sigma^m)},\end{aligned}$$

where $C(2M)$ is the constant appearing in Lemma 4.3.4 with $2M$ replacing M. Since $\|\tilde{\alpha}\|_{H^1_t} \leq M$, the estimate (4.45) follows from possibly choosing τ even smaller.
Finally, we show the continuity of the map $H^1(0,T) \to \Upsilon(0,T), \alpha \mapsto \psi(\alpha)$. Set

$$t_* := \inf\left\{0 \leq t \leq T : \limsup_{\tilde{\alpha}\to\alpha} \|\tilde{\psi} - \psi\|_{L^\infty(0,t;\Sigma^m)} > 0\right\},$$

with the convention $\inf\emptyset := +\infty$. We have to show that $t_* = +\infty$. Assuming $t_* \leq T < +\infty$, fix $M' \geq M$ such that $\|\psi\|_{L^\infty(0,T;\Sigma^m)} \leq M'$, let $\tau' = \tau(M'+1) > 0$ be chosen as above, with $M'+1$ replacing M. Furthermore let $\Delta t = \tau'/2$. The definition of of t_* yields

$$\limsup_{\tilde{\alpha}\to\alpha} \|\tilde{\psi} - \psi\|_{L^\infty(0,t_*-\Delta t;\Sigma^m)} = 0.$$

In particular, it holds that $\|\tilde{\psi}\|_{L^\infty(0,t_*-\Delta t;\Sigma^m)} \leq M' + 1$ for all $(\tilde{\alpha} - \alpha)$ small enough. But now we see that the Lipschitz continuity (4.45) is satisfied by $\tilde{\psi}$ and ψ and such controls $\tilde{\alpha}$, α on the interval $[t_* - \Delta t, t_* - \Delta t + \tau']$. Hence

$$\limsup_{\tilde{\alpha}\to\alpha} \|\tilde{\psi} - \psi\|_{L^\infty(0,t_*-\Delta t+\tau';\Sigma^m)} = 0,$$

a contradiction to the definition of t_*. Hence we must have $t_* = \infty$, and continuity holds. □

As a direct consequence of this continuity result, we obtain uniform boundedness of the solution $\psi(\alpha)$ on compact sets in $\alpha \in H^1(0,T)$. Of course, bounded sets in $H^1(0,T)$ are in general not compact and thus we have to restrict ourselves to finite-dimensional subsets.

Corollary 4.4.2. *Under the assumptions of Proposition 4.4.1, let* $\delta_\alpha \in H^1(0,T)$ *with* $\delta_\alpha(0) = 0$ *be a direction of change for* α *and let* $\psi(\alpha + \varepsilon\delta_\alpha)$ *be the solution to* (4.1) *with control* $\alpha + \varepsilon\delta_\alpha$ *and initial data* $\psi_0 \in \Sigma^m$, $m > d/2$. *Then there exists* $M < \infty$ *such that*

$$\|\psi(\alpha + \varepsilon\delta_\alpha)\|_{L^\infty(0,T;\Sigma^m)} \leq M, \quad \forall\, \varepsilon \in [-1,1].$$

Remark 4.4.3. This bound on finite dimensional subsets of $H^1(0,T)$ is the reason why we can only prove Gâteaux-differentiability. If we had a bound on $\psi(\alpha)$ in the Σ^m–norm which was uniform in $t \leq T$ and $\|\alpha\|_{H^1_t} \leq M$, we could prove Fréchet-differentiability. For our further analysis, however, this will not be of any consequence.

Now we are ready to prove Lipschitz-continuity of the solution $\psi(\alpha)$ with respect to the control parameter $\alpha \in H^1(0,T)$ on the whole control interval $[0,T]$.

Proposition 4.4.4. *Let* $\lambda \geq 0$, $\sigma \in \mathbb{N}$ *with* $\sigma < 2/(d-2)$, *and* $U \in C^\infty(\mathbb{R}^d)$ *be subquadratic. For* $m > d/2$, *let* $V \in W^{m,\infty}(\mathbb{R}^d)$, $\psi_0 \in \Sigma^m$, $\alpha \in H^1(0,T)$, *and* $\psi \equiv \psi(\alpha) \in L^\infty(0,T;\Sigma^m)$ *be the solution to* (4.1). *Set* $\tilde{\psi} \equiv \psi(\tilde{\alpha})$ *where for any* $\varepsilon \in [-1,1]$, *we let* $\tilde{\alpha} := \alpha + \varepsilon\delta_\alpha$ *with* $\delta_\alpha \in H^1(0,T)$ *such that* $\delta_\alpha(0) = 0$. *Then there exists a constant* $C > 0$, *such that*

$$\|\tilde{\psi} - \psi\|_{L^\infty(0,T;\Sigma^m)} \leq C\|\tilde{\alpha} - \alpha\|_{H^1(0,T)} = C|\varepsilon|\|\delta_\alpha\|_{H^1(0,T)}. \tag{4.46}$$

In other words, the solution to (4.1) *depends Lipschitz-continuously on the control* α *for each fixed direction* δ_α.

Proof. Since Corollary 4.4.2 provides a uniform (in ε) bound on $\|\tilde{\psi}\|_{L^\infty(0,T;\Sigma^m)}$, the quantity τ in the local Lipschitz estimate (4.45) is now independent of ϵ and t and the estimate indeed holds on every interval $[t, t+\tau]$, i.e.

$$\|\tilde{\psi} - \psi\|_{L^\infty(t,t+\tau;\Sigma^m)} \leq C\left(\|\tilde{\psi}(t) - \psi(t)\|_{\Sigma^m} + \|\tilde{\alpha} - \alpha\|_{H^1(t,t+\tau)}\right).$$

Since both solutions $\tilde{\psi}$ and ψ coincide at $t = 0$, finite summation of this estimate over intervals $[n\tau, (n+1)\tau]$ yields (4.46). □

4.4.2 Proof of differentiability and characterization of critical points

We are now in a position to state the second main result of this work.

Theorem 4.4.5. *Let $\lambda \geq 0$, $\sigma \in \mathbb{N}$ with $\sigma < 2/(d-2)$, and $U \in C^\infty(\mathbb{R}^d)$ be subquadratic. In addition, let $\psi_0 \in \Sigma^m$, $V \in W^{m,\infty}(\mathbb{R}^d)$ for some $m \in \mathbb{N}$, $m \geq 2$, and $\alpha \in H^1(0,T)$. Then the solution of* (4.1) *satisfies $\psi \in L^\infty(0,T;\Sigma^m)$ and the functional $\mathcal{J}(\alpha)$ is Gâteaux-differentiable for all $t \in [0,T]$, with*

$$\mathcal{J}'(\alpha) = \mathrm{Re} \int_{\mathbb{R}^d} \overline{\varphi}(t,x) V(x) \psi(t,x)\, dx - 2\frac{d}{dt}\left(\dot{\alpha}(t)\left(\gamma_2 + \gamma_1 \omega^2(t)\right)\right), \tag{4.47}$$

in the sense of distributions, where $\omega(t)$ is the weight factor defined in (4.9) *and $\varphi \in C([0,T];L^2(\mathbb{R}^d))$ is the solution of the adjoint equation*

$$\begin{aligned} i\partial_t \varphi = & -\frac{1}{2}\Delta\varphi + U(x)\varphi + \alpha(t)V(x)\varphi + \lambda(\sigma+1)|\psi|^{2\sigma}\varphi + \lambda\sigma|\psi|^{2\sigma-2}\psi^2\overline{\varphi} \\ & + 4\gamma_1 (\dot{\alpha}(t))^2\, \omega(t) V(x)\psi, \end{aligned} \tag{4.48}$$

subject to Cauchy data $\varphi(T,x) = 4i\langle \psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2_x} A\psi(T,x)$.

Remark 4.4.6. When compared to the assumptions of Theorem 4.2.1, the result of Theorem 4.4.5 requires additional regularity (and stronger decay) of the initial data ψ_0 and the potential V (plus, we need to restrict ourselves to $\sigma \in \mathbb{N}$). Note that the requirement $m \in \mathbb{N}$ and $m \geq 2$ implies $m > d/2$ for $d = 1,2,3$ spatial dimensions.

Proof. We need to prove that $\mathcal{J}'(\alpha)$ is of the form (4.4.2). For this purpose, let $\psi = \psi(\alpha)$, $\tilde{\psi} = \psi(\tilde{\alpha})$ with $\tilde{\alpha} = \alpha + \varepsilon\delta_\alpha$, satisfy the assumptions of Lemma 4.4.4 and consider the difference of the corresponding objective functionals $\mathcal{J}(\alpha), \mathcal{J}(\tilde{\alpha})$. This difference can be written as the sum of three terms

$$\mathcal{J}(\tilde{\alpha}) - \mathcal{J}(\alpha) = \mathrm{I} + \mathrm{II} + \mathrm{III},$$

where we define

$$\mathrm{I} := \langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle^2_{L^2_x} - \langle \psi(T), A\psi(T)\rangle^2_{L^2_x}, \quad \mathrm{II} := \gamma_2 \int_0^T (\dot{\tilde{\alpha}}(t))^2 - (\dot{\alpha}(t))^2\, dt,$$

and

$$\text{III} := \gamma_1 \int_0^T (\dot{\tilde{\alpha}}(t))^2 \left(\int_{\mathbb{R}^d} V(x) |\tilde{\psi}(t,x)|^2 \, dx \right)^2 dt \\ - \gamma_1 \int_0^T (\dot{\alpha}(t))^2 \left(\int_{\mathbb{R}^d} V(x) |\psi(t,x)|^2 \, dx \right)^2 dt.$$

The general strategy will be to use the Lipschitz property established in Lemma 4.4.4 and rewrite the terms I, II, and III in such a way that

$$\mathcal{J}(\tilde{\alpha}) - \mathcal{J}(\alpha) = \text{linear terms in } (\tilde{\alpha} - \alpha) + \mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}).$$

Since $\tilde{\alpha} = \alpha + \varepsilon \delta_\alpha$ and thus $\mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}) = \mathcal{O}(\varepsilon^2)$, the limit $\varepsilon \to 0$ then yields the desired functional derivative.

We start by considering the term I. It can be rewritten in the form

$$\begin{aligned} \text{I} &= \langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle^2_{L^2_x} - \langle \psi(T), A\psi(T)\rangle^2_{L^2_x} \\ &= 2\langle \psi(T), A\psi(T)\rangle_{L^2_x} \left(\langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle_{L^2_x} - \langle \psi(T), A\psi(T)\rangle_{L^2_x} \right) \\ &\quad + \left(\langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle_{L^2_x} - \langle \psi(T), A\psi(T)\rangle_{L^2_x} \right)^2. \end{aligned}$$

Using the essential self-adjointness of A, the terms within the parentheses yield

$$\begin{aligned} &\langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle_{L^2_x} - \langle \psi(T), A\psi(T)\rangle_{L^2_x} \\ &\quad = 2\langle \tilde{\psi}(T) - \psi(T), A\psi(T)\rangle_{L^2_x} + \langle \tilde{\psi}(T) - \psi(T), A(\tilde{\psi}(T) - \psi(T))\rangle_{L^2_x}. \end{aligned}$$

Using the Lipschitz-estimate (4.46), we obtain

$$\left| \langle \tilde{\psi}(T) - \psi(T), A(\tilde{\psi}(T) - \psi(T))\rangle_{L^2_x} \right| \leq \|A\|_{\mathcal{L}(\Sigma, L^2_x)} \|\tilde{\psi}(T) - \psi(T)\|^2_\Sigma \leq C\varepsilon^2 \|\delta_\alpha\|^2_{H^1_t},$$

and hence

$$\langle \tilde{\psi}(T), A\tilde{\psi}(T)\rangle_{L^2_x} - \langle \psi(T), A\psi(T)\rangle_{L^2_x} = 2\langle \tilde{\psi}(T) - \psi(T), A\psi(T)\rangle_{L^2_x} + \mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}).$$

Squaring the above result and plugging it into our expression for I consequently yields

$$\text{I} = 4\langle \psi(T), A\psi(T)\rangle_{L^2_x} \, \langle \tilde{\psi}(T) - \psi(T), A\psi(T)\rangle_{L^2_x} + \mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}). \tag{4.49}$$

Next we consider II, which can be written as

$$\begin{aligned}\mathrm{II} &= 2\gamma_2 \int_0^T \dot{\alpha}(t)\left(\dot{\tilde{\alpha}}(t) - \dot{\alpha}(t)\right) dt + \gamma_2 \int_0^T \left(\dot{\tilde{\alpha}}(t) - \dot{\alpha}(t)\right)^2 dt \\ &= 2\gamma_2 \int_0^T \dot{\alpha}(t)\left(\dot{\tilde{\alpha}}(t) - \dot{\alpha}(t)\right) dt + \mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}).\end{aligned}$$

The first term in the second line is thereby seen to be of the form given in (4.4.2). Finally we consider III, which in view of definition (4.9) can be written as

$$\begin{aligned}\mathrm{III} = \gamma_1 &\int_0^T \left((\dot{\tilde{\alpha}}(t))^2 - (\dot{\alpha}(t))^2\right)\omega^2(t)\, dt \\ &+ \gamma_1 \int_0^T (\dot{\tilde{\alpha}}(t))^2 \left(\left(\int_{\mathbb{R}^d} V(x)|\tilde{\psi}(t,x)|^2 dx\right)^2 - \omega^2(t)\right) dt.\end{aligned}$$

As before, we can expand these terms using quadratic expansions in both $\tilde{\psi}$ and $\tilde{\alpha}$. In view of the Lipschitz estimate (4.46), any quadratic error $\|\tilde{\psi} - \psi\|^2_{L^\infty_t L^2_x}$ is bounded by $\mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t})$ and hence we obtain

$$\begin{aligned}\mathrm{III} = 4\gamma_1 &\int_0^T (\dot{\alpha}(t))^2\, \omega(t) \left(\mathrm{Re} \int_{\mathbb{R}^d} \left((\overline{\tilde{\psi}} - \overline{\psi}) V \psi\right)(t,x)\, dx\right) dt \\ &+ \ 2\gamma_1 \int_0^T \left(\dot{\tilde{\alpha}}(t) - \dot{\alpha}(t)\right) \dot{\alpha}(t)\, \omega^2(t)\, dt + \mathcal{O}(\|\tilde{\alpha} - \alpha\|^2_{H^1_t}).\end{aligned} \tag{4.50}$$

Here the second term on the right hand side is linear in $(\tilde{\alpha} - \alpha)$ and hence of the desired form. In order to treat the first term, we note that the expression

$$4\gamma_1 \left((\dot{\alpha}(t))^2 \int_{\mathbb{R}^d} V(x)|\psi(t,x)|^2\, dx\right) V(x)\psi(t,x)$$

appears as a source term in the adjoint equation (4.48). Thus we obtain

$$\begin{aligned}4\gamma_1 &\int_0^T (\dot{\alpha}(t))^2\, \omega(t) \left(\mathrm{Re} \int_{\mathbb{R}^d} \left((\overline{\tilde{\psi}} - \overline{\psi}) V \psi\right)(t,x)\, dx\right) dt \\ &= \mathrm{Re} \int_0^T \int_{\mathbb{R}^d} \overline{\varphi}(t,x) \left(\partial_\psi P(\psi,\alpha)(\tilde{\psi} - \psi)\right)(t,x)\, dx \\ &\quad - \mathrm{Re} \int_{\mathbb{R}^d} i\, \overline{\varphi}(T,x)\big(\tilde{\psi}(T,x) - \psi(T,x)\big) dx,\end{aligned} \tag{4.51}$$

where we recall that $\partial_\psi P(\psi, \alpha)$ denotes the linearized Schrödinger operator obtained in (4.31). The last term on the right hand side of (4.51) stems from the boundary condition at $t = T$. Note that the boundary term at $t = 0$ vanishes since $\tilde{\psi}(0) = \psi_0 = \psi(0)$ by assumption. We recall that $\varphi \in C([0,T]; L^2(\mathbb{R}^d))$ and

$$\tilde{\psi}, \psi \in L^\infty(0,T;\Sigma^m) \cap W^{1,\infty}(0,T;\Sigma^{m-2}), \quad \text{with } m \geq 2,$$

and hence the right hand side of (4.51) is well-defined. In addition, since both $\tilde{\psi}$ and ψ solve the nonlinear Schrödinger equation (4.1), we can write

$$\begin{aligned}\partial_\psi P(\psi,\alpha)(\tilde{\psi}-\psi) &= i\partial_t(\tilde{\psi}-\psi) - H(\tilde{\psi}-\psi) - V(x)(\tilde{\alpha}(t)\tilde{\psi} - \alpha(t)\psi)\\ &\qquad + \lambda|\psi|^{2\sigma}\psi - \lambda|\tilde{\psi}|^{2\sigma}\tilde{\psi} + (\tilde{\alpha}(t)-\alpha(t))V(x)\tilde{\psi} + \varrho(\tilde{\psi},\psi)\\ &= (\tilde{\alpha}(t)-\alpha(t))V(x)\tilde{\psi} + \varrho(\tilde{\psi},\psi),\end{aligned} \tag{4.52}$$

where the remainder $\varrho(\tilde{\psi},\psi)$ is given by

$$\frac{1}{\lambda}\varrho(\tilde{\psi},\psi) = |\tilde{\psi}|^{2\sigma}\tilde{\psi} - |\psi|^{2\sigma}\psi - (\sigma+1)|\psi|^{2\sigma}(\tilde{\psi}-\psi) - \sigma|\psi|^{2\sigma-2}\psi^2\left(\overline{\tilde{\psi}} - \overline{\psi}\right).$$

Since $2\sigma \geq 2$ by assumption, $\|\tilde{\psi}\|_{L^\infty_t L^\infty_x}, \|\psi\|_{L^\infty_t L^\infty_x} \leq C$ in view of Corollary 4.4.2, and $\Sigma^m \hookrightarrow L^\infty(\mathbb{R}^d)$, the remainder can be bounded by

$$|\varrho(\tilde{\psi},\psi)| \leq C\left(|\tilde{\psi}|^{2\sigma-1} + |\psi|^{2\sigma-1}\right)|\tilde{\psi}-\psi|^2 \leq C|\tilde{\psi}-\psi|^2.$$

In addition, since $\varphi \in C([0,T]; L^2(\mathbb{R}^d))$ and $\Sigma^m \subset H^m(\mathbb{R}^d) \hookrightarrow L^4(\mathbb{R}^d)$, we find that

$$\int_{\mathbb{R}^d} |\varphi(t,x)||\tilde{\psi}(t,x)-\psi(t,x)|^2\,dx \leq \|\varphi\|_{L^\infty_t L^2_x}\|\tilde{\psi}-\psi\|^2_{L^\infty_t L^4_x} = O(\|\tilde{\alpha}-\alpha\|^2_{H^1_t}).$$

Furthermore, the contribution of $(\tilde{\alpha}(t)-\alpha(t))V(x)\tilde{\psi}$ in (4.52) equals

$$(\tilde{\alpha}(t)-\alpha(t))V(x)\psi + (\tilde{\alpha}(t)-\alpha(t))V(x)(\tilde{\psi}-\psi),$$

where the latter term can be estimated by $O(\|\tilde{\alpha}-\alpha\|^2_{H^1_t})$ as before. In summary, this shows that

$$\begin{aligned}(4.51) = \int_0^T (\tilde{\alpha}(t)-\alpha(t))\mathrm{Re}\int_{\mathbb{R}^d}\overline{\varphi}(t,x)V(x)\psi(t,x)dxdt + O(\|\tilde{\alpha}-\alpha\|^2_{H^1_t})\\ - 4\langle\psi(T), A\psi(T)\rangle_{L^2_x}\,\langle\tilde{\psi}(T)-\psi(T), A\psi(T)\rangle_{L^2_x},\end{aligned} \tag{4.53}$$

where we have used the fact that the data of the adjoint problem at $t = T$ is given by

$$\varphi(T,x) = 4i\langle\psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2_x}\,A\psi(T,x).$$

Thus, we infer that, up to quadratic errors, the second line in (4.53) cancels with the terms obtained in (4.49). Collecting all the expressions obtained for I, II, III and taking the limit $\varepsilon \to 0$, we have shown that $\mathcal{J}(\alpha)$ is Gâteaux-differentiable with derivative $\mathcal{J}'(\alpha)$ given by (4.4.2). This concludes proof of Theorem 4.4.5. □

Equation (4.47) yields the following characterization of the critical points $\alpha_* \in H^1(0,T)$, i.e. points where $\mathcal{J}'(\alpha_*) = 0$.

Corollary 4.4.7. *Let ψ_* be the solution of (4.1) with control α_*. Also, let φ_* be the corresponding solution of the adjoint equation (4.48), and denote by ω_* the function defined in (4.9) with ψ replaced by ψ_*. Then $\alpha_* \in C^2(0,T)$ is a classical solution of the following ordinary differential equation*

$$\frac{d}{dt}\left(\dot\alpha_*(t)\left(\gamma_2 + \gamma_1\omega_*^2(t)\right)\right) = \frac{1}{2}\,\mathrm{Re}\int_{\mathbb{R}^d} \overline{\varphi_*}(t,x)V(x)\psi_*(t,x)\,dx, \tag{4.54}$$

subject to $\alpha_*(0) = \alpha_0$, $\dot\alpha_*(T) = 0$.

Remark 4.4.8. In the case $\gamma_1 = 0$ this simplifies to the expression used in the physics literature; cf. [40].

Proof. Let $\mu \in C_0^\infty(0,T)$ be a test function with compact support in $(0,T)$. Then, Theorem 4.2.1 and Theorem 4.4.5 imply that there exists $\alpha_* \in H^1(0,T)$ such that $\mathcal{J}'(\alpha_*) = 0$, satisfying (4.47) in the sense of distributions, i.e.

$$\int_0^T \dot\alpha_*(t)\dot\mu(t)\left(\gamma_2 + \gamma_1\omega_*^2(t)\right)dt = \frac{1}{2}\mathrm{Re}\int_0^T\int_{\mathbb{R}^d}\mu(t)\overline{\varphi_*}(t,x)V(x)\psi_*(t,x)dxdt,$$

where we have used the fact that the boundary terms at $t=0$ and $t=T$ vanish due to the compact support of $\mu(t)$. We shall show that the weak solution α_* is in fact unique. This can be seen by considering two different $\alpha_*^1(t), \alpha_*^2(t)$, satisfying $\alpha_*^1(0) = \alpha_*^2(0) = \alpha_0$. Denoting their difference by $\beta_* = \alpha_*^1 - \alpha_*^2$, we have that $\beta_*(t)$ solves

$$\int_0^T \dot\beta_*(t)\dot\mu(t)\left(\gamma_2 + \gamma_1\omega_*^2(t)\right)dt = 0, \quad \text{for all } \mu \in C_0^\infty(0,T).$$

Since $\gamma_2 > 0$ and $\gamma_1 \geq 0$, this implies that $\dot\beta_*(t) = 0$ in the sense of distributions. However, since $\alpha_*^1, \alpha_*^2 \in H^1(0,T) \hookrightarrow C(0,T)$, we conclude that $\beta_* \in C(0,T)$ and thus $\beta_*(t) = \text{const}$ for all $t \in [0,T]$. Since $\beta_*(0) = 0$ by assumption, we infer uniqueness of the weak solution $\alpha_*(t)$. On the other hand, standard arguments imply that (4.54) admits a unique classical solution $\alpha_* \in C^2(0,T)$, provided $\omega_* \in C^1(0,T)$ and the (source term on the) right hand side is continuous in time. The latter is obviously true in view of Proposition 4.2.4 and Proposition 4.3.9. In addition, since $V \in W^{1,\infty}(\mathbb{R}^d)$, we infer that for all $\psi(t) \in \Sigma$ it holds that $\chi(t) := (V(x)\psi(t)) \in \Sigma$. From Proposition 4.2.4 it follows that

$$\dot\omega_*(t) = 2\mathrm{Re}\int_{\mathbb{R}^d} V(x)\partial_t\psi_*(t,x)\overline{\psi_*}(t,x)\,dx = 2\langle\chi(t), \dot\psi_*(t)\rangle_{\Sigma,\Sigma^*} < +\infty.$$

Thus, $\omega(t) \in C^1(0,T)$, yielding the existence of a unique classical solution $\alpha_* \in C^2(0,T)$. We therefore conclude that the unique weak solution α_* obtained above is in fact a classical solution, satisfying (4.54) subject to $\alpha_*(0) = \alpha_0$, $\dot{\alpha}_*(T) = 0$. □

We call $\alpha_* \in H^1(0,T)$ a *critical* or *stationary* point of the problem

$$\text{minimize} \quad \mathcal{J}(\alpha) \quad \text{over} \quad \alpha \in H^1(0,T), \tag{4.55}$$

if $\mathcal{J}'(\alpha_*) = 0$, where $\mathcal{J}'$ is given in Theorem 4.4.5. In order the check computationally whether α_* is critical, one needs to solve (4.1) for $\alpha = \alpha_*$ to obtain ψ_* and then the adjoint equation (4.48) with $\psi = \psi_*$ and $\alpha = \alpha_*$ to compute φ_*. Inserting $(\alpha, \psi, \varphi) = (\alpha_*, \psi_*, \varphi_*)$ in (4.47) yields $\mathcal{J}'(\alpha_*)$ which has to vanish for α_* to be critical, i.e., (4.54) is satisfied. We therefore call (4.1), (4.48) and (4.54) the first order optimality conditions associated with (4.55).

4.5 Numerical simulation of the optimal control problem

For our numerical treatment we simplify to the case $d = \sigma = 1$. In this case, the first order optimality conditions for our optimal control problem are given by:

$$\begin{cases} \dfrac{d}{dt}\left(\dot{\alpha}(t)\left(\gamma_2 + \gamma_1\omega^2(t)\right)\right) = \dfrac{1}{2}\operatorname{Re}\displaystyle\int_{\mathbb{R}^d} \overline{\varphi(t,x)}V(x)\psi(t,x)\,dx, \\ i\partial_t\psi + \dfrac{1}{2}\partial_x^2\psi = (U(x) + \alpha(t)V(x))\psi + \lambda|\psi|^2\psi, \\ i\partial_t\varphi + \dfrac{1}{2}\partial_x^2\varphi = (U(x) + \alpha(t)V(x))\varphi + 2\lambda|\psi|^2\varphi + \lambda\psi^2\overline{\varphi} + 4\gamma_1(\dot{\alpha})^2\,\omega(t)V(x)\psi, \end{cases}$$

subject to the following conditions: $\alpha(0) = \alpha_0$, $\dot{\alpha}(T) = 0$, and

$$\psi(0,x) = \psi_0(x), \quad \varphi(T,x) = 4i\langle\psi(T,\cdot), A\psi(T,\cdot)\rangle_{L^2_x} A\psi(T,x).$$

In our numerical simulations, we solve the minimization problem (4.55) iteratively, constructing a minimizing sequence $(\alpha_k)_k \subset H^1(0,T)$. We determine a sequence of descent directions $(\delta_\alpha^k)_k \subset H^1(0,T)$, i.e., for every $k \in \mathbb{N}$

$$\mathcal{J}(\alpha_k + \delta_\alpha^k) < \mathcal{J}(\alpha_k) = J(\psi(\alpha_k), \alpha_k) \tag{4.56}$$

is satisfied, where the iteration is given by $\alpha_{k+1} = \alpha_k + \delta_\alpha^k$. If α_k is such that there is no descent direction, α_k is indeed a (local) minimum of $\mathcal{J}$ and $\psi(\alpha_k)$ is the corresponding (locally) optimal solution to the NLS (4.1).

We solve the resulting Cauchy problems for Schrödinger–type equations by a *time-splitting spectral method* of second order (Strang-splitting), as can be found in Section 3.5 or, for instance, in [7]. This computational approach is unconditionally stable and allows for spectral accuracy in the resolution of the wave function $\psi(t,x)$. This is needed due to the highly oscillatory nature of solutions to (nonlinear) Schrödinger–type equations. We consequently perform our simulations on a *numerical domain* $\Omega \subset \mathbb{R}$, equipped with periodic boundary conditions. The trapping potential $U(x)$ is thereby chosen such that the "effective" (i.e. the numerically relevant) support of the wave function $\psi(t,x)$ stays away from the boundary. In doing so, the boundary conditions do not significantly influence our results. A good test of the accuracy of our numerical code is given by the fact that the Gross-Pitaevskii equation conserves the physical mass (i.e. the L^2-norm of $\psi(t)$). Indeed, in all our numerical examples presented in Section 4.5.3 below, we find that the L^2-norm is numerically preserved up to relative errors of the order 10^{-13}.

4.5.1 Gradient-related descent method

Once a suitable solver for the state and the adjoint equations is at hand, our gradient-related descent scheme operates as follows. Given $\alpha^k \in H^1(0,T)$, determine δ_α^k such that the condition (4.56) is satisfied. A simple Taylor expansion of $\mathfrak{J}$ around α_k shows that

$$\langle \mathfrak{J}'(\alpha_k), \delta_\alpha^k \rangle < 0$$

is sufficient for δ_α^k to be a descent direction for $\mathfrak{J}$ at α_k. We are in particular interested in gradient-related descent directions which satisfy

$$M\delta_\alpha^k = -\mathfrak{J}'(\alpha_k), \text{ where } M : H^1(0,T) \to H^1(0,T)^*$$

is a suitably chosen positive definite operator.

A rather straightforward choice of M is given by $M = \partial_\alpha^2 J(\psi, \alpha_k)$. In this case δ_α^k is obtained as the solution of the following ordinary differential equation (of second order):

$$\mathfrak{J}'(\alpha_k) = 2\frac{d}{dt}\left(\dot{\delta}_\alpha^k(t)\left(\gamma_2 + \gamma_1\left(\int_{\mathbb{R}} V(x)|\psi_k(t,x)|^2 dx\right)^2\right)\right),$$

with $\delta_\alpha^k(0) = 0$ and $\dot{\delta}_\alpha^k(T) = 0$. Here $\psi_k(t,x)$ denotes the solution of the Gross–Pitaevskii equation with $\alpha(t) = \alpha_k(t)$. With this choice of a descent direction, we then perform a *line search* in order to decide on the length of the step taken along δ_α^k. In fact, we seek for $\nu_k > 0$ such that

$$\mathfrak{J}(\alpha_k + \nu_k \delta_\alpha^k) \leq \mathfrak{J}(\alpha_k) + \mu\nu_k \langle \mathfrak{J}'(\alpha_k), \delta_\alpha^k \rangle \tag{4.57}$$

with some fixed $\mu \in (0,1)$. Within each line search, we determine ν_k iteratively by a backtracking strategy. Starting from $\nu_k^{(0)} > 0$, we iteratively test the condition (4.57); if it holds for $\nu_k^{(\ell)}$, then we accept $\alpha_{k+1} := \alpha_k + \nu_k^{(\ell)}\delta_\alpha^k$, and if not, we choose $\nu_k^{(\ell+1)} < \nu_k^{(\ell)}$ and repeat. Thus, the whole procedure amounts to an Armijo line search method with backtracking. Of course, more elaborate strategies based on interpolation or alternative line search criteria are possible; see for instance [69] for more details.

We stop the gradient descent method whenever

$$\|\mathfrak{J}'(\alpha_k)\|_{H_t^{-1}} \leq \mathrm{TOL} \cdot \|\mathfrak{J}'(\alpha_1)\|_{H_t^{-1}} \tag{4.58}$$

is satisfied for the first time. Here, $\mathrm{TOL} \in (0,1)$ is a given stopping tolerance and $\alpha_1 \in H^1(0,T)$ is the initial guess satisfying the boundary conditions $\alpha_1(0) = \alpha_0$ and $\dot{\alpha}_1(T) = 0$. As a safeguard, also an upper bound on the number of iterations is implemented.

In our tests, we observe the usual behavior of steepest descent type algorithms, i.e., the method exhibits rather fast progress towards a stationary point in early iterations, but then suffers from scaling effects reducing the convergence speed. Therefore, often the maximum number of iterations is reached. Thus, we connect the first-order, gradient method to a Newton-type method which relies on second derivatives or approximations thereof.

4.5.2 Newton method

The majority of iterations within our simulations are performed via a second order method, *Newton's method*, for which we use the full Hessian

$$M := D_\alpha^2 \mathfrak{J}(\alpha_k) : H^1(0,T) \times H^1(0,T) \to \mathbb{R},$$

or a sufficiently close positive definite approximation thereof. Note that we can also consider the Hessian as a map $D_\alpha^2\mathfrak{J} : H^1(0,T) \to H^1(0,T)^*$. Recall that the gradient-related method above simply uses $M = \partial_\alpha^2 J(\psi, \alpha_k)$.

We derive $D_\alpha^2\mathfrak{J}$ formally form the Lagrangian formulation; see Remark 4.3.1. The Lagrangian is given by

$$L(\psi, \alpha, \varphi) = J(\psi, \alpha) - \langle \varphi, P(\psi, \alpha)\rangle_{L^2_{t,x}},$$

where φ is the solution to the adjoint equation (4.48) and $P(\psi, \alpha)$ is the Gross–Pitaevksii operator written in abstract form. Proceeding formally, we find

$$\begin{aligned}\langle (D_\alpha^2\mathfrak{J})\delta_\alpha, \tilde{\delta}_\alpha\rangle_{L^2_t} = {}& \langle (\partial_\psi^2 L)\delta_\psi, \tilde{\delta}_\psi\rangle_{L^2_{t,x}} + \langle (\partial_{\psi\alpha} L)\delta_\alpha, \tilde{\delta}_\psi\rangle_{L^2_{t,x}} \\ &+ \langle (\partial_{\alpha\psi} L)\tilde{\delta}_\alpha, \delta_\psi\rangle_{L^2_t} + \langle (\partial_\alpha^2 L)\delta_\alpha, \tilde{\delta}_\alpha\rangle_{L^2_t},\end{aligned}$$

where δ_ψ and $\tilde{\delta}_\psi$ solve the linearized Gross–Pitaevksii equation with controls $\delta_\alpha, \tilde{\delta}_\alpha$, respectively. In view of the derivation given in Section 4.3.1 we have

$$\delta_\psi = \psi'(\alpha)\delta_\alpha = -\partial_\psi P(\psi(\alpha),\alpha)^{-1}\partial_\alpha P(\psi(\alpha),\alpha)\delta_\alpha,$$

and analogously for $\tilde{\delta}_\psi$. Hence we conclude that

$$\begin{aligned}(4.59)\qquad \langle (D^2_\alpha \mathfrak{J})\delta_\alpha, \tilde{\delta}_\alpha\rangle_{L^2_t} &= \langle (\partial^2_\psi J)\psi'(\alpha)\delta_\alpha, \psi'(\alpha)\tilde{\delta}_\alpha\rangle_{L^2_{t,x}} + \langle (\partial_{\alpha\psi} J)\delta_\alpha, \psi'(\alpha)\tilde{\delta}_\alpha\rangle_{L^2_{t,x}}\\ &+ \langle (\partial_{\psi\alpha} J)\psi'(\alpha)\delta_\alpha, \tilde{\delta}_\alpha\rangle_{L^2_t} + \langle (\partial^2_\alpha J)\delta_\alpha, \tilde{\delta}_\alpha\rangle_{L^2_t} - \langle \varphi, \big(D^2_\alpha P(\psi,\alpha)\delta_\alpha\big)\tilde{\delta}_\alpha\rangle_{L^2_{t,x}},\end{aligned}$$

where

$$\begin{aligned}(D^2_\alpha P(\psi,\alpha)\delta_\alpha)\tilde{\delta}_\alpha &= \big(\partial^2_\psi P(\psi,\alpha)(\psi'(\alpha)\delta_\alpha)\big)(\psi'(\alpha)\tilde{\delta}_\alpha)\\ &+ \big(\partial_{\alpha\psi} P(\psi,\alpha)\delta_\alpha\big)(\psi'(\alpha)\tilde{\delta}_\alpha) + \big(\partial_{\psi\alpha} P(\psi,\alpha)(\psi'(\alpha)\delta_\alpha)\big)\tilde{\delta}_\alpha,\end{aligned}$$

since $\partial^2_\alpha P(\psi,\alpha) = 0$. All of the terms appearing on the right hand side of (4.59) can be evaluated by replacing $\psi'(\alpha)\delta_\alpha$ by $-\partial_\psi P(\psi,\alpha)^{-1}\partial_\alpha P(\psi,\alpha)\delta_\alpha$. Consequently for calculating the action of the Hessian this requires to solve several linearized Schrödinger-type equations with different source terms and boundary data. For example, the term involving $(\partial_{\alpha\psi} J)$ can be evaluated by using

$$\chi := \partial_\psi P(\psi,\alpha)^{-*}((\partial_{\alpha\psi} J)\delta_\alpha),$$

which solves the following Cauchy problem

$$i\partial_t \chi + \frac{1}{2}\partial^2_x \chi = U(x)\chi + \alpha(t)V(x)\chi + 2\lambda|\psi|^2\chi + \lambda\psi^2\overline{\chi} + 8\gamma_1 h(t,x)\psi,$$

where $h(t,x) := \omega(t)\dot{\alpha}(t)\dot{\delta}_\alpha(t)V(x)$ and

$$\chi(T,x) = \frac{\delta^2 J(\psi,\alpha)}{\delta\psi(T,x)\,\delta\alpha(T)} = 0.$$

Bearing this in mind, we have to solve the following equation for $\delta^k_\alpha \in H^1(0,T)$:

$$(4.60)\qquad M\delta^k_\alpha = D^2_\alpha \mathfrak{J}\delta^k_\alpha = -\mathfrak{J}'(\alpha_k) \in H^1(0,T)^*.$$

Hence, we need to invert $D^2_\alpha \mathfrak{J}$, which, in view of (4.59) is not directly possible. Rather we resort to an iterative method, the *preconditioned MINRES algorithm*, see [70], with the preconditioner $(\partial^2_\alpha J(\psi,\alpha))^{-1} : H^1(0,T)^* \to H^1(0,T)$.

Remark 4.5.1. (1) Note that $D^2_\alpha \mathfrak{J}$ maps $H^1(0,T)$ to $H^1(0,T)^*$ and thus makes it necessary to precondition the iterative MINRES algorithm with a map $H^1(0,T) \to H^1(0,T)^*$.

The choice $\partial_\alpha^2 J(\psi(\alpha_k), \alpha_k)$ is easy to implement and can be expected to contain some of the features of the full Hessian $D_\alpha^2 \mathfrak{J}$, thus making the inversion problem for the MINRES algorithm better-conditioned.
(2) We choose here the MINRES algorithm over alternatives like the conjugated gradient (CG) method, because the Hessian $D_\alpha^2 \mathfrak{J}$ is symmetric but not necessarily positive definite. In this setting the MINRES algorithm is superior to the CG-method. Note that the partial derivative $\partial_\alpha^2 J(\psi(\alpha_k), \alpha_k)$ is indeed positive definite and therefore is a valid preconditioner.
(3) The map $\partial_\alpha^2 J(\psi(\alpha_k), \alpha_k)$ can also be understood as inducing a scalar product in the dual space $H^1(0,T)^*$. The correspondence between the scalar product in the dual space and the preconditioner of the MINRES algorithm has been investigated in [35].

The description of the MINRES-algorithm is given in Algorithm 1. Setting $\mathfrak{A} := D_\alpha^2 \mathfrak{J}(\alpha_k)$, $\mathfrak{R} := \partial_\alpha^2 J(\psi(\alpha_k), \alpha_k)^{-1}$, and $r_0 := -\mathfrak{J}'(\alpha_k)$, it seeks at the ℓ-th step to minimize the residual r^ℓ of $\mathfrak{A}\delta_{\alpha\ell} + \mathfrak{J}'(\alpha_k)$ with respect to the norm $\langle r^\ell, \mathfrak{R} r^\ell \rangle$ over all $\delta_\alpha \in r_0 + \operatorname{span}\{\mathfrak{A} r_0, \dots, \mathfrak{A}^\ell r_0\}$ using the result of the previous step. Here and in the description of Algorithm 1 the brackets $\langle \cdot, \cdot \rangle$ denote the dual product between $H^1(0,T)$ and $H^1(0,T)^*$.

We emphasize that here we aim to study the behavior of solutions of our control problem rather than at optimizing the respective solution algorithm or its implementation.

4.5.3 Numerical examples

In all our examples, we choose the numerical domain $\Omega = [-L, L]$ with $L = 20$ and periodic boundary conditions. The number of spatial grid points is $N = 256$. In addition, we set the final control time to be $T = 10$, and we use $M = 1024$ equidistant time steps. In order to avoid the influence of the boundary, we choose a trapping potential $U(x) = 30\left(\frac{x}{L}\right)^2$. The initial guess for the control is taken to be just $\alpha_1 \equiv 0$ in the linear case ($\lambda = 0$), whereas each algorithm in the nonlinear case ($\lambda \neq 0$) is started from the control obtained by solving the linear problem. In our tests of the first-order gradient method, we choose $\mathrm{TOL} = 10^{-8}$ in the terminating condition (4.58) for the whole algorithm, $\mu = 10^{-3}$, and a maximum number of 20000 iterations. For the Newton method, we likewise set $\mathrm{TOL} = 10^{-8}$ and we stop the algorithm after at most 45 Newton steps.

Example: shifting a linear wave packet

For validation purposes, we consider the time-evolution of a *linear* wave packet, i.e. $\lambda = 0$, whose center of mass we aim to shift towards a prescribed point $y_1 \in [-L, L]$. For this

Algorithm 1: Preconditioned MINRES algorithm

Given $\delta^k_{\alpha 0}$, set $r_0 := -\mathfrak{A}\delta^k_{\alpha 0} - \mathcal{J}'(\alpha_k)$, $z_1 = \mathfrak{R}r_0$, $\beta_1 = \langle r_0, z_1\rangle^{\frac{1}{2}}$, $z_1 = \frac{z_1}{\beta_1}$, $v_1 = \frac{r_0}{\beta_1}$,
$\gamma_0 = \gamma_1 = 1$, $\sigma_0 = \sigma_1 = 0$, $\eta = \beta_1$ **foreach** $\ell = 1, 2, \ldots$ **do**
  if $\eta < \mathrm{TOL}_{MINRES}$ **then**
    Stop, $\delta^k_\alpha := \delta^k_{\alpha\ell}$ is the solution to (4.60).
  else
    Set $\mu_\ell = \langle z_\ell, \mathfrak{R}z_\ell\rangle$,
    $v_{\ell+1} = \mathfrak{A}z_\ell - \beta_\ell v_\ell - \mu_\ell v_\ell$,
    $z_{\ell+1} = \mathfrak{R}v_{\ell+1}$,
    $\beta_{\ell+1} = \langle z_{\ell+1}, \mathfrak{R}z_{\ell+1}\rangle^{\frac{1}{2}}$,
    $z_{\ell+1} = \frac{z_{\ell+1}}{\beta_{\ell+1}}$,
    $v_{\ell+1} = \frac{v_{\ell+1}}{\beta_{\ell+1}}$,
    $\rho_0 = \gamma_\ell\mu_\ell - \sigma_\ell\gamma_{\ell-1}\beta_\ell$,
    $\rho_1 = \sqrt{\rho_0^2 + \beta_{\ell+1}^2}$,
    $\rho_2 = \sigma_\ell\mu_\ell + \gamma_{\ell-1}\gamma_\ell\beta_\ell$,
    $\rho_3 = \sigma_{\ell-1}\beta_\ell$,
    $\gamma_{\ell+1} = \frac{\rho_0}{\rho_1}$,
    $\sigma_{\ell+1} = \frac{\beta_{\ell+1}}{\rho_1}$,
    $w_{\ell+1} = \frac{1}{\rho_1}\big(z_{\ell+1} - \rho_3 w_{\ell-1} - \rho_2 w_\ell\big)$,
    $x_{\ell+1} = x_\ell + \gamma_{\ell+1}\eta w_{\ell+1}$,
    $\eta = -\sigma_{\ell+1}\eta$
  end
end

purpose consider a control potential

$$V(x) = \frac{3}{10} + \frac{3x}{200} \geq 0, \quad \forall x \in [-L, L],$$

and the observable

$$A(x) = 1 - e^{-(\kappa(x-y_1))^2/L^2}.$$

In this case, we find that the algorithm converges well even if we only invoke the first order gradient method. Indeed, as we decrease the regularization parameters $\gamma_1, \gamma_2 \ll 1$, we approach an optimal solution which, as it seems, cannot be improved upon. This optimal solution, or, more precisely, its spatial density $\rho = |\psi|^2$, is depicted in Figure 4.1 (right plot), where we denote by "target" the function proportional to $1 - A(x)$ with $\kappa = 0.07$ and $y_1 = -2L/8$, such that it has the same L^2–norm as ψ_0. The left plot shows the associated control.

Since this solution seems optimal, the choice of γ_1, γ_2 becomes negligible below a certain threshold. Thus, it suffices to consider $\gamma_1 = 0$ and only include the cost term proportional to γ_2. Similar results hold for any other given point $y_1 \in \Omega$, provided y_1 stays sufficiently

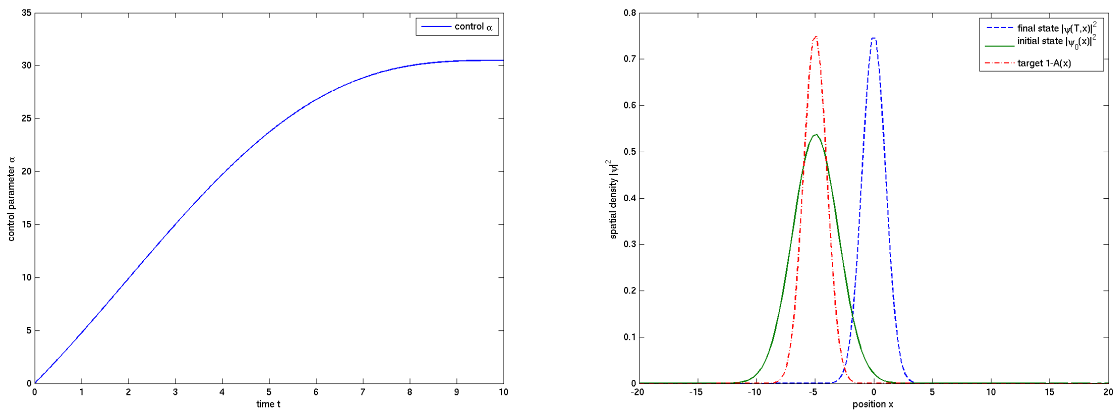

Figure 4.1: Shifting a linear wave paket

far away from the boundary.

Example: splitting a linear wave paket

We still consider the linear case, i.e., $\lambda = 0$, and aim to split a given initial wave packet into two separate packets centered around y_1 and y_2, respectively. The control potential is chosen as

$$V(x) = e^{-8x^2/L^2} \geq 0,$$

and the observable

$$A(x) = 1 - \left(e^{-(\kappa(x-y_1))^2/L^2} + e^{-(\kappa(x-y_2))^2/L^2} \right).$$

In the following we fix $\kappa = 0.07$, $y_1 = -2L/8$, and $y_2 = 2L/8$. In this case we find that the residual of the first order gradient method does not drop below the tolerance given in (4.58) before the maximum number of iterations is reached. With the Newton method, however, we find a (local) minimum of the objective functional $J(\psi, \alpha)$ in less than 20 Newton iterations. Of course there is no guarantee that this is a global minimum.

In order to illustrate our results, we consider the case where $\gamma_1 = 0$, $\gamma_2 = 1.5 \times 10^{-6}$. At the final control time $T = 10$ we then obtain:

$$\langle A\psi(T), \psi(T) \rangle^2_{L^2_x} \approx 2.261 \times 10^{-3}.$$

The spatial density $\rho = |\psi|^2$ of the corresponding solution is shown in the right plot of Figure 4.2. The associated control is depicted in the left plot. If, instead, we choose $\gamma_1 = 4 \times 10^{-5}$, $\gamma_2 = 1 \times 10^{-9}$, we find

$$\langle A\psi(T), \psi(T) \rangle^2_{L^2_x} \approx 2.269 \times 10^{-3},$$

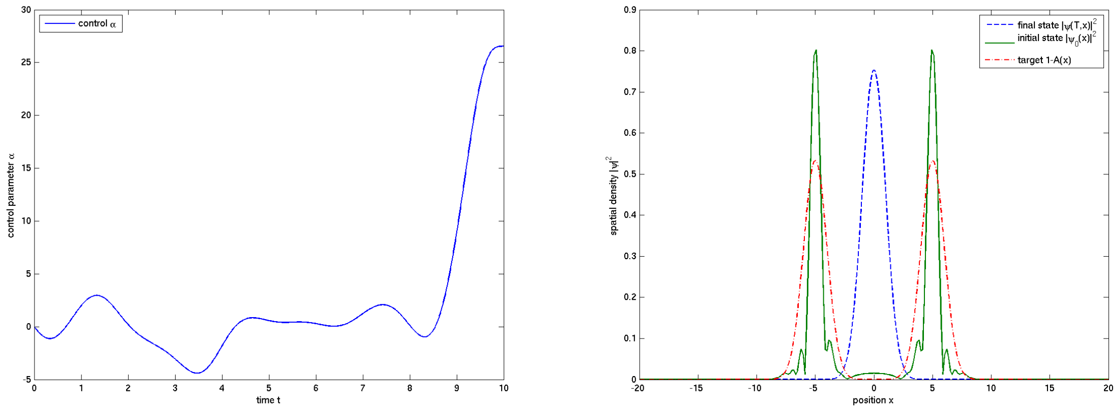

Figure 4.2: Splitting a linear wave paket with $\gamma_1 = 0$

and the corresponding solution is given in Figure 4.3. Here the intermediate state is a plot of $\rho(t)$ at $t = 4 = 0.4 \times T$.

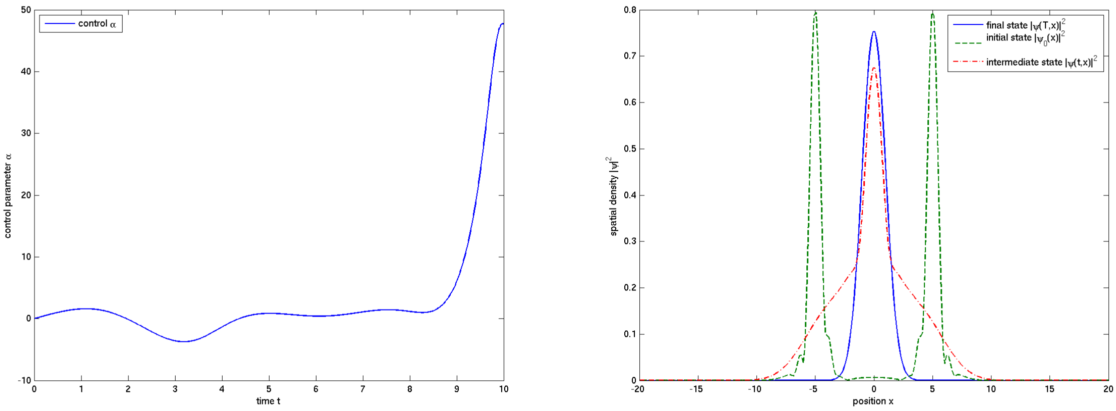

Figure 4.3: Splitting a linear wave paket with $\gamma_1 > 0$

A direct comparison of the (spatial densities of the) resulting wave functions and the respective controls is given in Figure 4.4. We see that the spatial densities are nearly identical, but the variability of the respective control parameters is not the same. This is, of course, related to time–evolution of the weight factor $\omega(t)$, defined in (4.9), which is shown in Figure 4.5 for the case of $\gamma_1 = 4 \times 10^{-5}$ and $\gamma_2 = 1 \times 10^{-9}$.

By construction, the time–integral of $\omega(t)$ can be interpreted as the physical work performed during the control process. We find that compared to the case $\gamma_1 > 0$, the term $\|E(\cdot)\|^2_{L^2_t}$ is around 30% larger (64.5 versus 49.1) and $\|\dot{E}(\cdot)\|^2_{L^2_t}$ is around twice as large (95.0 versus 43.4) in the case where $\gamma_1 = 0$, yielding a significant advantage of our control cost over terms considering the H^1-norm only; see [40] for the latter.

Finally, Figure 4.6 shows an example of the evolution of the objective functional $J(\psi, \alpha)$

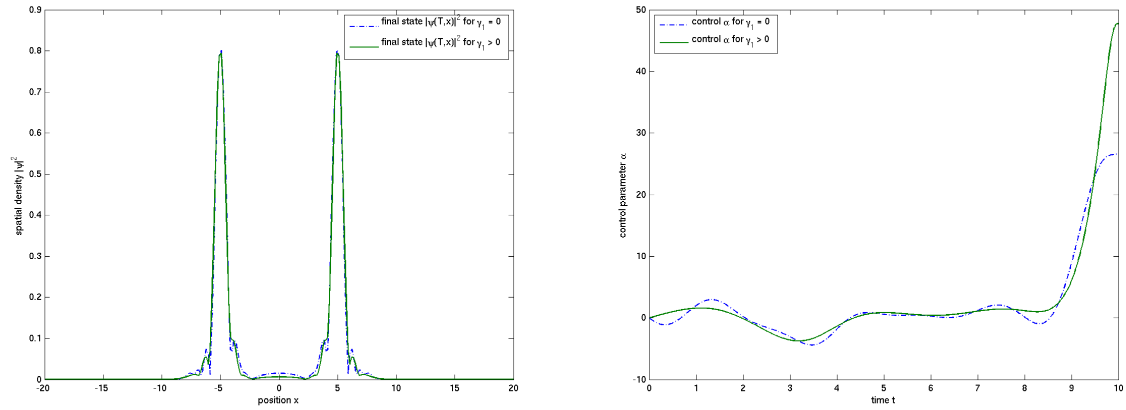

Figure 4.4: Direct comparison between results

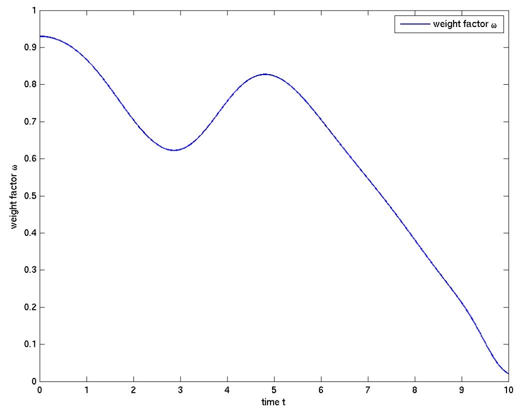

Figure 4.5: The weight factor $\omega = \int V|\psi|^2 dx$ over time

over the number of iterations of the Newton method, here for the case where $\gamma_1 = 0$.

Example: splitting a Bose–Einstein condensate

We consider the same situation as in the previous example, but with an additional (cubic) nonlinearity. More precisely, we choose $\lambda = 8 > 0$. It turns out that the conclusions are similar to the ones found in the linear case ($\lambda = 0$). Qualitatively, the main difference is that during the time–evolution, the wave function spreads out more because of the additionally repulsive (defocusing) nonlinearity. In the linear case, the widest extension of the wave packet is always comparable to its final value. Choosing as before $\gamma_1 = 4\times 10^{-5}$ and $\gamma_2 = 1 \times 10^{-9}$, we obtain the solution depicted in the right plot of Figure 4.7, where we show the spatial density at the times $t = 0$, $t = T = 10$ and at the intermediate time $t = 4$. The control is shown in the left plot. In comparison to the linear case ($\lambda = 0$), the

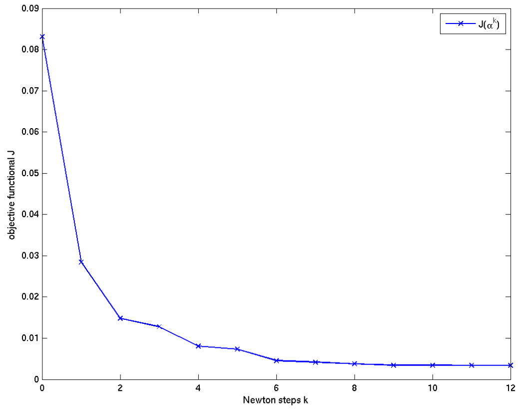

Figure 4.6: Value of $J(\psi, \alpha)$ over number of iterations

observable term in the objective functional $J(\psi, \alpha)$ is found to be slightly larger. Indeed, we obtain

$$\langle A\psi(T), \psi(T)\rangle^2_{L^2_x} \approx 3.720 \times 10^{-3}.$$

This seems to indicate that nonlinear effects counteract the influence of the control potential.

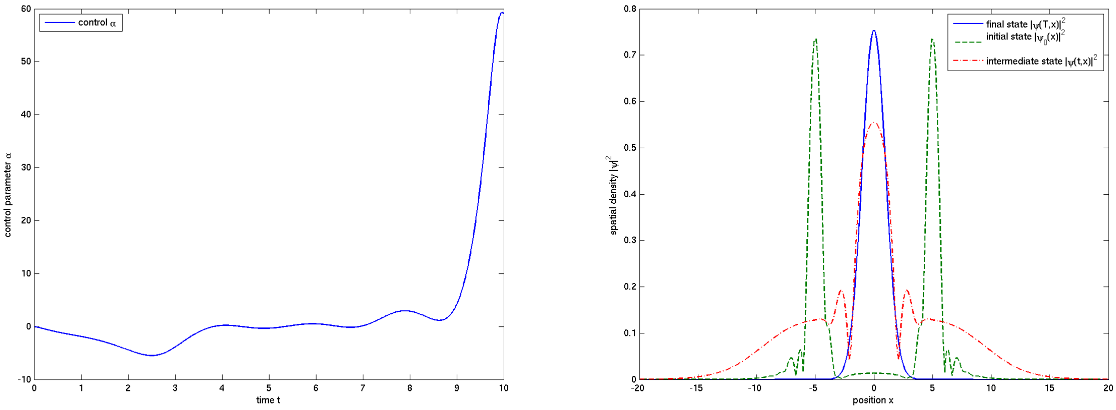

Figure 4.7: Splitting a condensate with $\gamma_1 > 0$

We again compare the present case with the one where $\gamma_1 = 0$ (i.e. no cost term proportional to the physical work) and $\gamma_2 = 1.5 \times 10^{-6}$. First, we find that

$$\langle A\psi(T), \psi(T)\rangle^2_{L^2_x} \approx 3.382 \times 10^{-3}.$$

Moreover, $\|\dot{E}\|^2_{L^2_t}$ is about 150% larger (172.1 versus 68.5) than in the case where $\gamma_1 \neq 0$. Similarly, the total energy $\|E\|^2_{L^2_t}$ is around 15% larger (91.8 versus 79.5).

Example: splitting an attractive Bose–Einstein condensate

Our numerical method allows us to go beyond the rigorous mathematical theory developed in the early chapters. In particular we may try to control the behavior of attractive condensates, which are modeled by (4.1) with $\lambda < 0$, i.e. a focusing nonlinearity. Here we choose $\lambda = -1$, whereas the parameters $\gamma_1 = 4 \times 10^{-5}$, $\gamma_2 = 1 \times 10^{-9}$ are the same as before. The results are shown in Figure 4.8 (control in the left plot and the state at times $t = 0, 10, 4$ in the right plot). The observable part of the objective functional satisfies

$$\langle A\psi(T), \psi(T)\rangle^2_{L^2_x} \approx 2.143 \times 10^{-3}.$$

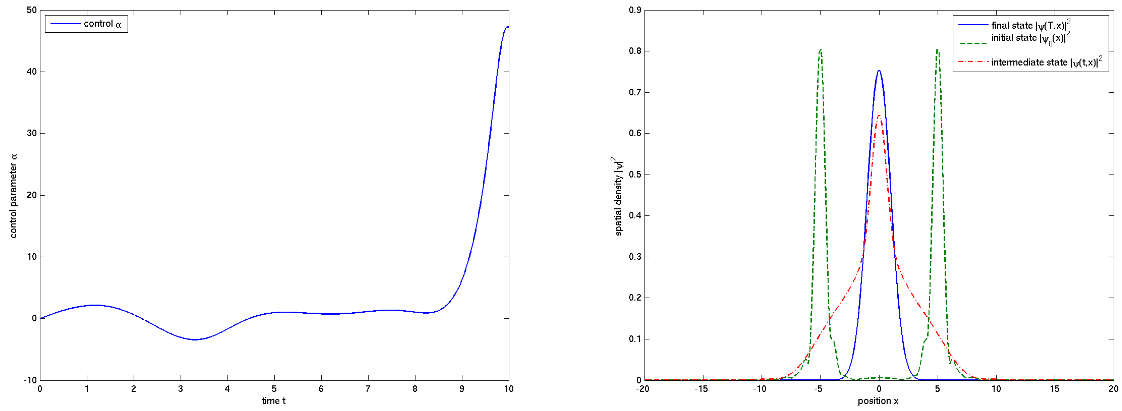

Figure 4.8: Splitting a focusing condensate with $\gamma_1 > 0$

In comparison to the case of a repulsive (defocusing) nonlinearity the final value for the observable term $\langle A\psi(T), \psi(T)\rangle^2_{L^2_x}$ is much smaller, confirming the basic intuition that an attractive condensate does not tend to spread out as much as in the repulsive case.

Chapter 5

Concluding remarks and future work

5.1 On the Cauchy-problem of nonlinear Schrödinger equations with angular momentum rotation term

In Chapter 3, we have investigated local and global existence for the nonlinear Schrödinger equation with angular momentum rotation term, generalizing earlier results in the literature [37, 38]. As we have seen there, equation (3.4) can be considered (upon a change of coordinates) as a special case of NLS with time-dependent potentials (sub-quadratic in x). This class of models has recently been studied in [18]. Following the arguments given therein, one could infer global in-time existence of (3.4) for *sufficiently small* initial data $\psi_0 \in \Sigma$, regardless of the sign of the nonlinearity. Moreover, growth rates for higher order (weighted) Sobolev norms can also be obtained as in [18]. In addition, we note that for a *repulsive*, isotropic quadratic potential $V(x) = -\frac{\gamma^2}{2}|x|^2$, the time-dependent change of coordinates is trivial and we could henceforth conclude global in-time existence for sufficiently large $\gamma > 0$ by following the arguments given in [16].

We also want to point out that for the usual NLS with $\sigma = 2/d$ there is an extra symmetry which has been successfully deployed in the study of blow-up (yielding explicit blow-up solutions and blow-up rates), see e.g. [76]. Using the so-called *Lens transform* [45] one can transfer (most of) these results to the case of NLS with isotropic time dependent quadratic potential $W(t,x) = \gamma(t)|x|^2$, see [18]. However, it is argued in [18] that such an approach is only feasible in the case of isotropic potentials and thus, we cannot expect from it any further insight on the possibility of blow-up in our case, when $(L \cdot \Omega)V(x) \neq 0$ and $|\Omega| > \underline{\gamma}$.

Finally, it is worth noting that the effect of the angular momentum rotation term in our model is very different from other situations. For example, it has been shown for the Euler equations with Coriolis force that blow-up can be delayed through a sufficiently strong rotation term [58] (see also as [4] for a related result). Clearly, the situation in our model is much more involved, and we can not expect an analogous result to be true (the counterexample being the case where $V(x)$ is axially symmetric).

In future work, we would like to numerically test the blow-up conditions of Theorem 3.2.3. In particular, we are intested in establishing whether the conditions are due to technical difficulties or present real obstacles to blow-up.

5.2 Optimal bilinear control of Gross-Pitaevskii equations

In Chapter 4, we have introduced a rigorous mathematical framework for optimal quantum control of linear and nonlinear Schrödinger equations of Gross-Pitaevskii type. We remark that in the physics literature, $L^2(\mathbb{R}^d)$ is usually considered as a complex Hilbert space, equipped with the inner product $\langle \varphi, \xi \rangle = \int_{\mathbb{R}^d} \varphi(x)\overline{\xi(x)}dx$, whereas we consider $L^2(\mathbb{R}^d)$ as a real Hilbert space (of complex functions), equipped with (4.12). Note, however, that the expectation value of any physical observable A and thus also $J(\psi, \alpha)$ is the same for both choices.

Let us briefly discuss possible generalizations for which our results remain valid. First, we point out that in our analysis above, we did not take advantage of the fact that $\gamma_1 > 0$ and hence all of our results remain true in the case $\gamma_1 = 0$. However, Example 4.5.3 shows a significant quantitative difference in the behavior of the cost functionals with and without the term proportional to γ_1.

Second, it is straightforward to extend our analysis to the case of *several* control parameters, i.e.

$$V(t,x) = \sum_{k=1}^{K} \alpha_k(t) V_k(x), \quad K \geq 2.$$

Clearly, for $V_k \in W^{m,\infty}(\mathbb{R}^d)$, $m \geq 2 > d/2$, all of our results remain valid. In addition, it is not difficult to extend our framework to cases of *more general control potentials* $V(\alpha(t), x)$, not necessarily given in the form of a product. Such potentials are of physical significance; see cf. [40]. From the mathematical point of view, all of our results still apply provided that

$$\|V(\alpha, \cdot)\|_{W^{m,\infty}_x} \leq C_1, \quad \|\partial^s_\alpha V(\alpha, \cdot)\|_{L^\infty_x} \leq C_2, \ \forall |s| \leq 2.$$

Note that in this case, the cost term in $J(\psi, \alpha)$, which is proportional to the physical work performed throughout the control process, reads

$$\int_0^T (\dot{E}(t))^2 dt = \int_0^T (\dot{\alpha}(t))^2 \left(\int_{\mathbb{R}^d} \partial_\alpha V(\alpha(t), x) |\psi(t,x)|^2 \, dx \right)^2 dt.$$

It is more problematic to provide a rigorous mathematical framework for control potentials $V(\alpha, x)$ which are *unbounded* with respect to $x \in \mathbb{R}^d$. Only in the case where $V(\alpha, x)$ is subquadratic with respect to x and in $L^\infty(\mathbb{R}^d)$ with respect to α, existence of a minimizer can be proved along the lines of the proof of Theorem 4.2.1. More general unbounded control potentials $V(\alpha, x)$ definitely require new mathematical techniques. Note that in this case, even the existence of solutions to the nonlinear Schrödinger equation is not obvious.

Finally, we want to mention that it is possible to extend our results (with some technical effort) to the case of *focusing nonlinearities*, $\lambda < 0$, provided $\sigma < 2/d$. The latter prohibits the appearance of finite-time blow-up in the dynamics of the Gross–Pitaevskii equation. Clearly, the optimal control problem ceases to make sense if the solution to the underlying partial differential equation no longer exists.

5.3 Uniform quantitative hydrodynamic limits

First and foremost, it remains to pursue the strategy outline in Section 2.7 to extend our results to general dimensions.
In Section 2.5, we showed, assuming initial convergence of the microscopic entropy towards the macroscopic entropy, this convergence is propagated along the evolution of the system. It would be interesting to prove uniformity in time of this convergence. The difficulty here lies in the fact that in general, the microscopic relative entropy $H^N(\mu_t^N | \nu_{f_\infty}^N)$ does not decay in t, since the weight of $\mathbb{P}_{\mu_t^N}(\sum_x \eta(x) = K)$ on the hyperplanes of constant particles is invariant under the evolution of the particle system. Thus as long as μ_0^N is not chosen exactly such that

$$\mathbb{P}_{\mu_t^N}\Big(\sum_x \eta(x) = K\Big) = \mathbb{P}_{\nu_{f_\infty}^N}\Big(\sum_x \eta(x) = K\Big),$$

we cannot take advantage of decay of the microscopic entropy. On the other hand, by the equivalence of ensembles, we expect that

$$\mathbb{P}_{\mu_t^N}\Big(\sum_x \eta(x) = K\Big) \approx \mathbb{P}_{\nu_{f_\infty}^N}\Big(\sum_x \eta(x) = K\Big)$$

and that we can still deduce a uniform-in-time convergence of the entropy. This remains to be clarified in future work. Another question, answered in Kosygina [50] for simple exclusion processes, is whether the entropies converge for all positive times even if we only assume a hydrodynamic limit (macroscopic profile) initially and no convergence of the initial entropies.

It should be possible to prove a strong conservation of local equilibrium using our techniques, see Remark 2.3.3 (4). In the case of attractive processes, this is a known result - however, our method has the advantage of yielding explicit uniform-in-time bounds on the rate of convergence.

Finally, it remains to be seen if this method can be extended to problems where the hydrodynamic limit is not yet known, especially limit equations that can exhibit shocks.

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