Dynamics of Patterns in Equivariant Hamiltonian Partial Differential Equations

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Contents

Introduction

In physics, many problems can be formulated as Hamiltonian systems with infinitely many degrees of freedom. These Hamiltonian partial differential equations possess conserved quantities, such as energy, mass, and momentum.

There is a wide range of physical applications. The nonlinear Schrödinger equation (NLS) appears in the description of laser propagation, free surface water waves, and plasma waves (see [22], [56], and [65]), the nonlinear Klein-Gordon equation (NLKG) arises in relativistic quantum mechanics (see [31], [63]), and nonlinear dispersive equations of Korteweg-de Vries (KdV) type are used to model oceanic waves, in particular tsunami waves (see [36], [55]).

This thesis deals with solitary wave solutions to these Hamiltonian partial differential equations and their stability. Our main interest is to analyze and implement a numerical method for the computation of solutions whose initial data are close to a solitary wave solution.

Let us first describe the setting. We consider an abstract evolution equation

$$u_t = F(u) \in X, \quad u(t) \in \mathcal{D}_F,$$

where the operator F is a Hamiltonian vector field defined on a dense subspace $\mathcal{D}_F$ of a Banach space $(X, \|\cdot\|)$ and maps into X. This means, there exists a $\mathcal{C}^2$ functional $H\colon X \to \mathbb{R}$ and a continuous symplectic form $\omega\colon X \times X \to \mathbb{R}$ such that

$$\omega(F(u), v) = \langle \mathrm{d}H(u), v\rangle$$

holds for all $u \in \mathcal{D}_F$ and $v \in X$. The evolution equation is then called a Hamiltonian system (see e.g. [1] and [45]), and the weak formulation in the dual space $X^\star$ takes the form

$$\omega(u_t, \cdot) = \mathrm{d}H(u).$$

The evolution in time of this autonomous dynamical system is completely determined by a scalar valued function, the Hamiltonian $H : X \to \mathbb{R}$. Since it does not depend explicitly on time, the Hamiltonian is a first integral of the system, which means that it remains constant on any solution. In physical applications, such as classical and quantum mechanics, the numerical value of the Hamiltonian equals the value of the total energy, which means Hamiltonian systems are systems with conserved energy.

As an additional structure, we assume the equation to be equivariant with respect to the action $a : G \to GL(X)$ of a finite-dimensional, but not necessarily

compact, Lie group G. Equivariance means that the Lie group G acts on X via a representation that is equivariant in the sense

$$F(a(\gamma)u) = a(\gamma)F(u)$$

for all $\gamma \in G$ and $u \in \mathcal{D}_F$, where $a(\gamma)\mathcal{D}_F \subseteq \mathcal{D}_F$ is assumed. However, in case of the weak formulation it is more convenient to express equivariance by the invariance of the Hamiltonian, which we write as

$$H(a(\gamma)u) = H(u).$$

From the physical point of view this is a symmetry, and it leads to a generalization of Noether's theorem from classical mechanics, which yields $d = \dim(G)$ conserved quantities.

In Hamiltonian partial differential equations dispersion and non-linearity can interact to produce solitary wave solutions, which maintain their shape $v_\star$ while rotating, oscillating or traveling at a constant speed $\mu_\star$. In the abstract setting of equivariant Hamiltonian systems they appear as relative equilibria, i.e., solutions of the form

$$u_\star(t) = a(e^{t\mu_\star})v_\star$$

with $\mu_\star \in \mathcal{A}$, $v_\star \in X$. Here $\mathcal{A}$ is the Lie algebra associated with G, and $\sigma \mapsto e^\sigma$ denotes the exponential map from $\mathcal{A}$ to G.

Solitary waves that are stable and travel over very large distances are a remarkable physical phenomenon as one usually assumes waves to either flatten out or steepen and collapse. Accordingly, the theory of solitary wave stability is a broad field of mathematical research. In terms of the nonlinear Schrödinger equations we refer to [15], [24], and [64]. The stability theory of solitary waves in an abstract setting can be found in [32], [38], [47], [52], and, in particular, in [33]. These approaches provide applications to a variety of Hamiltonian partial differential equations.

As stated before, our main objective is the long time behavior of numerical solutions of Hamiltonian partial differential equations with initial data close to a relative equilibrium. For these equivariant Hamiltonian systems, classical Lyapunov stability of steady states has to be weakened to orbital stability. A relative equilibrium $u_\star$ is called orbitally stable if solutions stay for all times close to the group orbit $a(G)u_\star$, provided their initial data are sufficiently close.

In numerical computations, this is not quite satisfactory. For example, a traveling wave solution $u_\star(t) = v_\star(\cdot - \mu_\star t)$ leaves the computational domain in finite time. This leads to additional difficulties in terms of spatial discretization and to undesirable issues with boundary conditions.

As an approach to tackle these problems we apply the so-called freezing method, introduced in [8] and independently in [50], to Hamiltonian systems. The freezing method has been successfully applied to parabolic equations and hyperbolic-parabolic systems with dissipative terms (see [6], [49], and the references therein), but its application to Hamitonian systems has not been studied at all.

The principal idea of the freezing method is to separate the time evolution of a solution into an evolution of the profile and an evolution in the Lie group by writing

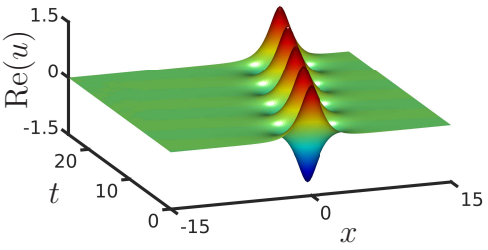
$$u(t) = a\big(\gamma(t)\big)v(t).$$

We assume that $\gamma \mapsto a(\gamma)v$ is smooth for v on a dense subset of X and denote its derivative at unity by $\mu \mapsto d[a(\mathbb{1})v]\mu$. The problem is then transformed into an equation of the form

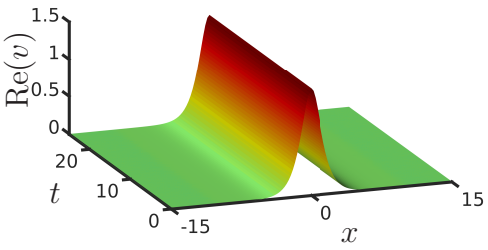
$$\omega(v_t, \cdot) = \mathrm{d}H(v) - \mathrm{d}Q(v)\mu,$$

where $v \mapsto \mathrm{d}Q(v)\mu$ is the continuous extension of the mapping $v \mapsto \omega(\mathrm{d}[a(\mathbb{1})v]\mu, \cdot)$ to $v \in X$. A phase condition $\psi(v, \mu) = 0$ is added in order to compensate for the additional unknown μ. In this way, a partial differential equation transforms into a partial differential algebraic equation (PDAE), and relative equilibria become steady states. Thereby, the freezing method yields additional information about the dynamics close to a relative equilibrium, in particular it provides a direct approximation of $\mu_\star$.

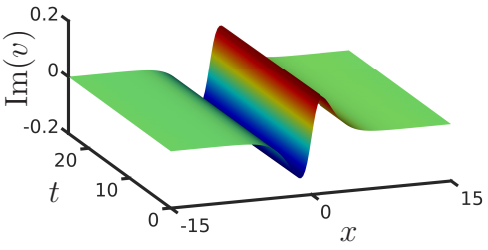
As a typical case, the following pictures contrast a solitary wave solution of the nonlinear Schrödinger equation with the corresponding steady state of the freezing system.



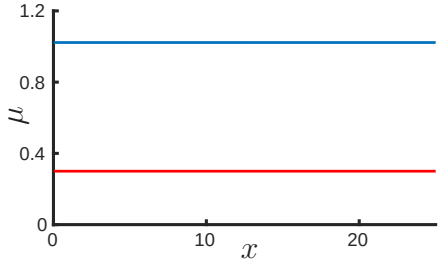
Solution of the original problem



Solution of the freezing system



Solution of the freezing system



Frequency and Velocity

The question arises whether such steady states are stable in the sense of Lyapunov, i.e., for any $\varepsilon > 0$ there exists $\delta > 0$ such that we have

$$\sup_{0 \le t < \infty} \Big[\|v(t) - v_\star\| + |\mu(t) - \mu_\star| \Big] < \varepsilon,$$

provided that the initial data are consistent and satisfy $\|v(0) - v_\star\| < \delta$. The stability analysis in Chapter 2 is based on the spectral stability assumptions that M. Grillakis, J. Shatah, and W. Strauss imposed in [33]. Our main result, Theorem 2.3.7, states that under these assumptions a steady state $(v_\star, \mu_\star)$ of the freezing system is Lyapunov stable.

The abstract stability theory is applied to the nonlinear Schrödinger equation

$$iu_t = -u_{xx} - |u|^2 u, \quad u_0 \in H^1(\mathbb{R}; \mathbb{C}),$$

which is invariant under the action of a two-parameter group of gauge transformations and translations, and to the nonlinear Klein-Gordon equation

$$u_{tt} = u_{xx} - u + |u|^2 u, \quad u_0 \in H^1(\mathbb{R}; \mathbb{R}^3) \times L^2(\mathbb{R}; \mathbb{R}^3)$$

with its four-dimensional Lie group of oscillations in the u-components and translations.

In Chapter 3 we put our focus on the discretization of the freezing system and the preservation of stability. Loosely following the approach of D. Bambusi, E. Faou, and B. Grébert in [3], we consider approximation parameters $\Gamma \in \mathfrak{P}$, finite-dimensional subspaces $X^\Gamma \subseteq X$, and an error function $\varepsilon\colon \mathfrak{P} \mapsto \mathbb{R}_{>0}$.

As examples, we take the finite difference and finite element method for the nonlinear Schrödinger equation. We restrict ourselves to two levels of approximation, namely, truncation to a finite domain with appropriate boundary conditions and spatial semi-discretization.

We do not analyze the time-integration of the freezing method and leave it as work in progress. This is despite the fact that orbital stability results for fully discrete approximations of the NLS are known. We refer to [3], and to [14] for results on conserved quantities. The main difficulty is the construction of a modified energy as in [21]. The underlying theory for ordinary differential equations can be found in [34].

Provided that $\varepsilon(\Gamma)$ is small enough, our analysis in Chapter 3 yields the existence and stability of steady states for the discretized freezing system

$$\begin{aligned} \omega^\Gamma(v_t^\Gamma, \cdot) &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma, \\ 0 &= \psi^\Gamma(v^\Gamma). \end{aligned}$$

These steady states $(v_\star^\Gamma, \mu_\star^\Gamma)$ are close to steady states of the continuous problem in the sense that

$$\left\|v_\star^\Gamma - v_\star\right\| + |\mu_\star^\Gamma - \mu_\star| \leq C\varepsilon(\Gamma).$$

Moreover, they are stable, i.e., for any $\varepsilon > 0$ there exists $\delta > 0$ such that we have

$$\sup_{0 \leq t < \infty} \left[\left\|v^\Gamma(t) - v_\star^\Gamma\right\|_\Gamma + \left|\mu^\Gamma(t) - \mu_\star^\Gamma\right| \right] < \varepsilon,$$

provided the initial data are consistent and satisfy $\left\|v^\Gamma(0) - v_\star^\Gamma\right\|_\Gamma < \delta$.

When it comes to the discretized nonlinear Schrödinger equation, the abstract theory currently applies only to solitary waves of the form $u_\star(t) = e^{i\mu_\star t} v_\star$, which

do not travel at all. It is quite challenging to set up a theory that treats truncation to finite domains and discretization for traveling solitary waves. That is why a comprehensive theory does not yet exist.

As a first step, we put our emphasis in Chapter 4 on the impact of boundary conditions and spatial discretization on the conservation properties of Hamiltonian systems. Here, we stay away from an abstract setting, but instead get insight via direct computations for the truncated and discretized freezing system for the NLS.

We first consider the continuous problem that is truncated to a finite interval, where we choose separated boundary conditions. However, it turns out that periodic boundary conditions lead to better results. In a second step, we analyze finite difference and spectral methods. Since the translation group does not act on a discrete grid, the conservation of momentum and energy is not even locally satisfied for finite differences. This issue can be bypassed by making use of spectral methods.

In Chapter 5 we support our abstract theoretical results by numerical experiments. Due to the superior conservation properties of periodic boundary conditions and spectral methods, we make use of the Strang splitting (see [53]). The principal idea is to decompose the vector field into two parts that can be efficiently evolved. The application of this method to the nonlinear Schrödinger equation with periodic boundary conditions has been analyzed in [20].

We consider these numerical computations rather as a benchmark test for solving the freezing system by a splitting algorithm, than an effort to find an optimized numerical scheme for a specific type of partial differential equation. Nevertheless, we still want to exploit the high efficiency for an equation that can be split into two analytically solvable parts (e.g. the NLS).

That is why we do not directly solve the PDAE system, but in each step compute the extra variables $\mu \in \mathcal{A}$ in a preliminary calculation. But, this does not come without a drawback. The numerical solution is no longer forced to stay exactly on the manifold that is given by the phase condition. As a consequence, we notice a high fluctuation in the values of μ. However, strictly enforcing the phase condition is not mandatory since it is artificial anyway.

We also use the Strang splitting for numerically solving the NLKG, where we do not solve the second order in time equation, but use the transformation to a first order system that is also used in our stability theory. Finally, we apply the freezing method to the Korteweg-de Vries equation

$$u_t = -u_{xxx} - 6uu_x, \quad u_0 \in H^1(\mathbb{R};\mathbb{R}).$$

Due to the third derivative, its geometric structure is different from the previous examples, and that is why it does not fit into our abstract setting, however, it almost does. Based on [10], we indicate a modification of our abstract approach, which allows us to treat this equation. Our numerical realization is based on the Strang splitting for the original problem, as analyzed in [37].

For each of the three equations, we notice a stable behavior of the steady states for the freezing system, at least for very small deviations. But, in contrast to parabolic problems, there is no asymptotic stability. That is why initial deviations

and computational errors are rather amplified, than die out over long times. This issue is unaffected by the freezing method.

Chapter 1

Equivariant Hamiltonian Systems

1.1 Hamiltonian Ordinary Differential Equations

Many problems in classical mechanics, for instance the motion of celestial objects, can be written as Hamiltonian ordinary differential equations. In the following, we give a brief overview of the principle concepts of Hamiltonian mechanics, where we focus on those aspects that reappear in Hamiltonian partial differential equations. In a second step, the Hamiltonian formalism is illustrated by a very basic example.

By $\left(\cdot,\cdot\right)_{\mathbb{R}^n}$ we denote the Euclidean inner product and by $\langle\cdot,\cdot\rangle$ the dual pairing of a Banach space X and its dual $X^\star$. In case of $X=\mathbb{R}^d$, the Riesz isomorphism is given by

$$\Theta_{\mathbb{R}^d}\colon \mathbb{R}^d \to \mathbb{R}^{d,\star}, \quad q \mapsto \left(q,\cdot\right)_{\mathbb{R}^d}.$$

If a function $f : \mathcal{D}_f \subseteq \mathbb{R}^d \to \mathbb{R}$ is differentiable at $x \in \mathcal{D}_f$, then its gradient is defined as

$$\nabla f(x) = \Theta_{\mathbb{R}^d}^{-1}\,\mathrm{d}f(x) \in \mathbb{R}^d.$$

Moreover, a vector $q \in \mathbb{R}^d$ is written as

$$q = \begin{pmatrix} q_1 \\ \vdots \\ q_d \end{pmatrix},$$

where each component q_j is a real number.

1.1.1 Hamiltonian Mechanics

In accordance with the historical construction, we introduce Hamiltonian mechanics as a reformulation of Lagrangian mechanics. As a starting point, let us consider generalized coordinates $q \in \mathbb{R}^d$, where d is the number of degrees of freedom, velocities $v \in \mathbb{R}^d$, and the Lagrangian

$$L(q,v) = T(q,v) - U(q),$$

which is defined as the difference between the kinetic energy T and the potential energy U. For a trajectory

$$q\colon [t_0, t_E] \to \mathbb{R}^d, \quad t \mapsto q(t)$$

the action S is defined by the integral of the Lagrangian of q and its time derivative q_t between the two instants of time t_0 and t_E, i.e.,

$$S(q) = \int_{t_0}^{t_E} L\big(q(t), q_t(t)\big)\mathrm{d}t.$$

According to Hamilton's principle the realization of a physical system is a stationary point of this action functional, which means $\mathrm{d}S(q) = 0$. Then, the calculus of variations leads to the Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[L_v(q, q_t)\Big] = L_q(q, q_t).$$

This is a d-dimensional system of second-order differential equations, which requires initial data for $q(t_0) \in \mathbb{R}^d$ and $v(t_0) = q_t(t_0) \in \mathbb{R}^d$.

The Legendre transform converts the Euler-Lagrange equations into a $2d$-dimensional system of first-order differential equations. The first step is to replace the generalized velocities with conjugate momenta. Define the generalized momentum $p(t) \in \mathbb{R}^d$ at time $t \in [0, T]$ corresponding to the position $q(t) \in \mathbb{R}^d$ and the velocity $q_t(t) \in \mathbb{R}^d$ by

$$p(t) = \nabla_v L(q(t), q_t(t)).$$

For simplicity, let us make the hypothesis (see [19]) that there exists a global implicit function $\hat{v} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ such that $v \in \mathbb{R}^d$, $p \in \mathbb{R}^d$, and $q \in \mathbb{R}^d$ satisfy the equation

$$p = \nabla_v L(q, v)$$

if and only if $v = \hat{v}(p, q)$. Rewriting the Euler-Lagrange equations in terms of q and p leads to Hamilton's equations

$$p_t = -\nabla_q H(p, q), \quad q_t = \nabla_p H(p, q), \tag{1.1.1}$$

where the scalar valued Hamiltonian is given by

$$H(p, q) = \big(p, \hat{v}(p, q)\big)_{\mathbb{R}^d} - L(q, \hat{v}(p, q)), \tag{1.1.2}$$

together with initial data for $q(t_0) \in \mathbb{R}^d$ and $p(t_0) \in \mathbb{R}^d$.

Let us show that Hamilton's equations (1.1.1) can be equivalently written as an abstract Hamiltonian system

$$\omega(u_t, \cdot) = \mathrm{d}H(u) \in X^\star, \tag{1.1.3}$$

where the phase space X is the $2d$-dimensional real vector space $\mathbb{R}^{2d}$, and the symplectic form $\omega\colon \mathbb{R}^{2d} \times \mathbb{R}^{2d} \to \mathbb{R}$ is defined by

$$\omega(u, v) = (Ju)^T v$$

with

$$J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \in \mathbb{R}^{2d \times 2d}.$$

Proposition 1.1.1. *Let $\mathcal{I} \subseteq \mathbb{R}$ be an open interval. Then $p : \mathcal{I} \to \mathbb{R}^d$ and $q : \mathcal{I} \to \mathbb{R}^d$ solve (1.1.1) if and only if $u : \mathcal{I} \to \mathbb{R}^{2d}$,*

$$u(t) = \begin{pmatrix} p(t) \\ q(t) \end{pmatrix}$$

is a solution of (1.1.3), where the Hamiltonian is defined in (1.1.2).

Proof. On the one hand, from (1.1.1) we obtain

$$\begin{aligned} \omega(u_t, v) = (Ju_t)^T v = \begin{pmatrix} q_t^T & -p_t^T \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \big(q_t, v_1\big)_{\mathbb{R}^d} - \big(p_t, v_2\big)_{\mathbb{R}^d} \\ = \big(\nabla_p H(u), v_1\big)_{\mathbb{R}^d} + \big(\nabla_q H(u), v_2\big)_{\mathbb{R}^d} = \langle \mathrm{d}H(u), v \rangle \end{aligned}$$

for $v \in \mathbb{R}^{2d}$. On the other hand, from

$$\omega(u_t, \cdot) = \mathrm{d}H(u) \in (\mathbb{R}^{2d})^\star$$

we conclude

$$u_t = J^{-1} \nabla H(u).$$

This is rewritten as

$$\begin{pmatrix} p_t \\ q_t \end{pmatrix} = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \begin{pmatrix} \nabla_p H(u) \\ \nabla_q H(u) \end{pmatrix} = \begin{pmatrix} \nabla_q H(u) \\ -\nabla_p H(u) \end{pmatrix},$$

which implies (1.1.1). □

Hamilton's equations possess several remarkable properties. Since we have

$$J^T = -J = J^{-1},$$

the matrix J is skew-symmetric and non-degenerate, which means ω is a symplectic form. This skew-symmetry has an immediate consequence for solutions of (1.1.3).

Proposition 1.1.2. *Let u be a solution of equation (1.1.3). Then H is a conserved quantity, i.e., $H(u(t)) = H(u(0))$ holds for all $t \geq 0$.*

Proof. Differentiating with respect to time gives us

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[H(u)\Big] = \langle \mathrm{d}H(u), u_t\rangle = \omega(u_t, u_t) = 0.$$

Since the derivative vanishes, the Hamiltonian is constant in time. □

Remark 1. A few notes on further references are as follows.

- Details on the Legendre transform can be found in [2] and [19].
- A more general situation in which J explicitly depends on u with $J(u)$ being singular is considered in [38] and [44].

1.1.2 Rain Gutter Dynamics

The following elementary example from [44] illustrates the notion of stability for relative equilibria in Hamiltonian systems. Consider a particle with position $q \in \mathbb{R}^2$ sliding along a rain gutter. The rain gutter is horizontally arranged, it is flat in q_1-direction and shaped as a parabola in q_2-direction.

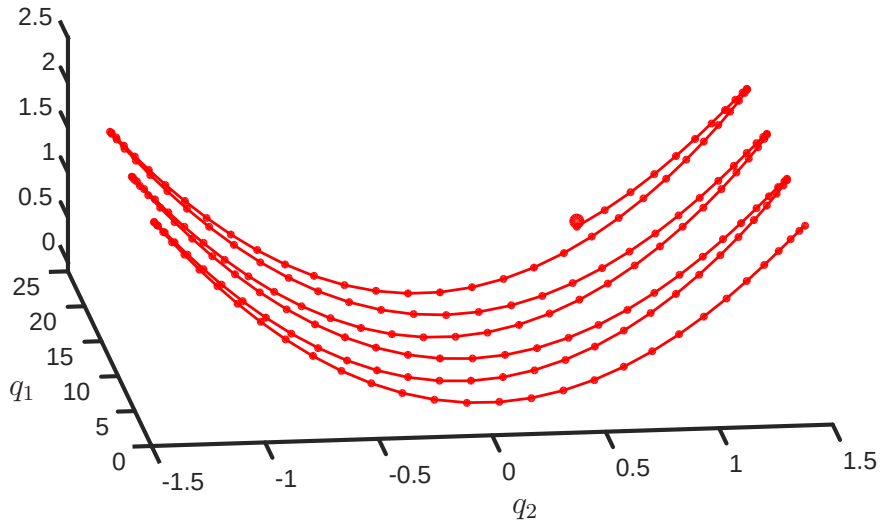


Figure 1.1.1: Motion of the particle

By compressing the q_1-axis, we get an impression of the steady lateral motion of the particle. The potential energy

$$U(q) = \frac{1}{2}q_2^2$$

represents this parabolic geometry. The kinetic energy $T(q, q_t)$, which is given by

$$T(q, v) = \frac{1}{2}(-v_1^2 + v_2^2),$$

appears non-physical, since in q_1-direction the functional does not increase as velocity squared, but decreases instead. However, no force acts in q_1-direction.

Hence, the particle undergoes a motion with constant velocity, and we deduce that $+v_1^2$ instead of $-v_1^2$ leads to exactly the same dynamics. But, the negative sign choice more closely mimics the stability problem of solitary waves in Hamiltonian PDEs.

The Lagrangian $L : \mathbb{R}^4 \to \mathbb{R}$ is given by

$$L(q, v) = T(q, v) - U(q) = \tfrac{1}{2}(-v_1^2 + v_2^2) - \tfrac{1}{2}q_2^2,$$

and its partial derivative with respect to the v-component writes as

$$\langle L_v(q, v), y\rangle = -v_1 y_1 + v_2 y_2$$

for $y \in \mathbb{R}^2$. This leads to the generalized momentum

$$p = \nabla_v L(q, q_t) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} q_t.$$

Solving

$$p = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} v$$

for $v \in \mathbb{R}^2$ gives us the implicit function

$$\hat{v}(p, q) = \begin{pmatrix} -p_1 \\ p_2 \end{pmatrix}.$$

The dot product of p and $\hat{v}(p, q)$ is given by $\big(p, \hat{v}(p, q)\big)_{\mathbb{R}^2} = -p_1^2 + p_2^2$. Hence, the Lagrangian in terms of p and q writes as

$$L(q, \hat{v}(p, q)) = \tfrac{1}{2}(-p_1^2 + p_2^2) - \tfrac{1}{2}q_2^2.$$

As a result, the Hamiltonian $H\colon \mathbb{R}^4 \to \mathbb{R}$ takes the form

$$H(q, p) = \big(p, \hat{v}(p, q)\big)_{\mathbb{R}^2} - L(q, q_t(p, q)) = \tfrac{1}{2}(q_2^2 - p_1^2 + p_2^2).$$

In conclusion, Hamilton's equations in (1.1.1) are given by

$$q_t = \nabla_p H(q, p) = \begin{pmatrix} -p_1 \\ p_2 \end{pmatrix},$$
$$p_t = -\nabla_q H(q, p) = \begin{pmatrix} 0 \\ -q_2 \end{pmatrix}.$$

To simplify the notation, we write

$$u = \begin{pmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix},$$

which leads to

$$u_t = J^{-1}\nabla H(u) = \begin{pmatrix} 0 \\ -u_4 \\ -u_1 \\ u_2 \end{pmatrix}, \tag{1.1.4}$$

where we have

$$J = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

As we have mentioned before, the momentum in q_1-direction is a conserved quantity. From the Newtonian point of view, this is a consequence of no force acting in this direction. However, the conservation can be directly deduced from equation (1.1.4). Indeed, the derivative of the functional

$$Q\colon \mathbb{R}^4 \to \mathbb{R}, \quad Q(u) = u_1$$

is given by

$$\langle \mathrm{d}Q(u), v\rangle = v_1$$

for $v \in \mathbb{R}^4$. Hence, equation (1.1.4) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q(u)\Big] = \langle \mathrm{d}Q(u), u_t\rangle = 0,$$

i.e., the functional Q is a conserved quantity. Relative equilibria of (1.1.4) that are associated with this conserved quantity are steady translations in q_1-direction, which can be written as

$$u_\star(t) = \begin{pmatrix} -\mu_\star \\ 0 \\ \mu_\star t + \delta_\star \\ 0 \end{pmatrix} = \begin{pmatrix} -\mu_\star \\ 0 \\ \delta_\star \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \mu_\star t \\ 0 \end{pmatrix} = v_\star + \begin{pmatrix} 0 \\ 0 \\ \mu_\star t \\ 0 \end{pmatrix}$$

for $\mu_\star, \delta_\star \in \mathbb{R}$. In order to analyze stability, we consider the functional

$$S(v) = H(v) - Q(v)\mu_\star. \tag{1.1.5}$$

Since

$$\mathrm{d}S(v_\star) = \mathrm{d}H(v_\star) - \mathrm{d}Q(v_\star)\mu_\star = 0$$

and all terms in (1.1.5) are at most quadratic, we find

$$S(v) - S(v_\star) = \tfrac{1}{2}\langle L_\star(v - v_\star), v - v_\star\rangle,$$

where we denote $L_\star = \mathrm{d}^2 S(v_\star)$. If $L_\star$ is positive definite, this leads to

$$S(v) - S(v_\star) \geq C\|v - v_\star\|^2,$$

and the Lyapunov stability follows as a direct consequence of the conservation of this functional. But in the case of the rain gutter, the matrix representation of $L_\star$ is given by the Hessian

$$L_\star = \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 0 & \\ & & & 1 \end{pmatrix}. \tag{1.1.6}$$

Its negative subspace is

$$W = \{\nabla Q(v_\star)\sigma \colon \sigma \in \mathbb{R}\} = \mathbb{R} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

This means W is spanned by the gradient of Q at $v_\star$, i.e., it consists of vectors orthogonal to the level set $\{v \in \mathbb{R}^4 : Q(v) = Q(v_\star)\}$. Since Q is a conserved quantity, which means that solutions cannot leave a level set of Q, the stability is unaffected by this negative subspace. Moreover, it is worth mentioning that the negative subspace is a result of the negative sign in the kinetic energy. The canonical choice $T(q, v) = \frac{1}{2}(v_1^2 + v_2^2)$ leads to W being a positive subspace.

In addition to the negative subspace, there is the non-trivial kernel

$$Z = \ker(L_\star) = \mathbb{R} \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},$$

which results from the fact that H and Q are invariant under the shift.

Now, the freezing method is applied to realize a splitting into these shift dynamics in q_1-direction and the evolution in q_2-direction. This is done by choosing a comoving frame, i.e., a different frame for each time t. More specifically, we write

$$v(t) = u(t) - \begin{pmatrix} 0 \\ 0 \\ \gamma(t) \\ 0 \end{pmatrix}.$$

We note that H and Q are both invariant under this transformation, i.e.,

$$\begin{aligned} H(v(t)) &= H(u(t)), \\ Q(v(t)) &= Q(u(t)). \end{aligned}$$

Moreover, the shift can be expressed in terms of the symplectic matrix J and the gradiant of Q as

$$J^{-1}\nabla Q(u) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

By combining these properties and defining $\mu = \gamma_t$, the system (1.1.4) is transformed into

$$v_t = u_t - \begin{pmatrix} 0 \\ 0 \\ \gamma_t \\ 0 \end{pmatrix} = J^{-1}\big(\nabla H(v) - \nabla Q(v)\mu\big) = \begin{pmatrix} 0 \\ -v_4 \\ -v_1 - \mu \\ v_2 \end{pmatrix}.$$

The arbitrariness in this representation is removed by introducing a so-called phase condition for the additional unknown μ. In this example, we can simply require the v_3-component to be constant for all times, i.e.,

$$0 = \psi(v) = v_3 - \widehat{\delta}$$

for some $\widehat{\delta} \in \mathbb{R}$. Physically speaking, the frame is attached to the particle in this direction. The transformed system

$$\begin{aligned} v_t &= J^{-1}\big(\nabla H(v) - \nabla Q(v)\mu\big), \\ 0 &= \psi(v) \end{aligned}$$

is a differential algebraic equation and has steady states of the form

$$v_\star = \begin{pmatrix} -\mu_\star \\ 0 \\ \widehat{\delta} \\ 0 \end{pmatrix}$$

for all $\mu_\star \in \mathbb{R}$. The Lyapunov stability of these steady states is a consequence of the conservation of Q and the phase condition, which reduce the dynamics of the transformed system to the q_2-component. In Chapter 2, we extend this freezing ansatz to abstract Hamiltonian systems.

1.2 Abstract Hamiltonian Systems

In the following, we introduce the basic framework that allows us to generalize the concept of Hamiltonian ODEs to abstract evolution equation with applications in Hamiltonian PDEs. Such an abstract evolution equation is of the form

$$u_t = F(u) \in X, \quad u(t) \in \mathcal{D}_F, \tag{1.2.1}$$

and it is assumed to be equivariant under the action of a finite-dimensional Lie group G. For more details on equivariant dynamical systems, we refer to [16], [23], and [46]. By $T_\gamma G$ we denote the tangent space of G at γ, in particular $\mathcal{A} = T_{\mathbb{1}} G$ is the tangent space of G at unity.

1.2.1 Basic Framework

In Section 1.1.1 we have only considered finite-dimensional Hamiltonian systems. The next step is to allow the phase space X to be infinite-dimensional. Let $(X, \|\cdot\|)$ be a separable Banach space over the field of real numbers. We equip this vector space with a continuous symplectic form

$$\omega\colon X \times X \to \mathbb{R}.$$

That is, the mapping ω is linear in each argument, alternating, and nondegenerate. Alternating means that $\omega(u,u) = 0$ for all $u \in X$, while nondegenerate refers to the property that $\omega(u,v) = 0$ for all $v \in X$ implies $u = 0$. As an immediate consequence of the alternation, the skew-symmetry

$$\omega(u,v) = -\omega(v,u)$$

for all $u, v \in X$ follows from

$$0 = \omega(u+v, u+v) = \omega(u,v) + \omega(v,u).$$

Lemma 1.2.1. *The mapping $u \mapsto \omega(u,\cdot)$ is one-to-one.*

Proof. Let $u \in X$ satisfy $\omega(u,\cdot) = 0 \in X^\star$, which means that $\omega(u,v) = 0$ for all $v \in X$. From the non-degeneracy of ω, we find $u = 0$. Hence, the mapping is one-to-one. □

In general, this mapping is not onto. This is a main difference compared to finite-dimensional Hamiltonian systems with symplectic matrices, which are invertible.

A differentiable operator $f\colon X \to X$ is called *symplectic* if it preserves the symplectic form, i.e.,

$$\omega\big(\mathrm{d}f(y)u, \mathrm{d}f(y)v\big) = \omega(u,v) \tag{1.2.2}$$

for all $y, u, v \in X$. In the finite-dimensional case (see Section 1.1), the equation (1.2.2) is equivalent to the matrix equation $\mathrm{d}f(y)^T J^{-1} \mathrm{d}f(y) = J^{-1}$.

This symplectic structure gives rise to the notion of Hamiltonian systems. An operator $F\colon \mathcal{D}_F \subseteq X \to X$ is called a Hamiltonian vector field if its domain $\mathcal{D}_F$ is dense in X, and if there exists a twice continuously differentiable functional $H : X \to \mathbb{R}$ such that

$$\omega(F(u), v) = \langle \mathrm{d}H(u), v\rangle \tag{1.2.3}$$

for all $u \in \mathcal{D}_F$ and $v \in X$. Provided that F is a Hamiltonian vector field, we can use the identity (1.2.3) to formally rewrite the abstract evolution equation (1.2.1) as a Hamiltonian system

$$\omega(u_t, \cdot) = \mathrm{d}H(u), \tag{1.2.4}$$

where the bilinear form ω defines a linear operator $u \mapsto \omega(u,\cdot)$ from X to its dual space $X^\star$.

Since we want equation (1.2.4) to possess additional symmetries, we require the existence of a finite-dimensional Lie group G that acts on X.

Assumption 1.2.2. The Lie group G acts on X via a homomorphism

$$a\colon G \to \mathrm{GL}(X),$$

whose images $a(g)$ are symplectic.

Remark 2. Assumption 1.2.2 is too restrictive for the rain gutter equation since

$$a(\gamma)v = v + \begin{pmatrix} 0 \\ 0 \\ \gamma \\ 0 \end{pmatrix}$$

for $\gamma \in G = \mathbb{R}$ is an affine transformation and not in $\mathrm{GL}(\mathbb{R}^4)$. However, the bijective functions from $\mathbb{R}^4$ to itself, together with the operation of composition, form a group, and a is a group homomorphism since

$$a(\gamma_1)[a(\gamma_2)v] = v + \begin{pmatrix} 0 \\ 0 \\ \gamma_2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \\ 0 \end{pmatrix} = a(\gamma_1 + \gamma_2)v.$$

Moreover, by setting $f(v) = a(\gamma)v$ for $v \in \mathbb{R}^4$, we get $\mathrm{d}f(y)v = v$ for all $y \in \mathbb{R}^4$, which means, that $a(\gamma)$ is symplectic for all $\gamma \in \mathbb{R}$. Since our main interest are Hamiltonian PDEs, where translations in space are linear mappings, we decide against keeping affine transformations in the general framework.

If it exists, the (Gâteaux) differential of $a(\cdot)v$ at unity in the direction of μ is denoted by $\mathrm{d}[a(\mathbb{1})v]\mu$ and

$$\mathcal{D}_\mu = \{v \in X\colon \text{The differential of } a(\cdot)v \text{ at unity in the direction of } \mu \text{ exists.}\}$$

denotes the domain of the operator $\mathrm{d}[a(\mathbb{1})\cdot]\mu\colon \mathcal{D}_\mu \to X$, $v \mapsto \mathrm{d}[a(\mathbb{1})v]\mu$. In general, the mapping $a(\cdot)v\colon G \to X$, $\gamma \mapsto a(\gamma)v$ is not smooth for all $v \in X$, but we require the operators $\mathrm{d}[a(\mathbb{1})\cdot]\mu$ for $\mu \in \mathcal{A}$ to have a common dense domain in X.

Assumption 1.2.3. The operator $F\colon \mathcal{D}_F \subseteq X \to X$ is densely defined and its domain is a subset of the intersection

$$\mathfrak{D}_a^1 = \bigcap_{\mu \in \mathcal{A}} \mathcal{D}_\mu.$$

Remark 3. Linearity of the differential allows us to pick a basis in $\mathcal{A}$, which leads to a finite intersection.

We deal with the lack of smoothness of the group action by making use of the weak formulation in (1.2.4).

Assumption 1.2.4. For all $\mu \in \mathcal{A}$ the mapping

$$v \mapsto \omega(\mathrm{d}[a(\mathbb{1})v]\mu, \cdot)$$

can be continuously extended to a bounded linear operator $B(\cdot)\mu\colon X \to X^\star$, which means

$$\langle B(v)\mu, u\rangle = \omega(\mathrm{d}[a(\mathbb{1})v]\mu, u)$$

holds for all $u \in X$ and $v \in \mathcal{D}_\mu$.

Before we discuss implications of this setting, we are left to impose our requirements on the Hamiltonian. A function $f : X \to V$ with images in a Banach space $\left(V, \|\cdot\|_V\right)$ is called *locally bounded* if for any $x \in X$ there exists a neighborhood $\mathcal{U}$ such that $\left\|f(\widetilde{x})\right\|_V \leq C$ holds uniformly for $\widetilde{x} \in \mathcal{U}$.

Assumption 1.2.5. The Hamiltonian $H : X \to \mathbb{R}$ is twice continuously differentiable with locally bounded derivatives and invariant with respect to the group action, i.e.,

$$H(a(\gamma)v) = H(v)$$

for all $v \in X$ and $\gamma \in G$.

Differentiating the identity $H(a(\gamma)v) = H(v)$ with respect to v yields

$$a(\gamma)^\star \mathrm{d}H(a(\gamma)v) = \langle \mathrm{d}H(a(\gamma)v), a(\gamma)\cdot\rangle = \mathrm{d}H(v) \in X^\star. \tag{1.2.5}$$

Let us show that due to this formula, an invariant Hamiltonian leads to an equivariant Hamiltonian system and vice versa, where equivariance is defined as follows. The evolution equation (1.2.1) is called equivariant if the inclusion

$$a(\gamma)\mathcal{D}_F \subseteq \mathcal{D}_F$$

holds for all $\gamma \in G$, and if

$$F(a(\gamma)v) = a(\gamma)F(v) \tag{1.2.6}$$

for all $v \in \mathcal{D}_F$ and $\gamma \in G$.

Proposition 1.2.6. *Given the Assumptions 1.2.2 and 1.2.3, suppose that we have $a(\gamma)v \in \mathcal{D}_F$ for all $v \in \mathcal{D}_F$ and $\gamma \in G$. Then $H(a(\gamma)v) = H(v)$ for all $v \in X$, $\gamma \in G$ if and only if (1.2.6) holds for all $v \in \mathcal{D}_F$, $\gamma \in G$.*

Proof. From the symplecticity of the group action and (1.2.5) we deduce

$$\begin{aligned}\omega(a(\gamma^{-1})F(a(\gamma)v), u) &= \omega(F(a(\gamma)v), a(\gamma)u) = \langle \mathrm{d}H(a(\gamma)v), a(\gamma)u\rangle \\ &= \langle \mathrm{d}H(v), u\rangle = \omega(F(v), u)\end{aligned}$$

for $v \in \mathcal{D}_F$ and $\gamma \in G$, while (1.2.6) follows from Lemma 1.2.1. In a similar way, we obtain from (1.2.6) the identity

$$a(\gamma)^\star \mathrm{d}H(a(\gamma)v) = \mathrm{d}H(v)$$

for $v \in \mathcal{D}_F$ and $\gamma \in G$. By continuity the validity of the formula extends to all $v \in X$. This implies that the mapping $v \mapsto H(a(\gamma)v) - H(v)$ is constant for fixed $\gamma \in G$. Since it vanishes for $v = 0 \in X$, the constant equals zero. □

Physically speaking, such symmetry properties lead by Noether's theorem to additional conserved quantities. For $\mu \in \mathcal{A}$ we define the functionals

$$Q(\cdot)\mu \colon X \to \mathbb{R}, \quad v \mapsto \tfrac{1}{2}\langle B(v)\mu, v\rangle, \tag{1.2.7}$$

where $v \mapsto B(v)\mu$ extends $v \mapsto \omega(\mathrm{d}[a(\mathbb{1})v]\mu, \cdot)$ as stated in Assumption 1.2.4. From (1.2.7) we obtain the identity

$$\langle \mathrm{d}Q(v)\mu, u\rangle = \omega(\mathrm{d}[a(\mathbb{1})v]\mu, u) \tag{1.2.8}$$

for all $\mu \in \mathcal{A}$, $v \in \mathcal{D}_\mu$, and $u \in X$. In the following, we write $\mathrm{d}Q(\cdot)\mu$ instead of $B(\cdot)\mu$.

The invariance of $Q(\cdot)\mu$ under the group action is a consequence of the symplecticity of $a(\gamma)$. However, in general, the invariance is only true for a suitable subgroup. This restriction arises from the fact that the Lie group G is not assumed to be commutative. Having this in mind, we treat the tangent space $\mathcal{A} = T_{\mathbb{1}}G$ as a Lie algebra together with the commutator

$$[\sigma, \mu] = \sigma\mu - \mu\sigma, \quad \sigma, \mu \in \mathcal{A}$$

as its Lie bracket. The centralizer of $\mu \in \mathcal{A}$ is defined to be

$$\mathrm{C}_{\mathcal{A}}(\mu) = \{\sigma \in \mathcal{A} \colon [\sigma, \mu] = 0\}.$$

Since $\mathrm{C}_{\mathcal{A}}(\mu)$ is a Lie subalgebra of $\mathcal{A}$, there exists a unique connected Lie subgroup, which has $\mathrm{C}_{\mathcal{A}}(\mu)$ as its Lie algebra and is generated by $e^{\mathrm{C}_{\mathcal{A}}(\mu)}$ (see e.g. [51]). We denote this subgroup by $G(e^{\mathrm{C}_{\mathcal{A}}(\mu)})$.

Proposition 1.2.7. *Given the Assumptions 1.2.2-1.2.4, the identity*

$$Q(a(\gamma)v)\mu = Q(v)\mu$$

holds for all $v \in X$, $\mu \in \mathcal{A}$, and $\gamma \in G(e^{\mathrm{C}_{\mathcal{A}}(\mu)})$.

Proof. By continuity it is sufficient to prove the invariance for $v \in \mathcal{D}_\mu$, which is dense in X by Assumption 1.2.3. Since $\gamma \in G(e^{\mathrm{C}_{\mathcal{A}}(\mu)})$ and $e^{t\mu}$ commute, we obtain

$$a(e^{t\mu})a(\gamma)v = a(\gamma)a(e^{t\mu})v.$$

Differentiating this identity with respect to time at $t = 0$ yields

$$\mathrm{d}[a(\mathbb{1})(a(\gamma)v)]\mu = a(\gamma)\mathrm{d}[a(\mathbb{1})v]\mu.$$

Therefore, we get

$$Q(a(\gamma)v)\mu = \tfrac{1}{2}\omega(\mathrm{d}[a(\mathbb{1})(a(\gamma)v)]\mu, a(\gamma)v) = \tfrac{1}{2}\omega(\mathrm{d}[a(\mathbb{1})v]\mu, v) = Q(v)\mu$$

by the symplecticity of the group action. □

The invariance of H and Q with respect to the group action has the following consequence.

Corollary 1.2.8. *Let the Assumptions 1.2.2-1.2.5 be satisfied. Then we have*

$$\langle \mathrm{d}H(v), \mathrm{d}[a(\mathbb{1})v]\sigma\rangle = 0 \tag{1.2.9}$$

for all $\sigma \in \mathcal{A}$ and $v \in \mathfrak{D}_a^1$. Moreover, if $[\mu, \sigma] = 0$ for $\mu \in \mathcal{A}$, we get

$$\langle \mathrm{d}Q(v)\mu, \mathrm{d}[a(\mathbb{1})v]\sigma\rangle = 0. \tag{1.2.10}$$

Proof. These two identities are obtained by differentiating at $\gamma = \mathbb{1}$ the equations $H(a(\gamma)v) = H(v)$ and $Q(a(\gamma)v)\mu = Q(v)\mu$. □

Since a is a symplectic group homomorphism, we also have

$$\omega\big(a(g)v, y\big) = \omega\big(a(\gamma)a(g)v, a(\gamma)y\big) = \omega\big(a(\gamma g)v, a(\gamma)y\big) \tag{1.2.11}$$

for all $\gamma, g \in G$ and $v, y \in X$. The right hand side of (1.2.11) involves the multiplication of the Lie group elements γ and g. In the proof of Proposition 1.2.7 we circumvented the differentiation with respect to a Lie group element by introducing the real variable t. In the following, it is preferable to directly analyze the Lie group operations. Denote the left multiplication with γ by L_γ, i.e.,

$$L_\gamma \colon G \to G, \quad g \mapsto \gamma g,$$

and write its derivative at $g \in G$ in the following way

$$\mathrm{d}L_\gamma(g) \colon T_gG \to T_{\gamma g}G, \quad \mu \mapsto \mathrm{d}L_\gamma(g)\mu.$$

The derivative at unity $\mathrm{d}L_\gamma(\mathbb{1})$ is a linear homeomorphism between the tangent spaces $\mathcal{A}$ and $T_\gamma G$ (see [1] for further details). In the same way a right multiplication R_γ and its derivative $\mathrm{d}R_\gamma$ are defined.

The identity (1.2.8) and differentiation of (1.2.11) at $g = \mathbb{1}$ give us

$$\langle \mathrm{d}Q(v)\mu, y\rangle = \omega\big(\mathrm{d}[a(\mathbb{1})v]\mu, y\big) = \omega\big(\mathrm{d}[a(\gamma)v]\mathrm{d}L_\gamma(\mathbb{1})\mu, a(\gamma)y\big) \tag{1.2.12}$$

for all $\mu \in \mathcal{A}$ and $v \in \mathcal{D}_\mu$, the domain of $\mathrm{d}[a(\mathbb{1})\cdot]\mu$. However, by Assumption 1.2.4, the derivative of Q exists for all $v \in X$. That is why the right hand side of (1.2.12) can be continously extended to the whole space.

Let us further show that the symmetry of $\mathrm{d}Q(\cdot)\mu$ is an immediate consequence of the symplecticity of the group action $a(\gamma)$ and Lemma A.2.1 from the Appendix.

Proposition 1.2.9. *Given the Assumptions 1.2.2-1.2.4, the operators*

$$\mathrm{d}Q(\cdot)\mu \colon X \to X^\star$$

are symmetric, i.e.,

$$\langle \mathrm{d}Q(v)\mu, u\rangle = \langle \mathrm{d}Q(u)\mu, v\rangle \tag{1.2.13}$$

for all $\mu \in \mathcal{A}$ and $v, u \in X$.

Proof. By continuity it suffices to prove the symmetry on the dense subset $\mathcal{D}_\mu$. From the symplecticity of the group action and the skew-symmetry of ω we conclude

$$\omega(a(\gamma)v, u) = \omega(v, a(\gamma^{-1})u) = -\omega(a(\gamma^{-1})u, v).$$

By Lemma A.2.1, differentiating with respect to γ at unity implies

$$\langle \mathrm{d}Q(v)\mu, u\rangle = \omega(\mathrm{d}[a(\mathbb{1})v]\mu, u) = \omega(\mathrm{d}[a(\mathbb{1})u]\mu, v) = \langle \mathrm{d}Q(u)\mu, v\rangle,$$

which finishes the proof. □

Due to these conserved quantities, many solutions of Hamiltonian systems possess specific spatio-temporal patterns. Physically speaking, these solutions are solitary waves, which take the form of relative equilibria in our abstract setting.

Definition 1.2.10. A solution $u\colon [0,\infty) \to X$ of (1.2.4) is called a relative equilibrium if there exist $v_\star \in X$ and $\mu_\star \in \mathcal{A}$ such that

$$u(t) = a(e^{t\mu_\star})v_\star \tag{1.2.14}$$

is satisfied for all $t \geq 0$.

We also use the notation $\gamma_\star(t) = e^{t\mu_\star}$, which means $u(t) = a(\gamma_\star(t))v_\star$.

1.2.2 Hamiltonian Evolution Equations

In Section 1.2.1 we considered a weak formulation of the problem (1.2.1) in the dual space $X^\star$, but with classical derivatives in time. However, solutions of partial differential equations may only be differentiable with respect to time in a generalized sense. This leads to the notion of a generalized solution as in [68].

Definition 1.2.11. Let $\mathcal{I} \subseteq \mathbb{R}$ be an interval. A continuous function $u\colon \mathcal{I} \to X$ is called a generalized solution of (1.2.4) if we have

$$-\int_{\mathcal{I}} \omega(u(t), y)\varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \langle \mathrm{d}H(u(t)), y\rangle \varphi(t)\mathrm{d}t \tag{1.2.15}$$

for all $y \in X$ and test functions $\varphi \in \mathcal{C}_0^\infty(\mathcal{I}^\circ; \mathbb{R})$, where $\mathcal{I}^\circ$ is the interior of $\mathcal{I}$.

Remark 4. If we set $\psi = \omega(\cdot, y) \in X^\star$, we obtain the definition of a weak solution as in [32]. However, we avoid the term weak solution since it may lead to confusion. In PDE applications, such as the nonlinear Schrödinger equation, a weak solution $u \in L^\infty(\mathcal{I}; L^2(\mathbb{R}; \mathbb{C}))$ must obey the integral formulation in the sense of Duhamel's principle. That is, the continuity with respect to time holds with images in $\mathcal{S}^\star(\mathbb{R}; \mathbb{C})$, the class of tempered distributions. If u is continuous in the $L^2(\mathbb{R}; \mathbb{C})$ topology, it is said to be a strong solution. See [58] for further details.

Having in mind transformations in time and space, it is convenient to make use of the following conclusion.

Lemma 1.2.12. *Let u be a generalized solution of (1.2.4). Then we have*

$$-\int_{\mathcal{I}} \omega\big(u(t), \Phi_t(t)\big)\mathrm{d}t = \int_{\mathcal{I}} \langle \mathrm{d}H(u(t)), \Phi(t)\rangle \mathrm{d}t \tag{1.2.16}$$

for all $\Phi \in \mathcal{C}_0^1(\mathcal{I}^\circ; X)$.

Proof. Since X is separable, we can approximate $\Phi \in \mathcal{C}_0^1(\mathcal{I}^\circ; X)$ arbitrarily closely by a sum $\sum_{k=1}^{N} \varphi_k y_k$, where we have $y_k \in X$, $\varphi_k \in \mathcal{C}_0^\infty(\mathcal{I}^\circ; \mathbb{R})$, and $N \in \mathbb{N}$. Then the assertion follows by linearity of (1.2.15) with respect to $\varphi(t)y$. □

So far, our notion of generalized solutions is nothing but a definition. We are left to prove that this is a generalization. In particular, we have to show that a smooth solution of (1.2.1) is a generalized solution in the sense of Definition 1.2.11, and under suitable regularity conditions, vice versa.

Proposition 1.2.13. *A function $u \in \mathcal{C}(\mathcal{I}; \mathcal{D}_F) \cap \mathcal{C}^1(\mathcal{I}^\circ; X)$ is a solution of (1.2.1) if and only if it is a generalized solution in the sense of Definition 1.2.11.*

Proof. If a smooth function u solves (1.2.1), i.e., we have $u_t = F(u)$, then it follows $\omega(u_t, \cdot) = \omega(F(u), \cdot) = \mathrm{d}H(u)$, which implies by integration by parts

$$-\int_{\mathcal{I}} \omega(u(t), y)\varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \omega(u_t(t), y)\varphi(t)\mathrm{d}t = \int_{\mathcal{I}} \langle \mathrm{d}H(u(t)), y\rangle \varphi(t)\mathrm{d}t$$

for all $y \in X$ and $\varphi \in \mathcal{C}_0^\infty(\mathcal{I}^\circ; \mathbb{R})$. Therefore, the function u is a generalized solution in the sense of Definition 1.2.11. On the other hand, given a generalized solution $u \in \mathcal{C}(\mathcal{I}; \mathcal{D}_F) \cap \mathcal{C}^1(\mathcal{I}^\circ; X)$, we find by applying integration by parts

$$\int_{\mathcal{I}} \omega(u_t(t), y)\varphi(t)\mathrm{d}t = -\int_{\mathcal{I}} \omega(u(t), y)\varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \langle \mathrm{d}H(u(t)), y\rangle \varphi(t)\mathrm{d}t$$

for all $y \in X$, $\varphi \in \mathcal{C}_0^\infty(\mathcal{I}^\circ; \mathbb{R})$. Now we make use of Lemma 1.2.1 together with a standard argument from the theory of distributions to conclude $u_t = F(u)$. □

Next, we collect our assumptions on local existence, uniqueness, continuous dependence, and persistence of regularity.

Assumption 1.2.14. The Banach space $(X, \|\cdot\|)$ is continuously embedded into another Banach space $(X_{-1}, \|\cdot\|_{-1})$, such that for each $u_0 \in X$ the following properties hold.

(a) There exist maximal existence times $T_{u_0}^- < 0$, $T_{u_0}^+ > 0$, and a unique function $u \in \mathcal{C}(\mathcal{I}; X) \cap \mathcal{C}^1(\mathcal{I}; X_{-1})$ satisfying (1.2.15) on $\mathcal{I} = (T_{u_0}^-, T_{u_0}^+)$ with the initial condition $u(0) = u_0$.

(b) For $M > 0$, there exist $T > 0$ and $\mathcal{R} < \infty$ such that the solutions with initial data $\|u_0\| \le M$ exist on $[0, T]$ and satisfy

$$\big\|u(t)\big\| + \big\|u_t(t)\big\|_{-1} \le \mathcal{R}$$

for all $t \in [0, T]$.

(c) Solutions depend continuously on their initial data in the following sense. For any solution $\widetilde{u}$ from (a) and any $\varrho > 0$ satisfying $[-\varrho, \varrho] \subseteq (T^-_{\widetilde{u}_0}, T^+_{\widetilde{u}_0})$, there exist $\delta, \mathcal{M} > 0$ such that solutions u with initial data $\|u_0 - \widetilde{u}_0\| \leq \delta$ exist on $[-\varrho, \varrho]$ and can be estimated by

$$\big\|u(t) - \widetilde{u}(t)\big\| + \big\|u_t(t) - \widetilde{u}_t(t)\big\|_{-1} \leq \mathcal{M}\|u_0 - \widetilde{u}_0\| \leq \mathcal{M}\delta.$$

(d) For $u_0 \in \mathcal{D}_F$ the solutions satisfy $u \in \mathcal{C}(T^-_{u_0}, T^+_{u_0}; \mathcal{D}_F) \cap \mathcal{C}^1(T^-_{u_0}, T^+_{u_0}; X)$.

Remark 5. We have simplified the notation by omitting the embedding, i.e., we formally assume $X \subseteq X_{-1}$. Moreover, it is worth mentioning that in some applications X_{-1} is the dual of X, while it is not in the general case.

Now, we deduce conservation laws, by exploiting these properties. It is a well-known fact that the solutions of a Hamiltonian system preserve the Hamiltonian $H\colon X \to \mathbb{R}$, i.e.,

$$H(u(t)) = H(u(0))$$

for all initial values $u(0) \in X$ and $t \in \mathcal{I}$. In other words, the Hamiltonian is a first integral, i.e.,

$$(H \circ u)_t = 0.$$

The formal proof for smooth solutions $u \in \mathcal{C}(\mathcal{I}; \mathcal{D}_F) \cap \mathcal{C}^1(\mathcal{I}; X)$ writes

$$(H \circ u)_t = \langle \mathrm{d}H(u), u_t \rangle = \omega(u_t, u_t) = 0,$$

where we have used (1.2.4) and the skew-symmetry of ω. The conservation property for generalized solutions is stated as a lemma.

Lemma 1.2.15. *Provided that Assumption 1.2.14 holds, let $E : X \to \mathbb{R}$ be a continuous function that is preserved by all smooth solutions $u \in \mathcal{C}(\mathcal{I}; \mathcal{D}_F) \cap \mathcal{C}^1(\mathcal{I}; X)$. Then it follows*

$$E(u(t)) = E(u(0))$$

for all $t \in \mathcal{I}$ and all generalized solutions $u \in \mathcal{C}(\mathcal{I}; X)$.

Proof. For $u \in \mathcal{C}(\mathcal{I}; X)$ we define

$$\mathfrak{A} = \{t \in \mathcal{I} : E(u(t)) = E(u(0))\}.$$

The first step is to show that $\mathfrak{A}$ is closed in $\mathcal{I}$. Let $t_n \in \mathfrak{A}$ be a sequence such that $t_n \to t \in \mathcal{I}$. From $u \in \mathcal{C}(\mathcal{I}; X)$ it follows $\|u(t_n) - u(t)\| \to 0$, which implies $E(u(t_n)) \to E(u(t))$ by the continuity of E. However, we have $E(u(t_n)) = E(u(0))$ due to $t_n \in \mathfrak{A}$. This yields $E(u(t)) = E(u(0))$, which means $t \in \mathfrak{A}$. Hence $\mathfrak{A}$ is closed in $\mathcal{I}$.

Next we show that $0 \in \mathfrak{A}$ is an interior point of $\mathfrak{A}$. By combining Assumption 1.2.14(c) and Assumption 1.2.14(d), there exists $\tau > 0$ and a sequence of functions

$u_n \in \mathcal{C}([-\tau,\tau];\mathcal{D}_F) \cap \mathcal{C}^1([-\tau,\tau];X)$ satisfying (1.2.15) with $\|u_n(t) - u(t)\| \to 0$ as $n \to \infty$ uniformly for $t \in [0,\tau]$. Then we have $E(u_n(0)) \to E(u(0))$ and $E(u_n(0)) = E(u_n(t)) \to E(u(t))$ for $t \in [0,\tau]$. By the uniqueness of the limit it follows $t \in \mathfrak{A}$ for $t \in [0,\tau]$.

Since an autonomous equation is invariant under time shifting, any point of $\mathfrak{A}$ is an interior point. Hence, we conclude $\mathfrak{A} = \mathcal{I}$. □

Likewise, other symmetries give rise to additional conserved quantities, where the word symmetry refers to some invariance under a Lie group of transformations. In particular, the functionals $Q(\cdot)\mu$ are conserved quantities. Indeed, by combining the identities (1.2.3), (1.2.8), and (1.2.9), we find

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q(u)\mu\Big] = \langle \mathrm{d}Q(u)\mu, u_t\rangle = \omega(\mathrm{d}[a(\mathbb{1})u]\mu, F(u)) = -\langle \mathrm{d}H(u), \mathrm{d}[a(\mathbb{1})u]\mu\rangle = 0,$$

provided $u \in \mathcal{C}(\mathcal{I};\mathcal{D}_F) \cap \mathcal{C}^1(\mathcal{I};X)$ holds. Then, by Lemma 1.2.15 we obtain the conservation of the functionals $Q(\cdot)\mu$ for the flows of all generalized solutions.

1.3 Partial Differential Equations as Hamiltonian Systems

Hamiltonian partial differential equations appear in many areas of physics. Some famous examples are the nonlinear Schrödinger equation

$$iu_t = -u_{xx} - |u|^2 u, \quad u(0,x) = u_0(x) \in H^1(\mathbb{R};\mathbb{C})$$

and the nonlinear Klein-Gordon equation

$$u_{tt} = u_{xx} - u + |u|^2 u, \quad u(0,x) = u_0(x) \in H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3).$$

In the following, we rewrite these equations as abstract Hamiltonian systems and discuss some of their relative equilibria. In terms of spatial variables we restrict ourselves to the one-dimensional case. As a consequence the stationary problems, which lead to relative equilibria, are ordinary differential equations. Moreover, the short and full notation will be used synonymously, i.e., $u = u(t) = u(t,x)$.

1.3.1 Nonlinear Schrödinger Equation (NLS)

The cubic nonlinear Schrödinger equation is given by

$$iu_t(t,x) = -u_{xx}(t,x) + \kappa|u(t,x)|^2 u(t,x), \quad u(0,x) = u_0(x), \tag{1.3.1}$$

where κ is a real constant. Moreover, we have $t \in \mathbb{R}_{>0}$, $x \in \mathbb{R}$, and $u(x,t) \in \mathbb{C}$. This equation is a nonlinear perturbation of the linear Schrödinger equation

$$iu_t + u_{xx} = 0,$$

which is used to describe the evolution of a quantum state in a physical system, while the NLS has applications to nonlinear optics and waves in dispersive media.

The choice of the parameter κ can be reduced to the two fundamental cases $\kappa = \pm 1$. In quantum mechanics these refer to the attractive and the repulsive case. The more common terms, however, arise from nonlinear optics, where the Kerr effect describes the change in the refractive index of a material in terms of the intensity of an applied electric field. Depending on the medium, a propagating laser beam has a self-focusing or self-defocusing effect, and as a result the medium acts as a focusing, respectively defocusing, lens. We refer to [22] and [41] for further details on this topic.

In case of the NLS, the relative sign of the linear (diffraction) term and the (Kerr-)nonlinearity matters. If they have the same sign, i.e., $\kappa < 0$, we are in the focusing case, whereas the defocusing case occurs for different signs, which means $\kappa > 0$.

The problem (1.3.1) fits into the abstract framework by using the Sobolev space

$$X = H^1(\mathbb{R}; \mathbb{C}),$$

which is a dense subspace of $L^2(\mathbb{R}; \mathbb{C})$. We equip $L^2(\mathbb{R}; \mathbb{C})$ with the real inner product

$$\big(u, v\big)_0 = \int_{\mathbb{R}} \big(u_1(x)v_1(x) + u_2(x)v_2(x)\big)\mathrm{d}x = \int_{\mathbb{R}} \mathrm{Re}\big(\bar{u}(x)v(x)\big)\mathrm{d}x. \tag{1.3.2}$$

That is, in principle, we handle $u = u_1 + iu_2$ by means of its real and imaginary part. However, we use the more convenient complex notation whenever possible.

The Sobolev spaces are defined via Fourier transform. For $s > 0$ we have

$$H^s(\mathbb{R}; \mathbb{C}) = \big\{v \in L^2(\mathbb{R}; \mathbb{C}) \colon \mathcal{F}^{-1} q_s \mathcal{F} v \in L^2(\mathbb{R}; \mathbb{C})\big\} \tag{1.3.3}$$

with $q_s(\xi) = (1 + |\xi|^2)^{\frac{s}{2}}$, and the corresponding norm is given by

$$\|v\|_s = \big\|\mathcal{F}^{-1} q_s \mathcal{F} v\big\|_0 .$$

The norm $\|\cdot\|_0$ coincides with the usual $L^2(\mathbb{R}; \mathbb{C})$-norm, and $X^\star = H^{-1}(\mathbb{R}; \mathbb{C})$ is the dual space of X. For $s = -1$, we have to replace $v \in L^2(\mathbb{R}; \mathbb{C})$ in (1.3.3) by $v \in \mathcal{S}^\star(\mathbb{R}; \mathbb{C})$, the space of tempered distributions. More details and alternative definitions can be found in [17].

By multiplying (1.3.1) with $-i$, the cubic nonlinear Schrödinger equation becomes

$$u_t = i(u_{xx} - \kappa |u|^2 u). \tag{1.3.4}$$

We write $F(v) = L(v) + N(v)$, where $L(v) = iv_{xx}$ and $N(v) = -i\kappa|v|^2 v$. Then (1.3.4) takes the abstract form $u_t = F(u)$, and we are left to specify a dense domain $\mathcal{D}_F \subseteq X$ such that $F \in \mathcal{C}(\mathcal{D}_F; H^1(\mathbb{R}; \mathbb{C}))$.

Lemma 1.3.1. *The differential operator $L : H^3(\mathbb{R}; \mathbb{C}) \to H^1(\mathbb{R}; \mathbb{C})$, $v \mapsto iv_{xx}$ is continous.*

Proof. We set $q_s(\xi) = (1+|\xi|^2)^{\frac{s}{2}}$ and $p_s(\xi) = |\xi|^s$. By Plancherel's theorem the Fourier transform is an isometry with respect to the L_2-Norm $\|\cdot\|_0$. Hence, from $q_1(\xi)p_2(\xi) \leq q_3(\xi)$ for all $\xi \in \mathbb{R}$, we conclude

$$\|L(v)\|_1 = \|v_{xx}\|_1 = \|\mathcal{F}^{-1}q_1\mathcal{F}v_{xx}\|_0 = \|\mathcal{F}^{-1}q_1p_2\mathcal{F}v\|_0 \leq \|\mathcal{F}^{-1}q_3\mathcal{F}v\|_0 = \|v\|_3,$$

which implies $L \in \mathcal{C}\big(H^3(\mathbb{R};\mathbb{C}); H^1(\mathbb{R};\mathbb{C})\big)$ by the linearity of the operator. □

For the nonlinear part we prove the stronger result $N \in \mathcal{C}\big(H^1(\mathbb{R};\mathbb{C}); H^1(\mathbb{R};\mathbb{C})\big)$, which is based on the properties of generalized Banach algebras. The following definition is taken from [67].

Definition 1.3.2. A Banach space $\big(X, \|\cdot\|\big)$ that at the same time is an associative algebra $\big(X, \cdot\big)$ is called a generalized Banach algebra if

$$\|u \cdot v\| \leq C\|u\|\|v\|$$

holds uniformly for all $u, v \in X$. We speak of a Banach algebra if $C = 1$.

In fact, the Sobolev space $H^s(\mathbb{R};\mathbb{C})$ for $s > \frac{1}{2}$ forms a generalized Banach algebra under the pointwise product. This result is due to Strichartz (see [54]).

Lemma 1.3.3. *The mapping $N : H^1(\mathbb{R};\mathbb{C}) \to H^1(\mathbb{R};\mathbb{C})$, $v \mapsto -i\kappa|v|^2v$ defines a continous operator.*

Proof. For $v \in H^1(\mathbb{R};\mathbb{C})$ we conclude $N(v) \in H^1(\mathbb{R};\mathbb{C})$ and $\|N(v)\|_1 \leq C\|v\|_1^3$, where we use the fact that $\|v\|_1 = \|\bar{v}\|_1$. For the (real) derivative of N we get

$$\|\mathrm{d}N(v)h\|_1 = \|2\bar{v}vh + v^2\bar{h}\|_1 \leq C\|v\|_1^2\,\|h\|_1$$

for any $h \in H^1(\mathbb{R};\mathbb{C})$ by the same argument. Now let $\|u - v\|_1 \leq \delta$ hold. Then

$$\|N(u) - N(v)\|_1 \leq C\big(\|v\|_1 + \delta\big)^2\|u - v\|_1$$

yields $N \in \mathcal{C}\big(H^1(\mathbb{R};\mathbb{C}); H^1(\mathbb{R};\mathbb{C})\big)$. □

The next step is to show that $F(v) = i(v_{xx} - \kappa|v|^2v)$ with $\mathcal{D}_F = H^3(\mathbb{R};\mathbb{C})$ yields a Hamiltonian vector field in the sense of (1.2.3).

Proposition 1.3.4. *Equation (1.3.4) is a Hamiltonian system with respect to*

$$H\colon H^1(\mathbb{R};\mathbb{C}) \to \mathbb{R}, \quad H(u) = \frac{1}{2}\int_{\mathbb{R}} \Big(|u_x(x)|^2 + \frac{\kappa}{2}|u(x)|^4\Big)\mathrm{d}x,$$

and the symplectic form

$$\omega\colon H^1(\mathbb{R};\mathbb{C}) \times H^1(\mathbb{R};\mathbb{C}) \to \mathbb{R}, \quad \omega(u,v) = \int_{\mathbb{R}} \mathrm{Im}\big(\bar{u}(x)v(x)\big)\mathrm{d}x = \big(iu, v\big)_0.$$

That is, these functions satisfy (1.2.3), where

$$F\colon H^3(\mathbb{R};\mathbb{C}) \to H^1(\mathbb{R};\mathbb{C}), \quad F(u) = i(u_{xx} - \kappa|u|^2u)$$

is the right hand side of the nonlinear Schrödinger equation.

Proof. We have to show

$$\omega(F(u),v) = \langle \mathrm{d}H(u), v\rangle$$

for all $u \in H^3(\mathbb{R};\mathbb{C})$ and $v \in H^1(\mathbb{R};\mathbb{C})$. By writing

$$H(u) = T(u) + U(u),$$

the Hamiltonian is split into two parts, the kinetic energy

$$T(u) = \frac{1}{2}\int_{\mathbb{R}} |u_x(x)|^2 \mathrm{d}x$$

and the potential energy

$$U(u) = \frac{\kappa}{4}\int_{\mathbb{R}} |u(x)|^4 \mathrm{d}x.$$

Analyzing the kinetic part, we obtain

$$\begin{aligned} T(u+v) &= \frac{1}{2}\int_{\mathbb{R}} \big(|u_x(x)|^2 + \bar{u}_x(x)v_x(x) + u_x(x)\bar{v}_x(x) + |v_x(x)|^2\big)\mathrm{d}x \\ &= T(u) + \int_{\mathbb{R}} \mathrm{Re}\big(\bar{u}_x(x)v_x(x)\big)\mathrm{d}x + \mathcal{O}(\|v\|_1^2), \end{aligned}$$

which yields the derivative

$$\langle \mathrm{d}T(u), v\rangle = \int_{\mathbb{R}} \mathrm{Re}\big(\bar{u}_x(x)v_x(x)\big)\mathrm{d}x = \big(u_x, v_x\big)_0. \tag{1.3.5}$$

Now, we study the potential part and note that

$$|z+\zeta|^4 = \big(|z|^2 + z\bar{\zeta} + \bar{z}\zeta + |\zeta|^2\big)^2 = |z|^4 + 2|z|^2(\bar{z}\zeta + z\bar{\zeta}) + \mathcal{O}(|\zeta|^2)$$

for $z, \zeta \in \mathbb{C}$. This leads to

$$\begin{aligned} U(u+v) &= U(u) + \frac{\kappa}{4}\int_{\mathbb{R}} 2\,|u(x)|^2\big(\bar{u}(x)v(x) + u(x)\bar{v}(x)\big)\mathrm{d}x + \mathcal{O}(\|v\|_1^2) \\ &= U(u) + \kappa\int_{\mathbb{R}} \mathrm{Re}\big(|u(x)|^2\bar{u}_x(x)v_x(x)\big)\mathrm{d}x + \mathcal{O}(\|v\|_1^2). \end{aligned}$$

Hence, the derivative takes the form

$$\langle \mathrm{d}U(u), v\rangle = \kappa\int_{\mathbb{R}} \mathrm{Re}\big(|u(x)|^2\bar{u}(x)v(x)\big)\mathrm{d}x = \big(\kappa|u|^2u, v\big)_0. \tag{1.3.6}$$

By combining (1.3.5) and (1.3.6), we get

$$\langle \mathrm{d}H(u), v\rangle = \langle \mathrm{d}T(u), v\rangle + \langle \mathrm{d}U(u), v\rangle = \big(u_x, v_x\big)_0 + \big(\kappa|u|^2u, v\big)_0,$$

which implies

$$\langle \mathrm{d}H(u), v\rangle = \big(-u_{xx} + \kappa|u|^2u, v\big)_0 = \omega(i(u_{xx} - \kappa|u|^2u), v) = \omega(F(u), v)$$

for $u \in H^3(\mathbb{R};\mathbb{C})$ and $v \in H^1(\mathbb{R};\mathbb{C})$ via integration by parts. □

In conclusion, the nonlinear Schrödinger equation written as a Hamiltonian system takes the form

$$\omega(u_t, y) = \big(iu_t, y\big)_0 = \big(u_x, y_x\big)_0 + \big(\kappa|u|^2u, y\big)_0 = \langle \mathrm{d}H(u), y\rangle$$

for $y \in X = H^1(\mathbb{R};\mathbb{C})$. According to Definition 1.2.11 a generalized solution to this equation is a function $u \in \mathcal{C}(\mathcal{I}; X)$ that satisfies

$$-\int_{\mathcal{I}} \big(iu(t), y\big)_0 \varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \Big(\big(u_x(t), y_x\big)_0 + \big(\kappa|u(t)|^2u(t), y\big)_0\Big)\varphi(t)\mathrm{d}t$$

for all $y \in X$ and $\varphi \in C_0^\infty(\mathcal{I}^\circ;\mathbb{R})$.

After the functional setting we consider symmetries of the nonlinear Schrödinger equation. For simplicity, we start with a one-parameter group of gauge transformations. The Lie group is $G = S^1$, the group action $a\colon G \to GL(X)$ is given by

$$a(\gamma)v = e^{-i\gamma}v$$

for $v \in X$ and $\gamma \in G$. Consequently, the derivative of $a(\cdot)v$ at $\mathbb{1}$ is

$$\mathrm{d}[a(\mathbb{1})v]\mu = -i\mu v$$

with $\mu \in \mathcal{A} = \mathbb{R}$. Moreover, we have $\mathrm{d}Q(v)\colon \mathcal{A} \to X^\star$ given by

$$\langle \mathrm{d}Q(v)\mu, y\rangle = \omega(\mathrm{d}([a(\mathbb{1})v])\mu, y) = \big(\mu v, y\big)_0$$

for $y \in X$, and

$$Q\colon X \times \mathcal{A} \to \mathbb{R}, \quad (v,\mu) \mapsto \frac{\mu}{2}\big\|v\big\|_0^2.$$

This group action is smooth for all $v \in X = H^1(\mathbb{R}; C)$. More generally, we consider the two-parameter group

$$a\colon G \to GL(X), \quad a(\gamma)v = e^{-i\gamma_1}v(\cdot - \gamma_2), \quad \gamma = (\gamma_1, \gamma_2) \in G = S^1 \times \mathbb{R}$$

of gauge transformations and translations. Here $\mathcal{A} = \mathbb{R} \oplus \mathbb{R}$ is the Lie-Algebra of G, such that we can write $\mu = \mu_1 e_1 + \mu_2 e_2 \in \mathcal{A}$, where $\{e_1, e_2\} = \{(1,0),(0,1)\}$ is a basis of $\mathcal{A}$. We decompose the derivative of the group action into

$$\mathrm{d}[a(\mathbb{1})v]\mu = \mu_1\mathcal{S}_1 v + \mu_2\mathcal{S}_2 v,$$

where we have

$$\begin{aligned}\mathcal{S}_1 v &= \mathrm{d}[a(\mathbb{1})v]e_1 = -iv,\\ \mathcal{S}_2 v &= \mathrm{d}[a(\mathbb{1})v]e_2 = -v_x.\end{aligned}$$

The focusing cubic nonlinear Schrödinger equation

$$iu_t = -u_{xx} - |u|^2u$$

possesses so-called solitary wave solutions. The initial value $u_0(x) = \frac{\sqrt{2}}{\cosh(x)}$ leads to the solution

$$u_\star(t,x) = \frac{\sqrt{2}}{\cosh(x)} e^{it}. \tag{1.3.7}$$

With (1.3.7) is associated a two-parameter family of solitary wave solution (see e.g. [18] and [20]). It is also known (see [24]) that the number of parameters can be reduced by using further symmetries of the NLS. Going the other way around, we deduce the two-parameter family by exploiting two additional symmetries. The first one is the scale invariance.

Proposition 1.3.5. *If u is a classical solution on $\mathcal{I} = [0,T]$, then so is $\widetilde{u}$ on the scaled interval $\widetilde{\mathcal{I}} = [0,\lambda^2 T]$, where $\widetilde{u}$ is given by*

$$\widetilde{u}(t,x) = \lambda u(\lambda^2 t, \lambda x)$$

for $\lambda > 0$.

Proof. Let us rewrite the NLS as $\mathfrak{L}v = 0$ with

$$\mathfrak{L}v = iv_t + v_{xx} + |v|^2 v. \tag{1.3.8}$$

This differential operator is equivariant in the sense that

$$\begin{aligned}\big[\mathfrak{L}\widetilde{u}\big](t,x) &= i\widetilde{u}_t(t,x) + \widetilde{u}_{xx}(t,x) + \big|\widetilde{u}(t,x)\big|^2\widetilde{u}(t,x)\\ &= i\lambda u_t(\lambda^2 t,\lambda x)\lambda^2 + \lambda u_{xx}(\lambda^2 t,\lambda x)\lambda^2 + \big|\lambda u(\lambda^2 t,\lambda x)\big|^2\lambda u(\lambda^2 t,\lambda x)\\ &= \lambda^3\big[\mathfrak{L}u\big](\lambda^2 t,\lambda x).\end{aligned}$$

This shows that $\widetilde{u}$ is a solution on $\widetilde{\mathcal{I}} = [0,\lambda^2 T]$ if u is a solution on $\mathcal{I} = [0,T]$. □

Remark 6. The scale invariance is very helpful in addressing the question of well-posedness, and the so-called criticality (with respect to scaling) denotes a significant transition in the behaviour of many partial differential equations. For more information on this see [59].

By applying the scaling with $\lambda > 0$, the solution (1.3.7) is transformed into

$$u_\star(t,x) = \lambda e^{i\lambda^2 t}\frac{\sqrt{2}}{\cosh(\lambda x)}. \tag{1.3.9}$$

The other symmetry is the Galilean invariance.

Proposition 1.3.6. *If u is a classical solution and $c \in \mathbb{R}$, then $\widetilde{u}$ given by*

$$\widetilde{u}(t,x) = e^{i\left(\frac{c}{2}x - \frac{c^2}{4}t\right)}u(t, x-ct)$$

is a solution to the same equation.

Proof. For the differential operator (1.3.8) and $g(t,x) = e^{i\left(\frac{c}{2}x - \frac{c^2}{4}t\right)}$ we find

$$\begin{aligned}\big[\mathfrak{L}\widetilde{u}\big](t,x) &= i\widetilde{u}_t(t,x) + \widetilde{u}_{xx}(t,x) + \big|\widetilde{u}(t,x)\big|^2\widetilde{u}(t,x)\\ &= ig(t,x)\big[-i\tfrac{c^2}{4}u + u_t - cu_x\big](t,x-ct)\\ &\quad + g(t,x)\big[(i\tfrac{c}{2})^2u + 2\tfrac{ic}{2}u_x + u_{xx}\big](t,x-ct)\\ &\quad + g(t,x)\big|u(t,x-ct)\big|^2u(t,x-ct)\\ &= g(t,x)\big[\mathfrak{L}u\big](t,x-ct),\end{aligned}$$

which shows that $\widetilde{u}$ is a solution if u is so. □

By exploiting the Galilean invariance, we get the two-parameter family of solutions

$$u_\star(t,x) = \lambda e^{i\left(\lambda^2 t + \frac{c}{2}x - \frac{c^2}{4}t\right)}\frac{\sqrt{2}}{\cosh(\lambda(x-ct))}, \quad \lambda > 0, c \in \mathbb{R}. \tag{1.3.10}$$

Let us change the notation by setting $\mu_1 = -\left(\lambda^2 + \frac{c^2}{4}\right)$ and $\mu_2 = c$. Then we find

$$\lambda^2 t + \tfrac{c}{2}x - \tfrac{c^2}{4}t = -\mu_1 t + \frac{\mu_2}{2}(x - \mu_2 t),$$

and (1.3.10) becomes

$$u_\star(t,x) = e^{-i\mu_1 t}v_\star(x - \mu_2 t) \tag{1.3.11}$$

with the profile

$$v_\star(x) = \sqrt{-\left(\mu_1 + \tfrac{\mu_2^2}{4}\right)}\cdot e^{i\frac{\mu_2}{2}x}\frac{\sqrt{2}}{\cosh\left(\sqrt{-\left(\mu_1 + \frac{\mu_2^2}{4}\right)}\cdot x\right)}.$$

1.3.2 Nonlinear Klein-Gordon Equation (NLKG)

Our next example are coupled nonlinear wave equations, namely the system

$$u_{tt}(t,x) = u_{xx}(t,x) - u(t,x) + |u(t,x)|^2u(t,x), \quad u(0,x) = u_0(x) \tag{1.3.12}$$

with $x \in \mathbb{R}$ and $u(x,t) \in \mathbb{R}^3$, where the Euclidean norm on $\mathbb{R}^3$ is denoted by $|\cdot|$. This is a nonlinear pertubation of the Klein-Gordon equation

$$u_{tt} = u_{xx} - mu,$$

where by rescaling spacetime, the mass m is normalized to equal one. In contrast to the Schrödinger equation, it is consistent with the laws of special relativity and has applications in quantum field theory (see e.g. [31], [63]).

Due to the wave operator, the nonlinear Klein-Gordon equation (NLGK) is a second order hyperbolic partial differential equation. However, by writing

$$u_t(t,x) = \begin{pmatrix}u_1(t,x)\\ u_2(t,x)\end{pmatrix} = \begin{pmatrix}u_2(t,x)\\ u_{1,xx}(t,x) - u_1(t,x) + |u_1(t,x)|^2u_1(t,x)\end{pmatrix}, \tag{1.3.13}$$

it is transformed to a first order system. The transformed equation (1.3.13) takes the abstract form

$$u_t = F(u)$$

with

$$F(v) = \begin{pmatrix} v_2 \\ v_{1,xx} - v_1 + |v_1|^2 v_1 \end{pmatrix}, \tag{1.3.14}$$

where $\mathcal{D}_F = H^2(\mathbb{R};\mathbb{R}^3) \times H^1(\mathbb{R};\mathbb{R}^3)$ is by definition the domain of (1.3.14). Let us show that the Hamiltonian

$$H(u) = \frac{1}{2}\int_{\mathbb{R}} \left(|u_2|^2 + |(u_1)_x|^2 + |u_1|^2 - \tfrac{1}{2}|u_1|^4\right)\mathrm{d}x \tag{1.3.15}$$

and the symplectic form

$$\omega(v,u) = \int_{\mathbb{R}} (v_1^T u_2 - v_2^T u_1)\mathrm{d}x \tag{1.3.16}$$

lead to a weak formulation of this problem, where the phase space is the Hilbert space

$$X = H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3)$$

with its dual space given by

$$X^\star = H^{-1}(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3).$$

Proposition 1.3.7. *Equation (1.3.13) is a Hamiltonian system with respect to (1.3.15), and the symplectic form is given by (1.3.16).*

Proof. We have to show that

$$\omega(F(u),v) = \langle \mathrm{d}H(u), v\rangle$$

for all $u \in \mathcal{D}_F = H^2(\mathbb{R};\mathbb{R}^3) \times H^1(\mathbb{R};\mathbb{R}^3)$ and $v \in X = H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3)$. Plugging (1.3.14) into (1.3.16) gives us

$$\begin{aligned}
\omega(F(u),v) &= \int_{\mathbb{R}} \Big(F_1(u)^T v_2 - F_2(u)^T v_1\Big)\mathrm{d}x \\
&= \int_{\mathbb{R}} \Big(u_2^T v_2 - \big(u_{1,xx} - u_1 + |u_1|^2 u_1\big)^T v_1\Big)\mathrm{d}x \\
&= \int_{\mathbb{R}} u_2^T v_2 \,\mathrm{d}x + \int_{\mathbb{R}} u_{1,x}^T v_{1,x}\,\mathrm{d}x + \int_{\mathbb{R}} u_1^T v_1\,\mathrm{d}x - \int_{\mathbb{R}} |u_1|^2 u_1^T v_1\,\mathrm{d}x.
\end{aligned}$$

We must compare this expression with the derivative of the Hamiltonian. First, we note that for $x, y \in \mathbb{R}^3$ with $|x| \le C$ it holds

$$\begin{aligned}
|x+y|^4 &= \big(|x+y|^2\big)^2 = \big(|x|^2 + 2x^T y + |y|^2\big)^2 \\
&= |x|^4 + 4|x|^2 x^T y + \mathcal{O}(|y|^2).
\end{aligned}$$

For fixed $u \in H^2(\mathbb{R};\mathbb{R}^3) \times H^1(\mathbb{R};\mathbb{R}^3)$ this implies

$$\begin{aligned} H(u+v) &= \frac{1}{2}\int_{\mathbb{R}} \big(|u_2+v_2|^2 + |u_{1,x}+v_{1,x}|^2 + |u_1+v_1|^2 - \tfrac{1}{2}|u_1+v_1|^4\big)\mathrm{d}x \\ &= \frac{1}{2}\int_{\mathbb{R}} \big(|u_2|^2 + |u_{1,x}|^2 + |u_1|^2 - \tfrac{1}{2}|u_1|^4\big)\mathrm{d}x \\ &\quad + \int_{\mathbb{R}} \big(u_2^T v_2 + u_{1,x}^T v_{1,x} + u_1^T v_1 - |u_1|^2 u_1^T v_1\big)\mathrm{d}x + \mathcal{O}(\|v\|^2). \end{aligned}$$

Hence, the derivative of the Hamiltonian takes the form

$$\langle \mathrm{d}H(u), v\rangle = \int_{\mathbb{R}} \big(u_2^T v_2 + u_{1,x}^T v_{1,x} + u_1^T v_1 - |u_1|^2 u_1^T v_1\big)\mathrm{d}x = \omega(F(u), v)$$

for all $u \in H^2(\mathbb{R};\mathbb{R}^3) \times H^1(\mathbb{R};\mathbb{R}^3)$ and $v \in H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3)$. □

The nonlinear Klein-Gordon equation is equivariant under the action of a four-dimensional Lie group of oscillations in u and translations in x. More precisely, the Lie group is given by

$$G = \mathrm{SO}(3) \times \mathbb{R}$$

and the corresponding group action takes the form

$$a\colon G \to GL(X), \quad \gamma \mapsto a(\gamma)v$$

with

$$a(\gamma)v = \big(Av_1(\cdot+\alpha), Av_2(\cdot+\alpha)\big)$$

for $\gamma = (A,\alpha) \in \mathrm{SO}(3) \times \mathbb{R}$ and $v = (v_1, v_2) \in H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3)$. Its derivative at unity along $\mu = (S, c) \in \mathfrak{so}(3) \times \mathbb{R}$ is given by

$$d[a(\mathbb{1})v]\mu = \big(Sv_1 + cv_{1,x}, Sv_2 + cv_{2,x}\big).$$

Before we consider solitary wave solutions, we recall that the product of a skew-symmetric 3×3 matrix with a vector $\nu \in \mathbb{R}^3$ can be rewritten as

$$S\nu = s \times \nu,$$

where we provide

$$S = \begin{pmatrix} 0 & -s_3 & s_2 \\ s_3 & 0 & -s_1 \\ -s_2 & s_1 & 0 \end{pmatrix}.$$

We thereby get an isomorphism from $\mathfrak{so}(3)$ to $\mathbb{R}^3$, which maps S as above to

$$s = \begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}.$$

In particular, if the vector $\nu \in \mathbb{R}^3$ is orthogonal to s, it follows

$$S^2\nu = S(s \times \nu) = s \times (s \times \nu) = -|s|^2\nu.$$

The solitary wave solutions of the nonlinear Klein-Gordon equation that correspond to the symmetry with respect to oscillations in u and translations in x are of the form

$$u_\star(t,x) = \big(e^{tS_\star}v_{\star,1}(x+c_\star t), e^{tS_\star}v_{\star,2}(x+c_\star t)\big), \tag{1.3.17}$$

where $S_\star \in \mathfrak{so}(3)$ is a non-zero skew-symmetric 3×3 matrix, and we have $|c_\star| < 1$. Plugging the ansatz (1.3.17) into (1.3.13) leads to the stationary problem

$$0 = v_2 - S_\star v_1 - c_\star v_{1,x}, \tag{1.3.18a}$$
$$0 = v_{1,xx} - v_1 + |v_1|^2 v_1 - S_\star v_2 - c_\star v_{2,x}. \tag{1.3.18b}$$

The top equation (1.3.18a) can be solved for v_2, and by substituting $S_\star v_1 + c_\star v_{1,x}$ for v_2, the bottom equation (1.3.18b) is transformed into

$$0 = (1-c_\star^2)v_{1,xx} - v_1 + |v_1|^2 v_1 - S_\star^2 v_1 - 2c_\star S_\star v_{1,x}. \tag{1.3.19}$$

Next, we change variables by writing

$$v_1(x) = e^{\alpha_\star x S_\star}\xi(x),$$

where $\alpha_\star \in \mathbb{R}$ is a free variable. Since the first and second derivative of v_1 are given by

$$v_{1,x}(x) = e^{\alpha_\star x S_\star}\Big[\xi_x(x) + \alpha_\star S_\star \xi(x)\Big],$$
$$v_{1,xx}(x) = e^{\alpha_\star x S_\star}\Big[\xi_{xx}(x) + 2\alpha_\star S_\star \xi_x(x) + \alpha_\star^2 S_\star^2 \xi(x)\Big],$$

the stationary equation (1.3.19) is transformed into

$$0 = (1-c_\star^2)\xi_{xx} + k_1(\alpha_\star, c_\star)S_\star\xi_x - k_2(\alpha_\star, c_\star)S_\star^2\xi - \xi + |\xi|^2\xi \tag{1.3.20}$$

with coefficients given by

$$k_1(\alpha, c) = 2\alpha(1-c^2) - 2c,$$
$$k_2(\alpha, c) = 1 - \alpha^2(1-c^2) + 2\alpha c.$$

By choosing $\alpha_\star = \dfrac{c_\star}{1-c_\star^2}$, we get $k_1(\alpha_\star, c_\star) = 0$, $k_2(\alpha_\star, c_\star) = \dfrac{1}{1-c_\star^2}$, and thereby simplify (1.3.20) to

$$0 = (1-c_\star^2)\xi_{xx} - (1-c_\star^2)^{-1}S_\star^2\xi - \xi + |\xi|^2\xi. \tag{1.3.21}$$

The final step is to restrict ourselves to solutions of the form

$$\eta(x)\nu = \xi(x) = e^{-\alpha_\star x S_\star}v_1(x),$$

where η is a scalar function and $\nu \in \mathbb{R}^3$ is a vector of unit length and orthogonal to $s_\star$. Consequently, the system (1.3.21) is reduced to the scalar equation

$$0 = (1 - c_\star^2)\eta_{xx} + (1 - c_\star^2)^{-1}|s_\star|^2\eta - \eta + \eta^3. \tag{1.3.22}$$

The solution of (1.3.22) is given by

$$\eta_\star(x) = \frac{\sqrt{2\beta_\star}}{\cosh(\delta_\star x)}$$

with $\beta_\star = 1 - \dfrac{|s_\star|^2}{1 - c_\star^2}$ and $\delta_\star = \sqrt{\dfrac{\beta_\star}{1 - c_\star^2}}$. As in case of the NLS, this is a positive function with exponential decay as $|x| \to \infty$.

Chapter 2

Analysis of the Freezing Method

2.1 Derivation of the PDAE Formulation

We now apply the freezing method (see [8], [50]) to equivariant Hamiltonian evolution equations. The idea of this approach is to decompose the evolution into a group action and profile part. This is done by minimizing the temporal changes of the spatial profile of the solutions. During the numerical process, a moving coordinate frame is determined, and the partial differential equation is rewritten as a partial differential-algebraic equation with additional variables.

2.1.1 General Principle

In the following, the approach of [8] is transfered to the Hamiltonian setting. Before we go into technical details and discuss the application of the freezing method to generalized solutions, we start with the principal idea. Consider a smooth solution $u \in \mathcal{C}^1(\mathcal{I}; X)$ of

$$\omega(u_t, \cdot) = \mathrm{d}H(u), \tag{2.1.1}$$

a function $\gamma \in \mathcal{C}^1(\mathcal{I}; G)$ with $\gamma(0) = \mathbb{1}$, and define another function $v \in \mathcal{C}^1(\mathcal{I}; X)$ via $u(t) = a(\gamma(t))v(t)$. Differentiation with respect to time gives us

$$u_t = \mathrm{d}[a(\gamma)v]\gamma_t + a(\gamma)v_t, \tag{2.1.2}$$

provided v is in the domain of the operator $\mathrm{d}[a(\gamma)\cdot]\gamma_t$. Next, we make use of the symplectic structure and rewrite (2.1.2) in the weak form

$$\omega\big(u_t, \cdot\big) = \omega\big(\mathrm{d}[a(\gamma)v]\gamma_t, \cdot\big) + \omega\big(a(\gamma)v_t, \cdot\big) \in X^\star.$$

In particular, we have

$$\omega\big(u_t, a(\gamma)y\big) = \omega\big(\mathrm{d}[a(\gamma)v]\gamma_t, a(\gamma)y\big) + \omega\big(a(\gamma)v_t, a(\gamma)y\big) \tag{2.1.3}$$

for all $y \in X$. Due to (1.2.5) and (2.1.1), the left hand side can be expressed in terms of the derivative of the Hamiltonian, i.e.,

$$\langle \mathrm{d}H(v), y\rangle = \langle \mathrm{d}H(a(\gamma)v), a(\gamma)y\rangle = \langle \mathrm{d}H(u), a(\gamma)y\rangle = \omega\big(u_t, a(\gamma)y\big).$$

On the right hand side, however, the symplecticity of the group action yields

$$\omega\big(a(\gamma)v_t, a(\gamma)y\big) = \omega\big(v_t, y\big).$$

Hence, the indentity in (2.1.3) takes the form

$$\langle \mathrm{d}H(v), y\rangle = \omega\big(\mathrm{d}[a(\gamma)v]\gamma_t, a(\gamma)y\big) + \omega(v_t, y). \tag{2.1.4}$$

Using the Lie group structure, we shift the derivative of $a(\cdot)v$ at γ to its derivative at unity. As in [6] and [60], we choose a function $\mu : \mathcal{I} \to \mathcal{A}$ that satisfies

$$\gamma_t = \mathrm{d}L_\gamma(\mathbb{1})\mu, \quad \gamma(0) = \mathbb{1}.$$

Since $\mathrm{d}L_\gamma(\mathbb{1})$ is a linear homeomorphism between $\mathcal{A}$ and $T_\gamma G$, the function μ is uniquely defined by this equation. Then (1.2.12) becomes

$$\langle \mathrm{d}Q(v)\mu, y\rangle = \omega\big(\mathrm{d}[a(\gamma)v]\gamma_t, a(\gamma)y\big),$$

and (2.1.4) takes the form

$$\langle \mathrm{d}H(v), y\rangle = \langle \mathrm{d}Q(v)\mu, y\rangle + \omega(v_t, y)$$

for all $y \in X$. Written as a system for v and γ, the freezing approach yields

$$\omega(v_t, \cdot) = \mathrm{d}H(v) - \mathrm{d}Q(v)\mu, \quad v(0) = u_0, \tag{2.1.5a}$$

$$\gamma_t = \mathrm{d}L_\gamma(\mathbb{1})\mu, \qquad \gamma(0) = \mathbb{1}. \tag{2.1.5b}$$

We define a generalized solution to this problem in a similar way as in (1.2.15).

Definition 2.1.1. Let $\mathcal{I} \subseteq \mathbb{R}$ be an interval and $\mu\colon \mathcal{I} \to \mathcal{A}$ a continuous mapping. A continuous function $v\colon \mathcal{I} \to X$ is called a generalized solution of (2.1.5a) if we have

$$-\int_{\mathcal{I}} \omega(v(t), y)\varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \big\langle \mathrm{d}H(v(t)) - \mathrm{d}Q(v(t))\mu(t), y\big\rangle \varphi(t)\mathrm{d}t$$

for all $y \in X$, $\varphi \in C_0^\infty(\mathcal{I}^\circ; \mathbb{R})$, where $\mathcal{I}^\circ$ is the interior of $\mathcal{I}$.

We are left to prove that the equivalence of the evolution equation (1.2.4) and the freezing system (2.1.5) remains true for generalized solutions. In order to do so, we need to rewrite the generalized derivative of $\omega\big(a(\gamma(t))u(t), \cdot\big)$ in terms of $\mathrm{d}H$ and $\mathrm{d}Q$. This can be done by applying the chain rule to $\Phi(t) = a(\gamma(t))\varphi(t)y$ for appropriate test functions φ and y.

For $y \in \mathfrak{D}_a^1$ and $\varphi \in \mathcal{C}_0^\infty(\mathcal{I}^\circ; \mathbb{R})$ we find $t \mapsto \Phi(t) = a(\gamma(t))\varphi(t)y \in \mathcal{C}_0^1(\mathcal{I}^\circ; X)$, where $\mathfrak{D}_a^1$ is defined in Assumption 1.2.3, and by the chain rule we get

$$\Phi_t(t) = a(\gamma(t))\varphi_t(t)y + \mathrm{d}[a(\gamma(t))\varphi(t)y]\gamma_t(t). \tag{2.1.6}$$

This allows us to prove the equivalence of the evolution equation and the freezing system.

Theorem 2.1.2. *Given the Assumptions 1.2.2-1.2.5, let $\gamma \in \mathcal{C}^1(\mathbb{R};G)$ satisfy $\gamma(0)=\mathbb{1}$, and let $\mu \in \mathcal{C}(\mathbb{R};G)$ be defined by (2.1.5b). Furthermore, let u and v be continuous functions from $\mathcal{I}$ to the Banach space X, such that $u(t)=a(\gamma(t))v(t)$ holds for all $t\in\mathcal{I}$. Then v is a generalized solution of (2.1.5) if and only if u is a generalized solution of (1.2.4).*

Proof. By using (1.2.5), (1.2.16) with Φ as above, the skew-symmetry of ω, (2.1.6), (1.2.12), the symplecticity of the group action and (1.2.13), we obtain

$$\begin{aligned}
\int_{\mathcal{I}}\langle \mathrm{d}H(v(t)),\varphi(t)y\rangle \mathrm{d}t &= \int_{\mathcal{I}}\langle a(\gamma(t))^{\star}\mathrm{d}H(u(t)),\varphi(t)y\rangle \mathrm{d}t = \int_{\mathcal{I}}\langle \mathrm{d}H(u(t)),\Phi(t)\rangle \mathrm{d}t\\
&= -\int_{\mathcal{I}}\omega\big(u(t),\Phi_t(t)\big)\mathrm{d}t = \int_{\mathcal{I}}\omega\big(\Phi_t(t),u(t)\big)\mathrm{d}t\\
&= \int_{\mathcal{I}}\omega\big(a(\gamma(t))y,u(t)\big)\varphi_t(t)\mathrm{d}t\\
&\quad + \int_{\mathcal{I}}\omega\big(\mathrm{d}[a(\gamma(t))y]\gamma_t(t),u(t)\big)\varphi(t)\mathrm{d}t\\
&= -\int_{\mathcal{I}}\omega\big(u(t),a(\gamma(t))y\big)\varphi_t(t)\mathrm{d}t\\
&\quad + \int_{\mathcal{I}}\langle \mathrm{d}Q(y)\mu(t),v(t)\rangle\varphi(t)\mathrm{d}t\\
&= -\int_{\mathcal{I}}\omega(v(t),y)\varphi_t(t)\mathrm{d}t + \int_{\mathcal{I}}\langle \mathrm{d}Q(v(t))\mu(t),y\rangle\varphi(t)\mathrm{d}t.
\end{aligned}$$

The only-if-part is proven in a similar way, where (1.2.16) is replaced by

$$-\int_{\mathcal{I}}\omega\big(v(t),\Phi_t(t)\big)\mathrm{d}t = \int_{\mathcal{I}}\big\langle \mathrm{d}H(v(t)) - \mathrm{d}Q(v(t))\mu(t),\Phi(t)\big\rangle \mathrm{d}t \tag{2.1.7}$$

with $\Phi(t)=a(\gamma(t)^{-1})\varphi(t)y$. For a weak solution v of (2.1.5), this identity is verified in the same way as in Lemma 1.2.12, and by applying Lemma A.2.1 to deal with the derivative of the inverse, we obtain

$$a(\gamma(t)^{-1})\varphi_t(t)y = \Phi_t(t) + \mathrm{d}[a(\gamma(t)^{-1})\varphi(t)y]\gamma_t(t). \tag{2.1.8}$$

Then, by using the symplecticity of the group action, (2.1.8), (2.1.7), the skew-symmetry of ω, (1.2.12), (1.2.13), and (1.2.5), we find

$$\begin{aligned}
-\int_{\mathcal{I}}\omega\big(u(t),y\big)\varphi_t(t)\mathrm{d}t &= -\int_{\mathcal{I}}\omega\big(v(t),a(\gamma(t)^{-1})\varphi_t(t)y\big)\mathrm{d}t\\
&= -\int_{\mathcal{I}}\omega(v(t),\Phi_t(t))\mathrm{d}t\\
&\quad - \int_{\mathcal{I}}\omega\big(v(t),\mathrm{d}[a(\gamma(t)^{-1})\varphi(t)y]\gamma_t(t)\big)\mathrm{d}t\\
&= \int_{\mathcal{I}}\big\langle \mathrm{d}H(v(t)) - \mathrm{d}Q(v(t))\mu(t),\Phi(t)\big\rangle\mathrm{d}t\\
&\quad + \int_{\mathcal{I}}\big\langle \mathrm{d}Q(v(t))\mu(t),\Phi(t)\big\rangle\mathrm{d}t\\
&= \int_{\mathcal{I}}\langle \mathrm{d}H(u(t)),y\rangle\varphi(t)\mathrm{d}t,
\end{aligned}$$

which finishes the proof. □

In general, we cannot expect the solution of the freezing equation (2.1.5) to be unique. Therefore, we impose a phase condition, which is defined by $\psi(v, \mu) = 0$ with some mapping

$$\psi \colon X \times \mathcal{A} \to \mathcal{A}^\star,$$

where $\mathcal{A}^\star$ is the dual space of $\mathcal{A}$. Using this approach, we get a differential-algebraic equation for $v(t) \in X$, $\gamma(t) \in G$, $\mu(t) \in \mathcal{A}$, which reads

$$\begin{aligned} \omega(v_t, \cdot) &= \mathrm{d}H(v) - \mathrm{d}Q(v)\mu, & v(0) &= u_0, \\ 0 &= \psi(v, \mu), & & \\ \gamma_t &= \mathrm{d}L_\gamma(\mathbb{1})\mu, & \gamma(0) &= \mathbb{1}. \end{aligned} \tag{2.1.9}$$

Suitable choices for the phase condition are based on various minimization principles (see [6], [8], [60]).

2.1.2 Fixed Phase Condition

As an example, we consider the fixed phase condition with a set-up as follows. We embed the Banach space X in a Hilbert space X_0 with inner product $\big(\cdot, \cdot\big)_0$ and corresponding norm $\|\cdot\|_0$ and obtain a Gelfand triple

$$X \hookrightarrow X_0 = X_0^\star \hookrightarrow X^\star,$$

where we apply the Riesz representation theorem to identify X_0 and $X_0^\star$. Moreover, we denote by

$$\iota \colon X \to X_0, \quad v \mapsto \iota v,$$

the inclusion mapping from X to X_0. Its adjoint operator

$$\iota^\star \colon X_0 \to X^\star, \quad u \mapsto \iota^\star u,$$

with respect to $\big(\cdot, \cdot\big)_0$ is given by

$$\langle \iota^\star u, v \rangle = \big(u, \iota v\big)_0 \tag{2.1.10}$$

for all $u \in X_0$ and $v \in X$. In other words, the duality pairing between X and $X^\star$ is compatible with the inner product on X_0. However, we prefer to simplify the notation by omitting ι.

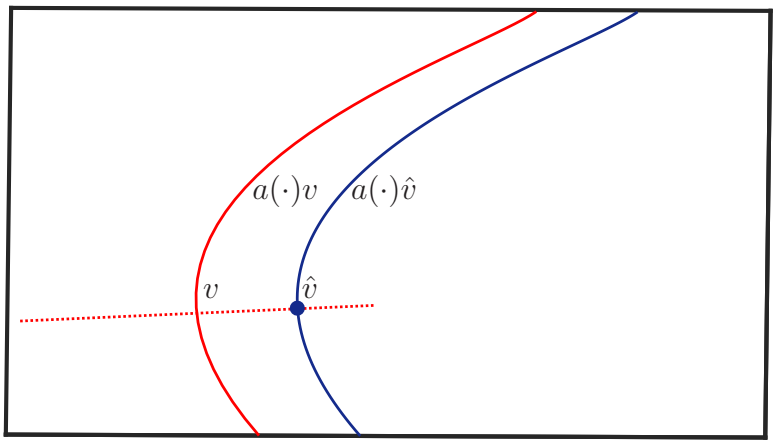


Figure 2.1.1: Fixed phase condition

Now, we select a template function, for instance $\hat{v} = u_0$, provided that the initial value is smooth enough, and require at any time instance the distance

$$\big\|a(g)\hat{v} - v\big\|_0^2$$

to attain its minimum with respect to $g \in G$ at $g = \mathbb{1}$.

This means that among the points forming the group orbit

$$a(G)\hat{v} = \{a(g)\hat{v} : g \in G\}$$

the template function $\hat{v}$ is closest to v. As a necessary condition we get

$$\big(\mathrm{d}[a(\mathbb{1})\hat{v}]\sigma, \hat{v} - v\big)_0 = 0$$

for all $\sigma \in \mathcal{A}$. However, the operators $\mathrm{d}[a(\mathbb{1})\cdot]\sigma$ are skew-symmetric, which yields

$$\big\langle \iota^\star \mathrm{d}[a(\mathbb{1})\hat{v}]\sigma, v\big\rangle = \big(\mathrm{d}[a(\mathbb{1})\hat{v}]\sigma, v\big)_0 = 0.$$

2.2 Preliminaries and Spectral Hypotheses

Our stability proof is based on a modification of the Grillakis-Shatah-Strauss stability approach. In [32] and [33] the authors have established a general theory of stability in the following sense.

Definition 2.2.1. A relative equilibrium $u_\star(t) = a(e^{t\mu_\star})v_\star$, $t \geq 0$ is called orbitally stable if for any $\varepsilon > 0$ there exists $\delta > 0$ with the following property. For any initial value $u_0 \in X$ with $\|u_0 - v_\star\| \leq \delta$ equation (1.2.4) has a unique generalized solution $u\colon [0,\infty) \to X$, $u(0) = u_0$ that satisfies

$$\sup_{0<t<\infty} \inf_{g\in G} \|u(t) - a(g)v_\star\| \leq \varepsilon. \tag{2.2.1}$$

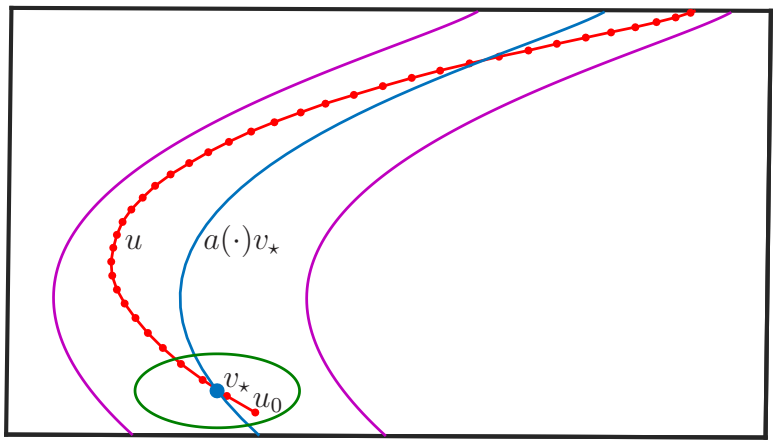


Figure 2.2.1: Orbital stability

Let us first derive a simple consequence of Definition 2.2.1, namely the preservation of orbital stability by the freezing method. Given the orbital stability (2.2.1), it follows

$$\begin{aligned}\sup_{0<t<\infty}\inf_{g\in G}\|v(t)-a(g)v_\star\| &= \sup_{0<t<\infty}\inf_{g\in G}\|a(\gamma(t))u(t)-a(g)v_\star\|\\ &= \sup_{0<t<\infty}\inf_{g\in G}\|u(t)-a(\gamma(t)^{-1}g)v_\star\|\le\varepsilon,\end{aligned}$$

where we assume that the group action is a unitary representation of G on X. That is, the identity $\|a(g)v\|=\|v\|$ holds for all $g\in G$ and $v\in X$.

However, our aim with the freezing method and the fixed phase condition is to ensure Lyapunov stability of the steady state $v_\star$, i.e.,

$$\sup_{0<t<\infty}\|v(t)-v_\star\|\le\varepsilon.$$

Such a stability result is not that surprising at first glance. Indeed, assume

$$\|u(t)-a\big(g(t)\big)v_\star\|\le\varepsilon$$

for some $t>0$. Then the minimality requirement in the fixed phase condition and $u(t)=a\big(\gamma(t)\big)v(t)$ imply

$$\big\|v(t)-\hat v\big\|\le\big\|v(t)-a\big(\gamma(t)^{-1}g(t)\big)\hat v\big\|=\big\|a(\gamma(t)^{-1})u(t)-a\big(\gamma(t)^{-1}g(t)\big)\hat v\big\|,$$

where we require $X=X_0$. If, in addition to that, the template function satisfies

$$\|\hat v-v_\star\|\le\varepsilon,$$

we conclude

$$\begin{aligned}\big\|v(t)-v_\star\big\| &\le \big\|v(t)-\hat v\big\|+\big\|\hat v-v_\star\big\|\\ &\le \big\|a\big(\gamma(t)^{-1}\big)u(t)-a\big(\gamma(t)^{-1}g(t)\big)\hat v\big\|+\big\|\hat v-v_\star\big\|\\ &\le \big\|u(t)-a\big(g(t)\big)\hat v\big\|+\big\|\hat v-v_\star\big\|\\ &\le \big\|u(t)-a\big(g(t)\big)v_\star\big\|+2\big\|\hat v-v_\star\big\|\le 3\varepsilon.\end{aligned}$$

However, the interpretation as stability of the freezing method is questionable. First of all, the term $\|\hat{v} - v_\star\|$ does not vanish as the initial value u_0 goes to $v_\star$. While it does for the special choice $\hat{v} = u_0$, the template function $\hat{v}$ occurs in the algebraic part of the differential-algebraic equation and must be considered as a constant term in a stability proof. Second, this approach is very restrictive in terms of the phase condition. It is highly unlikely to work in more general cases. In addition to that, the norms $\|\cdot\|$ and $\|\cdot\|_0$ have to be the same. Therefore, a more extensive analysis of the stability problem is necessary.

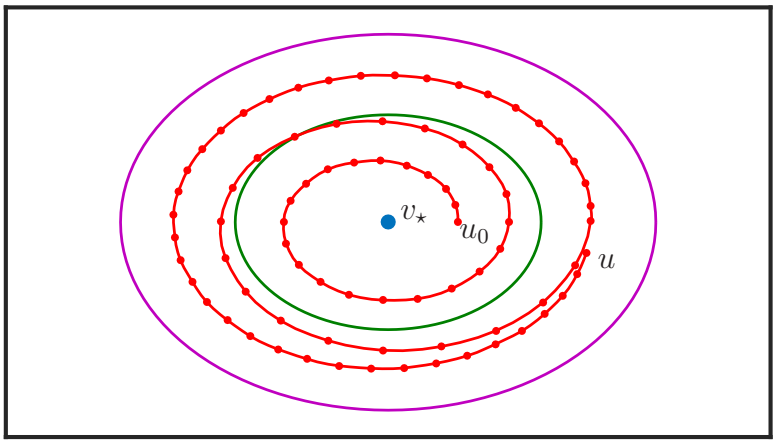


Figure 2.2.2: Lyapunov stability of a steady state

For the sake of completeness we repeat the assumptions and basic properties from [33], which are sufficient for orbital stability of $u_\star$, and which we require in the following. From now on, let $a(e^{t\mu_\star})v_\star$ be a fixed relative equilibrium. To shorten the notation, we denote by $\mathcal{A}_0$ the centralizer of $\mu_\star$, i.e.,

$$\mathcal{A}_0 = C_{\mathcal{A}}(\mu_\star) = \{\sigma \in \mathcal{A} : [\sigma, \mu_\star] = 0\}.$$

Moreover, let $\{e_1, ..., e_{d_\star}\}$ with $d_\star = \dim(\mathcal{A}_0)$ denote a basis of $\mathcal{A}_0$, and by c and C we denote generic positive constants.

A prominent feature of an equivariant Hamiltonian system is the existence of a family of relative equilibria, which can be parametrized by $\mu \in \mathcal{A}_0$. We refer to Section 1.3 for specific examples, while the general assumption is due to [33]. For μ close to $\mu_\star$, we write $a(e^{t\mu})\phi(\mu)$ for the corresponding relative equilibrium. This means in particular $v_\star = \phi(\mu_\star)$.

Assumption 2.2.2. There exists an open subset $\mathcal{U} \subseteq \mathcal{A}_0$ containing $\mu_\star$ and a continuously differentiable mapping $\phi\colon \mathcal{U} \to X$ such that the properties

(a) $\mathrm{d}H(\phi(\mu)) - \mathrm{d}Q(\phi(\mu))\mu = 0$ for all $\mu \in \mathcal{U}$,

(b) $\phi(\mu) \in \mathfrak{D}_a^1$ for all $\mu \in \mathcal{U}$

are fulfilled.

By Assumption 1.2.5 and 2.2.2 we can differentiate

$$\mathrm{d}H(\phi(\mu)) - \mathrm{d}Q(\phi(\mu))\mu = 0$$

at $\mu = \mu_\star$. The differentiation along $\sigma \in \mathcal{A}_0$ yields

$$L_\star \mathrm{d}\phi(\mu_\star)\sigma = \mathrm{d}Q(v_\star)\sigma, \tag{2.2.2}$$

where we have

$$L_\star \colon X \to X^\star, \quad L_\star = \mathrm{d}^2 H(v_\star) - \mathrm{d}^2 Q(v_\star)\mu_\star. \tag{2.2.3}$$

This operator is the right hand side of the linearization of the freezing equation

$$\omega(v_t, \cdot) = \mathrm{d}H(v) - \mathrm{d}Q(v)\mu$$

around its equilibrium $(v_\star, \mu_\star)$. In order to obtain stability, we are left to impose spectral conditions on $L_\star$. In the rain gutter example, the operator in (1.1.6) is positive on $Y = (W + Z)^\perp$, where

$$Z = \{\mathrm{d}[a(\mathbb{1})v_\star]\sigma \colon \ \sigma \in \mathbb{R}\}$$

is its kernel, and its negative subspace is given by

$$W = \{\nabla Q(v_\star)\sigma \colon \ \sigma \in \mathbb{R}\}.$$

Since the gradient $\nabla Q(v_\star)$ is perpendicular to the level set of Q at $v_\star$, we can exploit the conservation of Q (see Proposition 1.2.7) in order to obtain stability. In case of partial differential equations, we cannot check directly the orthogonality to level sets. Instead, we follow the approach of [33] and make use of the Lagrange functions

$$\ell(\mu) = H(\phi(\mu)) - Q(\phi(\mu))\mu, \tag{2.2.4}$$

in particular

$$\ell_\star = \ell(\mu_\star) = H(v_\star) - Q(v_\star)\mu_\star. \tag{2.2.5}$$

By Assumption 2.2.2 we can differentiate (2.2.4) at $\mu \in \mathcal{U}$ along $\sigma \in \mathcal{A}_0$, and due to $\mathrm{d}H(\phi(\mu)) - \mathrm{d}Q(\phi(\mu))\mu = 0$, we get

$$\mathrm{d}\ell(\mu)\sigma = \big\langle \mathrm{d}H(\phi(\mu)) - \mathrm{d}Q(\phi(\mu))\mu, \mathrm{d}\phi(\mu)\sigma \big\rangle - Q(\phi(\mu))\sigma = -Q(\phi(\mu))\sigma. \tag{2.2.6}$$

Differentiating (2.2.6) at $\mu = \mu_\star$ along $\tau \in \mathcal{A}_0$, it follows for the second derivative

$$\langle \mathrm{d}^2\ell(\mu_\star)\sigma, \tau\rangle = -\langle \mathrm{d}Q(v_\star)\sigma, \mathrm{d}\phi(\mu_\star)\tau\rangle,$$

and (2.2.2) leads to

$$\langle \mathrm{d}^2\ell(\mu_\star)\sigma, \tau\rangle = -\langle L_\star \mathrm{d}\phi(\mu_\star)\sigma, \mathrm{d}\phi(\mu_\star)\tau\rangle \tag{2.2.7}$$

for any pair $\sigma, \tau \in \mathcal{A}_0$. We thereby obtain

$$\langle L_\star \mathrm{d}\phi(\mu_\star)\sigma, \mathrm{d}\phi(\mu_\star)\sigma\rangle < 0$$

for each eigenvector $\sigma \in \mathcal{A}_0$ of $\mathrm{d}^2\ell(\mu_\star)$ that belongs to a positive eigenvalue.

Assumption 2.2.3. The Banach space X is decomposed as a direct sum

$$X = W \oplus Y \oplus Z,$$

where we have $\dim W = d_\star$,

$$\big\langle \mathrm{d}Q(v_\star)\sigma, y \big\rangle = 0 \tag{2.2.8}$$

for all $\sigma \in \mathcal{A}_0$ and $y \in Y$. Furthermore, the subspace

$$Z = \{\mathrm{d}[a(\mathbb{1})v_\star]\sigma \colon \sigma \in \mathcal{A}_0\} \tag{2.2.9}$$

equals the kernel of $L_\star$, and the operator

$$d[a(\mathbb{1})v_\star] \colon \mathcal{A}_0 \to X$$

is one-to-one.

Remark 7. To be precise, Assumption 2.2.3 can be slightly weakened.

- If $X \hookrightarrow X_0 \hookrightarrow X^\star$ is a Gelfand triple, the decomposition is given by the orthogonal projections onto Z and W.
- We only have to ensure that the kernel is not larger than Z. The other inclusion $Z \subseteq \ker(L_\star)$ is an immediate consequence of the previous set-up. Indeed, differentiating $\mathrm{d}H(a(e^{t\sigma})v_\star) - \mathrm{d}Q(a(e^{t\sigma})v_\star)\mu_\star = 0$ at $t = 0$ yields $L_\star \mathrm{d}[a(\mathbb{1})v_\star]\sigma = \mathrm{d}^2H(v_\star)\mathrm{d}[a(\mathbb{1})v_\star]\sigma - \mathrm{d}^2Q(v_\star)\mu_\star \mathrm{d}[a(\mathbb{1})v_\star]\sigma = 0$, which was to be proven.

Since (1.2.10) states $\langle \mathrm{d}Q(v_\star)\sigma, z\rangle = 0$ for all $\sigma \in \mathcal{A}_0$ and $z \in Z$, we are only left to analyze $\big\langle \mathrm{d}Q(v_\star)\sigma, w \big\rangle$ for $w \in W$.

Lemma 2.2.4. *Given the Assumptions 1.2.2-1.2.5 and 2.2.3, there exists an isomorphism*

$$\Omega \colon \mathcal{A}_0 \to W, \quad \sigma \mapsto \Omega\sigma$$

such that $\Big[\mathrm{d}Q(v_\star)e_i\Big]_{i=1}^{d_\star}$ *is the dual basis of* $\Big[\Omega e_i\Big]_{i=1}^{d_\star}$, *i.e.,*

$$\big\langle \mathrm{d}Q(v_\star)e_i, \Omega e_j \big\rangle = \delta_{i,j}.$$

Proof. We have to show that

$$\{\mathrm{d}Q(v_\star)\sigma \colon \sigma \in \mathcal{A}_0\}$$

is a $d_\star$-dimensional subspace of $X^\star$. Assume that there is $\sigma \in \mathcal{A}_0$ such that

$$0 = \mathrm{d}Q(v_\star)\sigma = \omega(\mathrm{d}[a(\mathbb{1})v_\star]\sigma, \cdot) \in X^\star.$$

By Lemma 1.2.1, the mapping $u \mapsto \omega(u, \cdot)$ is one-to-one, which leads to

$$0 = \mathrm{d}[a(\mathbb{1})v_\star]\sigma \in Z.$$

However, Assumption 2.2.3 implies $\sigma = 0$. Hence, the matrix

$$\Big[\big\langle \mathrm{d}Q(v_\star)e_i, w_j \big\rangle\Big]_{i,j}^{d_\star}$$

is invertible, where $w_1, \ldots, w_{d_\star}$ is a basis of W, and Ω is given by its inverse. □

In (1.1.6) the operator $L_\star$ is a matrix with one zero, one negative, and two positive eigenvalues. The generalization of positive and negative subspaces to infinite dimensional spaces is as follows.

Definition 2.2.5. Let X be a Banach space and $T\colon X \to X^\star$ a bounded linear operator. A closed subspace Z of X is called positive if we have

$$\langle Tz, z\rangle \geq c\|z\|^2$$

for all $z \in Z$ and some $c > 0$. It is called negative if we have

$$\langle Tz, z\rangle \leq -c\|z\|^2.$$

Remark 8. Here, positive always means strongly positive, also called coercive. Otherwise, we speak of a non-negative subspace. We use the same terminology for negative and non-positve subspaces.

Subsets are partially ordered by inclusion, so we can speak of maximal positive and maximal negative subspaces. Thereby, we obtain an analog for the number of positive and negative eigenvalues, which is called the positive and negative index of an operator.

Definition 2.2.6. Let X be a Banach space and $T\colon X \to X^\star$ a bounded linear operator. If Z is a maximal positive subspace, then $\mathfrak{p}(T) = \dim(Z)$ is called the positive index of T. If Z is a maximal negative subspace, then $\mathfrak{n}(T) = \dim(Z)$ is called the negative index of T. Moreover, the null index of T is the dimension of the kernel, i.e., $\mathfrak{z}(T) = \dim(\ker(T))$.

The positive and negative indices, finite or infinite, are well-defined since they do not depend on the choice of the positive (or negative) subspace (see e.g. [30]). Now, the principal idea is to make use of (2.2.7) to obtain positivity of the linearized operator $L_\star$ for the entire subspace Y, provided that $\mathrm{d}^2\ell(\mu_\star)$ has sufficiently many positive eigenvalues.

Assumption 2.2.7. The inequality

$$\mathfrak{n}(L_\star) \leq \mathfrak{p}(\mathrm{d}^2\ell(\mu_\star))$$

holds for the negative index of $L_\star$ and the positive index of $\mathrm{d}^2\ell(\mu_\star)$.

Here, we remark that the strict inequality cannot occur. However, this is of no relevance for a stability result. It is also worth mentioning that this assumption means $\mathfrak{n}(L_\star) < \infty$, and by Assumption 2.2.2 we have $\mathfrak{z}(L_\star) = \dim(Z) < \infty$.

A direct sum comes with natural projectors, the coordinate mappings $\mathcal{P}_W$, $\mathcal{P}_Y$, $\mathcal{P}_Z$, and their complementary counterparts. As an exmaple, for $v = w + y + z$ with $w \in W$, $y \in Y$, and $z \in Z$ we get $\mathcal{P}_{Y\oplus Z}v = y + z$. Now, we consider the spectral properties of the operator

$$L_\star|_{Y\oplus Z}\colon Y \oplus Z \to (Y \oplus Z)^\star. \tag{2.2.10}$$

Lemma 2.2.8. *Provided that the Assumptions 1.2.2-1.2.5, 2.2.2, 2.2.3, and 2.2.7 hold, the subspace Z lies in the kernel of the operator $L_\star|_{Y\oplus Z}$, which means in particular*

$$\mathfrak{z}(L_\star) \leq \mathfrak{z}(L_\star|_{Y\oplus Z}). \tag{2.2.11}$$

Moreover, the only negative subspace of $L_\star|_{Y\oplus Z}$ is trivial, i.e.,

$$\mathfrak{n}(L_\star|_{Y\oplus Z}) = 0. \tag{2.2.12}$$

Proof. The inclusion $Z = \ker(L_\star) \subseteq \ker(L_\star|_{Y\oplus Z})$ is an immediate consequence of the definition of $L_\star|_{Y\oplus Z}$ as a restriction of $L_\star$, and (2.2.11) follows. Moreover, a maximal non-positive subspace of $L_\star|_{Y\oplus Z}$ is a subset of $Y\oplus Z$, and it forms a non-positive subspace of $L_\star$ of finite dimension $\mathfrak{n}(L_\star|_{Y\oplus Z}) + \mathfrak{z}(L_\star|_{Y\oplus Z})$. Furthermore, from (2.2.7) and (2.2.2) we get

$$\langle \mathrm{d}^2\ell(\mu_\star)\tau, \tau\rangle = -\langle L_\star \mathrm{d}\phi(\mu_\star)\tau, \mathrm{d}\phi(\mu_\star)\tau\rangle = -\langle \mathrm{d}Q(v_\star)\tau, \mathrm{d}\phi(\mu_\star)\tau\rangle$$

for $\tau \in \mathcal{A}_0$. But, by construction of the direct sum $W \oplus Y \oplus Z$, we have

$$\langle \mathrm{d}Q(v_\star)\tau, \mathrm{d}\phi(\mu_\star)\tau\rangle = 0,$$

provided $\mathrm{d}\phi(\mu_\star)\tau \in Y \oplus Z$. Consequently, there exists a negative subspace of $L_\star$ of dimension $\mathfrak{p}(\mathrm{d}^2\ell(\mu_\star))$ that is included in W, and since $Y \oplus Z$ and W are complements, there exists a non-positive subspace of $L_\star$ of dimension $\mathfrak{n}(L_\star|_{Y\oplus Z}) + \mathfrak{z}(L_\star|_{Y\oplus Z}) + \mathfrak{p}(\mathrm{d}^2\ell(\mu_\star))$, which implies

$$\mathfrak{n}(L_\star|_{Y\oplus Z}) + \mathfrak{z}(L_\star|_{Y\oplus Z}) + \mathfrak{p}(\mathrm{d}^2\ell(\mu_\star)) \leq \mathfrak{n}(L_\star) + \mathfrak{z}(L_\star). \tag{2.2.13}$$

From (2.2.11), (2.2.13), and Assumption 2.2.7 we conclude

$$0 \leq \mathfrak{n}(L_\star|_{Y\oplus Z}) \leq \mathfrak{n}(L_\star) - \mathfrak{p}(\mathrm{d}^2\ell(\mu_\star)) + \mathfrak{z}(L_\star) - \mathfrak{z}(L_\star|_{Y\oplus Z}) \leq 0.$$

Hence, the negative index of $L_\star|_{Y\oplus Z}$ must be zero. □

From Lemma 2.2.8 we can see that the existence of sufficiently many positive eigenvalues of $\mathrm{d}^2\ell(\mu_\star)$ leads to $\mathfrak{n}(L_\star|_{Y\oplus Z})$ being zero, and hence, the negative subspace of $L_\star|_{Y\oplus Z}$ being trivial.

Lemma 2.2.9. *Provided that the Assumptions 1.2.2-1.2.5, 2.2.2, 2.2.3, and 2.2.7 hold, we obtain the estimate*

$$\langle L_\star y, y\rangle \geq c\|y\|^2$$

for all $y \in Y$.

Proof. From Lemma 2.2.8 we get $\mathfrak{n}(L_\star|_{Y\oplus Z}) = 0$. Furthermore, we see that the kernel of $L_\star|_{Y\oplus Z}$ equals Z, since the dimensions are the same and $Z \subseteq \ker(L_\star|_{Y\oplus Z})$ is due to Lemma 2.2.8. Hence, we have

$$\langle L_\star y, y\rangle = \langle L_\star|_{Y\oplus Z}\, y, y\rangle \geq c\|y\|^2$$

for all $y \in Y$. □

The positivity in Lemma 2.2.9 is fundamental for orbital stability. To be more precise, the Grillakis-Shatah-Strauss stability approach is based on having

$$a(g)u - v_\star$$

in the (orthogonal) complement of Z for some $g \in G$. It is our aim with the freezing method to provide an adaptive algorithm such that

$$v - v_\star = a(\gamma^{-1})u - v_\star$$

is in the complement of a suitable approximation of Z.

Theorem 2.2.10. *Let $\hat{Z}^\star = \operatorname{span}(\hat{z}_1^\star, ..., \hat{z}_{d_\star}^\star)$ be a subspace of $X^\star$ such that*

$$\Big[\big\langle \hat{z}_i^\star, \mathrm{d}[a(\mathbb{1})v_\star]e_j \big\rangle\Big]_{i,j=1}^{d_\star} \tag{2.2.14}$$

is non-singular. Under the Assumptions 1.2.2-1.2.5, 2.2.2, 2.2.3, and 2.2.7, there exists a constant $\hat{c} > 0$ such that we get

$$\langle L_\star \hat{y}, \hat{y} \rangle \geq \hat{c}\|\hat{y}\|^2$$

for all $\hat{y}$ that lie in the subspace

$$\hat{Y} = \big\{ \hat{y} \in X : \big\langle \mathrm{d}Q(v_\star)e_j, \hat{y} \big\rangle = \langle \hat{z}_j^\star, \hat{y} \rangle = 0 \text{ for } j = 1, ..., d_\star \big\}. \tag{2.2.15}$$

Proof. We write $\hat{y} \in \hat{Y}$ as $\hat{y} = w + y + z$ with $w \in W$, $y \in Y$, and $z \in Z$. However, combining (1.2.10) and (2.2.8) implies

$$0 = \big\langle \mathrm{d}Q(v_\star)\sigma, \hat{y} \big\rangle = \langle \mathrm{d}Q(v_\star)\sigma, w \rangle$$

for all $\sigma \in \mathcal{A}_0$, and Lemma 2.2.4 leads to $w = 0$. Moreover, from the invertibility of the matrix (2.2.14) and

$$\big\langle \hat{z}^\star, y + z \big\rangle = \big\langle \hat{z}^\star, \hat{y} \big\rangle = 0,$$

we get the estimate

$$\eta\|z\| \leq \big|\big\langle \hat{z}^\star, z \big\rangle\big| = \big|\langle \hat{z}^\star, y \rangle\big| \leq \|y\|$$

for some $\eta > 0$, which is independent of $z \in Z$ and $y \in Y$, and for some functional $\hat{z}^\star \in \hat{Z}^\star$ of unit length. Due to the triangle inequality, this implies

$$\|y + z\| \leq \|y\| + \|z\| \leq (1 + C)\|y\|,$$

which leads to

$$\|y\|^2 \geq \frac{1}{(1+C)^2}\|y + z\|^2.$$

Hence, we obtain from Lemma 2.2.9 the inequality

$$\langle L_\star(y + z), (y + z) \rangle = \langle L_\star y, y \rangle \geq c\|y\|^2 \geq \frac{c}{(1+C)^2}\|y + z\|^2,$$

which was to be proven. □

Having in mind the fixed phase conditions, we impose requirements for the phase condition in the abstract setting. Up to this point, we have not made use of the space $(X_{-1}, \|\cdot\|_{-1})$ from Assumption 1.2.14. The freezing approach in general, in particular Theorem 2.1.2, is valid for any generalized solutions in the sense of Definition 2.1.1. However, when it comes to phase conditions of the form $\psi(v) = 0$, we require solutions $u \in \mathcal{C}(\mathcal{I}; X) \cap \mathcal{C}^1(\mathcal{I}; X_{-1})$. Furthermore, we simplify the notation by writing

$$G_0 = G(e^{\mathcal{A}_0}) \tag{2.2.16}$$

for the Lie subgroup of G that is generated by $\mathcal{A}_0$.

Assumption 2.2.11. The mapping $\psi : X \to \mathcal{A}_0^\star$ is twice continuously differentiable with locally bounded derivatives and satisfies the properties

(a) $\psi(v_\star) = 0$,

(b) the matrix $\Big[\big\langle \mathrm{d}\psi(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big\rangle\Big]_{i,j=1}^{d_\star}$ is invertible,

(c) the mapping $\mathfrak{F}\colon G_0 \times X_{-1} \to \mathcal{A}_0^\star$, $(g,u) \mapsto \mathfrak{F}(g,u)$ that continuously expands $(g,u) \mapsto \psi(a(g)u)$ is continuously differentiable.

The above allows us to consider $v_\star$ as a local minimum of H subject to constraints for Q and ψ. More precisely, the method of Lagrange multipliers leads to the modified stationary problem

$$\begin{aligned} 0 &= \mathrm{d}H(v) - \mathrm{d}Q(v)\mu - \mathrm{d}\psi(v)\lambda, \\ 0 &= Q(v) - Q(v_\star), \\ 0 &= \psi(v) \end{aligned} \tag{2.2.17}$$

which possesses the solution $\big(v_\star, \mu_\star, 0\big)$. Next, we show that $\lambda_\star = 0$ is not a coincidence, but an immediate consequence of the invariance of H and Q with respect to the group action.

Lemma 2.2.12. *Given the Assumptions 1.2.2-1.2.5 and 2.2.11, let $(v_\star, \mu_\star, \lambda_\star)$ be a solution of (2.2.17) with $v_\star \in \mathfrak{D}_a^1$. Then it follows $\lambda_\star = 0$, which means*

$$0 = \mathrm{d}H(v_\star) - \mathrm{d}Q(v_\star)\mu_\star.$$

Proof. From (1.2.9), (1.2.10), and

$$0 = \langle \mathrm{d}H(v_\star) - \mathrm{d}Q(v_\star)\mu_\star - \mathrm{d}\psi(v_\star)\lambda_\star, \mathrm{d}[a(\mathbb{1})v_\star]\sigma\rangle$$

for all $\sigma \in \mathcal{A}_0$, we conclude

$$0 = \langle \mathrm{d}\psi(v_\star)\lambda_\star, \mathrm{d}[a(\mathbb{1})v_\star]\sigma\rangle,$$

and $\lambda_\star = 0$ follows from Assumption 2.2.11. □

The modified stationary problem is set in the product space $\mathfrak{X} = X \times \mathcal{A}_0 \times \mathcal{A}_0$, which is a Banach space with respect to the norm

$$\big\|(v,\mu,\lambda)\big\|_{\mathfrak{X}} = \big\|v\big\|_X + \big|\mu\big|_{\mathcal{A}_0} + \big|\lambda\big|_{\mathcal{A}_0},$$

and we denote the dual space by $\mathfrak{X}^\star$. Then, the equation (2.2.17) is of the form

$$\mathfrak{S}(v,\mu,\lambda) = 0, \tag{2.2.18}$$

where the function

$$\mathfrak{S}\colon \mathfrak{X} \to \mathfrak{X}^\star, \quad \mathfrak{S}(v,\mu,\lambda) = \Big(\mathfrak{S}_1(v,\mu,\lambda), \mathfrak{S}_2(v,\mu,\lambda), \mathfrak{S}_3(v,\mu,\lambda)\Big)$$

is given by

$$\begin{aligned}
\mathfrak{S}_1(v,\mu,\lambda) &= \mathrm{d}H(v) - \mathrm{d}Q(v)\mu - \mathrm{d}\psi(v)\lambda,\\
\mathfrak{S}_2(v,\mu,\lambda) &= Q(v) - Q(v_\star),\\
\mathfrak{S}_3(v,\mu,\lambda) &= \psi(v).
\end{aligned}$$

The linearization of (2.2.18) around the steady state $(v_\star, \mu_\star, 0)$ is denoted by

$$\mathfrak{L} = \mathrm{d}\mathfrak{S}(v_\star,\mu_\star,0)\colon \mathfrak{X} \to \mathfrak{X}^\star. \tag{2.2.19}$$

Proposition 2.2.13. *Under the Assumptions 1.2.2-1.2.5, 2.2.2, 2.2.3, 2.2.7, and 2.2.11, the linear operator $\mathfrak{L}$ given by (2.2.19) is one-to-one.*

Proof. We have to show that the kernel of $\mathfrak{L}$ is trivial. Let

$$\mathfrak{L}(v,\mu,\lambda) = 0$$

for $v = w + y + z \in W \oplus Y \oplus Z$, $\mu \in \mathcal{A}_0$, and $\lambda \in \mathcal{A}_0$. This means that for all $(\widetilde{v},\widetilde{\mu},\widetilde{\lambda}) \in \mathfrak{X}$ we have

$$\begin{aligned}
0 = \langle \mathfrak{L}(v,\mu,\lambda), (\widetilde{v},\widetilde{\mu},\widetilde{\lambda})\rangle = \langle L_\star v, \widetilde{v}\rangle + \langle \mathrm{d}Q(v_\star)\mu, \widetilde{v}\rangle + \langle \mathrm{d}\psi(v_\star)\lambda, \widetilde{v}\rangle\\
+ \langle \mathrm{d}Q(v_\star)\widetilde{\mu}, v\rangle + \langle \mathrm{d}\psi(v_\star)\widetilde{\lambda}, v\rangle.
\end{aligned} \tag{2.2.20}$$

Next, we decompose $\widetilde{v} = \widetilde{w} + \widetilde{y} + \widetilde{z}$ and rewrite (2.2.20) for specific choices of $(\widetilde{v},\widetilde{\mu},\widetilde{\lambda}) \in \mathfrak{X}$. First of all, we choose $\widetilde{w} = \widetilde{y} = 0$ and $\widetilde{\mu} = \widetilde{\lambda} = 0$. Since $\widetilde{z}$ is in the kernel of $L_\star$ by Assumption 2.2.3, and since it is a zero of $dQ(v_\star)\mu$ by (1.2.10), we conclude

$$0 = \big\langle \mathfrak{L}(v,\mu,\lambda), (\widetilde{z},0,0)\big\rangle = \langle L_\star v, \widetilde{z}\rangle + \langle \mathrm{d}Q(v_\star)\mu, \widetilde{z}\rangle + \langle \mathrm{d}\psi(v_\star)\lambda, \widetilde{z}\rangle = \langle \mathrm{d}\psi(v_\star)\lambda, \widetilde{z}\rangle$$

for all $\widetilde{z} \in Z$, which means $\lambda = 0$ due to Assumption 2.2.11.

Moreover, by choosing $\widetilde{v} = 0$ and $\widetilde{\lambda} = 0$, we find

$$0 = \big\langle \mathfrak{L}(v,\mu,0), (0,\widetilde{\mu},0)\big\rangle = \langle \mathrm{d}Q(v_\star)\widetilde{\mu}, v\rangle = \langle \mathrm{d}Q(v_\star)\widetilde{\mu}, w\rangle$$

as a consequence of Assumption 2.2.3 and (1.2.10). Hence, we obtain $w = 0$, which means $v = y + z \in Y \oplus Z$.

The next choice is $\widetilde{v} = y$ and $\widetilde{\mu} = \widetilde{\lambda} = 0$. In the same way as before, we make use of $L_\star z = 0$ and (2.2.8) to obtain

$$0 = \big\langle \mathfrak{L}(y+z,\mu,0),(y,0,0)\big\rangle = \langle L_\star(z+y),y\rangle + \langle \mathrm{d}Q(v_\star)\mu, y\rangle = \langle L_\star y, y\rangle.$$

It follows $y = 0$ from Lemma 2.2.9, which means $v = z \in Z$.

But $z = 0$ is obtained from choosing $\widetilde{v} = 0$ and $\widetilde{\mu} = 0$, which leads to

$$0 = \big\langle \mathfrak{L}(z,\mu,0),(0,0,\widetilde{\lambda})\big\rangle = \langle \mathrm{d}\psi(v_\star)\widetilde{\lambda}, z\rangle$$

for all $\widetilde{\lambda} \in \mathcal{A}_0$, and part (b) of Assumption 2.2.11.

Finally, we pick $\widetilde{v} = \widetilde{w}$ and $\widetilde{\mu} = \widetilde{\lambda} = 0$. This results in

$$0 = \big\langle \mathfrak{L}(0,\mu,0),(\widetilde{w},0,0)\big\rangle = \langle \mathrm{d}Q(v_\star)\mu, \widetilde{w}\rangle$$

for all $\widetilde{w} \in W$, and Assumption 2.2.3 leads to $\mu = 0$. □

2.3 Stability of the PDAE Formulation

In the following we use the implicit function theorem to express the phase condition in terms of an implicit function $\hat{g}$, such that $v = a(\hat{g}(u))u$.

Lemma 2.3.1. *Provided the Assumptions 1.2.2, 1.2.3, and 2.2.11 hold, there exist open neighborhoods $\mathfrak{U}_\star \subseteq G_0 \times X_{-1}$ of $(\mathbb{1}, v_\star)$ and $U_\star \subseteq X_{-1}$ of $v_\star$ and a smooth function*

$$\hat{g}\colon U_\star \to G_0,$$

such that $\mathfrak{F}(g,u) = 0$ and $(g,u) \in \mathfrak{U}_\star$ if and only if $g = \hat{g}(u)$ and $u \in U_\star$. Moreover, we have

$$d\hat{g}(u) = -\big[\mathfrak{F}_g(\hat{g}(u),u)\big]^{-1}\mathfrak{F}_u(\hat{g}(u),u). \tag{2.3.1}$$

Proof. The idea of this proof is to apply Lemma A.3.1. Due to Assumption 2.2.11(c), we have $\mathfrak{F}(\mathbb{1}, v_\star) = \psi(v_\star) = 0$, and the mapping

$$\mathfrak{F}\colon G_0 \times X_{-1} \to \mathcal{A}_0^\star, \quad (g,u) \mapsto \mathfrak{F}(g,u) \tag{2.3.2}$$

is continuously differentiable with the partial derivative at $(\mathbb{1}, v_\star)$ given by

$$\mathfrak{F}_g(\mathbb{1},v_\star)\colon \mathcal{A}_0 \to \mathcal{A}_0^\star, \quad \langle \mathfrak{F}_g(\mathbb{1},v_\star)\sigma,\mu\rangle = \langle \mathrm{d}\psi(v_\star)\sigma, \mathrm{d}[a(\mathbb{1})v_\star]\mu\rangle$$

for any $\sigma,\mu \in \mathcal{A}_0$. With respect to the basis $\{e_j\}_{i=1}^{d_\star}$ this derivative is represented by the Jacobian submatrix

$$\Big[\big\langle \mathrm{d}\psi(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big\rangle\Big]_{i,j=1}^{d_\star},$$

which is invertible by Assumption 2.2.11(b). □

Remark 9. For $u \in X \cap U_\star$ it follows $\psi(u) = \mathfrak{F}(\mathbb{1}, u) = 0$ if and only if $\hat{g}(u) = \mathbb{1}$.

Next, we combine this with Theorem 2.1.2 to ensure that the freezing system has a local solution. By a solution we mean functions $v \in \mathcal{C}(\mathcal{I}; X) \cap \mathcal{C}^1(\mathcal{I}; X_{-1})$ and $\mu \in \mathcal{C}(\mathcal{I}; \mathcal{A}_0)$, where $\mathcal{I}$ is an open interval containing $t_0 = 0$, that form a generalized solution of the transformed evolution equation in the sense of Definition 2.1.1 and satisfy the phase condition $\psi(v(t)) = 0$ for all $t \in \mathcal{I}$.

Theorem 2.3.2. *Under the Assumptions 1.2.2-1.2.14, 2.2.3, and 2.2.11, for any initial value $u_0 \in X \cap U_\star$ such that $\psi(u_0) = 0$ the freezing system*

$$\begin{aligned} \omega(v_t, \cdot) &= \mathrm{d}H(v) - \mathrm{d}Q(v)\mu, \quad v(0) = u_0, \\ 0 &= \psi(v) \end{aligned} \tag{2.3.3}$$

has a unique local solution $v \in \mathcal{C}(\mathcal{I}; X) \cap \mathcal{C}^1(\mathcal{I}; X_{-1})$, $\mu \in \mathcal{C}(\mathcal{I}; \mathcal{A}_0)$ in the sense of Definition 2.1.1. Furthermore, the conservation laws

$$\begin{aligned} H(v(t)) &= H(u_0), \\ Q(v(t))\sigma &= Q(u_0)\sigma, \quad \sigma \in \mathcal{A}_0, \end{aligned}$$

hold for all $t \in \mathcal{I}$, and we have the following blow-up alternative. If $(\mathcal{T}^-, \mathcal{T}^+)$ is the maximal interval of existence such that $v(t)$ remains in $X \cap U_\star$ and we have $\mathcal{T}^+ < \infty$, then

$$\min\left(\operatorname{dist}_{\|\cdot\|_{-1}}\left(v(t), \partial U_\star\right), \frac{1}{\|v(t)\|} \right) \to 0$$

as $t \to \mathcal{T}^+$.

Proof. Let $\mathcal{T}_0^+ > 0$ be small enough. By Assumption 1.2.14 there exists a unique solution $u\colon [0, \mathcal{T}_0^+] \to X$ of the problem

$$\omega(u_t, \cdot) = \mathrm{d}H(u), \quad u(0) = u_0 \in X \cap U_\star, \tag{2.3.4}$$

which is continuously differentiable on $(0, \mathcal{T}_0^+)$ with respect to $\|\cdot\|_{-1}$ and has images in $U_\star$. Hence, the mapping $\gamma : [0, \mathcal{T}_0^+] \to G_0$, $t \mapsto \left[\hat{g}(u(t))\right]^{-1}$ is continuously differentiable as a composition of continuously differentiable mappings, where $\hat{g}$ is the implicit function from Lemma 2.3.1. By writing

$$u(t) = a(\gamma(t))v(t), \quad \gamma_t = \mathrm{d}L_\gamma(\mathbb{1})\mu, \quad \gamma(0) = \mathbb{1}$$

and applying Theorem 2.1.2, we get a local solution $v\colon [0, \mathcal{T}_0^+] \to X \cap U_\star$, $\mu\colon [0, \mathcal{T}_0^+] \to \mathcal{A}_0$ of the freezing system (2.3.3).

Now assume $z\colon [0, \mathcal{T}_0^+] \to X \cap U_\star$, $\sigma\colon [0, \mathcal{T}_0^+] \to \mathcal{A}_0$ is another solution of (2.3.3). Define $\eta : [0, \mathcal{T}_0^+] \to G_0$ via $\eta_t = \mathrm{d}L_\eta(\mathbb{1})\sigma$, $\eta(0) = \mathbb{1}$. From Theorem 2.1.2 we conclude that $t \mapsto a(\eta(t))z(t)$ solves (2.3.4), and due to the uniqueness in Assumption 1.2.14, it follows

$$a(\eta(t))z(t) = u(t) = a(\gamma(t))v(t).$$

The uniqueness of the implicit function in Lemma 2.3.1 gives us $\eta(t) = \gamma(t)$, which implies $z(t) = v(t)$.

The conservation laws are proven in a similar way as in Lemma 1.2.15. The set $\mathfrak{A} = \{t \in \mathcal{I} \colon H(v(t)) = H(u_0)\}$ is closed since $v \mapsto H(v)$ and $t \mapsto v(t)$ are continuous. Due to the invariance of H under the group action by Assumption 1.2.5 and $H(u(t)) = H(u_0)$ by Lemma 1.2.15, it is also open. Hence, we conclude $\mathfrak{A} = \mathcal{I}$. In case of the conservation of Q, where the invariance under the group action is due to Proposition 1.2.7, we proceed in the same way.

In order to prove the blow-up alternative, we first show that $\mathcal{T}_0^+$ can be chosen in such a way that it only depends on $\xi_0, M_0 > 0$ satisfying $\operatorname{dist}_{\|\cdot\|_{-1}}\left(u_0, \partial U_\star\right) \leq \xi_0$ and $\|u_0\| \leq M_0$. For $u_0 \in X \cap U_\star$ let $u \in \mathcal{C}(T_{u_0}^-, T_{u_0}^+; X)$ be the unique solution of (2.3.4) in the sense of Assumption 1.2.14(a). Since we want to apply Lemma 2.3.1, we shrink the time interval to make sure that the solution stays inside of $U_\star$. From Assumption 1.2.14(b) we get T_0 and R_0 depending only on M_0 such that it holds $\left\|u_t(t)\right\|_{-1} \leq R_0$ for $t \in [0, T_0]$, which implies

$$\left\|u(t) - u_0\right\|_{-1} \leq \int_0^t \left\|u_t(s)\right\|_{-1} \mathrm{d}s \leq tR_0.$$

By choosing

$$\mathcal{T}(\xi_0, M_0) = \min\left(\frac{\xi_0}{R_0}, T_0\right),$$

we get $u(t) \in X \cap U_\star$ for all $t \in [0, \mathcal{T}(\xi_0, M_0)]$, and we conclude that the freezing system has a solution $v \colon [0, \mathcal{T}(\xi_0, M_0)] \to X$, $\mu \colon [0, \mathcal{T}(\xi_0, M_0)] \to \mathcal{A}_0$, where $\mathcal{T}(\xi_0, M_0)$ only depends on ξ_0 and M_0.

Now, let $(\mathcal{T}^-, \mathcal{T}^+)$ be the maximal interval of existence of the PDAE (2.3.3) such that $v(t)$ remains in $X \cap U_\star$. Assume that $\mathcal{T}^+ < \infty$ holds and that there exists a sequence $t_j \to \mathcal{T}^+$ as $j \to \infty$ such that $\operatorname{dist}_{\|\cdot\|_{-1}}\left(v(t_j), \partial U_\star\right) \geq \xi$ and $\|v(t_j)\| \leq M$ for some constants $\xi > 0$ and $M \in \mathbb{R}$.

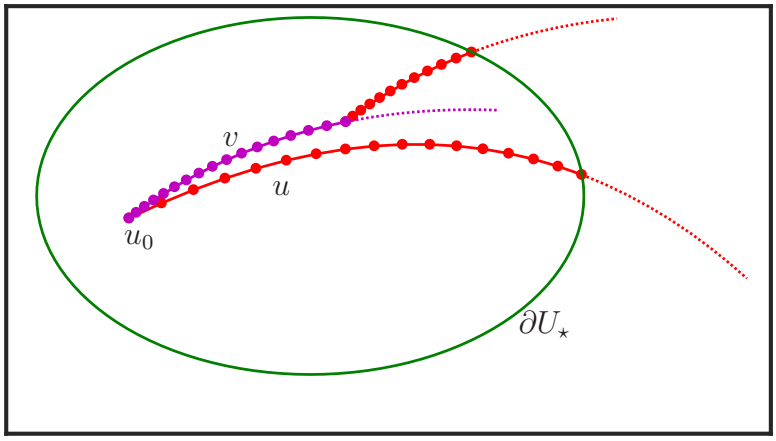


Figure 2.3.1: Extension of solution

Using the same construction as above, i.e., solving (2.3.4) with respect to the initial data $u(0) = v(t_k) \in X \cap U_\star$ and transforming to the freezing coordinates, we extend the solution (v, μ) to a larger time interval $[0, t_k + \mathcal{T}(\xi, M)]$, where $\mathcal{T}(\xi, M)$ only depends on ξ and M. However, for large enough k we obtain $t_k + \mathcal{T}(\xi, M) > \mathcal{T}^+$, which is a contradiction to $(\mathcal{T}^-, \mathcal{T}^+)$ being the maximal interval of existence. □

Denote by $\mathcal{B}_\zeta(v_\star)$ the (open) Ball in X of radius $\zeta > 0$ centered at $v_\star \in X$. From $U_\star \subseteq X_{-1}$ open and $X \hookrightarrow X_{-1}$, it follows $\mathcal{B}_\zeta(v_\star) \subseteq X \cap U_\star$ for $\zeta > 0$ small enough.

Corollary 2.3.3. *Let the Assumptions 1.2.2-1.2.14, 2.2.3, and 2.2.11 be satisfied. For any $\varepsilon > 0$ there exists $\zeta > 0$ such that $u_0 \in \mathcal{B}_\zeta(v_\star)$ satisfying $\psi(u_0) = 0$ implies*

$$|\mu(0; u_0) - \mu_\star| < \varepsilon,$$

where $t \mapsto \big(v(t; u_0), \mu(t; u_0)\big)$ denotes the solution of (2.3.3).

Proof. Let $t \mapsto u(t; u_0)$ solve (2.3.4) and let $\mathcal{T}_0^-, \mathcal{T}_0^+$ be small enough such that we have $u(t; u_0) \in X \cap U_\star$ for all $t \in (\mathcal{T}_0^-, \mathcal{T}_0^+)$. As in the proof of Theorem 2.3.2, this yields a function $g(t; u_0) = \hat{g}\big(u(t; u_0)\big)$, where $\hat{g}$ is given by Lemma 2.3.1, and from (2.3.1) we get by the chain rule

$$g_t = -\big[\mathfrak{F}_g(g, u)\big]^{-1} \mathfrak{F}_u(g, u) u_t. \tag{2.3.5}$$

We define $\gamma(t; u_0) = \big[\hat{g}(u(t; u_0))\big]^{-1} = \big[g(t; u_0)\big]^{-1}$ and obtain $\mu(t; u_0)$ by solving $\gamma_t = dL_\gamma(\mathbb{1})\mu$. Since the group operations of multiplication and inversion are smooth maps, for $\varepsilon > 0$ there exist $\xi > 0$ such that the inequality

$$|\mu(0; u_0) - \mu_\star| = |\mu(0; u_0) - \mu(0; v_\star)| < \varepsilon$$

holds, provided that we have

$$|g_t(0; u_0) - g_t(0; v_\star)| < \xi. \tag{2.3.6}$$

We are left to show that for $\xi > 0$ there exist $\zeta > 0$ such that $u_0 \in \mathcal{B}_\zeta(v_\star)$ implies (2.3.6). From $\psi(v_\star) = 0$, we get $g(0; v_\star) = \hat{g}(v_\star) = \mathbb{1}$. This implies

$$g_t(0; v_\star) = -\big[\mathfrak{F}_g(\mathbb{1}, v_\star)\big]^{-1} \mathfrak{F}_u(\mathbb{1}, v_\star) u_t(0; v_\star),$$

where the matrix

$$\Big[\big\langle \mathfrak{F}_g(\mathbb{1}, v_\star) e_i, e_j \big\rangle\Big]_{i,j=1}^{d_\star} = \Big[\big\langle \mathrm{d}\psi(v_\star) e_i, \mathrm{d}[a(\mathbb{1}) v_\star] e_j \big\rangle\Big]_{i,j=1}^{d_\star}$$

is non-singular by Assumption 2.2.11. Assumption 1.2.14(c) gives us the estimate

$$\big\| u_t(0; u_0) - u_t(0; v_\star) \big\|_{-1} \leq \mathcal{M} \|u_0 - v_\star\| \leq \mathcal{M}\zeta,$$

and the mapping $\mathfrak{F} \colon G_0 \times X_{-1} \to \mathcal{A}_0^\star$ is continuously differentiable by Assumption 2.2.11. Furthermore, we have $\|u(0; u_0) - v_\star\| = \|u_0 - v_\star\| \leq \zeta$, and the identity $g(0; u_0) = \hat{g}(u_0) = \mathbb{1}$ follows from $\psi(u_0) = 0$. Hence, we apply Banach's Lemma to obtain (2.3.6), provided that $\zeta > 0$ was chosen small enough. □

In the following, the perturbed version of Y from (2.2.15) in Theorem 2.2.10 is chosen as

$$\hat{Y} = \big\{\hat{y} \in X \colon \big\langle \mathrm{d}Q(v_\star)e_j, \hat{y}\big\rangle = \langle \mathrm{d}\psi(v_\star)e_j, \hat{y}\rangle = 0 \text{ for } j = 1, ..., d_\star\big\}, \tag{2.3.7}$$

i.e., $z_j^\star = \mathrm{d}\psi(v_\star)e_j$. In general, the desired property $v(t) - v_\star \in \hat{Y}$ fails to be true for the solutions of (2.3.3). However, this difficulty is circumvented by adding corrective terms in W and Z, i.e.,

$$\hat{y}(t) = v(t) - v_\star - \Omega\hat{\alpha}(v(t)) - \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v(t))$$

with Ω as in Lemma 2.2.4. Choosing $\hat{\alpha}$ and $\hat{\beta}$ as follows allows us to apply Theorem 2.2.10 to $\hat{y}(t) \in \hat{Y}$.

Lemma 2.3.4. *Provided the Assumptions 1.2.2-1.2.5, 2.2.3, and 2.2.11 hold, there exist uniquely defined smooth functions*

$$\hat{\alpha} \colon X \to \mathcal{A}_0,$$
$$\hat{\beta} \colon X \to \mathcal{A}_0,$$

such that $\mathfrak{G}(\alpha, \beta, v) = 0$ if and only if $\alpha = \hat{\alpha}(v)$, $\beta = \hat{\beta}(v)$, where

$$\mathfrak{G} = \begin{bmatrix} \mathfrak{G}^1 \\ \mathfrak{G}^2 \end{bmatrix}$$

is given by

$$\mathfrak{G}^1(\alpha, \beta, v) = \Big[\big\langle \mathrm{d}Q(v_\star)e_i, v - v_\star - \Omega\alpha - \mathrm{d}[a(\mathbb{1})v_\star]\beta\big\rangle\Big]_{i=1}^{d_\star},$$
$$\mathfrak{G}^2(\alpha, \beta, v) = \Big[\big\langle \mathrm{d}\psi(v_\star)e_i, v - v_\star - \Omega\alpha - \mathrm{d}[a(\mathbb{1})v_\star]\beta\big\rangle\Big]_{i=1}^{d_\star}.$$

Moreover, we obtain

$$|\hat{\alpha}(v)| + |\hat{\beta}(v)| \le C\|v - v_\star\|^2 \tag{2.3.8}$$

for all $v \in X \cap U_\star$ that satisfy $Q(v)e_j = Q(v_\star)e_j$ and $\psi(v)e_j = 0$ for $j = 1, ..., d_\star$.

Proof. Since $\mathfrak{G}$ is linear in α and β, the Jacobian submatrix

$$\begin{bmatrix} \mathfrak{G}^1_\alpha & \mathfrak{G}^1_\beta \\ \mathfrak{G}^2_\alpha & \mathfrak{G}^2_\beta \end{bmatrix} \tag{2.3.9}$$

is constant, and we have to show that it is invertible. First of all, the matrix $\mathfrak{G}^1_\alpha$ is non-singular by Lemma 2.2.4. Second, the other diagonal entry $\mathfrak{G}^2_\beta$ is invertible by Assumption 2.2.11(b). Third, due to (1.2.10), the off-diagonal block $\mathfrak{G}^1_\beta$ is the zero matrix. Hence, the matrix (2.3.9) is invertible.

We are left to verify the estimate for $\hat{\alpha}(v)$ and $\hat{\beta}(v)$. Denote $\sigma = \frac{\hat{\alpha}(v)}{|\hat{\alpha}(v)|} \in \mathcal{A}_0$ and $\lambda = \frac{\hat{\beta}(v)}{|\hat{\beta}(v)|} \in \mathcal{A}_0$. Due to $Q(v)\sigma = Q(v_\star)\sigma$, Taylor expansion of $Q(v)\sigma$ at $v_\star$ leads to

$$0 = Q(v)\sigma - Q(v_\star)\sigma = \big\langle \mathrm{d}Q(v_\star)\sigma, v - v_\star\big\rangle + \mathcal{O}(\|v - v_\star\|^2),$$

and because of Assumption 2.2.11(a), we have

$$0 = \psi(v)\lambda - \psi(v_\star)\lambda = \big\langle \mathrm{d}\psi(v_\star)\lambda, v - v_\star \big\rangle + \mathcal{O}(\|v - v_\star\|^2).$$

Then by using the identities

$$\begin{aligned} \big\langle \mathrm{d}Q(v_\star)\sigma, v - v_\star - \Omega\hat{\alpha}(v) - \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v) \big\rangle &= 0, \\ \big\langle \mathrm{d}\psi(v_\star)\lambda, v - v_\star - \Omega\hat{\alpha}(v) - \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v) \big\rangle &= 0 \end{aligned}$$

from the first part, we get

$$\begin{aligned} \big\langle \mathrm{d}Q(v_\star)\sigma, \Omega\hat{\alpha}(v) + \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v) \big\rangle &= \mathcal{O}(\|v - v_\star\|^2), \\ \big\langle \mathrm{d}\psi(v_\star)\lambda, \Omega\hat{\alpha}(v) + \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v) \big\rangle &= \mathcal{O}(\|v - v_\star\|^2). \end{aligned}$$

Combining (1.2.10) and Assumption 2.2.11(b), this leads to (2.3.8). □

The proof of stability is now based on estimating the distance $\|v - v_\star\|$ in terms of $H(v) - H(v_\star)$. This is obtained by Taylor expansion of $H(v) - Q(v)\mu_\star$ at $v_\star$, where we make use of Theorem 2.2.10 and the estimate (2.3.8) for $\hat{\alpha}(v)$ and $\hat{\beta}(v)$.

Lemma 2.3.5. *Let $v \in X \cap U_\star$ satisfy $Q(v)e_j = Q(v_\star)e_j$ and $\psi(v) = 0$ for $j = 1, ..., d_\star$. Provided the Assumptions 1.2.2-1.2.5, 2.2.2, 2.2.3, 2.2.7, and 2.2.11 hold, we have*

$$H(v) - H(v_\star) \geq c\|v - v_\star\|^2.$$

Proof. As before, we write $H(v_\star) - Q(v_\star)\mu_\star = \ell_\star$ and $\mathrm{d}^2H(v_\star) - \mathrm{d}^2Q(v_\star)\mu_\star = L_\star$. Together with $\mathrm{d}H(v_\star) - \mathrm{d}Q(v_\star)\mu_\star = 0$ we obtain by Taylor expansion at $v_\star$ the identity

$$H(v) - Q(v)\mu_\star = \ell_\star + \tfrac{1}{2}\big\langle L_\star(v - v_\star), v - v_\star \big\rangle + o(\|v - v_\star\|^2),$$

which can be rewritten as

$$H(v) - Q(u)\mu_\star = \ell_\star + \tfrac{1}{2}\langle L_\star\hat{y}, \hat{y}\rangle + \mathcal{R}(v), \tag{2.3.10}$$

where $\hat{y} = v - v_\star - \Omega\hat{\alpha}(v) - \mathrm{d}[a(\mathbb{1})v_\star]\hat{\beta}(v) \in \hat{Y}$ with $\hat{\alpha}$, $\hat{\beta}$ from Lemma 2.3.4, and the higher order terms are of the form

$$\mathcal{R}(v) = \mathcal{O}\Big(\big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)\|\hat{y}\| + \big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)^2\Big) + o(\|v - v_\star\|^2).$$

Next, we subtract $H(v_\star) - Q(v_\star)\mu_\star = \ell_\star$ from (2.3.10), make use of

$$Q(v)\mu_\star = Q(v_\star)\mu_\star, \tag{2.3.11}$$

and obtain

$$H(v) - H(v_\star) = \tfrac{1}{2}\langle L_\star\hat{y}, \hat{y}\rangle + \mathcal{R}(v). \tag{2.3.12}$$

The positivity of $L_\star$ on $\hat{Y}$, which we get from Theorem 2.2.10 and Assumption 2.2.11(b), gives us

$$\tfrac{1}{2}\langle L_\star \hat{y}, \hat{y}\rangle \geq c\|\hat{y}\|^2 \geq c\|v - v_\star\|^2 - C\Big(\big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)\|\hat{y}\| + \big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)^2\Big),$$

and by plugging this into (2.3.12), we find

$$H(v) - H(v_\star) \geq c\|v - v_\star\|^2 - C\Big(\big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)\|\hat{y}\| + \big(|\hat{\alpha}(v)| + |\hat{\beta}(v)|\big)^2\Big).$$

Since $\hat{y} = v - v_\star + \mathcal{O}(|\hat{\alpha}(v)| + |\hat{\beta}(v)|)$, we can make use of Lemma A.4.1 and get

$$H(v) - H(v_\star) \geq c\|v - v_\star\|^2 - C\big(|\hat{\alpha}(v)|^2 + |\hat{\beta}(v)|^2\big). \tag{2.3.13}$$

Due to (2.3.11) and $\psi(v) = 0$, the estimate (2.3.8) holds for $\hat{\alpha}(v)$ and $\hat{\beta}(v)$. Hence, the inequality in (2.3.13) takes the form

$$H(v) - H(v_\star) \geq c\|v - v_\star\|^2,$$

which is our claim. □

In the case of $Q(v(0))\sigma = Q(v_\star)\sigma$, the stability of $v_\star$ is a direct consequence of Lemma 2.3.5 and the preservation of the Hamiltonian. For the general case, we need an additional Lemma.

Lemma 2.3.6. *Provided the Assumptions 1.2.2-1.2.5, 2.2.3, and 2.2.11 hold, there exists $\varepsilon > 0$ such that for all $v \in \mathcal{B}_\varepsilon(v_\star)$ there are $\hat{w}(v) \in W$ and $\hat{z}(v) \in Z$ such that we have*

$$Q\big(v + \hat{w}(v) + \hat{z}(v)\big)\sigma = Q(v_\star)\sigma, \tag{2.3.14a}$$
$$\psi\big(v + \hat{w}(v) + \hat{z}(v)\big)\sigma = \psi(v_\star)\sigma \tag{2.3.14b}$$

for all $\sigma \in \mathcal{A}_0$ and the estimate

$$\|\hat{w}(v)\| + \|\hat{z}(v)\| \leq C\Big(\big|Q(v) - Q(v_\star)\big|_{\mathcal{A}_0^\star} + \big|\psi(v) - \psi(v_\star)\big|_{\mathcal{A}_0^\star}\Big). \tag{2.3.15}$$

Proof. Consider the mapping

$$\mathfrak{Q} = \begin{bmatrix}\mathfrak{Q}^1\\ \mathfrak{Q}^2\end{bmatrix} : X \times W \times Z \to \mathbb{R}^{2d_\star}$$

given by

$$\mathfrak{Q}^1 : X \times W \times Z \to \mathbb{R}^{d_\star}, \quad (v, w, z) \mapsto \Big[Q(v + w + z)e_i - Q(v_\star)e_i\Big]_{i=1}^{d_\star},$$
$$\mathfrak{Q}^2 : X \times W \times Z \to \mathbb{R}^{d_\star}, \quad (v, w, z) \mapsto \Big[\psi(v + w + z)e_i - \psi(v_\star)e_i\Big]_{i=1}^{d_\star}.$$

The Jacobian submatrix of $\mathfrak{Q}$ with respect to w and z evaluated at $(v_\star, 0, 0)$ takes the form

$$\mathfrak{Q}_{(w,z)} = \begin{bmatrix}\mathfrak{Q}^1_w & \mathfrak{Q}^1_z\\ \mathfrak{Q}^2_w & \mathfrak{Q}^2_z\end{bmatrix}$$

with

$$\begin{aligned}
\mathfrak{Q}_w^1 &= \Big[\big\langle \mathrm{d}Q(v_\star)e_i, \Omega e_j\big\rangle\Big]_{i,j=1}^{d_\star},\\
\mathfrak{Q}_z^1 &= \Big[\big\langle \mathrm{d}Q(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big\rangle\Big]_{i,j=1}^{d_\star},\\
\mathfrak{Q}_w^2 &= \Big[\big\langle \mathrm{d}\psi(v_\star)e_i, \Omega e_j\big\rangle\Big]_{i,j=1}^{d_\star},\\
\mathfrak{Q}_z^2 &= \Big[\big\langle \mathrm{d}\psi(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big\rangle\Big]_{i,j=1}^{d_\star}.
\end{aligned}$$

We have already seen in Lemma 2.3.4 that it is invertible. Hence, we apply the implicit function theorem to obtain $\big(\hat{w}(v), \hat{z}(v)\big) \in W \times Z$. We are left to show (2.3.15). The mean value theorem gives us

$$\begin{aligned}
\mathfrak{Q}(v_\star, 0, 0) - \mathfrak{Q}(v, 0, 0) &= \mathfrak{Q}(v, \hat{w}(v), \hat{z}(v)) - \mathfrak{Q}(v, 0, 0)\\
&= \int_0^1 \mathfrak{Q}_{(w,z)}\big(v, t\hat{w}(v), t\hat{z}(v)\big)\mathrm{d}t \cdot \big(\hat{w}(v), \hat{z}(v)\big),
\end{aligned}$$

which implies

$$\|\hat{w}(v)\| + \|\hat{z}(v)\| \leq C\big|\mathfrak{Q}(v_\star, 0, 0) - \mathfrak{Q}(v, 0, 0)\big|$$

since $\mathfrak{Q}_{(w,z)}$ has a uniformly bounded inverse in a neighborhood of $v_\star$. □

The preliminary work allows us now to prove the main theorem of this chapter.

Theorem 2.3.7. *Under the Assumptions 1.2.2-1.2.5, 1.2.14, 2.2.2, 2.2.3, 2.2.7, and 2.2.11, the steady state $(v_\star, \mu_\star) \in X \times \mathcal{A}_0$ is stable in the Lyapunov sense. That is, for any $\varepsilon > 0$ there exists $\delta > 0$ such that the solution (v, μ) of the freezing system (2.3.3) exists for all times, and*

$$\|v(t) - v_\star\| + |\mu(t) - \mu_\star| < \varepsilon$$

holds for all $t \in [0, \infty)$, provided the initial data satisfy $\|v(0) - v_\star\| < \delta$.

Proof. Assume first that the v-component is not stable and choose $\varepsilon > 0$ small enough such that Lemma 2.3.1 and Lemma 2.3.6 can be applied. In particular $\|v - v_\star\| < \varepsilon$ must guarantee $v \in U_\star \subseteq X_{-1}$. Then there exists a sequence of intervals $\mathcal{I}_n$ and solutions $v_n \in \mathcal{C}(\mathcal{I}_n; X) \cap \mathcal{C}^1(\mathcal{I}_n; X_{-1})$ of (2.3.3), $n \in \mathbb{N}$, such that we have $\|v_n(0) - v_\star\| \to 0$ as $n \to \infty$, but $\sup_{t \in \mathcal{I}_n} \|v_n(t) - v_\star\| \geq \varepsilon$ for all $n \in \mathbb{N}$.

By continuity of the solutions we can define t_n to be the first time such that $\|v_n(t_n) - v_\star\| = \frac{\varepsilon}{2}$. In particular, this means $[0, t_n] \subseteq \mathcal{I}_n$. Since H and Q are continuous and conserved quantities (see Theorem 2.3.2), we have

$$\begin{aligned}
H(v_n(t_n)) = H(v_n(0)) \quad &\to H(v_\star),\\
Q(v_n(t_n))e_j = Q(v_n(0))e_j &\to Q(v_\star)e_j
\end{aligned}$$

as $n \to \infty$ for all $j = 1, ..., d_\star$. From Lemma 2.3.6 we obtain $w_n \in W$ and $z_n \in Z$ such that the identities

$$\begin{aligned} Q(v_n(t_n) + w_n + z_n)e_j &= Q(v_\star)e_j, \\ \psi(v_n(t_n) + w_n + z_n)e_j &= \psi(v_\star)e_j = 0 \end{aligned}$$

hold for $j = 1, ..., d_\star$ and such that

$$\|w_n\| + \|z_n\| \leq C\Big(\big|Q(v_n(t_n)) - Q(v_\star)\big|_{\mathcal{A}_0^\star} + \big|\psi(v_n(t_n))\big|_{\mathcal{A}_0^\star}\Big)$$

is satisfied. Due to $Q(v_n(t_n))e_j \to Q(v_\star)e_j$ and $\psi(v_n(t_n))e_j = 0$ for $j = 1, ..., d_\star$, it follows $\|w_n\| + \|z_n\| \to 0$ as $n \to \infty$. Furthermore, Lemma 2.3.5 gives us

$$H(v_n(t_n) + w_n + z_n) - H(v_\star) \geq c\big\|v_n(t_n) + w_n + z_n - v_\star\|^2,$$

where $H(v_n(t_n) + w_n + z_n) \to H(v_\star)$ is due to continuity of H and $\|w_n + z_n\| \to 0$. This implies

$$\|v_n(t_n) - v_\star\| \to 0,$$

which contradicts the assumption.

Now, we consider the μ-component. Given $t \geq 0$, let $s \mapsto \big(z(s), \sigma(s)\big)$ solve

$$\begin{aligned} \omega(z_s, \cdot) = \mathrm{d}H(z) - \mathrm{d}Q(z)\sigma, \quad z(0) = v(t), \\ 0 = \psi(z). \end{aligned}$$

From the uniqueness in Theorem 2.3.2, we conclude $\sigma(0) = \mu(t)$. According to Corollary 2.3.3, for any $\varepsilon > 0$ there exists $\zeta \in (0, \frac{\varepsilon}{2})$ such that we obtain

$$|\mu(t) - \mu_\star| = |\sigma(0) - \mu_\star| < \frac{\varepsilon}{2},$$

provided that we have $z(0) \in \mathcal{B}_\zeta(v_\star)$. By the first part, we know that there exists $\delta > 0$ such that initial data satisfying $\|v(0) - v_\star\| < \delta$ lead to

$$\|v(t) - v_\star\| < \zeta$$

for all $t \in [0, \infty)$, which implies $z(0) \in \mathcal{B}_\zeta(v_\star)$. □

2.4 Application to the NLS

The next proposition shows that the cubic nonlinear Schrödinger equation

$$iu_t = -u_{xx} + \kappa|u|^2 u$$

together with its two-parameter group

$$a\colon G \to GL(X), \quad [a(\gamma)v](x) = e^{-i\gamma_1}v(x - \gamma_2), \quad \gamma = (\gamma_1, \gamma_2) \in G = S^1 \times \mathbb{R}$$

fits into the abstract setting. In Proposition 1.3.4 we have already seen that the Hamiltonian is given by

$$H(v) = \frac{1}{2}\int_{\mathbb{R}} \Big(|v_x|^2 + \frac{\kappa}{2}|v|^4\Big)\mathrm{d}x.$$

Moreover, the corresponding spaces are given by

$$X = H^1(\mathbb{R};\mathbb{C}), \quad X_{-1} = X^\star = H^{-1}(\mathbb{R};\mathbb{C}).$$

Proposition 2.4.1. *For the NLS the Assumptions 1.2.2-1.2.5 and 1.2.14 are fulfilled.*

Proof. We start with Assumption 1.2.2. The mapping $a : G \to GL(X)$ is a group homomorphism since

$$\begin{aligned} a(\gamma g)v &= e^{-i(\gamma_1+g_1)}v(\cdot-\gamma_2-g_2) = e^{-i\gamma_1}e^{-ig_1}v(\cdot-g_2-\gamma_2)\\ &= e^{-i\gamma_1}[a(g)v](\cdot-\gamma_2) = a(\gamma)a(g)v \end{aligned}$$

for all $\gamma, g \in G$. We are left to prove the symplecticity of the group action. For $z = e^{-i\gamma_1}$ we have $\bar{z}z = 1$. This implies $(zu, zv)_0 = (\bar{z}zu, v)_0 = (u, v)_0$, where the inner product is given by (1.3.2). Due to the translation invariance of the integral, this leads to

$$\begin{aligned} \omega(a(\gamma)v, a(\gamma)u) &= \big(ia(\gamma)v, a(\gamma)u\big)_0 = \big(ie^{-i\gamma_1}v(\cdot-\gamma_2), e^{-i\gamma_1}u(\cdot-\gamma_2)\big)_0\\ &= \big(iv(\cdot-\gamma_2), u(\cdot-\gamma_2)\big)_0 = \big(iv, u\big)_0 = \omega(v,u) \end{aligned}$$

for all $v, u \in X$.

In order to verify Assumption 1.2.3, it suffices to show that the intersection

$$\mathcal{D}_{e_1} \cap \mathcal{D}_{e_2}$$

is contained in $\mathcal{D}_F$ and a dense subset of X, where we denote by $\mathcal{D}_{e_1}$ the domain of $\mathrm{d}[a(\mathbb{1})v]e_1 = -iv$ and by $\mathcal{D}_{e_2}$ the domain of $\mathrm{d}[a(\mathbb{1})v]e_2 = -v_x$. This is obtained by setting $\mathcal{D}_{e_1} = H^1(\mathbb{R};\mathbb{C})$, $\mathcal{D}_{e_2} = H^2(\mathbb{R};\mathbb{C})$, and $\mathcal{D}_F = H^3(\mathbb{R};\mathbb{C})$.

Since $v_x \in L^2(\mathbb{R};\mathbb{C})$ holds for all $v \in H^1(\mathbb{R};\mathbb{C})$, the mapping

$$\omega(\mathrm{d}[a(\mathbb{1})v]\mu, u) = \omega(-iv\mu_1 - v_x\mu_2, u) = \big(v\mu_1 - iv_x\mu_2, u\big)_0$$

extends to $v \in H^1(\mathbb{R};\mathbb{C})$. Hence, Assumption 1.2.4 is fulfilled, where we remark that

$$\langle B(v)\mu, u\rangle = \big(v\mu_1 - iv_x\mu_2, u\big)_0$$

implies

$$Q(v)\mu = \tfrac{1}{2}\langle B(v)\mu, v\rangle = \tfrac{1}{2}\mu_1\|v\|_0^2 - \tfrac{1}{2}\mu_2\big(iv_x, v\big)_0,$$

which can be rewritten as

$$Q(v)\mu = \frac{1}{2}\int_{\mathbb{R}} \mathrm{Re}\big(\mu_1|v|^2 + i\mu_2\bar{v}_x v\big)\mathrm{d}x.$$

For Assumption 1.2.5 we have to prove that $H \in \mathcal{C}^2(X;\mathbb{R})$ holds with locally bounded derivatives and that H is invariant with respect to the group action. Combining (1.3.5) and (1.3.6), we have

$$\langle \mathrm{d}H(u), v\rangle = \int_{\mathbb{R}} \mathrm{Re}\big(\bar{u}_x(x)v_x(x)\big)\mathrm{d}x + \kappa \int_{\mathbb{R}} \mathrm{Re}\big(|u(x)|^2\bar{u}(x)v(x)\big)\mathrm{d}x$$

for all $u, v \in H^1(\mathbb{R};\mathbb{C})$. Due to the Cauchy-Schwarz inequality, this is locally bounded by

$$|\langle \mathrm{d}H(u), v\rangle| \leq C(\|u\|_1 + \kappa\|u\|_1^3) \cdot \|v\|_1$$

since $H^1(\mathbb{R};\mathbb{C})$ is a generalized Banach algebra and $\|u\|_1 = \|\bar{u}\|_1$. For the second derivative we note that

$$\begin{aligned} |z+\zeta|^2(\bar{z}+\bar{\zeta}) &= (|z|^2 + \bar{z}\zeta + z\bar{\zeta} + |\zeta|^2)(\bar{z}+\bar{\zeta}) \\ &= |z|^2\bar{z} + \bar{z}^2\zeta + 2|z|^2\bar{\zeta} + 2\bar{z}|\zeta|^2 + z\bar{\zeta}^2 + |\zeta|^2\bar{\zeta} \end{aligned}$$

for all $z, \zeta \in \mathbb{C}$. This implies

$$\begin{aligned} \langle \mathrm{d}H(u+h), v\rangle = \langle \mathrm{d}H(u), v\rangle &+ \int_{\mathbb{R}} \mathrm{Re}\big(\bar{h}_x(x)v_x(x)\big)\mathrm{d}x \\ &+ 2\kappa \int_{\mathbb{R}} \mathrm{Re}\big(|u(x)|^2\bar{h}(x)v(x)\big)\mathrm{d}x + \kappa \int_{\mathbb{R}} \mathrm{Re}\big(\bar{u}(x)^2h(x)v(x)\big)\mathrm{d}x \\ &+ \mathfrak{O}\big(u(x), v(x), h(x)\big) \end{aligned}$$

with

$$\big|\mathfrak{O}\big(u, v, h\big)\big| \leq C\big(\|h\|_1 + 3\|u\|_1\big)\|h\|_1\|v\|_1.$$

Hence, the second derivative is given by

$$\langle \mathrm{d}^2H(u)v, h\rangle = \big(h_x, v_x\big)_0 + 2\kappa\big(|u|^2h, v\big)_0 + \kappa\big(u^2, hv\big)_0,$$

which is locally bounded as follows

$$|\langle \mathrm{d}^2H(u)v, h\rangle| \leq C(1 + 3\kappa\|u\|_1^2) \cdot \|v\|_1\|h\|_1.$$

The invariance of the Hamiltonian under the group action is due to

$$\begin{aligned} H(a(\gamma)u) &= \frac{1}{2}\int_{\mathbb{R}} \Big(|a(\gamma)u_x(x)|^2 + \frac{\kappa}{2}|a(\gamma)u(x)|^4\Big)\mathrm{d}x \\ &= \frac{1}{2}\int_{\mathbb{R}} \Big(\big|e^{-i\gamma_1}u_x(x-\gamma_2)\big|^2 + \frac{\kappa}{2}\big|e^{-i\gamma_1}u(x-\gamma_2)\big|^4\Big)\mathrm{d}x \\ &= \frac{1}{2}\int_{\mathbb{R}} \Big(|u_x(x-\gamma_2)|^2 + \frac{\kappa}{2}|u(x-\gamma_2)|^4\Big)\mathrm{d}x \\ &= \frac{1}{2}\int_{\mathbb{R}} \Big(|u_x(z)|^2 + \frac{\kappa}{2}|u(z)|^4\Big)\mathrm{d}z = H(u), \end{aligned}$$

where we have $z = x - \gamma_2$.

For local existence, uniqueness, continuous dependence, and regularity in Assumption 1.2.14 we refer to [15], [27], and [39]. Since a strong $H^1(\mathbb{R};\mathbb{C})$-solution satisfies the NLS in $H^{-1}(\mathbb{R};\mathbb{C})$-sense for all $t \in \mathcal{I}$, we obtain $\|u_t\|_{-1}$ estimates in terms of $\|u\|$, and the same is true for continuous dependence. □

Next, we discuss the spectral hypotheses that are imposed on the linear operator

$$L_\star\colon X \to X^\star, \quad L_\star = \mathrm{d}^2 H(v_\star) - \mathrm{d}^2 Q(v_\star)\mu_\star.$$

This is an integral part of the Grillakis-Shatah-Strauss stability approach. Their seminal article [33] comes with a series of examples, including the nonlinear Schrödinger equation. That is why we do not cover all details.

Proposition 2.4.2. *The linerization of the NLS at a relative equilibrium (1.3.10) satisfies the Assumptions 2.2.2, 2.2.3, and 2.2.7.*

Proof. Starting with Assumption 2.2.2, we note that the family of relative equilibria is given by (1.3.11).

The decomposition in Assumption 2.2.3 is verified by making use of the Gelfand triple

$$H^1(\mathbb{R};\mathbb{C}) \hookrightarrow L^2(\mathbb{R};\mathbb{C}) \hookrightarrow H^{-1}(\mathbb{R};\mathbb{C}),$$

where the natural embedding

$$\iota\colon H^1(\mathbb{R};\mathbb{C}) \to L^2(\mathbb{R};\mathbb{C}), \quad v \mapsto v$$

is a consequence of the subset relation $H^1(\mathbb{R};\mathbb{C}) \subseteq L^2(\mathbb{R};\mathbb{C})$, and where the operator

$$\iota^\star\colon L^2(\mathbb{R};\mathbb{C}) \to H^{-1}(\mathbb{R};\mathbb{C}), \quad v \mapsto \big(v, \cdot\big)_0$$

is obtained by using the Riesz representation on $L^2(\mathbb{R};\mathbb{C})$. While the composition $\iota^\star\iota$ of these mappings is not onto, the preimages

$$[\iota^\star\iota]^{-1}\mathrm{d}Q(v_\star)\sigma = \sigma_1 v_\star - \sigma_2 i v_{\star,x} \in H^1(\mathbb{R};\mathbb{C})$$

of the functionals

$$\mathrm{d}Q(v_\star)\sigma = \big(\sigma_1 v_\star - \sigma_2 i v_{\star,x}, \cdot\big)_0$$

exist for all $\sigma \in \mathcal{A}_0$ due to the smoothness of the profile $v_\star$. Now we define

$$W = \big\{[\iota^\star\iota]^{-1}\mathrm{d}Q(v_\star)\sigma\colon \sigma \in \mathcal{A}_0\big\}$$

and

$$Y = (W \oplus Z)^\perp,$$

where Z is the kernel of $L_\star$. This gives us a decomposition

$$X = W \oplus Y \oplus Z,$$

which satisfies

$$\dim(W) = 2 = d_\star$$

and

$$\big\langle \mathrm{d}Q(v_\star)e_i, y\big\rangle = \big([\iota^\star\iota]^{-1}\mathrm{d}Q(v_\star)e_i, y\big)_0 = 0$$

by construction.

For the remaining (spectral) hypotheses in Assumption 2.2.3 and Assumption 2.2.7 we refer to [33] since the proof is based on the Sturmian theory of oscillations, which we do not want to repeat. □

For the NLS the fixed phase condition

$$\psi\colon X \to (\mathcal{A}_0)^\star$$

is given by

$$\psi(v)\sigma = \big(i\sigma_1\hat{v}, v\big)_0 + \big(\sigma_2\hat{v}_x, v\big)_0$$

for $v \in X$ and $\sigma \in \mathcal{A}_0$.

Proposition 2.4.3. *The fixed phase condition satisfies the parts (b) and (c) of Assumption 2.2.11 for any template function $\hat{v} \in H^3(\mathbb{R};\mathbb{C})$, provided that $\|\hat{v}-v_\star\|$ is small enough.*

Proof. The mapping $\psi\colon X \to (\mathcal{A}_0)^\star$ is a bounded linear operator, which implies continuous differentiability, for any template function $\hat{v} \in H^1(\mathbb{R};\mathbb{C})$.

For any template function $\hat{v} \in H^1(\mathbb{R};\mathbb{C})$ the preimages

$$[\iota^\star\iota]^{-1}\mathrm{d}\psi(v_\star)\sigma = \sigma_1 i\hat{v} + \sigma_2\hat{v}_x \in L^2(\mathbb{R};\mathbb{C})$$

exist. By choosing the template function in such a way that $\|\hat{v} - v_\star\|$ is small enough, the matrix

$$-\Big[\big([\iota^\star\iota]^{-1}\mathrm{d}\psi(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big)_0\Big]_{i,j=1}^{d_\star} = \begin{bmatrix} (i\hat{v}, iv_\star)_0 & (i\hat{v}, v_{\star,x})_0 \\ (\hat{v}_x, iv_\star)_0 & (\hat{v}_x, v_{\star,x})_0 \end{bmatrix}$$

is invertible by Banach's Lemma as a small perturbation of

$$\Big[\big(\mathrm{d}[a(\mathbb{1})v_\star]e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big)_0\Big]_{i,j=1}^{d_\star} = \begin{bmatrix} (iv_\star, iv_\star)_0 & (iv_\star, v_{\star,x})_0 \\ (v_{\star,x}, iv_\star)_0 & (v_{\star,x}, v_{\star,x})_0 \end{bmatrix},$$

which is non-singular by Assumption 2.2.3.

For $u \in H^1(\mathbb{R};\mathbb{C})$ the mapping $(g,u) \mapsto \psi(a(g)u)$ is continuously differentiable. The derivative can be continuously expanded to $u \in H^{-1}(\mathbb{R};C)$ if we have $\hat{v} \in H^3(\mathbb{R};\mathbb{C})$. Indeed, for $\hat{v} \in H^3(\mathbb{R};\mathbb{C})$ it holds $[\iota^\star\iota]^{-1}\mathrm{d}\psi(u)\sigma \in H^2(\mathbb{R};\mathbb{C})$ for any $\sigma \in \mathcal{A}$, and the differentials of the group action can be continuously extended to mappings from $H^{-1}(\mathbb{R};C)$ to $H^{-2}(\mathbb{R};C)$. □

Remark 10. If Assumption 2.2.11(a) fails, the stability is with respect to some other element of the orbit $a(G_0)v_\star$, which satisfies the phase condition. We only imposed this assumption to avoid technical difficulties.

2.5 Application to the NLKG

Next, we verify the hypothesis in case of the nonlinear Klein-Gordon equation

$$u_t = \begin{pmatrix} u_2 \\ u_{1,xx} - u_1 + |u_1|^2 u_1 \end{pmatrix}.$$

The corresponding spaces are given by

$$\begin{aligned} X &= H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3), \quad & X^\star &= H^{-1}(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3), \\ X_0 &= L^2(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3), \quad & X_{-1} &= L^2(\mathbb{R};\mathbb{R}^3) \times H^{-1}(\mathbb{R};\mathbb{R}^3), \end{aligned}$$

and the Hamiltonian takes the form

$$H(v) = \frac{1}{2}\int_{\mathbb{R}} \big(|v_2|^2 + |v_{1,x}|^2 + |v_1|^2 - \tfrac{1}{2}|v_1|^4\big)\mathrm{d}x.$$

Moreover, the equivariance is with respect to the group action

$$a\colon G \to GL(X), \quad a(\gamma)v = \big(Av_1(\cdot+\alpha), Av_2(\cdot+\alpha)\big) \tag{2.5.1}$$

for $\gamma = (A,\alpha) \in G = \mathrm{SO}(3) \times \mathbb{R}$, and the additional conserved quantities are

$$Q(v)\mu = \int_{\mathbb{R}} (Sv_1)^T v_2 \mathrm{d}x + c\int_{\mathbb{R}} v_{1,x}^T v_2 \mathrm{d}x, \quad \mu = (S,c) \in \mathcal{A},$$

where $\mathcal{A} = \mathfrak{so}(3) \times \mathbb{R}$ is the Lie algebra.

Proposition 2.5.1. *The NLKG satisfies the Assumptions 1.2.2-1.2.5 and 1.2.14.*

Proof. We start with Assumption 1.2.2 and show that (2.5.1) is a group homomorphism. By writing group elements $\gamma, g \in G$ as $\gamma = (A,\alpha)$, $g = (B,\beta)$, we obtain

$$a(\gamma g)v = \big(ABv_1(\cdot+\alpha+\beta), ABv_2(\cdot+\alpha+\beta)\big) = a(\gamma)a(g)v.$$

Next, we prove for any $\gamma = (A,\alpha) \in \mathrm{SO}(3)\times\mathbb{R}$ the symplecticity of the images $a(\gamma)v = Av(\cdot+\alpha)$ with respect to the symplectic form

$$\omega(v,u) = \int_{\mathbb{R}} (v_1^T u_2 - v_2^T u_1)\mathrm{d}x.$$

Any orthogonal matrix $A \in \mathrm{SO}(3)$ satisfies $A^TA = \mathrm{id}_{\mathbb{R}^{3\times3}}$, and by the translation of the integral it follows

$$\begin{aligned} \omega\big(a(\gamma)v, a(\gamma)u\big) &= \int_{\mathbb{R}} \Big((Av_1(\cdot+\alpha))^T Au_2(\cdot+\alpha) - (Av_2(\cdot+\alpha))^T Au_1(\cdot+\alpha)\Big)\mathrm{d}x \\ &= \int_{\mathbb{R}} \big(v_1^T A^T Au_2 - v_2^T A^T Au_1\big) = \int_{\mathbb{R}} \big(v_1^T u_2 - v_2^T u_1\big) = \omega(v,u) \end{aligned}$$

for all $v, u \in X$.

In order to verify Assumption 1.2.3, we have to specify the domain $\mathcal{D}_F$ of

$$F(v) = \begin{pmatrix} v_2 \\ v_{1,xx} - v_1 + |v_1|^2 v_1 \end{pmatrix}$$

and the common domain $\mathfrak{D}_a^1$ of

$$\mathrm{d}[a(\mathbb{1})v]\mu = Sv + cv_x, \quad \mu = (S, c) \in \mathfrak{so}(3) \times \mathbb{R}.$$

A suitable choice is $\mathcal{D}_F = \mathfrak{D}_a^1 = H^2(\mathbb{R}; \mathbb{R}^3) \times H^1(\mathbb{R}; \mathbb{R}^3)$, which is dense in X.

The composition of the symplectic form and the differential of the group action

$$\omega(\mathrm{d}[a(\mathbb{1})v]\mu, u) = \int_{\mathbb{R}} \big((Sv_1)^T u_2 + cv_{1,x}^T u_2 - (Sv_2)^T u_1 - cv_{2,x}^T u_1\big)\mathrm{d}x$$

extends to a bounded linear operator

$$B(\cdot)\mu \colon X \to X^\star, \quad v \mapsto B(v)\mu.$$

Indeed, for $v = (v_1, v_2) \in H^1(\mathbb{R}; \mathbb{R}^3) \times L^2(\mathbb{R}; \mathbb{R}^3)$ it holds $v_{1,x} \in L^2(\mathbb{R}; \mathbb{R}^3)$ and $v_{2,x} \in H^{-1}(\mathbb{R}; \mathbb{R}^3)$. Hence, we obtain

$$B(v)\mu \in H^{-1}(\mathbb{R}; \mathbb{R}^3) \times L^2(\mathbb{R}; \mathbb{R}^3).$$

Due to the linearity of the integral, we get a bounded linear operator, and Assumption 1.2.4 is fulfilled. Moreover, from the skew-symmetry of S and the differential operator $v \mapsto v_x$ it follows that the conserved quantities $Q : X \times \mathcal{A} \to \mathbb{R}$ in (1.2.7) take the form

$$Q(v)\mu = \frac{1}{2}\omega(\mathrm{d}[a(\mathbb{1})v]\mu, v) = \int_{\mathbb{R}} (Sv_1)^T v_2 \mathrm{d}x + c\int_{\mathbb{R}} v_{1,x}^T v_2 \mathrm{d}x.$$

According to Proposition 1.2.7 it holds

$$Q(a(e^\sigma)v)\mu = Q(v)\mu$$

for those $\sigma, \mu \in \mathcal{A}$ that commute, but not in general. Let us show that for this specific example the invariance with respect to the group action is indeed subject to some restriction. Direct computation with $\gamma = (A, c) \in \mathrm{SO}(3) \times \mathbb{R}$ and $\mu = (S, c) \in \mathfrak{so}(3) \times \mathbb{R}$ yields

$$\begin{aligned} Q(a(\gamma)v)\mu &= \int_{\mathbb{R}} \big(SAv_1(x + c)\big)^T Av_2(x + c)\mathrm{d}x \\ &\quad + c\int_{\mathbb{R}} \big(Av_{1,x}(x + c)\big)^T Av_2(x + c)\mathrm{d}x \\ &= \int_{\mathbb{R}} \big(SAv_1(x)\big)^T Av_2(x)\mathrm{d}x + c\int_{\mathbb{R}} \big(v_{1,x}(x)\big)^T v_2(x)\mathrm{d}x, \end{aligned}$$

i.e., we can only ensure the invariance if $SA = AS$, which is true for any $\gamma = (A, c) \in G(\mu)$, the Lie group generated by $C_{\mathcal{A}}(\mu)$.

Next, we consider Assumption 1.2.5, i.e., the smoothness and invariance of the Hamiltonian. The first derivative

$$\langle \mathrm{d}H(u), v\rangle = \int_{\mathbb{R}} \big(u_2^T v_2 + u_{1,x}^T v_{1,x} + u_1^T v_1 - |u_1|^2 u_1^T v_1\big)\mathrm{d}x$$

is locally bounded by

$$|\langle \mathrm{d}H(u), v\rangle| \leq C(\|u\| + \|u\|^3) \cdot \|v\|.$$

This is obtained by applying the Cauchy-Schwarz inequality and using fact that $H^1(\mathbb{R};\mathbb{R}^3)$ is a generalized Banach algebra. The second derivative takes the form

$$\langle \mathrm{d}^2 H(u)v, h\rangle = \int_{\mathbb{R}} \big(h_2^T v_2 + h_{1,x}^T v_{1,x} + h_1^T v_1 - \mathfrak{N}(u_1, v_1, h_1)\big)\mathrm{d}x,$$

where the nonlinear term is given by

$$\mathfrak{N}(u, v, h) = h^T u u^T v + u^T h u^T v + u^T u h^T v.$$

Consequently, a local estimate for the second derivative is given by

$$|\langle \mathrm{d}^2 H(u)v, h\rangle| \leq C(1 + \|u\|^2) \cdot \|v\| \cdot \|h\|.$$

The invariance of Hamiltonian under the group action, i.e., $H(a(\gamma)u) = H(u)$ for all $\gamma \in \mathrm{SO}(3) \times \mathbb{R}$, follows from the shift invariance of the L^2-norm and the property

$$|Sv|^2 = v^T S^T S v = |v|^2, \quad S \in \mathrm{SO}(3).$$

Moreover, we refer to [28] and [29] for the hypotheses on local existence, uniqueness, continuous dependence, and regularity in Assumption 1.2.14. Since a strong solution satisfies the NLKG in X_{-1}-sense for all $t \in \mathcal{I}$, we obtain $\|u_t\|_{-1}$ estimates in terms of $\|u\|$, and the same is true for continuous dependence. □

Next, we discuss the spectral hypotheses that are imposed on the linear operator

$$L_\star \colon X \to X^\star, \quad L_\star = \mathrm{d}^2 H(v_\star) - \mathrm{d}^2 Q(v_\star)\mu_\star.$$

Proposition 2.5.2. *The linerization of the NLKG at a relative equilibrium (1.3.17) satisfies the Assumptions 2.2.2, 2.2.3, and 2.2.7.*

Proof. Similar to the NLS, a Gelfand triple is given by

$$H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3) \hookrightarrow L^2(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3) \hookrightarrow H^{-1}(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3),$$

together with the embeddings

$$\begin{aligned} \iota &\colon H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3) \to L^2(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3), \quad v \mapsto v, \\ \iota^\star &\colon L^2(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3) \to H^{-1}(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3), \quad v \mapsto \big(v, \cdot\big)_0, \end{aligned}$$

where the inner product is given by

$$\big(v,y\big)_0 = \int_{\mathbb{R}} \big(v_1^T y_1 + v_2^T y_2\big)\mathrm{d}x.$$

The preimages of the composition

$$[\iota^\star\iota]^{-1}\mathrm{d}Q(v_\star)\sigma = \Big(\big[Sv_{\star,2}\big]^T + c\big[v_{\star,2}\big]_x^T, \big[Sv_{\star,1}\big]^T + c\big[v_{\star,1}\big]_x^T\Big), \quad \sigma \in \mathcal{A}_0$$

of the functionals

$$\langle \mathrm{d}Q(v_\star)\mu, y\rangle = \int_{\mathbb{R}} \Big(\big[Sv_{\star,1}\big]^T y_2 + c\big[v_{\star,1}\big]_x^T y_2 - \big[Sv_{\star,2}\big]^T y_1 - c\big[v_{\star,2}\big]_x^T y_1\Big)\mathrm{d}x$$

exist as functions in $H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3)$ due to the smoothness of $v_\star$. In the same way as for the NLS, we define $W = \big\{[\iota^\star\iota]^{-1}\mathrm{d}Q(v_\star)\sigma\colon \sigma \in \mathcal{A}_0\big\}$ and $Y = (W \oplus Z)^\perp$, where Z is the kernel of $L_\star$, to decompose $X = W \oplus Y \oplus Z$.

For the other parts of the Assumptions 2.2.2, 2.2.3, and 2.2.7, we refer to [33] since we do not want to repeat the Sturmian theory of oscillations. □

Let us discuss the fixed phase condition for the NLKG. By choosing $\sigma_1, \sigma_2 \in \mathbb{R}$ and by writing

$$\sigma = (\sigma_1 S_\star, \sigma_2),$$

we identify the Lie subalgebra $\mathcal{A}_0 = \{\sigma \in \mathcal{A}\colon [\sigma, \mu_\star] = 0\}$ with $\mathbb{R}^2$. Then

$$\psi\colon X \to \mathcal{A}_0^\star$$

is given by

$$\psi(v)\sigma = \big(\sigma_1 S_\star \hat{v}, v\big)_0 + \big(\sigma_2 \hat{v}_x, v\big)_0, \quad v \in X, \sigma \in \mathcal{A}_0.$$

We have to emphasize that this approach is only applicable if the Lie subalgebra $\mathcal{A}_0$ is explicitly known. That is why our numerical scheme deviates from this analytical approach. According to our experience, the freezing method is robust enough to handle commutator errors of small magnitude. Hence, in numerical computations, we let $\mu(t)$ be any element of the entire Lie algebra $\mathcal{A}$, rather than restricting it to $\mathcal{A}_0$.

Proposition 2.5.3. *The fixed phase condition satisfies the parts (b) and (c) of Assumption 2.2.11 for any template function $\hat{v} = (\hat{v}_1, 0)$, $\hat{v}_1 \in H^2(\mathbb{R};\mathbb{R}^3)$, provided that $\|\hat{v}_1 - v_{\star,1}\|_{H^1(\mathbb{R};\mathbb{R}^3)}$ is small enough.*

Proof. We have to prove the invertibility of

$$\Big[\big([\iota^\star\iota]^{-1}\mathrm{d}\psi(v_\star)e_i, \mathrm{d}[a(\mathbb{1})v_\star]e_j\big)_0\Big]_{i,j=1}^{d_\star},$$

where

$$[\iota^\star\iota]^{-1}\mathrm{d}\psi(v_\star)\sigma = \sigma_1 S_\star \hat{v} + \sigma_2 \hat{v}_x \in H^1(\mathbb{R};\mathbb{R}^3) \times L^2(\mathbb{R};\mathbb{R}^3).$$

Let us apply Banach's Lemma using the fact that $\|\hat{v}_1 - v_{\star,1}\|_{H^1(\mathbb{R};\mathbb{R}^3)}$ is small. Here, it suffices to show that $S_\star v_{\star,1}$ and $\left[v_{\star,1}\right]_x$ span a two-dimensional subspace of $H^1(\mathbb{R};\mathbb{R}^3)$. This can be verified by assuming the contrary. From

$$\mathfrak{v}_x = rS_\star\mathfrak{v}$$

for some $r \in \mathbb{R}$ and $\mathfrak{v} = v_{\star,1}$, it follows

$$|\mathfrak{v}(x)| = \left|e^{rS_\star x}\mathfrak{v}(0)\right| = |\mathfrak{v}(0)|$$

for all $x \in \mathbb{R}$, which implies $\mathfrak{v} = 0 \in H^1(\mathbb{R};\mathbb{R}^3)$. The rest of the proof is done in the same way as for the NLS.

□

Chapter 3

Preservation of Solitary Waves and Their Stability

In this chapter, we consider the spatial semi-discretization of the freezing system. Our primary goal is to impose reasonable assumptions that ensure the existence and stability of steady states $(v_\star^\Gamma, \mu_\star^\Gamma)$ for the discrete freezing system that are close to the steady states $(v_\star, \mu_\star)$ of the continuous problem.

3.1 Motivating Examples

Let us start with two numerical methods for the spatial semi-discretization of the freezing problem for the nonlinear Schrödinger equation

$$\begin{aligned} iv_t(t,x) &= -v_{xx}(t,x) - |v(t,x)|^2 v(t,x) - \mu(t)v(t,x), \\ 0 &= \psi(v(t,x)) \end{aligned} \tag{3.1.1}$$

set in the space of even functions

$$X = \{v \in H^1(\mathbb{R};\mathbb{C})\colon v(x) = v(-x)\}.$$

As in [3], the reason for choosing this space is the preservation of the symmetry relation under the flow of the nonlinear Schrödinger equation. Consequently, the translational equivariance is broken, which simplifies the stability analysis.

In terms of notation, we label the approximation parameters as $\Gamma = (\Delta x, K)$, where Δx is the stepsize of a symmetric and equidistant grid

$$\mathfrak{G}^\Gamma = \{x_j = j\Delta x\colon |j| \le K\}.$$

Moreover, we emphasize that c and C denote generic positive constants that do not depend on Γ.

3.1.1 Finite Difference Method

In a finite difference method for (3.1.1) the derivatives are approximated by difference quotients. In the simplest case, the spatial discretization of the second

derivative is the central difference quotient

$$(\partial^2 v^\Gamma)_j = \frac{v^\Gamma_{j+1} - 2v^\Gamma_j + v^\Gamma_{j-1}}{\Delta x^2}, \quad j \in \mathbb{Z}.$$

By adding Dirichlet boundary conditions $v^\Gamma_{-K} = 0 = v^\Gamma_K$, we obtain an ordinary differential-algebraic system of the form

$$\begin{aligned} i(v^\Gamma_t)_j &= -(\partial^2 v^\Gamma)_j - |v^\Gamma_j|^2 v^\Gamma_j - \mu^\Gamma v^\Gamma_j, \quad |j| < K, \\ 0 &= v^\Gamma_{-K} = v^\Gamma_K, \\ 0 &= \psi^\Gamma(v^\Gamma). \end{aligned} \tag{3.1.2}$$

The fixed phase condition with respect to some discrete template function $\hat{v}^\Gamma$ is given by

$$\psi^\Gamma(v^\Gamma) = \big(i\hat{v}^\Gamma, v^\Gamma\big)^\Gamma_0.$$

Here, the inner product $\big(\cdot,\cdot\big)^\Gamma_0$ is the discrete analog of the L^2-inner product, which takes the form

$$\big(v^\Gamma, y^\Gamma\big)^\Gamma_0 = \Delta x \sum_{|j|\le K} \mathrm{Re}(\bar{v}^\Gamma_j y^\Gamma_j).$$

Following [4], we set the problem in the space

$$X^\Gamma = \{v^\Gamma \in X^{\Delta x} \colon v^\Gamma(x) = 0 \text{ for } |x| \ge K\Delta x\}, \tag{3.1.3}$$

where

$$X^{\Delta x} = \{v^{\Delta x} \in X \colon v^{\Delta x}|_{(x_j, x_{j+1})} \text{ is an affine function for all } j \in \mathbb{Z}\} \tag{3.1.4}$$

is the finite element subspace of X that consists of piecewise linear functions. Here, the identification of a vector $\big(v^\Gamma_j\big)_{j\in\mathbb{Z}}$ and $v^\Gamma \in X^\Gamma$ is given by

$$v^\Gamma(x) = \sum_{|j|<K} \mathfrak{f}\Big(\frac{x}{\Delta x} - j\Big) v^\Gamma_j,$$

where the function $\mathfrak{f}\colon \mathbb{R} \to \mathbb{R}$ is defined as

$$\mathfrak{f}(x) = \begin{cases} 0, & |x| > 1, \\ 1 - x, & -1 \le x \le 0, \\ 1 + x, & 0 \le x \le 1. \end{cases}$$

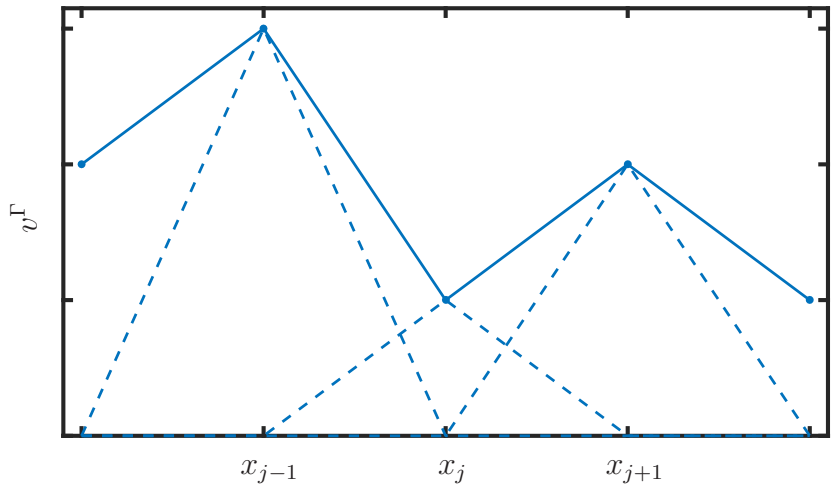


Figure 3.1.1: Piecewise linear function

By using the forward difference quotient

$$(\partial^+ v^\Gamma)_j = \frac{v^\Gamma_{j+1} - v^\Gamma_j}{\Delta x},$$

we equip the space X^Γ with a discretized version of the H^1 inner product, namely

$$\big(v^\Gamma, y^\Gamma\big)^\Gamma = \big((\partial^+ v)^\Gamma, (\partial^+ y)^\Gamma\big)^\Gamma_0 + \big(v^\Gamma, y^\Gamma\big)^\Gamma_0,$$

and its corresponding norm, which is denoted by $\|\cdot\|^\Gamma$. We further note that the backward difference quotient leads to exactly the same formulas.

3.1.2 Finite Element Method

The finite element method is based on the weak formulation of (3.1.1), i.e.,

$$\begin{aligned}\big(iv_t, y\big)_0 &= (-v_x, y_x)_0 + (-|v|^2 v - \mu v, y)_0,\\ 0 &= \big(i\hat{v}, v\big)_0,\end{aligned}$$

which is set in the Hilbert space

$$X = \{v \in H^1(\mathbb{R};\mathbb{C})\colon v(x) = v(-x) \text{ for all } x \in \mathbb{R}\}.$$

In order to discretize the second derivative, we introduce a linear mapping

$$A^\Gamma\colon X^\Gamma \to X^{\Gamma,\star},$$

which is implicitly defined by

$$\big\langle A^\Gamma v^\Gamma, y^\Gamma\big\rangle = \big(v^\Gamma_x, y^\Gamma_x\big)_0 \tag{3.1.5}$$

for $v^\Gamma, y^\Gamma \in X^\Gamma$. While the finite element space X^Γ is the same as for the finite difference method, the main difference of the Galerkin finite element approach

is the discretization of the nonlinear part. The standard idea is the orthogonal projection

$$P^\Gamma \colon X \to X^\Gamma$$

onto X^Γ. For any $v \in X$ the error $v - P^\Gamma v$ of the projection is orthogonal to the subspace X^Γ, which means

$$0 = \left(v - P^\Gamma v, y^\Gamma\right)_0 \tag{3.1.6}$$

for all $y^\Gamma \in X^\Gamma$. Then the corresponding ordinary differential-algebraic system takes the form

$$\begin{aligned} i v_t^\Gamma &= A^\Gamma v^\Gamma - P^\Gamma\left(|v^\Gamma|^2 v^\Gamma\right) - \mu^\Gamma v^\Gamma, \\ 0 &= \left(i\hat{v}^\Gamma, v^\Gamma\right)_0^\Gamma, \end{aligned} \tag{3.1.7}$$

where the inner product $\left(\cdot,\cdot\right)_0^\Gamma$ is the restriction of the L^2-inner product to the subspace X^Γ. Moreover, for the stability analysis, we equip the space X^Γ with the restriction of the H^1-inner product and the corresponding norm $\|\cdot\|^\Gamma$.

3.2 Abstract Setting

In order to embed the above examples into an abstract setting, we loosely follow the approach presented in [3]. That is, the discrete problem is considered to be a small perturbation of the continuous problem. Throughout the entire Chapter 3, we take the Assumptions 1.2.2-1.2.5, 1.2.14, 2.2.2, 2.2.3, 2.2.7, and 2.2.11 from the previous chapters as given, without further reference.

Let $\mathfrak{P}$ be a set of approximation parameters. For any $\Gamma \in \mathfrak{P}$ we denote by X^Γ a finite-dimensional subspace of X, which we equip with a norm $\left\|\cdot\right\|_\Gamma$ and a symplectic form

$$\omega^\Gamma \colon X^\Gamma \times X^\Gamma \to \mathbb{R}.$$

In analogy to the continuous case, the discrete problem is written as

$$\omega^\Gamma(u_t^\Gamma, \cdot) = \mathrm{d}H^\Gamma(u^\Gamma), \tag{3.2.1}$$

where

$$H^\Gamma \colon X^\Gamma \to \mathbb{R} \tag{3.2.2}$$

is called the discrete Hamiltonian. In order to get additional conserved quantities

$$Q^\Gamma \colon X^\Gamma \to \mathcal{A}^\star, \tag{3.2.3}$$

the finite-dimensional Lie group G is assumed to act on the subspaces X^Γ via symplectomorphisms.

Assumption 3.2.1. For any $\Gamma \in \mathfrak{P}$ the Lie Group G acts on X^Γ via a homomorphism

$$a^\Gamma \colon G \to \mathrm{GL}(X^\Gamma), \quad \gamma \mapsto a(\gamma)\big|_{X^\Gamma},$$

whose images are symplectic with respect to ω^Γ. In particular $a(\gamma)v^\Gamma \in X^\Gamma$ holds for all $\gamma \in G$ and $v^\Gamma \in X^\Gamma$. Moreover, we have $\mathrm{d}[a(\mathbb{1})v^\Gamma]\sigma \in X^\Gamma$ for all $v^\Gamma \in X^\Gamma$ and $\sigma \in \mathcal{A}$.

The mapping (3.2.3) is the discrete analog of (1.2.7), i.e., we may also write $Q^\Gamma(\cdot)\sigma$ for $\sigma \in \mathcal{A}$. Furthermore, the discrete freezing system takes the form

$$\begin{aligned} \omega^\Gamma(v_t^\Gamma, \cdot) &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma, \\ 0 &= \psi^\Gamma(v^\Gamma). \end{aligned} \tag{3.2.4}$$

Further key aspects of the setting are the approximation estimates that we collect in the following. Given $k \geq 0$, a smooth functional $E \colon X^\Gamma \to \mathbb{R}$, and an open subset $V^\Gamma \subseteq X^\Gamma$, we define its $\|\cdot\|_{C^k(V^\Gamma)}$-norm to be

$$\|E\|_{C^k(V^\Gamma)} = \sup_{j\in\{0,\dots,k\}} \sup_{v^\Gamma \in V^\Gamma} \sup_{y_0^\Gamma,\dots,y_j^\Gamma \in X^\Gamma\setminus\{0\}} \frac{\left|\mathrm{d}^j E(v^\Gamma)[y_1^\Gamma,\dots,y_j^\Gamma]\right|}{\prod_{\nu=1}^j \|y_\nu^\Gamma\|_\Gamma}.$$

As in Chapter 2, we fix a steady state $(v_\star, \mu_\star) \in X \times \mathcal{A}$, which is stable by Theorem 2.3.7. We denote by $\mathcal{A}_0$ the centralizer of $\mu_\star \in \mathcal{A}$ and by $\{e_1, \dots, e_{d_\star}\}$ a basis of $\mathcal{A}_0$.

Moreover, we introduce an error function $\varepsilon \colon \mathfrak{P} \to \mathbb{R}_{>0}$. If there exists $\varepsilon_{\max} > 0$ such that an estimate holds uniformly for all $\Gamma \in \mathfrak{P}$ with $\varepsilon(\Gamma) \leq \varepsilon_{\max}$, then we say that it holds for $\varepsilon(\Gamma)$ small enough.

Assumption 3.2.2. For any $\varepsilon_0 > 0$ there exists $\Gamma_0 \in \mathfrak{P}$ such that we have $\varepsilon(\Gamma_0) \leq \varepsilon_0$. In addition to that, the following properties hold for $\varepsilon \colon \mathfrak{P} \to \mathbb{R}_{>0}$ and all $\Gamma \in \mathfrak{P}$ with $\varepsilon(\Gamma)$ small enough.

(a) The discrete Hamiltonian (3.2.2) and the discrete quantities $Q^\Gamma(\cdot)e_j$ for $j = 1, \dots, d_\star$, which are determined by (3.2.3), are invariant under the group action.

(b) There exists $\vartheta^\Gamma \in X^\Gamma$ that satisfies

$$\|\vartheta^\Gamma - v_\star\| \leq C\varepsilon(\Gamma),$$

where $(v_\star, \mu_\star) \in X \times \mathcal{A}_0$ is the steady state of the continuous problem.

(c) There exists a constant $R > 0$ such that the discrete Hamiltonian (3.2.2) and the discrete quantities $Q^\Gamma(\cdot)e_j$, $j = 1, \dots, d_\star$, which are determined by (3.2.3), satisfy

$$\begin{aligned} \|H - H^\Gamma\|_{C^2(\mathcal{B}_R^\Gamma(\vartheta^\Gamma))} &\leq C\varepsilon(\Gamma), \\ \|Q(\cdot)e_j - Q^\Gamma(\cdot)e_j\|_{C^2(\mathcal{B}_R^\Gamma(\vartheta^\Gamma))} &\leq C\varepsilon(\Gamma) \end{aligned}$$

on $\mathcal{B}_R^\Gamma(\vartheta^\Gamma)$, where C depends only on R.

(d) The discrete and the continuous norm are equivalent in the sense that

$$c\|v^\Gamma\| \leq \|v^\Gamma\|_\Gamma \leq C\|v^\Gamma\|$$

holds uniformly for $v^\Gamma \in X^\Gamma$.

Without loss of generality, we may assume that $\varepsilon(\Gamma)$ is small compared to R. Next, we impose a similar condition as in Assumption 3.2.2(c) on the discrete version of our phase condition.

Assumption 3.2.3. For any $\Gamma \in \mathfrak{P}$ the mapping

$$\psi^\Gamma \colon X^\Gamma \to \mathcal{A}_0^\star$$

is twice continuously differentiable and satisfies

$$\|\psi(\cdot)e_j - \psi^\Gamma(\cdot)e_j\|_{\mathcal{C}^2(\mathcal{B}_R^\Gamma(\vartheta^\Gamma))} \leq C\varepsilon(\Gamma)$$

for $j = 1, ..., d_\star$.

The local well-posedness of an ordinary differential equation with smooth right hand side follows from the Picard-Lindelöf theorem. However, in general, estimates depend on the discretization parameters Γ. That is why we introduce an additional space X_{-1}^Γ.

Assumption 3.2.4. For any $\Gamma \in \mathfrak{P}$ with $\varepsilon(\Gamma)$ small enough there exists a space $\left(X_{-1}^\Gamma, \|\cdot\|_{X_{-1}^\Gamma}\right)$ such that Assumption 1.2.14 holds for the discretized version of the original problem (3.2.1), where the constants for embedding and continuous dependence are independent of Γ. Moreover, the mapping

$$\mathfrak{F}^\Gamma \colon G_0 \times X_{-1}^\Gamma \to \mathcal{A}_0^\star$$

that extends $(g, v^\Gamma) \mapsto \psi^\Gamma(a(g)v^\Gamma)$ is continuously differentiable.

An additional approximation property is needed for our proof of existence of the discrete steady states. It can be considered as a weaker version of Assumption 3.2.2(b) in such a way that it covers all $v \in X$. The stronger version for $v_\star \in X$ remains unaffected by this.

Assumption 3.2.5. For any $v \in X$ and any sequence Γ_n in $\mathfrak{P}$ that satisfies $\varepsilon(\Gamma_n) \to 0$ there exists a sequence $v^{\Gamma_n} \in X^{\Gamma_n}$ such that $\|v^{\Gamma_n} - v\| \to 0$ as $n \to \infty$.

3.3 Positivity Estimates

We recall that by Lemma 2.2.9, the linearization around the relative equilibrium of the continuous problem

$$L_\star = \mathrm{d}^2 H(v_\star) - \mathrm{d}^2 Q(v_\star)\mu_\star$$

is positive on a subspace $Y \subseteq X$, which is of codimension $d_\star + d_\star$. To be more precise, by Assumption 2.2.3 the Banach space X is decomposed into the direct sum $X = W \oplus Y \oplus Z$, where W is given by Lemma 2.2.4 and where, due to (2.2.9), the kernel of $L_\star$ is given by

$$Z = \{\mathrm{d}[a(\mathbb{1})v_\star]\sigma \colon \sigma \in \mathcal{A}_0\}.$$

Now, we consider a discrete approximation $Y^\Gamma \subseteq X^\Gamma$ of this positive subspace.

Lemma 3.3.1. *Let $W^{\Gamma,\star} = \operatorname{span}\left(w_1^{\Gamma,\star}, ..., w_{d_\star}^{\Gamma,\star}\right)$ and $Z^{\Gamma,\star} = \operatorname{span}(z_1^{\Gamma,\star}, ..., z_{d_\star}^{\Gamma,\star})$ be subspaces of $X^{\Gamma,\star}$, the dual space of X^Γ, such that the estimates*

$$\left\|\mathrm{d}Q(v_\star)e_j - w_j^{\Gamma,\star}\right\|_{X^{\Gamma,\star}} \leq C\varepsilon(\Gamma) \tag{3.3.1}$$

and

$$\left\|\mathrm{d}\psi(v_\star)e_j - z_j^{\Gamma,\star}\right\|_{X^{\Gamma,\star}} \leq C\varepsilon(\Gamma) \tag{3.3.2}$$

are satisfied. Provided the Assumptions 3.2.1 and 3.2.2 hold and $\varepsilon(\Gamma)$ is small enough, we obtain $c > 0$ independent of Γ such that

$$\langle L_\star y^\Gamma, y^\Gamma\rangle \geq c\|y^\Gamma\|^2$$

holds for all

$$y^\Gamma \in Y^\Gamma = \left\{y^\Gamma \in X^\Gamma \colon \left\langle w_j^{\Gamma,\star}, y^\Gamma\right\rangle = \left\langle z_j^{\Gamma,\star}, y^\Gamma\right\rangle = 0 \text{ for } j = 1, ..., d_\star\right\}.$$

Proof. Let us write $y^\Gamma \in Y^\Gamma$ as $y^\Gamma = w + y + z$ with $w \in W$, $y \in Y$, and $z \in Z$. From Lemma 2.2.4 we obtain $\lambda \in \mathcal{A}_0$ with $\|\mathrm{d}Q(v_\star)\lambda\|_{X^\star} = 1$ such that

$$\begin{aligned}\|w\| &= \langle \mathrm{d}Q(v_\star)\lambda, w\rangle = \langle \mathrm{d}Q(v_\star)\lambda, y + z + w\rangle = \langle \mathrm{d}Q(v_\star)\lambda, y^\Gamma\rangle \\ &= \left\langle w^{\Gamma,\star}, y^\Gamma\right\rangle + \left\langle \mathrm{d}Q(v_\star)\lambda - w^{\Gamma,\star}, y^\Gamma\right\rangle\end{aligned} \tag{3.3.3}$$

for any $w^{\Gamma,\star} \in W^{\Gamma,\star}$, where $\langle \mathrm{d}Q(v_\star)\lambda, y + z\rangle = 0$ is due to (1.2.10) and (2.2.8). But, by definition of Y^Γ it holds

$$\left\langle w^{\Gamma,\star}, y^\Gamma\right\rangle = 0. \tag{3.3.4}$$

By combining (3.3.1), (3.3.3), (3.3.4), and $w^{\Gamma,\star} = \sum_{j=1}^{d_\star} \lambda_j w_j^{\Gamma,\star}$ it follows

$$\|w\| \leq C\sum_{j=1}^{d_\star} |\lambda_j| \left|\left\langle \mathrm{d}Q(v_\star)e_j - w_j^{\Gamma,\star}, y^\Gamma\right\rangle\right| \leq C\varepsilon(\Gamma)\sum_{j=1}^{d_\star} |\lambda_j|\, \|y^\Gamma\|.$$

Due to $\|\mathrm{d}Q(v_\star)\lambda\|_{X^\star} = 1$, we conlcude

$$\|w\| \leq C\varepsilon(\Gamma)\|y^\Gamma\|. \tag{3.3.5}$$

In addition to that, there exists $\sigma \in \mathcal{A}_0$ with $\|\mathrm{d}\psi(v_\star)\sigma\|_{X^\star} = 1$ such that we have

$$\begin{aligned} \eta\|z\| &\leq \big|\langle \mathrm{d}\psi(v_\star)\sigma, z\rangle\big| = \big|\langle \mathrm{d}\psi(v_\star)\sigma, y^\Gamma - w - y\rangle\big| \\ &\leq \big|\langle \mathrm{d}\psi(v_\star)\sigma - z^{\Gamma,\star}, y^\Gamma\rangle\big| + \big|\langle z^{\Gamma,\star}, y^\Gamma\rangle\big| + \|y + w\| \end{aligned} \tag{3.3.6}$$

for any $z^{\Gamma,\star} \in Z^{\Gamma,\star}$, where $\eta > 0$ is obtained in the same way as in the proof of Theorem 2.2.10. However, by definition of Y^Γ it holds

$$\langle z^{\Gamma,\star}, y^\Gamma\rangle = 0. \tag{3.3.7}$$

In the same way as above, the combination of (3.3.2), (3.3.6), and (3.3.7) yields

$$\|z\| \leq C\big(\|y\| + \varepsilon(\Gamma)\|y^\Gamma\|\big).$$

Due to the triangle inequality, the estimates for $\|w\|$ and $\|z\|$ imply

$$\|y^\Gamma\| = \|w + y + z\| \leq \|w\| + \|y\| + \|z\| \leq C\|y\| + C\varepsilon(\Gamma)\|y^\Gamma\|,$$

which leads to

$$\|y\|^2 \geq c\|y^\Gamma\|^2 - C\varepsilon(\Gamma)\|y^\Gamma\|^2$$

by Lemma A.4.1. Hence, we obtain, again by Lemma A.4.1 and the positivity of $L_\star$ on Y (see Lemma 2.2.9), the estimate

$$\begin{aligned} \big\langle L_\star y^\Gamma, y^\Gamma\big\rangle = \big\langle L_\star(w+y), w+y\big\rangle &\geq c\|y\|^2 - C_{L_\star}\big(2\|y\|\|w\| + \|w\|^2\big) \\ &\geq c\|y^\Gamma\|^2 - C\varepsilon(\Gamma)\|y^\Gamma\|^2, \end{aligned}$$

where the last inequality is due to (3.3.5), and where the uniform bound by $C_{L_\star} > 0$ is obtained from Assumption 3.2.2(c). □

When we handle pertubations of $L_\star$, the extended notation

$$L(v,\mu) = \mathrm{d}^2 H(v) - \mathrm{d}^2 Q(v)\mu$$

is more suitable, where the relation to the short notation is given by the identity $L_\star = L(v_\star, \mu_\star)$. Now, we linearize the right hand side of the discrete problem (3.2.4) and obtain

$$L^\Gamma(v^\Gamma, \mu^\Gamma) = \mathrm{d}^2 H^\Gamma(v^\Gamma) - \mathrm{d}^2 Q^\Gamma(v^\Gamma)\mu^\Gamma$$

for $v^\Gamma \in X^\Gamma$ and $\mu^\Gamma \in \mathcal{A}_0$.

Theorem 3.3.2. *Under the assumptions of Lemma 3.3.1 there exists $r_{\max} > 0$ such that we have*

$$\big\langle L^\Gamma(v^\Gamma, \mu^\Gamma)y^\Gamma, y^\Gamma\big\rangle \geq c\big\|y^\Gamma\big\|_\Gamma^2$$

for all $y^\Gamma \in Y^\Gamma$ and $\varepsilon(\Gamma)$ small enough. The constant c does not depend on Γ and holds uniformly for $v^\Gamma \in X^\Gamma$, $\mu^\Gamma \in \mathcal{A}_0$ satisfying $|\mu^\Gamma - \mu_\star| + \big\|v^\Gamma - \vartheta^\Gamma\big\|_\Gamma \leq r_{\max}$.

Proof. From Assumption 3.2.2(c) we get

$$\left|\left\langle L(v^\Gamma,\mu^\Gamma)y^\Gamma,y^\Gamma\right\rangle-\left\langle L^\Gamma(v^\Gamma,\mu^\Gamma)y^\Gamma,y^\Gamma\right\rangle\right|\leq C\varepsilon(\Gamma)\left\|y^\Gamma\right\|_\Gamma^2 \tag{3.3.8}$$

for any $v^\Gamma, y^\Gamma \in X^\Gamma$ and $\mu \in \mathcal{A}_0$ such that $|\mu^\Gamma-\mu_\star|+\left\|v^\Gamma-\vartheta^\Gamma\right\|_\Gamma \leq r_{\max}$. Since both the Hamiltonian H and the additional conserved quantities $Q(\cdot)\mu$ of the continuous problem are smooth in a neighborhood of $v_\star$ with bounded derivatives, we further have

$$\left|\left\langle L(v^\Gamma,\mu^\Gamma)y^\Gamma,y^\Gamma\right\rangle-\left\langle L_\star y^\Gamma,y^\Gamma\right\rangle\right|\leq C(\varepsilon(\Gamma)+r_{\max})\left\|y^\Gamma\right\|_\Gamma^2, \tag{3.3.9}$$

provided that $|\mu^\Gamma-\mu_\star|+\|v^\Gamma-\vartheta^\Gamma\|^\Gamma\leq r_{\max}$ holds. Then, the estimate

$$\left\langle L_\star y^\Gamma,y^\Gamma\right\rangle\geq c\left\|y^\Gamma\right\|_\Gamma^2$$

for $y^\Gamma \in Y^\Gamma$, which follows from Assumption 3.2.2(d) and Lemma 3.3.1, implies

$$\left\langle L^\Gamma(v^\Gamma,\mu^\Gamma)y^\Gamma,y^\Gamma\right\rangle\geq\big(c-C(\varepsilon(\Gamma)+r_{\max})\big)\left\|y^\Gamma\right\|_\Gamma^2.$$

Consequently, for $r_{\max}\geq 0$ small enough, the positivity remains true with a different constant. □

Let us apply Lemma 3.3.1 and Theorem 3.3.2 to

$$\begin{aligned} w_j^{\Gamma,\star}&=\mathrm{d}Q^\Gamma(\vartheta^\Gamma)e_j,\\ z_j^{\Gamma,\star}&=\mathrm{d}\psi^\Gamma(\vartheta^\Gamma)e_j \end{aligned}$$

and conclude that $L^\Gamma(\vartheta^\Gamma,\mu_\star)$ is positive on a subspace of codimension $d_\star+d_\star$ in X^Γ, which takes the form

$$Y^\Gamma=\big\{y^\Gamma\in X^\Gamma\colon\left\langle w_j^{\Gamma,\star},y^\Gamma\right\rangle=\left\langle z_j^{\Gamma,\star},y^\Gamma\right\rangle=0\text{ for }i=1,\dots,d_\star\big\}. \tag{3.3.10}$$

Indeed, the Assumptions 3.2.2(b)-(d) give us

$$\left\|\mathrm{d}Q(v_\star)e_j-\mathrm{d}Q^\Gamma(\vartheta^\Gamma)e_j\right\|_{X^{\Gamma,\star}}\leq C\varepsilon(\Gamma) \tag{3.3.11}$$

for $j=1,\dots,d_\star$, and we make use of the Assumptions 3.2.2(b), 3.2.2(d), and 3.2.3 to obtain

$$\left\|\mathrm{d}\psi(v_\star)e_j-\mathrm{d}\psi^\Gamma(\vartheta^\Gamma)e_j\right\|_{X^{\Gamma,\star}}\leq C\varepsilon(\Gamma). \tag{3.3.12}$$

3.4 Existence of Discrete Steady States

As we have discussed in Section 2.2, the modified stationary problem (2.2.17) possesses a locally unique solution $\big(v_\star,\mu_\star,0\big)$, where $\big(v_\star,\mu_\star\big)$ is a steady state of the freezing system.

In this section, we are primarily interested in finding a solution to the discretized version of the modified stationary problem, which takes the form

$$\begin{aligned} 0 &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma - \mathrm{d}\psi(v^\Gamma)\lambda^\Gamma, \\ 0 &= Q^\Gamma(v^\Gamma) - Q(v_\star), \\ 0 &= \psi^\Gamma(v^\Gamma). \end{aligned}$$

This problem is set in the space $\mathfrak{X}^\Gamma = X^\Gamma \times \mathcal{A}_0 \times \mathcal{A}_0$ with its norm denoted by

$$\left\|(v^\Gamma, \mu^\Gamma, \lambda^\Gamma)\right\|_{\mathfrak{X}^\Gamma} = \left\|v^\Gamma\right\|_{X^\Gamma} + \left|\mu^\Gamma\right|_{\mathcal{A}_0} + \left|\lambda^\Gamma\right|_{\mathcal{A}_0}.$$

In the same way as for the continuous case, it can be written as

$$\mathfrak{S}^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma) = 0, \tag{3.4.1}$$

where the function $\mathfrak{S}^\Gamma \colon \mathfrak{X}^\Gamma \to \mathfrak{X}^{\Gamma,\star}$ takes the form

$$\mathfrak{S}^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma) = \Big(\mathfrak{S}_1^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma), \mathfrak{S}_2^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma), \mathfrak{S}_3^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma)\Big)$$

with

$$\begin{aligned} \mathfrak{S}_1^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma) &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma - \mathrm{d}\psi^\Gamma(v^\Gamma)\lambda^\Gamma, \\ \mathfrak{S}_2^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma) &= Q^\Gamma(v^\Gamma) - Q(v_\star), \\ \mathfrak{S}_3^\Gamma(v^\Gamma, \mu^\Gamma, \lambda^\Gamma) &= \psi^\Gamma(v^\Gamma). \end{aligned}$$

The linerization of (3.4.1) at $(\vartheta^\Gamma, \mu_\star, 0) \in X^\Gamma \times \mathcal{A}_0 \times \mathcal{A}_0$ is denoted by

$$\mathfrak{L}^\Gamma = \mathrm{d}\mathfrak{S}^\Gamma(\vartheta^\Gamma, \mu_\star, 0) \colon \mathfrak{X}^\Gamma \to \mathfrak{X}^{\Gamma,\star} \tag{3.4.2}$$

and can be written as a bordered operator

$$\mathfrak{L}^\Gamma = \begin{pmatrix} L^\Gamma(\vartheta^\Gamma, \mu_\star) & \mathfrak{L}_{1,2}^\Gamma & \mathfrak{L}_{1,3}^\Gamma \\ \mathfrak{L}_{2,1}^\Gamma & 0 & 0 \\ \mathfrak{L}_{3,1}^\Gamma & 0 & 0 \end{pmatrix}$$

with

$$\left\langle \mathfrak{L}_{1,2}^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle = \left\langle \mathfrak{L}_{2,1}^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle = \left\langle \mathrm{d}Q^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle$$

and

$$\left\langle \mathfrak{L}_{1,3}^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle = \left\langle \mathfrak{L}_{3,1}^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle = \left\langle \mathrm{d}\psi^\Gamma(\vartheta^\Gamma)\sigma, y^\Gamma \right\rangle$$

for all $\sigma \in \mathcal{A}_0$ and $y^\Gamma \in X^\Gamma$. For $\varepsilon(\Gamma)$ small enough, the positivity of L^Γ on the $2d_\star$-codimensional subspace (3.3.10) is uniform. In addition to that, we obtain uniform bounds for $\|\mathfrak{L}^\Gamma\|_{\mathfrak{X}^{\Gamma,\star} \leftarrow \mathfrak{X}^\Gamma}$ from Assumption 3.2.2 and Assumption 3.2.3. Hence, Lemma A.5.1 grants us a decomposition $\mathfrak{L}^\Gamma = \mathfrak{A}^\Gamma + \mathfrak{B}^\Gamma$ into a positive operator $\mathfrak{A}^\Gamma$ and a rank-$4d_\star$-operator $\mathfrak{B}^\Gamma$, which are uniformly bounded for $\varepsilon(\Gamma)$ small enough. In the same way, we apply Lemma A.5.1 to decompose

$$\mathfrak{L} = \mathrm{d}\mathfrak{S}(v_\star, \mu_\star, 0) \colon \mathfrak{X} \to \mathfrak{X}^\star,$$

which is obtained via linearization of the continuous problem, into the sum of a positive operator $\mathfrak{A}$ and a rank-$4d_\star$-operator $\mathfrak{B}$, i.e., $\mathfrak{L} = \mathfrak{A} + \mathfrak{B}$.

Lemma 3.4.1. *Provided the Assumptions 3.2.1-3.2.3 hold and $\varepsilon(\Gamma)$ is small enough, the inequality*

$$\left\|\mathfrak{A}^{\Gamma}\chi^{\Gamma}-\mathfrak{A}\chi^{\Gamma}\right\|_{\mathfrak{X}^{\Gamma,\star}}+\left\|\mathfrak{B}^{\Gamma}\chi^{\Gamma}-\mathfrak{B}\chi^{\Gamma}\right\|_{\mathfrak{X}^{\Gamma,\star}}\leq C\varepsilon(\Gamma)\left\|\chi^{\Gamma}\right\|_{\mathfrak{X}^{\Gamma}}$$

is satisfied for all $\chi^{\Gamma}\in\mathfrak{X}^{\Gamma}$.

Proof. From (3.3.9), (3.3.11), (3.3.12), and Assumption 3.2.2 we get

$$\left\|\mathfrak{L}^{\Gamma}\chi^{\Gamma}-\mathfrak{L}\chi^{\Gamma}\right\|_{\mathfrak{X}^{\Gamma,\star}}\leq C\varepsilon(\Gamma)\left\|\chi^{\Gamma}\right\|_{\mathfrak{X}^{\Gamma}}.$$

The same inequality for $\mathfrak{B}^{\Gamma}-\mathfrak{B}$ follows due to (A.5.1), and the estimate for $\mathfrak{A}^{\Gamma}-\mathfrak{A}$ is a consequence of the triangle inequality. □

This estimate is a key step in showing that the linear operator in (3.4.2) has a uniformly bounded inverse with respect to Γ.

Lemma 3.4.2. *Provided the Assumptions 3.2.1-3.2.3 hold and $\varepsilon(\Gamma)$ is small enough, for the inverse of $\mathfrak{L}^{\Gamma}$ we have the estimate*

$$\left\|\left(\mathfrak{L}^{\Gamma}\right)^{-1}\right\|_{\mathfrak{X}^{\Gamma}\leftarrow\mathfrak{X}^{\Gamma,\star}}\leq C.$$

Proof. Assume on the contrary that $\Gamma_m\in\mathfrak{P}$ and $\chi^{\Gamma_m}\in X^{\Gamma_m}$, $m\in\mathbb{N}$, form sequences such that $\varepsilon(\Gamma_m)\to 0$ and $\left\|\chi^{\Gamma_m}\right\|_{\mathfrak{X}^{\Gamma_m}}=\rho>0$, but

$$\left\|\mathfrak{L}^{\Gamma_m}\chi^{\Gamma_m}\right\|_{\mathfrak{X}^{\Gamma_m,\star}}=\left\|(\mathfrak{A}^{\Gamma_m}+\mathfrak{B}^{\Gamma_m})\chi^{\Gamma_m}\right\|_{\mathfrak{X}^{\Gamma_m,\star}}\to 0. \tag{3.4.3}$$

Since $\mathfrak{B}$ is a compact operator, there exists a converging subsequence $\mathfrak{B}\chi^{\Gamma_n}\to\zeta^{\star}$, $n\in\mathcal{N}\subseteq\mathbb{N}$. Moreover, from Lemma 3.4.1 we get

$$\left\|\mathfrak{B}^{\Gamma_n}\chi^{\Gamma_n}-\mathfrak{B}\chi^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\leq C\varepsilon(\Gamma_n)\to 0,$$

which implies

$$\left\|\mathfrak{B}^{\Gamma_n}\chi^{\Gamma_n}-\zeta^{\star}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0$$

and, as a consequence of (3.4.3),

$$\left\|\mathfrak{A}^{\Gamma_n}\chi^{\Gamma_n}+\zeta^{\star}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0. \tag{3.4.4}$$

In order to get the limit of χ^{Γ_n}, let us show that

$$\mathfrak{A}\chi=-\zeta^{\star}$$

has a unique solution in $\mathfrak{X}$. Indeed, the bilinear form

$$\mathfrak{a}\colon\mathfrak{X}\times\mathfrak{X}\to\mathbb{R},\quad(\chi_1,\chi_2)\mapsto\langle\mathfrak{A}\chi_1,\chi_2\rangle$$

is bounded and coercive. Hence, the statement follows from the Lax-Milgram theorem (see [48]). The solution can be written as $\chi=(v,\mu,\lambda)\in X\times\mathcal{A}_0\times\mathcal{A}_0$. By Assumption 3.2.5, there exists a sequence $\widetilde{\chi}^{\Gamma_n}=(v_n^{\Gamma},\mu,\lambda)$ such that

$$\left\|\widetilde{\chi}^{\Gamma_n}-\chi\right\|_{\mathfrak{X}}\to 0, \tag{3.4.5}$$

which implies

$$\left\|\mathfrak{A}\widetilde{\chi}^{\Gamma_n}+\zeta^\star\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0. \tag{3.4.6}$$

Furthermore, the triangle inequality, Lemma 3.4.1, and (3.4.4) yield

$$\left\|\mathfrak{A}\chi^{\Gamma_n}+\zeta^\star\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\leq\left\|\mathfrak{A}\chi^{\Gamma_n}-\mathfrak{A}^{\Gamma_n}\chi^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}+\left\|\mathfrak{A}^{\Gamma_n}\chi^{\Gamma_n}+\zeta^\star\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0,$$

which, due to (3.4.6), gives us

$$\left\|\mathfrak{A}\widetilde{\chi}^{\Gamma_n}-\mathfrak{A}\chi^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0.$$

Consequently, we get

$$\left\|\chi^{\Gamma_n}-\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n}}\leq C\left\|\mathfrak{A}\chi^{\Gamma_n}-\mathfrak{A}\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n,\star}}\to 0$$

from

$$\left\langle\mathfrak{A}(\chi^{\Gamma_n}-\widetilde{\chi}^{\Gamma_n}),\chi^{\Gamma_n}-\widetilde{\chi}^{\Gamma_n}\right\rangle\geq c\left\|\chi^{\Gamma_n}-\widetilde{\chi}^{\Gamma_n}\right\|^2_{\mathfrak{X}^{\Gamma_n}}.$$

Hence, combining Lemma 3.4.1 with the inequality

$$\left\|(\mathfrak{A}+\mathfrak{B})\chi^{\Gamma_n}-(\mathfrak{A}+\mathfrak{B})\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma,\star}}\leq C\left\|\chi^{\Gamma_n}-\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n}}$$

yields

$$\left\|(\mathfrak{A}^{\Gamma_n}+\mathfrak{B}^{\Gamma_n})\chi^{\Gamma_n}-(\mathfrak{A}+\mathfrak{B})\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma,\star}}\to 0.$$

This implies

$$\left\|(\mathfrak{A}+\mathfrak{B})\widetilde{\chi}^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma,\star}}\to 0$$

due to (3.4.3), and we obtain $(\mathfrak{A}+\mathfrak{B})\chi=0$ from (3.4.5). Since $\chi=0$ follows from Proposition 2.2.13, we conclude

$$\left\|\chi^{\Gamma_n}\right\|_{\mathfrak{X}^{\Gamma_n}}\to 0,$$

which contradicts the assumption. □

Next, we show that (3.4.1) has a locally unique solution $\left(v^\Gamma_\star,\mu^\Gamma_\star,\lambda^\Gamma_\star\right)$ and, after that, deduce $\lambda^\Gamma_\star=0$.

Lemma 3.4.3. *Provided the Assumptions 3.2.1-3.2.3 hold and $\varepsilon(\Gamma)$ is small enough, the modified stationary problem*

$$\begin{aligned}0&=\mathrm{d}H^\Gamma(v^\Gamma)-\mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma-\mathrm{d}\psi^\Gamma(v^\Gamma)\lambda^\Gamma,\\0&=Q^\Gamma(v^\Gamma)-Q(v_\star),\\0&=\psi^\Gamma(v^\Gamma)\end{aligned}$$

possesses a locally unique solution $(v^\Gamma_\star,\mu^\Gamma_\star,\lambda^\Gamma_\star)$ that satisfies

$$\|v^\Gamma_\star-v_\star\|+|\mu^\Gamma_\star-\mu_\star|+|\lambda^\Gamma_\star-\lambda_\star|\leq C\varepsilon(\Gamma).$$

Proof. The main idea is to apply Lemma A.6.1 with the operators

$$L = \mathfrak{L}^\Gamma \colon \mathfrak{X}^\Gamma \to \mathfrak{X}^{\Gamma,\star}$$

and

$$L + F = \mathfrak{S}^\Gamma \colon \mathfrak{X}^\Gamma \to \mathfrak{X}^{\Gamma,\star}.$$

We are left to verify the requirements. First of all, from Lemma 3.4.2 we get

$$\frac{1}{\big\|(\mathfrak{L}^\Gamma)^{-1}\big\|_{\mathfrak{X}^\Gamma \leftarrow \mathfrak{X}^{\Gamma,\star}}} \geq c_1.$$

Second, provided that $\delta > 0$ is small enough, the mean value theorem implies

$$\begin{aligned}\big\|F(\chi_1^\Gamma) - F(\chi_2^\Gamma)\big\|_{\mathfrak{X}^{\Gamma,\star}} &= \big\|\mathfrak{S}^\Gamma(\chi_1^\Gamma) - \mathfrak{L}^\Gamma\chi_1^\Gamma - \mathfrak{S}^\Gamma(\chi_2^\Gamma) - \mathfrak{L}^\Gamma\chi_2^\Gamma\big\|_{\mathfrak{X}^{\Gamma,\star}} \\ &\leq \sup_{\zeta^\Gamma \in \mathfrak{B}_\delta^\Gamma} \big\|\mathrm{d}\mathfrak{S}^\Gamma(\zeta^\Gamma) - \mathfrak{L}^\Gamma\big\|_{\mathfrak{X}^{\Gamma,\star} \leftarrow \mathfrak{X}^\Gamma} \big\|\chi_1^\Gamma - \chi_2^\Gamma\big\|_{\mathfrak{X}^\Gamma} \\ &\leq \frac{c_1}{2}\big\|\chi_1^\Gamma - \chi_2^\Gamma\big\|_{\mathfrak{X}^\Gamma}\end{aligned}$$

for $\chi_1, \chi_2 \in \mathfrak{B}_\delta^\Gamma$. Here, we denote by $\mathfrak{B}_\delta^\Gamma$ the ball around $(\vartheta^\Gamma, \mu_\star, 0) \in \mathfrak{X}^{\Gamma,\star}$ with radius δ, and $\mathrm{d}\mathfrak{S}^\Gamma$ is equicontinuous in $(\vartheta^\Gamma, \mu_\star, 0)$ because of Assumption 3.2.2 and Assumption 3.2.3. Third, for $\varepsilon(\Gamma)$ small enough, we obtain the estimate

$$\big\|(L+F)(\vartheta^\Gamma, \mu_\star, 0)\big\|_{\mathfrak{X}^\Gamma} = \big\|\mathfrak{S}^\Gamma(\vartheta^\Gamma, \mu_\star, 0)\big\|_{\mathfrak{X}^\Gamma} \leq C\varepsilon(\Gamma) \leq \delta\frac{c_1}{2}$$

by combining Assumption 3.2.2 and Assumption 3.2.3. Finally, we make use of

$$\|v_\star^\Gamma - v_\star\| \leq \|v_\star^\Gamma - \vartheta^\Gamma\| + \|\vartheta^\Gamma - v_\star\| \leq C\big\|v_\star^\Gamma - \vartheta^\Gamma\big\|_\Gamma + C\varepsilon(\Gamma),$$

which is due to Assumption 3.2.2. □

In order to show $\lambda_\star^\Gamma = 0$, we adjust Lemma 2.2.12 to the discretized problem. This is possible due to the invariance properties from Assumption 3.2.2(a).

Theorem 3.4.4. *Under the Assumptions 3.2.1-3.2.3 and for $\varepsilon(\Gamma)$ small enough, the stationary problem*

$$\begin{aligned}0 &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma, \\ 0 &= Q^\Gamma(v^\Gamma) - Q(v_\star), \\ 0 &= \psi^\Gamma(v^\Gamma)\end{aligned}$$

possesses a locally unique solution $(v_\star^\Gamma, \mu_\star^\Gamma)$ that satisfies

$$\|v_\star^\Gamma - v_\star\| + |\mu_\star^\Gamma - \mu_\star| \leq C\varepsilon(\Gamma).$$

Proof. By taking $(v_\star^\Gamma, \mu_\star^\Gamma, \lambda_\star^\Gamma)$ from Lemma 3.4.3, we only have to show $\lambda_\star^\Gamma = 0$. Due to Assumption 3.2.2(a) the discrete Hamiltonian is invariant under the group action. Differentiating at $\gamma = \mathbb{1}$ the identity

$$H^\Gamma\big(a(\gamma)v_\star^\Gamma\big) = H^\Gamma(v_\star^\Gamma)$$

gives us

$$\langle \mathrm{d}H^\Gamma(v_\star^\Gamma), \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]\sigma\rangle = 0 \tag{3.4.7}$$

for all $\sigma \in \mathcal{A}_0$. In the same way, we get

$$\langle \mathrm{d}Q^\Gamma(v_\star^\Gamma)\mu_\star^\Gamma, d[a(\mathbb{1})v_\star^\Gamma]\sigma\rangle = 0. \tag{3.4.8}$$

Since the solution $(v_\star^\Gamma, \mu_\star^\Gamma, \lambda_\star^\Gamma)$ of the modified stationary problem satisfies

$$0 = \big\langle \mathrm{d}H^\Gamma(v_\star^\Gamma) - \mathrm{d}Q^\Gamma(v_\star^\Gamma)\mu_\star^\Gamma - \mathrm{d}\psi^\Gamma(v_\star^\Gamma)\lambda_\star^\Gamma, \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]\sigma\big\rangle$$

for all $\sigma \in \mathcal{A}_0$, the identities (3.4.7) and (3.4.8) give us

$$\langle \mathrm{d}\psi^\Gamma(v_\star^\Gamma)\lambda_\star, \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]\sigma\rangle = 0.$$

Finally, the Assumptions 2.2.11, 3.2.2, 3.2.3, and Lemma 3.4.3 taken together imply $\lambda_\star = 0$. □

Remark 11. In [3] the authors follow a slightly different strategy to prove the existence of a discrete relative equilibrium. Their proof is very elegant and much shorter than ours since it is adapted to the specific case of the one-dimensional Lie group of gauge transformations $\sigma \mapsto e^{i\sigma}$ and the resulting explicit formulas. Even though this is the main application, we want to keep the abstract setting as general as possible.

3.5 Stability of Discrete Steady States

The question arises, whether the steady state $(v_\star^\Gamma, \mu_\star^\Gamma)$ of the discretized freezing system is stable in the sense of Lyapunov. In our proof of stability, we proceed in a similar way as for the continuous problem in Section 2.3. This is why, we indicate the main steps, but we do not go through all technical details. The first step is to ensure the existence of solutions of the discrete freezing system with initial data close to the steady state, where, in analogy to Lemma 2.3.1, the phase condition is solved by an implicit function.

Lemma 3.5.1. *Provided $\varepsilon(\Gamma)$ is small enough and the Assumptions 3.2.1-3.2.4 hold, there exist open neighborhoods $\mathfrak{U}_\star^\Gamma \subseteq G_0 \times X_{-1}^\Gamma$ of $(\mathbb{1}, v_\star^\Gamma)$ and $U_\star^\Gamma \subseteq X_{-1}^\Gamma$ of $v_\star^\Gamma$ and a smooth function*

$$g^\Gamma \colon U_\star^\Gamma \to G,$$

such that $\mathfrak{F}^\Gamma(g, u^\Gamma) = 0$ and $(g, u^\Gamma) \in \mathfrak{U}_\star^\Gamma$ if and only if $g = g^\Gamma(u^\Gamma)$ and $u^\Gamma \in U_\star^\Gamma$. These neighborhoods have Γ-independent size in the sense that there exists $\xi > 0$

such that $\operatorname{dist}_G(\mathbb{1}, g) \le \xi$ *and* $\left\|v^\Gamma - v_\star^\Gamma\right\|_\Gamma \le \xi$ *imply* $(g, v^\Gamma) \in \mathfrak{U}_\star^\Gamma$ *and* $v^\Gamma \in U_\star^\Gamma$. *Moreover, we have*

$$dg^\Gamma(u^\Gamma) = -\left[\mathfrak{F}_g^\Gamma(g^\Gamma(u^\Gamma), u^\Gamma)\right]^{-1} \mathfrak{F}_{u^\Gamma}(g^\Gamma(u^\Gamma), u^\Gamma). \tag{3.5.1}$$

Proof. As in Lemma 2.3.1, we apply Lemma A.3.1. Due to the Assumptions 3.2.2 and 3.2.3, the mapping $\mathfrak{F}^\Gamma$ from Assumption 3.2.2 is continuously differentiable and there exists a Γ-independent local bound for its derivative. For the same reason and Theorem 3.4.4, the Jacobian submatrix

$$\left[\left\langle \mathrm{d}\psi^\Gamma(v_\star^\Gamma)e_i, \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]e_j \right\rangle\right]_{i,j=1}^d$$

is a small perturbation of the matrix in Assumption 2.2.11(b). Hence, its inverse is uniformly bounded by Banach's Lemma. Moreover, the Lie subgroup G_0 and the Lie subalgebra $\mathcal{A}_0$ do not depend on Γ, and that is why the coordinate representation is Γ-independent. Following the proof of Lemma A.3.1 in [61], we conlude that $\mathfrak{U}_\star^\Gamma$ and $U_\star^\Gamma$ have Γ-independent size. □

Theorem 2.1.2 together with the implicit function g^Γ allows us to show that the freezing system is locally well-posed for initial data close to the relative equilibrium, where the distance is measured in the $\left\|\cdot\right\|_{X_{-1}^\Gamma}$-norm, which is weaker than the $\left\|\cdot\right\|_\Gamma$-norm.

Lemma 3.5.2. *Provided the Assumptions 3.2.1-3.2.4 hold, for any initial value* $u_0^\Gamma \in X^\Gamma \cap U_\star^\Gamma$ *such that* $\psi^\Gamma(u_0^\Gamma) = 0$ *the freezing system*

$$\begin{aligned} \omega^\Gamma(v_t^\Gamma, \cdot) &= \mathrm{d}H^\Gamma(v^\Gamma) - \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma, \quad v^\Gamma(0) = u_0^\Gamma, \\ 0 &= \psi^\Gamma(v^\Gamma) \end{aligned} \tag{3.5.2}$$

has a unique local solution $v^\Gamma \in \mathcal{C}(\mathcal{I}^\Gamma; X^\Gamma) \cap \mathcal{C}^1(\mathcal{I}^\Gamma; U_\star^\Gamma)$, $\mu^\Gamma \in \mathcal{C}(\mathcal{I}^\Gamma; \mathcal{A}_0)$ *on an open interval* $\mathcal{I}^\Gamma$. *Furthermore, the conservation laws*

$$\begin{aligned} H^\Gamma(v^\Gamma(t)) &= H^\Gamma(u_0^\Gamma), \\ Q^\Gamma(v^\Gamma(t))\sigma &= Q^\Gamma(u_0^\Gamma)\sigma, \quad \sigma \in \mathcal{A}_0, \end{aligned}$$

hold for all $t \in \mathcal{I}^\Gamma$, *and we have the following blow-up alternative. If* $(\mathcal{T}^{\Gamma,-}, \mathcal{T}^{\Gamma,+})$ *is the maximal interval of existence such that* $v^\Gamma(t)$ *remains in* $X^\Gamma \cap U_\star^\Gamma$ *and* $\mathcal{T}^{\Gamma,+} < \infty$, *then*

$$\min\left(\operatorname{dist}_{\|\cdot\|_{X_{-1}^\Gamma}}\left(v^\Gamma(t), \partial U_\star^\Gamma\right), \frac{1}{\left\|v^\Gamma(t)\right\|_\Gamma} \right) \to 0$$

as $t \to \mathcal{T}^{\Gamma,+}$.

Proof. By Assumption 3.2.2(a), the quantities H^Γ and $Q^\Gamma(\cdot)\sigma$ are invariant under the group action. Hence, Theorem 2.1.2 can be applied to the discrete problem and yields a local solution $v^\Gamma \colon \mathcal{I}^\Gamma \to X^\Gamma$, $\mu^\Gamma \colon \mathcal{I}^\Gamma \to \mathcal{A}$ of the freezing system (3.5.2). Since no uniformity in Γ is required, we proceed in the same way as in the proof of Theorem 2.3.2. □

In the same way as for the continuous problem, the distance $|\mu^\Gamma(0) - \mu_\star^\Gamma|$ depends continuously on $\|u_0^\Gamma - v_\star^\Gamma\|$.

Lemma 3.5.3. *Let the Assumptions 3.2.1-3.2.4 be satisfied and $\varepsilon(\Gamma)$ be small enough. For any $\xi > 0$ there exists $\zeta > 0$, which does not depend on Γ, such that $u_0^\Gamma \in \mathcal{B}_\zeta^\Gamma(v_\star^\Gamma)$ satisfying $\psi^\Gamma(u_0^\Gamma) = 0$ implies*

$$\left|\mu^\Gamma(0; u_0^\Gamma) - \mu_\star^\Gamma\right| < \xi,$$

where the solution of (3.5.2) is denoted by $t \mapsto \left(v^\Gamma(t; u_0^\Gamma), \mu^\Gamma(t; u_0^\Gamma)\right)$.

Proof. The group operations do not depend on Γ, the continuous dependence on the initial data is independent of Γ (see Assumption 3.2.4), and the estimates on (3.5.1) are uniform, as discussed in the proof of Lemma 3.5.1. This is why, we proceed as in the proof of Corollary 2.3.3. □

The proof of stability is now based on the linearized operator

$$L_\star^\Gamma = L^\Gamma(v_\star^\Gamma, \mu_\star). \tag{3.5.3}$$

Due to Lemma 3.3.1, it is positive on the subspace

$$\hat{Y}^\Gamma = \left\{\hat{y}^\Gamma \in X^\Gamma : \left\langle \mathrm{d}Q^\Gamma(v_\star^\Gamma)\sigma, \hat{y}^\Gamma \right\rangle = \left\langle \mathrm{d}\psi^\Gamma(v_\star^\Gamma)\sigma, \hat{y}^\Gamma \right\rangle = 0 \text{ for all } \sigma \in \mathcal{A}_0\right\}. \tag{3.5.4}$$

Indeed, combining Theorem 3.4.4 and the Assumptions 3.2.2(b)-(d) yields

$$\left\|\mathrm{d}Q(v_\star)\sigma - \mathrm{d}Q^\Gamma(v_\star^\Gamma)\sigma\right\|_{X^{\Gamma,\star}} \le C\varepsilon(\Gamma)|\sigma|,$$

and together with Assumption 3.2.3 we obtain

$$\left\|\mathrm{d}\psi(v_\star)\sigma - \mathrm{d}\psi^\Gamma(v_\star^\Gamma)\sigma\right\|_{X^{\Gamma,\star}} \le C\varepsilon(\Gamma)|\sigma|.$$

Next, in accordance with the setting for the continuous problem, we choose Ω^Γ such that $\left\{dQ^\Gamma(v_\star^\Gamma)e_1, ..., dQ^\Gamma(v_\star^\Gamma)e_{d_\star}\right\}$ is the dual basis of $\left\{\Omega^\Gamma e_1, ..., \Omega^\Gamma e_{d_\star}\right\}$. What follows is an analog of Lemma 2.3.4.

Lemma 3.5.4. *Provided $\varepsilon(\Gamma)$ is small enough and the Assumptions 3.2.1-3.2.3 hold, there exist uniquely defined smooth functions*

$$\alpha^\Gamma : X^\Gamma \to \mathcal{A}_0,$$
$$\beta^\Gamma : X^\Gamma \to \mathcal{A}_0,$$

such that $\mathfrak{G}^\Gamma(\alpha, \beta, v^\Gamma) = 0$ if and only if $\alpha = \alpha^\Gamma(v^\Gamma)$, $\beta = \beta^\Gamma(v^\Gamma)$, where

$$\mathfrak{G}^\Gamma = \begin{bmatrix} \mathfrak{G}^{\Gamma,1} \\ \mathfrak{G}^{\Gamma,2} \end{bmatrix}$$

is given by

$$\mathfrak{G}^{\Gamma,1}(\alpha, \beta, v^\Gamma) = \left[\left\langle \mathrm{d}Q^\Gamma(v_\star^\Gamma)e^i, v^\Gamma - v_\star^\Gamma - \Omega^\Gamma\alpha - \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]\beta \right\rangle\right]_{i=1}^{d_\star},$$
$$\mathfrak{G}^{\Gamma,2}(\alpha, \beta, v^\Gamma) = \left[\left\langle \mathrm{d}\psi^\Gamma(v_\star^\Gamma)e^i, v^\Gamma - v_\star^\Gamma - \Omega^\Gamma\alpha - \mathrm{d}[a(\mathbb{1})v_\star^\Gamma]\beta \right\rangle\right]_{i=1}^{d_\star}.$$

Moreover, we have the estimate

$$\big\|\alpha^\Gamma(v^\Gamma)\big\|_\Gamma + \big\|\beta^\Gamma(v^\Gamma)\big\|_\Gamma \leq C\big\|v^\Gamma - v_\star^\Gamma\big\|_\Gamma^2 \tag{3.5.5}$$

for all $v^\Gamma \in X^\Gamma \cap U_\star^\Gamma$ *that satisfy* $Q^\Gamma(v^\Gamma)e_j = Q^\Gamma(v_\star^\Gamma)e_j$ *and* $\psi^\Gamma(v^\Gamma)e_j = 0$ *for* $j = 1, ..., d_\star$.

Proof. By Assumption 3.2.2, Assumption 3.2.3, and Theorem 3.4.4 the Jacobian submatrix with respect to α and β is invertible by Banach's Lemma as a small perturbation of (2.3.9). The estimate (3.5.5) is Γ-independent due to the Γ-independent approximations of the continuous functionals (see Assumptions 3.2.2 and 3.2.3). □

Now, we make use of the positivity of $L_\star^\Gamma$ on $\hat{Y}^\Gamma$, where the former is given by (3.5.3) and the latter by (3.5.4), to estimate $\big\|v^\Gamma - v_\star^\Gamma\big\|_\Gamma$ in terms of the difference of the discrete Hamiltonian of v^Γ and $v_\star^\Gamma$.

Lemma 3.5.5. *Let* $v^\Gamma \in X^\Gamma \cap U_\star^\Gamma$ *satisfy* $Q^\Gamma(v^\Gamma)e_j = Q^\Gamma(v_\star^\Gamma)e_j$ *and* $\psi^\Gamma(v^\Gamma)e_j = 0$ *for* $j = 1, ..., d_\star$. *Provided the Assumptions 3.2.1-3.2.4 hold, we obtain*

$$H^\Gamma(v^\Gamma) - H^\Gamma(v_\star^\Gamma) \geq c\big\|v^\Gamma - v_\star^\Gamma\big\|_\Gamma^2$$

for $\varepsilon(\Gamma)$ *small enough.*

Proof. We proceed in the same way as in the proof of Lemma 2.3.5, where we have to make sure that the constant $c > 0$ does not depend on Γ. From the Assumptions 3.2.2(c) and 3.2.3, we conclude that the estimates for the remainders of the Taylor expansions of $H^\Gamma(v^\Gamma) - Q^\Gamma(v^\Gamma)\mu_\star^\Gamma$ around $v_\star^\Gamma$ are uniform with respect to Γ. Due to Lemma 3.3.1 and Theorem 3.3.2, the same holds for the positivity of the linearized operator $L_\star^\Gamma = \mathrm{d}^2 H^\Gamma(v_\star^\Gamma) - \mathrm{d}^2 Q^\Gamma(v_\star^\Gamma)\mu_\star^\Gamma$ and uniform estimates for α^Γ and β^Γ from Lemma 3.5.4 are given by (3.5.5). □

In general, the initial data do no satisfy $Q^\Gamma(u_0^\Gamma)e_j = Q^\Gamma(v_\star^\Gamma)e_j$ for $j = 1, ..., d_\star$. But, the error can be estimated in terms of the distance between u_0^Γ and $v_\star^\Gamma$.

Lemma 3.5.6. *Provided* $\varepsilon(\Gamma)$ *is small enough and the Assumptions 3.2.1-3.2.3 hold, there exists* $\xi > 0$ *such that for all* $v^\Gamma \in \mathcal{B}_\xi^\Gamma(v_\star^\Gamma)$ *there are* $w^\Gamma(v^\Gamma) \in W^\Gamma$ *and* $z^\Gamma(v^\Gamma) \in Z^\Gamma$ *that satisfy*

$$\begin{aligned} Q^\Gamma\big(v^\Gamma + w^\Gamma(v^\Gamma) + z^\Gamma(v^\Gamma)\big)\sigma &= Q^\Gamma(v_\star^\Gamma)\sigma, \\ \psi^\Gamma\big(v^\Gamma + w^\Gamma(v^\Gamma) + z^\Gamma(v^\Gamma)\big)\sigma &= \psi^\Gamma(v_\star^\Gamma)\sigma \end{aligned}$$

for all $\sigma \in \mathcal{A}_0$ *and can be estimated by*

$$\big\|w^\Gamma(v^\Gamma)\|_\Gamma + \|z^\Gamma(v^\Gamma)\big\|_\Gamma \leq C\Big(\big|Q^\Gamma(v^\Gamma) - Q^\Gamma(v_\star^\Gamma)\big|_{\mathcal{A}_0^\star} + \big|\psi^\Gamma(v^\Gamma) - \psi^\Gamma(v_\star^\Gamma)\big|_{\mathcal{A}_0^\star}\Big).$$

Proof. As in the proof of Lemma 3.5.6, we make use of the implicit function theorem. Due to the Assumptions 3.2.2 and 3.2.3, the size of the neighborhoods $\xi > 0$ does not depend on Γ, which is shown in the same way as in Lemma 3.5.1. In the second step, we obtain the uniform estimate due to the Assumption 3.2.2 and 3.2.3. □

Theorem 3.5.7. *Under the Assumptions 3.2.1-3.2.4, the discrete relative equilibrium $(v_\star^\Gamma, \mu_\star^\Gamma)$ is stable in the following sense. For any $\xi > 0$ there exists $\delta > 0$ such that for all $t \in [0, \infty)$ the solution (v^Γ, μ^Γ) exists and satisfies*

$$\left\|v^\Gamma(t) - v_\star^\Gamma\right\|_\Gamma + \left|\mu^\Gamma(t) - \mu_\star^\Gamma\right| \leq \xi,$$

provided $\varepsilon(\Gamma)$ is small enough and the initial satisfy $\left\|v^\Gamma(0) - v_\star^\Gamma\right\|_\Gamma \leq \delta$.

Proof. As in the proof of Theorem 2.3.7, we assume first that the v^Γ-component is not stable, i.e., there exists a sequence of intervals $\mathcal{I}_n$ and solutions $v_n^{\Gamma_n}$, such that we have $\left\|v_n^{\Gamma_n}(0) - v_\star^{\Gamma_n}\right\|_{\Gamma_n} \leq \frac{1}{n}$, but $\sup_{t\in\mathcal{I}_n} \left\|v_n^{\Gamma_n}(t) - v_\star^{\Gamma_n}\right\|_{\Gamma_n} \geq \xi$ for all $n \in \mathbb{N}$. Let t_n be the first time such that $\left\|v_n^{\Gamma_n}(t_n) - v_\star^{\Gamma_n}\right\|_{\Gamma_n} = \frac{\xi}{2}$. Since the discrete quantities H^Γ and Q^Γ are equicontinuous with respect to Γ by Assumption 3.2.2 and conserved quantities by Lemma 3.5.2, we conclude

$$\begin{aligned} H^{\Gamma_n}\big(v_n^{\Gamma_n}(t_n)\big) - H^{\Gamma_n}(v_\star^{\Gamma_n}) &= H^{\Gamma_n}\big(v_n^{\Gamma_n}(0)\big) - H^{\Gamma_n}(v_\star^{\Gamma_n}) \quad \to 0, \\ Q^{\Gamma_n}\big(v_n^{\Gamma_n}(t_n)\big)e_j - Q^{\Gamma_n}(v_\star^{\Gamma_n})e_j &= Q^{\Gamma_n}\big(v_n^{\Gamma_n}(0)\big)e_j - Q^{\Gamma_n}(v_\star^{\Gamma_n})e_j \to 0 \end{aligned}$$

as $n \to \infty$ for $j = 1, ..., d_\star$. By Lemma 3.5.6 there exist sequences $w_n^{\Gamma_n} \in W^{\Gamma_n}$ and $z_n^{\Gamma_n} \in Z^{\Gamma_n}$, such that the two identities

$$\begin{aligned} Q^{\Gamma_n}(v_n^{\Gamma_n}(t_n) + w_n^{\Gamma_n} + z_n^{\Gamma_n})e_j &= Q^{\Gamma_n}(v_\star^{\Gamma_n})e_j, \\ \psi^{\Gamma_n}(v_n^{\Gamma_n}(t_n) + w_n^{\Gamma_n} + z_n^{\Gamma_n})e_j &= \psi^{\Gamma_n}(v_\star^{\Gamma_n})e_j = 0 \end{aligned}$$

hold for $j = 1, ..., d_\star$ and such that

$$\left\|w_n^{\Gamma_n}\right\|_{\Gamma_n} + \left\|z_n^{\Gamma_n}\right\|_{\Gamma_n} \leq C\Big(\left|Q^{\Gamma_n}(v_n^{\Gamma_n}(t_n)) - Q^{\Gamma_n}(v_\star^{\Gamma_n})\right|_{\mathcal{A}_0^\star} + \left|\psi^{\Gamma_n}(v_n^{\Gamma_n}(t_n))\right|_{\mathcal{A}_0^\star}\Big)$$

is satisfied. From $Q^{\Gamma_n}(v_n^{\Gamma_n}(t_n))e_j - Q^{\Gamma_n}(v_\star^{\Gamma_n}(t_n))e_j \to 0$ and $\psi^{\Gamma_n}(v_n^{\Gamma_n}(t_n))e_j = 0$ for $j = 1, ..., d_\star$, it follows $\left\|w_n^{\Gamma_n}\right\|_{\Gamma_n} + \left\|z_n^{\Gamma_n}\right\|_{\Gamma_n} \to 0$ as $n \to \infty$. Furthermore, the inequality in Lemma 3.5.5 takes the form

$$H^{\Gamma_n}(v_n^{\Gamma_n}(t_n) + w_n^{\Gamma_n} + z_n^{\Gamma_n}) - H^{\Gamma_n}(v_\star^{\Gamma_n}) \geq c\left\|v_n^{\Gamma_n}(t_n) + w_n^{\Gamma_n} + z_n^{\Gamma_n} - v_\star^{\Gamma_n}\right\|_{\Gamma_n}^2.$$

By combining $\left\|w_n^{\Gamma_n} + z_n^{\Gamma_n}\right\|_{\Gamma_n} \to 0$ and $H^{\Gamma_n}(v_n^{\Gamma_n}(t_n) + w_n^{\Gamma_n} + z_n^{\Gamma_n}) - H^{\Gamma_n}(v_\star^{\Gamma_n}) \to 0$, which is due to equicontinuity of H^Γ, it follows

$$\left\|v_n^{\Gamma_n}(t_n) - v_\star^{\Gamma_n}\right\|_{\Gamma_n} \to 0,$$

which contradicts the assumption. Finally, by using Lemma 3.5.3, the stability of the μ-component is proven in the same way as for the continuous case. □

3.6 Verification of the Hypotheses

Let us show that the finite difference method and the finite elements method from Section 3.1 fit into the abstract setting. In both cases, the approximation

parameters $\Gamma = (\Delta x, K)$ determine grid spacing and grid size, and we have $\Gamma \in \mathfrak{P} = \mathbb{R}_{>0} \times \mathbb{N}$. Moreover, the discrete spaces X^Γ are given by (3.1.3), and the group actions

$$a^\Gamma : G \to \mathrm{GL}(X^\Gamma), \quad \gamma \mapsto a(\gamma)\big|_{X^\Gamma} \tag{3.6.1}$$

take the form

$$a(\gamma)v^\Gamma = e^{-i\gamma}v^\Gamma.$$

The Lie group $G = S^1$ is abelian, and its Lie algebra is given by $\mathcal{A} = \mathbb{R}$.

At first, we put our focus on the finite difference method from Section 3.1.1, where we recall that the forward difference quotient is written as

$$(\partial^+ v^\Gamma)_j = \frac{v^\Gamma_{j+1} - v^\Gamma_j}{\Delta x}.$$

Proposition 3.6.1. *Provided that the phase condition of the continuous problem (2.3.3) is of the form $0 = \big(i\hat{v}, v\big)_0$, where the template function $\hat{v} \in H^1(\mathbb{R};\mathbb{C})$ decays exponentially as $|x| \to \infty$, the finite difference method with the error function*

$$\varepsilon(\Gamma) = \Delta x + \frac{1}{\Delta x^2} e^{-\nu K \Delta x} \tag{3.6.2}$$

for some $\nu > 0$, which depends only on the decay rates of $\hat{v}$ and $v_\star$, satisfies the Assumptions 3.2.1-3.2.4. Furthermore, the mass functional is given by

$$Q^\Gamma(v^\Gamma)\mu^\Gamma = \frac{\mu^\Gamma}{2}\Delta x \sum_{j\in\mathbb{Z}} |v^\Gamma_j|^2, \tag{3.6.3}$$

and the Hamiltonian takes the form

$$H^\Gamma(v^\Gamma) = \Delta x \sum_{j\in\mathbb{Z}} \left(\frac{|(\partial^+ v^\Gamma)_j|^2}{2} - \frac{|v^\Gamma_j|^4}{4} \right). \tag{3.6.4}$$

Proof. Let us start with Assumption 3.2.1. From the definition of X^Γ in (3.1.3), we conclude that $v^\Gamma \in X^\Gamma$ implies $e^{-i\gamma}v^\Gamma \in X^\Gamma$ for any $\gamma \in G$. Hence, the mapping a^Γ in (3.6.1) exists. Moreover, it is a group homomorphism since $a^\Gamma(\gamma)$ is the restriction of $a(\gamma)$ from X to the smaller space X^Γ. The discrete symplectic form on X^Γ is given by

$$\omega^\Gamma(v^\Gamma, y^\Gamma) = \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Im}(\bar{v}^\Gamma_j y^\Gamma_j).$$

For any given $\gamma \in G$ we write $\zeta = e^{i\gamma}$, and since we have $\bar{\zeta}\zeta = 1$, it follows

$$\omega^\Gamma(\zeta v^\Gamma, \zeta y^\Gamma) = \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Im}(\bar{\zeta}\bar{v}^\Gamma_j \zeta y^\Gamma_j) = \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Im}(\bar{v}^\Gamma_j y^\Gamma_j) = \omega^\Gamma(v^\Gamma, y^\Gamma),$$

which means the images of a^Γ are symplectic with respect to ω^Γ. In addition to that, we get

$$d[a(\mathbb{1})v^\Gamma]\sigma = -i\sigma v^\Gamma \in X^\Gamma$$

for any $\sigma \in \mathcal{A}$.

Next, we consider Assumption 3.2.2. Given any $\varepsilon_0 > 0$, we choose $K_0 \in \mathbb{N}$ such that the inequality

$$K_0 \geq \frac{2}{\nu\,\varepsilon_0} \ln\left(\frac{8}{\varepsilon_0^3}\right)$$

holds. By plugging this into (3.6.2), we get $\varepsilon(\Gamma_0) \leq \varepsilon_0$ for

$$\Gamma_0 = \left(\frac{\varepsilon_0}{2}, K_0\right).$$

Furthermore, differentiating (3.6.3) and (3.6.4) gives us

$$\left\langle \mathrm{d}Q^\Gamma(v^\Gamma)\mu^\Gamma, y^\Gamma \right\rangle = \frac{\mu^\Gamma}{2}\Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar{v}_j^\Gamma y_j^\Gamma)$$

and

$$\left\langle \mathrm{d}H^\Gamma(v^\Gamma), y^\Gamma \right\rangle = \Delta x \sum_{j\in\mathbb{Z}} \left(\frac{1}{\Delta x^2} \mathrm{Re}\big((-\bar{v}_{j+1}^\Gamma + 2\bar{v}_j^\Gamma - \bar{v}_{j-1}^\Gamma) y_j^\Gamma\big) - \mathrm{Re}\big(|v_j^\Gamma|^2 \bar{v}_j^\Gamma y_j^\Gamma\big) \right).$$

These terms coincide with (3.1.2), and the invariance under the group action follows directly from $e^{i\gamma}e^{-i\gamma} = 1$ for all $\gamma \in G$. The estimate in part (b) has been proven in [3], where $\vartheta^\Gamma \in X^\Gamma$ is determined by

$$\vartheta_j^\Gamma = v_\star(x_j), \quad j \in \mathbb{Z}.$$

In addition to that, part (c) has been proven in [4], and (d) is due to [3].

Next, we verify Assumption 3.2.3. As the discrete template function we pick

$$\hat{v}_j^\Gamma = \hat{v}(x_j), \quad j \in \mathbb{Z}.$$

Since

$$\left(v^\Gamma, y^\Gamma\right)_0^\Gamma = \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar{v}_j^\Gamma y_j^\Gamma) \tag{3.6.5}$$

is a (real) inner product, the mapping $\psi^\Gamma \colon X^\Gamma \to \mathcal{A}^\star$, which is given by

$$\psi^\Gamma(y^\Gamma)\sigma = \left(i\sigma\hat{v}^\Gamma, y^\Gamma\right)_0^\Gamma, \quad \sigma \in \mathcal{A},$$

is linear. Let us consider the difference between $\big(v^\Gamma, y^\Gamma\big)_0^\Gamma$ and $\big(v^\Gamma, y^\Gamma\big)_0$ for any $v^\Gamma, y^\Gamma \in X^\Gamma$. Since the L^2-inner product for piecewise linear functions yields

$$\begin{aligned}\big(v^\Gamma, y^\Gamma\big)_0 &= \Delta x \sum_{j\in\mathbb{Z}} \int_0^1 \mathrm{Re}\big((t\bar v_j^\Gamma + (1-t)\bar v_{j+1}^\Gamma)(t y_j^\Gamma + (1-t) y_{j+1}^\Gamma)\big)\mathrm{d}t \\ &= \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar v_j^\Gamma y_j^\Gamma) \int_0^1 2t^2 \mathrm{d}t + \Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar v_{j+1}^\Gamma y_j^\Gamma) \int_0^1 2(1-t)t\,\mathrm{d}t \\ &= \frac{2}{3}\Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar v_j^\Gamma y_j^\Gamma) + \frac{1}{3}\Delta x \sum_{j\in\mathbb{Z}} \mathrm{Re}(\bar v_{j+1}^\Gamma y_j^\Gamma),\end{aligned}$$

we obtain the inequality

$$\begin{aligned}\Big|\big(v^\Gamma, y^\Gamma\big)_0^\Gamma - \big(v^\Gamma, y^\Gamma\big)_0\Big| &= \frac{1}{3}\Delta x \Big|\sum_{j\in\mathbb{Z}} \mathrm{Re}\big((\bar v_{j+1}^\Gamma - \bar v_j^\Gamma) y_j^\Gamma\big)\Big| \\ &\le \frac{1}{3}\Delta x \big\|\partial^+ v^\Gamma\big\|_{\Gamma,0} \big\|y^\Gamma\big\|_{\Gamma,0} \\ &\le C\varepsilon(\Gamma)\big\|v^\Gamma\big\|_\Gamma \big\|y^\Gamma\big\|_\Gamma.\end{aligned}$$

For $e_1 = 1$ this implies

$$\begin{aligned}\big|\psi^\Gamma(y^\Gamma)e_1 - \psi(y^\Gamma)e_1\big| &\le \Big|\big(i\hat v^\Gamma, y^\Gamma\big)_0^\Gamma - \big(i\hat v^\Gamma, y^\Gamma\big)_0\Big| + \Big|\big(i(\hat v^\Gamma - \hat v), y^\Gamma\big)_0\Big| \\ &\le C\varepsilon(\Gamma)\big\|y^\Gamma\big\|_\Gamma,\end{aligned}$$

where we applied the Cauchy-Schwarz inequality and the estimate

$$\big\|\hat v^\Gamma - \hat v\big\|_{L^2(\mathbb{R};\mathbb{C})} \le C\varepsilon(\Gamma),$$

which is obtained in the same way as in Assumption 3.2.2(b).

Assumption 3.2.4 holds for $X_{-1}^\Gamma = X^{\Gamma,\star}$. The linear part of the discretized NLS is represented by a bounded, symmetric operator $A^\Gamma\colon X^\Gamma \to X^{\Gamma,\star}$. For any $t \in \mathbb{R}$ the evolution of this linear part leads to an isometry $v^\Gamma \mapsto e^{itA^\Gamma} v^\Gamma$, and due to Assumption 3.2.2(d), estimates for the nonlinear part are uniform with respect to Γ. Hence, uniform estimates for the continuous dependence follow from Duhamel's formula and Gronwall's inequality. Moreover, the mapping $\mathfrak{F}^\Gamma\colon G \times X^\Gamma \to \mathcal{A}^\star$ that extends

$$\psi^\Gamma(a(\gamma)v^\Gamma) = \big(i\hat v^\Gamma, e^{i\gamma} v^\Gamma\big)_0^\Gamma$$

is smooth with respect to γ and linear in v^Γ.

We are left to consider Assumption 3.2.5, i.e., we pick a sequence v^{Γ_n} and show that for any $\xi > 0$ there exists $N \in \mathbb{N}$ such that $n > N$ implies

$$\big\|v^{\Gamma_n} - v\big\|_{H^1(\mathbb{R};\mathbb{C})} < \xi. \tag{3.6.6}$$

Due to $v \in H^1(\mathbb{R};\mathbb{C})$, for $\xi > 0$ and any $\rho > 0$ there exists $M = M(\xi,\rho) > 1$ such that the inequalities

$$\big\|v\big\|_{H^1(-\infty,-M;\mathbb{C})} + \big\|v\big\|_{H^1(M,\infty;\mathbb{C})} < \tfrac{\xi}{12} \tag{3.6.7}$$

and

$$\sup\big\{|v(x)|\colon\ -M+1<x<M-1\big\}<\rho \tag{3.6.8}$$

hold. We choose $\rho=\frac{\xi}{12}$ and $\tilde{v}\in H^2(-M,M;\mathbb{C})$ satisfying the estimate

$$\big\|\tilde{v}-v\big\|_{H^1(-M,M;\mathbb{C})}<\tfrac{\xi}{12}. \tag{3.6.9}$$

Furthermore, we pick $m\in(0,1)$ and a sequence v^{Γ_n} such that $(\Delta x)_n<m$ and $(\Delta x)_nK_n>M$ imply

$$\big\|v^{\Gamma_n}-\tilde{v}\big\|_{H^1(-M,M;\mathbb{C})}<\tfrac{\xi}{12} \tag{3.6.10}$$

and

$$\big\|v^{\Gamma_n}\big\|_{H^1(-\infty,-M;\mathbb{C})}+\big\|v^{\Gamma_n}\big\|_{H^1(M,\infty;\mathbb{C})}<\tfrac{3}{4}\xi. \tag{3.6.11}$$

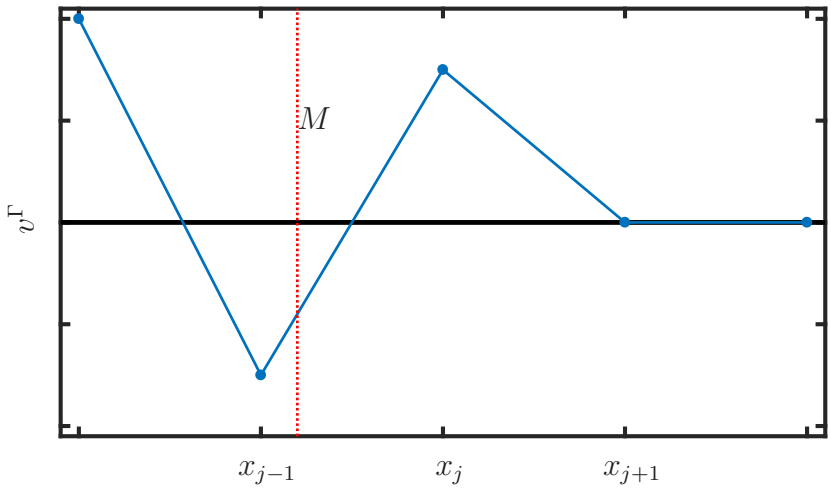


Figure 3.6.1: Cut-off for v^Γ

While the former is due to finite element interpolation on bounded intervals, the latter is obtained from (3.6.8) and by choosing $v^{\Gamma_n}(x_j)=0$ if $x_{j+1}\le -M$ or $M\le x_{j-1}$. Indeed, this gives us

$$\big\|v^{\Gamma_n}\big\|_{L^2(-\infty,-M;\mathbb{C})}+\big\|v^{\Gamma_n}\big\|_{L^2(M,\infty;\mathbb{C})}<2\big(m+\tfrac{m}{2}\big)\tfrac{\xi}{12}\le\tfrac{\xi}{4}$$

and

$$\big\|v_x^{\Gamma_n}\big\|_{L^2(-\infty,-M;\mathbb{C})}+\big\|v_x^{\Gamma_n}\big\|_{L^2(M,\infty;\mathbb{C})}<2\cdot(2+1)\tfrac{\xi}{12}=\tfrac{\xi}{2}.$$

From (3.6.2) and $\varepsilon(\Gamma_n)\to 0$, we get $(\Delta x)_n\to 0$ and $K_n(\Delta x)_n\to\infty$. Hence, there exists $N\in\mathbb{N}$ such that $n>N$ gives us $(\Delta x)_n<m$ and $(\Delta x)_nK_n>M$. By combining (3.6.7), (3.6.9), and (3.6.10)), we obtain (3.6.6) for $n>N$, which finishes the proof. □

Next, we turn our focus to the discretization via finite elements and verify the same assumptions.

Proposition 3.6.2. *Provided that the phase condition of the continuous problem (2.3.3) is of the form* $0 = \big(i\hat{v}, v\big)_0$, *where the template function* $\hat{v} \in H^1(\mathbb{R};\mathbb{C})$ *decays exponentially as* $|x| \to \infty$, *the Assumptions 3.2.1-3.2.4 are fulfilled for the finite element method with the error function (3.6.2). The constant* $\nu > 0$ *in (3.6.2) depends only on the decay rates of* $\hat{v}$ *and* $v_\star$. *Moreover, the discrete Hamiltonian* $H^\Gamma = H\big|_{X^\Gamma}$ *and the discrete mass* $Q^\Gamma = Q\big|_{X^\Gamma}$ *are given by the restriction of* H *and* Q.

Proof. The Lie group G, the group action (3.6.1), and the space X^Γ are the same as for the finite difference method. Furthermore, we can select the same $\vartheta^\Gamma \in X^\Gamma$. Hence, the Assumptions 3.2.1, 3.2.2(b), and 3.2.5 were already verified in Proposition 3.6.1. Differentiating

$$H(v^\Gamma) = \int_{\mathbb{R}} \Big(\tfrac{1}{2}|v_x^\Gamma(x)|^2 - \tfrac{1}{4}|v^\Gamma|^4\Big)\mathrm{d}x$$

gives us

$$\begin{aligned}\langle \mathrm{d}H(v^\Gamma), y^\Gamma\rangle &= \big(v_x^\Gamma, y_x^\Gamma\big)_0 - \big(|v^\Gamma|^2 v^\Gamma, y^\Gamma\big)_0 \\ &= \big(A^\Gamma v^\Gamma, y^\Gamma\big)_0 - \big(P^\Gamma(|v^\Gamma|^2 v^\Gamma), y^\Gamma\big)_0,\end{aligned}$$

where the last step is due to (3.1.5) and (3.1.6). Moreover, differentiating

$$Q(v^\Gamma) = \int_{\mathbb{R}} \tfrac{1}{2}|v^\Gamma|^2 \mathrm{d}x$$

yields

$$\langle \mathrm{d}Q(v^\Gamma)\mu^\Gamma, y^\Gamma\rangle = \mu^\Gamma\big(v^\Gamma, y^\Gamma\big)_0.$$

Hence, the discretization (3.1.7) is obtained by restricting H and Q to X^Γ. Furthermore, as restrictions of H and Q, the discrete Hamiltonian $H^\Gamma = H\big|_{X^\Gamma}$ and the discrete mass $Q^\Gamma = Q\big|_{X^\Gamma}$ are invariant under the group action. The inequalities in (c) follow from $H^\Gamma = H\big|_{X^\Gamma}$ and $Q^\Gamma = Q\big|_{X^\Gamma}$, and from $\big\|v^\Gamma\big\|_\Gamma = \|v^\Gamma\|$ for all $v^\Gamma \in X^\Gamma$ we get (d). Moreover, the template function in Assumption 3.2.3 can be chosen as in Proposition 3.6.1. Finally, Assumption 3.2.4 is satisfied by choosing the space $X_{-1}^\Gamma = X^{\Gamma,\star}$. The proof is done in the same way as in Proposition 3.6.1. □

Chapter 4

Truncation and Discretization for the NLS

4.1 Analysis of Boundary Conditions

In Section 1.3.1 we have seen that due to the scaling property and the Galilean invariance, the solitary wave solutions of the nonlinear Schrödinger equation appear as a two-parameter family of the form

$$u_\star(t,x) = e^{-i\mu_1 t} v_\star(x - \mu_2 t).$$

However, applied to this specific problem, the stability result in Chapter 3 is subject to the restriction $\mu_2 = 0$ with symmetric perturbations $\widetilde{v}(x) = \widetilde{v}(-x)$. As pointed out in [3], the general case is far more complicated since the action of the group of translations is much harder to handle. This is no different for the freezing method.

In the following, we study the impact of discrete approximations on the conservation of energy, mass and momentum, which is a key aspect of the stability theory in Hamiltonian systems. However, as an intermediate step, we start with the restriction of the freezing system to a finite interval.

While we take as a model problem the nonlinear Schrödinger equation, similar computations can be made for other problems, such as the nonlinear Klein-Gordon equation.

In contrary to Chapter 3 we omit in our notation the impact of perturbation parameters Γ. Since there is no risk of confusion, we write v instead of v^Γ for functions on the finite interval $[x_-, x_+]$. Moreover, we note that the suppressed notation $v = v(t) = v(t,x)$ is used once more.

4.1.1 Separated Boundary Conditions

With the freezing ansatz $u(t) = a(\gamma(t))v(t)$ the cubic nonlinear Schrödinger equation on a finite interval with separated boundary conditions is transformed into

$$\begin{aligned} iv_t(t,x) &= -v_{xx}(t,x) - |v(t,x)|^2 v(t,x) - \mu_1(t)v(t,x) + i\mu_2(t)v_x(t,x), \\ v_x(t,x_\pm) &= g_\pm(v(t,x_\pm)), \end{aligned} \tag{4.1.1}$$

where we have $t \in \mathcal{I}$ and $x \in (x_-, x_+)$. On the real line, the skew-symmetry

$$\int_{\mathbb{R}} \operatorname{Re}(\bar{v}_x y)\mathrm{d}x = -\int_{\mathbb{R}} \operatorname{Re}(\bar{v} y_x)\mathrm{d}x$$

of the differential operator

$$\frac{\mathrm{d}}{\mathrm{d}x}\colon H^1(\mathbb{R};\mathbb{C}) \to L^2(\mathbb{R};\mathbb{C}), \quad v \mapsto v_x$$

simplifies the weak formulation. In contrary, adjoint differential operators on finite intervals contain additional terms, which depend on the boundary conditions. To be more precise, we take a function

$$v \in \mathcal{C}\big(\mathcal{I}; H^2\big((x_-, x_+);\mathbb{C}\big)\big) \cap \mathcal{C}^1\big(\mathcal{I}; L^2\big((x_-, x_+);\mathbb{C}\big)\big)$$

that satisfies equation (4.1.1) in $L^2\big((x_-, x_+);\mathbb{C}\big)$-sense and $y \in H^1\big((x_-, x_+);\mathbb{C}\big)$. Then the complex conjugation $\bar{i} = -i$ and integration by parts lead to

$$\begin{aligned}
\int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_t y)\mathrm{d}x &= \int_{x_-}^{x_+} \operatorname{Re}(\bar{v}_{xx} y)\mathrm{d}x + \int_{x_-}^{x_+} \operatorname{Re}(|v|^2 \bar{v} y)\mathrm{d}x \\
&\quad + \mu_1 \int_{x_-}^{x_+} \operatorname{Re}(\bar{v} y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_x y)\mathrm{d}x \\
&= \operatorname{Re}(\bar{v}_x y)\Big|_{x_-}^{x_+} - \int_{x_-}^{x_+} \operatorname{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \operatorname{Re}(|v|^2 \bar{v} y)\mathrm{d}x \\
&\quad + \mu_1 \int_{x_-}^{x_+} \operatorname{Re}(\bar{v} y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_x y)\mathrm{d}x \\
&= \operatorname{Re}\big(\bar{g}_+(v(\cdot, x_+))y(x_+)\big) - \operatorname{Re}\big(\bar{g}_-(v(\cdot, x_-))y(x_-)\big) \\
&\quad - \int_{x_-}^{x_+} \operatorname{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \operatorname{Re}(|v|^2 \bar{v} y)\mathrm{d}x \\
&\quad + \mu_1 \int_{x_-}^{x_+} \operatorname{Re}(\bar{v} y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_x y)\mathrm{d}x,
\end{aligned}$$

which is the weak formulation of (4.1.1).

Proposition 4.1.1. *The weak formulation is a generalization of (4.1.1) in the following sense. A function $v \in \mathcal{C}\big(\mathcal{I}; H^2\big((x_-, x_+);\mathbb{C}\big)\big) \cap \mathcal{C}^1\big(\mathcal{I}; L^2\big((x_-, x_+);\mathbb{C}\big)\big)$ is a solution of (4.1.1) if and only if it fulfills the weak formulation.*

Proof. The only-if-part has already been proven. In order to show the if-part, we only consider $y \in H_0^1\big((x_-, x_+);\mathbb{C}\big)$. Hence, we get $y(x_\pm) = 0$ and conclude

$$\operatorname{Re}\big(\bar{g}_\pm(v(\cdot, x_\pm))y(x_\pm)\big) = 0.$$

Consequently, the weak formulation takes the form

$$\begin{aligned}
\int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_t y)\mathrm{d}x &= -\int_{x_-}^{x_+} \operatorname{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \operatorname{Re}(|v|^2 \bar{v} y)\mathrm{d}x \\
&\quad + \mu_1 \int_{x_-}^{x_+} \operatorname{Re}(\bar{v} y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \operatorname{Re}(i\bar{v}_x y)\mathrm{d}x.
\end{aligned}$$

Integration by parts leads to

$$\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_t y)\mathrm{d}x = \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_{xx} y)\mathrm{d}x + \int_{x_-}^{x_+} \mathrm{Re}(|v|^2\bar{v}y)\mathrm{d}x + \mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x,$$

which is rewritten as

$$\begin{aligned} 0 &= \int_{x_-}^{x_+} \mathrm{Re}\big((i\bar{v}_t - \bar{v}_{xx} - |v|^2\bar{v} - \mu_1\bar{v} - i\mu_2\bar{v}_x)y\big)\mathrm{d}x \\ &= -\int_{x_-}^{x_+} \mathrm{Re}\big(\bar{y}(iv_t + v_{xx} + |v|^2 v + \mu_1 v - i\mu_2 v_x)\big)\mathrm{d}x. \end{aligned}$$

Since $H_0^1\big((x_-, x_+); \mathbb{C}\big)$ is dense in $L^2\big((x_-, x_+); \mathbb{C}\big)$, we obtain

$$iv_t = -v_{xx} - |v|^2 v - \mu_1 v + i\mu_2 v_x \tag{4.1.2}$$

in $L^2\big((x_-, x_+); \mathbb{C}\big)$-sense.

We are left to verify the boundary conditions. For the right boundary, we define a function

$$y : (x_-, x_+) \to \mathbb{R}, \quad x \mapsto x - x_-. \tag{4.1.3}$$

Since (4.1.2) holds in $L^2\big((x_-, x_+); \mathbb{C}\big)$-sense and $y(x_-) = 0$, we have

$$\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_t y)\mathrm{d}x = \mathrm{Re}(\bar{v}_x(\cdot, x_+)y(x_+)) - \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \mathrm{Re}(|v|^2\bar{v}y)\mathrm{d}x + \mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x.$$

However, the weak formulation gives us

$$\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_t y)\mathrm{d}x = \mathrm{Re}\big(\bar{g}_+(v(\cdot, x_+))y(x_+)\big) - \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \mathrm{Re}(|v|^2\bar{v}y)\mathrm{d}x + \mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x.$$

Subtraction of these formulas yields

$$\mathrm{Re}(\bar{v}_x(\cdot, x_+)) = \mathrm{Re}\big(\bar{g}_+(v(\cdot, x_+))\big)$$

since we have $y(x_+) = x_+ - x_- \in \mathbb{R}_{>0}$. Furthermore, replacing (4.1.3) by

$$y : (x_-, x_+) \to \mathbb{R}, \quad x \mapsto i(x - x_-),$$

gives us the identity

$$\mathrm{Im}(\bar{v}_x(\cdot, x_+)) = \mathrm{Im}\big(\bar{g}_+(v(\cdot, x_+))\big).$$

Hence, the right boundary condition is verified. The left boundary condition can be handled in the same way. □

Now, we are ready to discuss the impact of the boundary on the time evolution of mass, momentum and energy. Since all these functionals are continuous on $H^1\big((x_-,x_+);\mathbb{C}\big)$, it suffices to consider a dense subset of initial data with solutions in $\mathcal{C}\big(\mathcal{I};H^2\big((x_-,x_+);\mathbb{C}\big)\big)\cap\mathcal{C}^1\big(\mathcal{I};L^2\big((x_-,x_+);\mathbb{C}\big)\big)$, and due to Proposition 4.1.1 the cubic nonlinear Schrödinger equation in $L^2\big((x_-,x_+);\mathbb{C}\big)$-sense is equivalent to its weak formulation.

On a finite interval (x_-,x_+) the mass is given by the formula

$$Q_1(v)=\int_{x_-}^{x_+}\tfrac{1}{2}|v|^2\mathrm{d}x.$$

Hence, its derivative takes the form

$$\langle \mathrm{d}Q_1(v),y\rangle=\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}y)\mathrm{d}x.$$

For the total derivative with respect to time this means

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big]&=\langle \mathrm{d}Q_1(v),v_t\rangle=\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}v_t)\mathrm{d}x\\&=\int_{x_-}^{x_+}\mathrm{Re}\big(\bar{v}(iv_{xx}+i|v|^2v+i\mu_1v+\mu_2v_x)\big)\mathrm{d}x,\end{aligned}\tag{4.1.4}$$

provided that $v\in\mathcal{C}\big(\mathcal{I};H^2\big((x_-,x_+);\mathbb{C}\big)\big)\cap\mathcal{C}^1\big(\mathcal{I};L^2\big((x_-,x_+);\mathbb{C}\big)\big)$ solves (4.1.1). The linearity of the integral allows us to analyze each term in (4.1.4) separately. First of all, we note that the second and third term can be rewritten as

$$\int_{x_-}^{x_+}\mathrm{Re}\big(\bar{v}\,i|v|^2v\big)\mathrm{d}x=\int_{x_-}^{x_+}\mathrm{Re}\big(i|v|^4\big)\mathrm{d}x$$

and

$$\int_{x_-}^{x_+}\mathrm{Re}\big(\bar{v}\,i\mu_1v\big)\mathrm{d}x=\int_{x_-}^{x_+}\mathrm{Re}\big(i\mu_1|v|^2\big)\mathrm{d}x.$$

However, these expressions vanish since $|v|^4$ and $\mu_1|v|^2$ are real-valued. Second, the same argument and integration by parts give us

$$\begin{aligned}\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}\,iv_{xx})\mathrm{d}x&=\mathrm{Re}(\bar{v}iv_x)\Big|_{x_-}^{x_+}-\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}_x\,iv_x)\mathrm{d}x\\&=\mathrm{Re}(\bar{v}iv_x)\Big|_{x_-}^{x_+}-\int_{x_-}^{x_+}\mathrm{Re}(i|v_x|^2)\mathrm{d}x\\&=-\mathrm{Re}(i\bar{v}_xv)\Big|_{x_-}^{x_+}\end{aligned}\tag{4.1.5}$$

for the first term. The remaining term is slighly more difficult to handle. We state as a Lemma the general formula for the inner product of u_x and $|u|^{2\sigma}u$.

Lemma 4.1.2. *For $u \in H^1\big((x_-, x_+); \mathbb{C}\big)$ and $\sigma \in \mathbb{N}$ we have*

$$\int_{x_-}^{x_+} \mathrm{Re}(\bar{u}_x |u|^{2\sigma} u)\mathrm{d}x = \frac{1}{2\sigma+2}|u|^{2\sigma+2}\Big|_{x_-}^{x_+}.$$

Proof. By writing $u = a + ib$, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}\Big[|u|^{2\sigma+2}\Big] &= \frac{\mathrm{d}}{\mathrm{d}x}\Big[\big(a^2+b^2\big)^{\sigma+1}\Big] = (\sigma+1)(a^2+b^2)^{\sigma}(2aa_x + 2bb_x)\\ &= (\sigma+1)(a^2+b^2)^{\sigma}\mathrm{Re}\big(2(a_x - ib_x)(a+ib)\big) = (\sigma+1)|u|^{2\sigma}\mathrm{Re}(2\bar{u}_x u)\\ &= (2\sigma+2)\mathrm{Re}(\bar{u}_x|u|^{2\sigma}u).\end{aligned}$$

This implies

$$\begin{aligned}\int_{x_-}^{x_+} \mathrm{Re}\big(\bar{u}_x(x)|u(x)|^{2\sigma}u(x)\big)\mathrm{d}x &= \int_{x_-}^{x_+} \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0}\frac{1}{2\sigma+2}|u(x+\varepsilon)|^{2\sigma+2}\mathrm{d}x\\ &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0}\int_{x_-}^{x_+}\frac{1}{2\sigma+2}|u(x+\varepsilon)|^{2\sigma+2}\mathrm{d}x\\ &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0}\int_{x_-+\varepsilon}^{x_++\varepsilon}\frac{1}{2\sigma+2}|u(x)|^{2\sigma+2}\mathrm{d}x\\ &= \frac{1}{2\sigma+2}|u(x)|^{2\sigma+2}\Big|_{x_-}^{x_+},\end{aligned}$$

which was to be proven. □

Applying Lemma 4.1.2 with $\sigma = 0$ gives us

$$\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}\mu_2 v_x)\mathrm{d}x = \mu_2\int_{x_-}^{x_+}\mathrm{Re}(\bar{v}_x v)\big)\mathrm{d}x = \frac{\mu_2}{2}|v|^2\Big|_{x_-}^{x_+}. \tag{4.1.6}$$

Summing up (4.1.5) and (4.1.6), the identity in (4.1.4) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big] = \mathrm{Re}(\bar{v}iv_x)\Big|_{x_-}^{x_+} + \frac{\mu_2}{2}|v|^2\Big|_{x_-}^{x_+}. \tag{4.1.7}$$

The mass is conserved if this derivative vanishes. In case of seperated boundary conditions this means

$$\mathrm{Re}\Big(\bar{v}(\cdot,x_+)\big(iv_x(\cdot,x_+) + \frac{\mu_2}{2}v(\cdot,x_+)\big)\Big) = 0,$$

which is true if and only if $v(\cdot,x_+) = 0$ or

$$v_x(\cdot,x_+) = \Big(i\frac{\mu_2}{2} + r_+\Big)\,v(\cdot,x_+)$$

holds for some $r_+ \in \mathbb{R}$. Here, we have to remark that a boundary condition

$$v_x(\cdot,x_+) = g_+\big(\mu_2, v(\cdot,x_+)\big)$$

is slightly more general than our initial approach. The left boundary is handled in the same way.

There is still some freedom in the choice of the parameter $r_+ \in \mathbb{R}$, whence we turn our focus to the conservation of the next functional. The momentum is defined as

$$\begin{aligned} Q_2(v) &= \frac{i}{4}\int_{x_-}^{x_+} (\bar{v}_x v - \bar{v} v_x)\mathrm{d}x = \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Im}(\bar{v} v_x)\mathrm{d}x \\ &= -\frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v} v_x) = \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x v)\mathrm{d}x. \end{aligned}$$

Since the derivative of this functional is given by

$$\begin{aligned} \langle \mathrm{d}Q_2(v), y\rangle &= \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{y}_x v)\mathrm{d}x + \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x \\ &= \frac{1}{2}\mathrm{Re}(i\bar{y} v)\Big|_{x_-}^{x_+} - \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{y} v_x)\mathrm{d}x + \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x \\ &= -\frac{1}{2}\mathrm{Re}(i\bar{v} y)\Big|_{x_-}^{x_+} + \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x + \frac{1}{2}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x \\ &= -\frac{1}{2}\mathrm{Re}(i\bar{v} y)\Big|_{x_-}^{x_+} + \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x, \end{aligned}$$

the total derivative with respect to time takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] = \langle \mathrm{d}Q_2(v), v_t\rangle = -\frac{1}{2}\mathrm{Re}(i\bar{v} v_t)\Big|_{x_-}^{x_+} + \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x v_t)\mathrm{d}x. \tag{4.1.8}$$

The computation of the right hand side requires the evaluation of v_t at the boundary $x_\pm$. Even if this time derivative at these points exists in a suitable sense, we do not know its values.

In an attempt to bypass this problem, the question arises whether we can modify Q_2 by adding a boundary functional Q_2^b such that the boundary terms in (4.1.8) cancel out, i.e.,

$$\langle \mathrm{d}Q_2^b(v), y\rangle = \frac{1}{2}\mathrm{Re}(i\bar{v} y)\Big|_{x_-}^{x_+}.$$

Let us check the Schwarz integrability condition for such a functional. By setting $v(x_\pm) = a_\pm + ib_\pm$ and $y(x_\pm) = c_\pm + id_\pm$, we get

$$\begin{aligned} \frac{1}{2}\mathrm{Re}\big(i\bar{v}(x_\pm)y(x_\pm)\big) &= \frac{1}{2}\mathrm{Re}\big(i(a_\pm - ib_\pm)(c_\pm + id_\pm)\big) = \frac{1}{2}(b_\pm c_\pm - a_\pm d_\pm) \\ &= \frac{1}{2}\begin{pmatrix} b_\pm & -a_\pm \end{pmatrix}\begin{pmatrix} c_\pm \\ d_\pm \end{pmatrix}, \end{aligned}$$

which leads to

$$\frac{1}{2}\mathrm{Re}(i\bar{v} y)\Big|_{x_-}^{x_+} = \frac{1}{2}\begin{pmatrix} -b_- & a_- & b_+ & -a_+ \end{pmatrix}\begin{pmatrix} c_- \\ d_- \\ c_+ \\ d_+ \end{pmatrix}.$$

But, from

$$\nabla Q_2^b(a_-, b_-, a_+, b_+) = \frac{1}{2}\begin{pmatrix} -b_- \\ a_- \\ b_+ \\ -a_+ \end{pmatrix},$$

we conclude that the second derivative is represented by the Hessian matrix

$$\frac{1}{2}\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

which fails to be symmetric. This contradicts the integrability assumption.

4.1.2 Periodic Boundary Conditions

This issue can be avoided by choosing periodic instead of separated boundary conditions. In terms of the nonlinear Schrödinger equation these boundary conditions are a very popular choice. For the local well-posedness we refer to [13], while the existence and stability of ground states has been proven in [11] and [12]. The weak formulation of

$$\begin{aligned} iv_t(t,x) &= -v_{xx}(t,x) - |v(t,x)|^2 v(t,x) - \mu_1(t)v(t,x) + i\mu_2(t)v_x(t,x), \\ 0 &= v(t,x_+) - v(t,x_-), \\ 0 &= v_x(t,x_+) - v_x(t,x_-) \end{aligned} \tag{4.1.9}$$

for $t \in \mathcal{I}$ and $x \in (x_-, x_+)$ is given by

$$\begin{aligned} \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_t y)\mathrm{d}x = &- \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \mathrm{Re}(|v|^2\bar{v}y)\mathrm{d}x \\ &+ \mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x. \end{aligned} \tag{4.1.10}$$

Here the corresponding space of test functions is $H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$, and we consider generalized solutions $v \in \mathcal{C}\big(\mathcal{I}; H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)\big)$. Due to the periodicity, the boundary term in (4.1.8) vanishes, and we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] = \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x v_t)\mathrm{d}x. \tag{4.1.11}$$

Again, there is no loss of generality in choosing a dense subset of initial data that leads to sufficiently smooth solutions since the conservation property for generalized solutions follows by continuity of the momentum functional.

Proposition 4.1.3. *For $v \in \mathcal{C}\big(\mathcal{I}; H^2\big((x_-,x_+);\mathbb{C}\big)\big) \cap \mathcal{C}^1\big(\mathcal{I}; L^2\big((x_-,x_+);\mathbb{C}\big)\big)$ the strong formulation (4.1.9) and the weak formulation (4.1.10) are equivalent.*

Proof. If $v \in \mathcal{C}\big(\mathcal{I}; H^2\big((x_-,x_+);\mathbb{C}\big)\big) \cap \mathcal{C}^1\big(\mathcal{I}; L^2\big((x_-,x_+);\mathbb{C}\big)\big)$ solves (4.1.9), then integration by parts yields

$$\begin{aligned}\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_t y)\mathrm{d}x = \mathrm{Re}(\bar{v}_x y)\Big|_{x_-}^{x_+} - \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x y_x)\mathrm{d}x + \int_{x_-}^{x_+} \mathrm{Re}(|v|^2\bar{v}y)\mathrm{d}x \\ + \mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}y)\mathrm{d}x + \mu_2 \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x,\end{aligned} \tag{4.1.12}$$

and the boundary term vanishes for any $y \in H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$. Moreover, we have $v \in \mathcal{C}\big(\mathcal{I}; H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)\big)$ due to the boundary conditions.

Now, let $v \in \mathcal{C}\big(\mathcal{I}; H^2\big((x_-,x_+);\mathbb{C}\big)\big) \cap \mathcal{C}^1\big(\mathcal{I}; L^2\big((x_-,x_+);\mathbb{C}\big)\big)$ solve (4.1.10). For any test function $y \in H^1_0\big((x_-,x_+);\mathbb{C}\big) \cap H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$ we rewrite the weak formulation (4.1.10) as

$$\begin{aligned}0 &= \int_{x_-}^{x_+} \mathrm{Re}\big((i\bar{v}_t - \bar{v}_{xx} - |v|^2\bar{v} - \mu_1\bar{v} - i\mu_2\bar{v}_x)y\big)\mathrm{d}x \\ &= -\int_{x_-}^{x_+} \mathrm{Re}\big(\bar{y}(iv_t + v_{xx} + |v|^2 v + \mu_1 v - i\mu_2 v_x)\big)\mathrm{d}x.\end{aligned}$$

Since $H^1_0\big((x_-,x_+);\mathbb{C}\big) \cap H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$ is a dense subset of $L^2\big((x_-,x_+);\mathbb{C}\big)$, the differential equation in (4.1.9) holds, and we are left to check the boundary conditions. The first boundary condition, i.e., $v(t,x_+) = v(t,x_-)$, is fulfilled by any $v(t,\cdot) \in H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$. In order to verify the second boundary condition, we subtract (4.1.10) from (4.1.12) and obtain

$$0 = \mathrm{Re}(\bar{v}_x y)\Big|_{x_-}^{x_+}$$

for all $y \in H^1_{\mathrm{per}}\big((x_-,x_+);\mathbb{C}\big)$. Then it follows $v_x(t,x_+) = v_x(t,x_-)$. □

Due to this equivalence, we can consider (4.1.11) in L^2-sense for smooth enough initial data. Replacing iv_t by the right hand side of the differential equation in (4.1.9) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] = \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x v_t)\mathrm{d}x = \int_{x_-}^{x_+} \mathrm{Re}\big(\bar{v}_x(-v_{xx} - |v|^2 v - \mu_1 v + i\mu_2 v_x)\big).$$

As before, we analyze each term separately. First of all, we have

$$\int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x\mu_2 v_x)\mathrm{d}x = \int_{x_-}^{x_+} \mathrm{Re}\big(i\mu_2|v_x|^2\big)\mathrm{d}x = 0$$

since $\mu_2|v_x|^2$ is real-valued. Second, we apply Lemma 4.1.2 with $\sigma = 1$ and $\sigma = 0$, which gives us

$$-\int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x|v|^2 v)\mathrm{d}x = -\frac{1}{4}|v|^4\Big|_{x_-}^{x_+} \tag{4.1.13}$$

and

$$-\mu_1 \int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x v)\mathrm{d}x = -\frac{\mu_1}{2}|v|^2\Big|_{x_-}^{x_+}, \tag{4.1.14}$$

respectively. Finally, Lemma 4.1.2 applied to v_x and $\sigma = 0$ yields

$$-\int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_x\, v_{xx})\mathrm{d}x = -\int_{x_-}^{x_+} \mathrm{Re}(\bar{v}_{xx}\, v_x)\mathrm{d}x = -\frac{1}{2}|v_x|^2\Big|_{x_-}^{x_+}. \tag{4.1.15}$$

For periodic boundary conditions all these terms vanish, so that the momentum Q_2 is a conserved quantity.

Let us address the question whether it is possible to find other boundary conditions with the same property. First, we recall that the term $\mathrm{Re}(i\bar{v}y)\Big|_{x_-}^{x_+}$ in

$$\langle \mathrm{d}Q_2(v), y\rangle = \int_{x_-}^{x_+} \mathrm{Re}(i\bar{v}_x y)\mathrm{d}x - \frac{1}{2}\mathrm{Re}(i\bar{v}y)\Big|_{x_-}^{x_+}$$

must vanish for all times. Hence, we require

$$|v(t,x_+)|^2 - |v(t,x_-)|^2 = 0,$$

which means that (4.1.13) and (4.1.14) equal zero. Since (4.1.15) is left, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] = \langle \mathrm{d}Q_2(v), v_t\rangle = -\frac{1}{2}|v_x|^2\Big|_{x_-}^{x_+},$$

and the resulting requirement is

$$|v_x(t,x_+)|^2 - |v_x(t,x_-)|^2 = 0.$$

This leads to periodic boundary conditions, except for some freedom in the choice of the complex argument.

We are left to consider the conservation of the Hamiltonian

$$H(v) = \int_{x_-}^{x_+} \left(\tfrac{1}{2}|v_x|^2 - \tfrac{1}{4}|v|^4\right)\mathrm{d}x$$

with its derivative given by

$$\begin{aligned}\langle \mathrm{d}H(v), y\rangle &= \int_{x_-}^{x_+} \mathrm{Re}\big(\bar{v}_x y_x - |v|^2\bar{v}y\big)\mathrm{d}x \\ &= \mathrm{Re}(\bar{v}_x y)\Big|_{x_-}^{x_+} - \int_{x_-}^{x_+} \mathrm{Re}\big((\bar{v}_{xx} + |v|^2\bar{v})y\big)\mathrm{d}x.\end{aligned}$$

For the total derivative with respect to time it follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big[H(v)\Big] = \langle \mathrm{d}H(v), v_t\rangle = -\int_{x_-}^{x_+} \mathrm{Re}\big((\bar{v}_{xx} + |v|^2\bar{v})v_t\big)\mathrm{d}x.$$

Again, we replace v_t by $i(v_{xx} + |v|^2 v + \mu_1 v) + \mu_2 v_x$ and split the sum into three terms. The first integral

$$-\int_{x_-}^{x_+} \mathrm{Re}\big(i\big(\bar{v}_{xx} + |v|^2\bar{v}\big)\big(v_{xx} + |v|^2 v\big)\big)\mathrm{d}x = -\int_{x_-}^{x_+} \mathrm{Re}\Big(i\big|v_{xx} + |v|^2 v\big|^2\Big)\Big|_{x_-}^{x_+}$$

equals zero since $\big|v_{xx} + |v|^2\bar{v}\big|^2$ is real-valued. Moreover, integration by parts and the above argument applied to $|v_x|^2$ and $|v|^4$ yield

$$-\int_{x_-}^{x_+} \mathrm{Re}\big(i\big(\bar{v}_{xx} + |v|^2\bar{v}\big)\mu_1 v\big)\mathrm{d}x = -\mu_1 \mathrm{Re}(i\bar{v}_x v)\Big|_{x_-}^{x_+}. \tag{4.1.16}$$

In order to rewrite the last term, we apply Lemma 4.1.2 to v_x with $\sigma = 0$ and to v with $\sigma = 1$, which results in

$$-\int_{x_-}^{x_+} \mathrm{Re}\big(\big(\bar{v}_{xx} + |v|^2\bar{v}\big)\mu_2 v_x\big)\mathrm{d}x = -\frac{\mu_2}{2}|v_x|^2\Big|_{x_-}^{x_+} - \frac{\mu_2}{4}|v|^4\Big|_{x_-}^{x_+}. \tag{4.1.17}$$

After summing up (4.1.16) and (4.1.17), we end up with the following proposition for the time dependency of mass, momentum, and energy.

Proposition 4.1.4. *For the mass Q_1, the momentum Q_2, and the energy H we get the identities*

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big] &= \frac{\mu_2}{2}|v|^2\Big|_{x_-}^{x_+} - \mathrm{Re}(i\bar{v}_x v)\Big|_{x_-}^{x_+},\\
\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] &= -\frac{1}{2}\mathrm{Re}(i\bar{v}v_t)\Big|_{x_-}^{x_+} - \frac{1}{4}|v|^4\Big|_{x_-}^{x_+} - \frac{\mu_1}{2}|v|^2\Big|_{x_-}^{x_+} - \frac{1}{2}|v_x|^2\Big|_{x_-}^{x_+},\\
\frac{\mathrm{d}}{\mathrm{d}t}\Big[H(v)\Big] &= \mathrm{Re}(\bar{v}_x v_t)\Big|_{x_-}^{x_+} - \mu_1\mathrm{Re}(i\bar{v}_x v)\Big|_{x_-}^{x_+} - \frac{\mu_2}{2}|v_x|^2\Big|_{x_-}^{x_+} - \frac{\mu_2}{4}|v|^4\Big|_{x_-}^{x_+}.
\end{aligned}$$

The following table collects the conservation properties of homogeneous Dirichlet, Neumann and periodic boundary conditions.

	Mass	Momentum	Energy
Dirichlet	✓		
Neumann			
Periodic	✓	✓	✓

4.2 Spatial Discretization

Next, we study the system that arises by spatial discretization of the freezing equation, where we put emphasis on the case of periodic boundary conditions. As in Section 4.1 we omit in our notation the impact of perturbation parameters Γ and write v instead of v^Γ for functions in discrete spaces. Our first approach is a finite difference discretization on a bounded spatial grid.

4.2.1 Finite Difference Method

The very basic idea of the finite difference method is to approximate derivatives in differential equations with corresponding difference formulas. The central difference quotient ∂^1 is defined by

$$(\partial^1 u)_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x},$$

and the second order central difference quotient ∂^2 is given by

$$(\partial^2 u)_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}.$$

Replacing the first and the second derivative in the freezing equation leads to

$$iu_t = -\partial^2 u - |u|^2 u - \mu_1 u + i\mu_2 \partial^1 u,$$

which rewrites as

$$u_t = i\partial^2 u + i|u|^2 u + i\mu_1 u + \mu_2 \partial^1 u.$$

We impose this equation pointwise on a spatial grid x_j with $j \in \mathbb{Z}$. The easiest way to obtain periodic boundary conditions is to identify x_j and x_{N+j}, in particular $x_0 = x_N$ and $x_1 = x_{N+1}$.

As before, we are interested in the time evolution of mass, momentum and energy. The discrete version of mass is given by

$$Q_1(v) = \frac{\Delta x}{2} \sum_{j=1}^{N} |v_j|^2,$$

and differentiation leads to

$$\langle \mathrm{d}Q_1(v), y \rangle = \Delta x \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j y_j).$$

Hence, the derivative with respect to time takes the form

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big] &= \langle \mathrm{d}Q_1(v), v_t \rangle = \langle \mathrm{d}Q_1(v), i\partial^2 v + i|v|^2 v + i\mu_1 v + \mu_2 \partial^1 v \rangle \\ &= \Delta x \sum_{j=1}^{N} \mathrm{Re}\big(\bar{v}_j (i\partial^2 v_j + i|v_j|^2 v_j + i\mu_1 v_j + \mu_2 \partial^1 v_j)\big). \end{aligned}$$

The two sums

$$\Delta x \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j \, i|v_j|^2 v_j) = \Delta x \sum_{j=1}^{N} \mathrm{Re}(i|v_j|^4)$$

and

$$\Delta x \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j \, i\mu_1 v_j) = \Delta x \sum_{j=1}^{N} \mathrm{Re}(i\mu_1 |v_j|^2)$$

vanish since $|v_j|^4$ and $\mu_1|v_j|^2$ are real-valued. By the same argument as before, an index shift and the skew-symmetry

$$\mathrm{Re}(i\bar{v}y) = -\mathrm{Re}(i\bar{y}v),$$

we get

$$\begin{aligned} \Delta x \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j \, i\partial^2 v_j) &= \Delta x \sum_{j=1}^{N} \mathrm{Re}\Big(i\bar{v}_j \frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2} \Big) \\ &= \frac{1}{\Delta x}\Big(\sum_{j=1}^{N} \mathrm{Re}(i\bar{v}_j v_{j+1}) + \sum_{j=1}^{N} \mathrm{Re}(i\bar{v}_j v_{j-1}) \Big) \\ &= \frac{1}{\Delta x}\big(\mathrm{Re}(i\bar{v}_N v_{N+1}) - \mathrm{Re}(i\bar{v}_0 v_1) \big). \end{aligned} \tag{4.2.1}$$

Moreover, the above index shift and the symmetry

$$\mathrm{Re}(\bar{v}_{j+1} v_j) = \mathrm{Re}(\bar{v}_j v_{j+1})$$

lead to

$$\begin{aligned} \Delta x \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j \, \mu_2 \partial^1 v_j) &= \Delta x \sum_{j=1}^{N} \mathrm{Re}\Big(\mu_2 \bar{v}_j \frac{v_{j+1} - v_{j-1}}{2\Delta x} \Big) \\ &= \frac{\mu_2}{2} \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j v_{j+1}) - \frac{\mu_2}{2} \sum_{j=1}^{N} \mathrm{Re}(\bar{v}_j v_{j-1}) \\ &= \frac{\mu_2}{2}\big(\mathrm{Re}(\bar{v}_N v_{N+1}) - \mathrm{Re}(\bar{v}_0 v_1) \big). \end{aligned} \tag{4.2.2}$$

Due to the periodic boundary conditions, both (4.2.1) and (4.2.2) equal zero. Hence, the discrete mass is a conserved quantity. We continue with the discrete momentum, which is given by

$$\begin{aligned} Q_2(v) &= \frac{\Delta x}{2} \sum_{j=1}^{N} \mathrm{Re}\big(i(\partial^1 \bar{v})_j v_j \big) = \frac{\Delta x}{2} \sum_{j=1}^{N} \mathrm{Re}\Big(i \frac{\bar{v}_{j+1} - \bar{v}_{j-1}}{2\Delta x} v_j \Big) \\ &= \frac{1}{4} \sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1}) v_j \big). \end{aligned}$$

The j-th partial derivative takes the form

$$\begin{aligned} \langle \mathrm{d}Q_2(v), y_j \rangle &= \tfrac{1}{4}\mathrm{Re}\big(i\bar{y}_j v_{j-1} \big) - \tfrac{1}{4}\mathrm{Re}\big(i\bar{y}_j v_{j+1} \big) + \tfrac{1}{4}\mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1}) y_j \big) \\ &= \tfrac{1}{4}\mathrm{Re}\big(i\bar{v}_{j+1} y_j \big) - \tfrac{1}{4}\mathrm{Re}\big(i\bar{v}_{j-1} y_j \big) + \tfrac{1}{4}\mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1}) y_j \big) \\ &= \tfrac{1}{2}\mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1}) y_j \big), \end{aligned}$$

and summing up leads to

$$\langle \mathrm{d}Q_2(v), y\rangle = \frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1})y_j\big).$$

Hence, we conclude that the total derivative with respect to time takes the form

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] &= \langle \mathrm{d}Q_2(v), v_t\rangle = \langle \mathrm{d}Q_2(v), i\partial^2 v + i|v|^2 v + i\mu_1 v + \mu_2\partial^1 v\rangle \\ &= \frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\Big(i(\bar{v}_{j+1} - \bar{v}_{j-1})(i\partial^2 v_j + i|v_j|^2 v_j + i\mu_1 v_j + \mu_2\partial^1 v_j)\Big).\end{aligned}$$

Again we consider the terms one after another, and first observe that

$$\begin{aligned}\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1})\mu_2\partial^1 v_j\big) &= \frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\Big(i(\bar{v}_{j+1} - \bar{v}_{j-1})\mu_2\frac{v_{j+1} - v_{j-1}}{2\Delta x}\Big) \\ &= \frac{\mu_2}{4\Delta x}\sum_{j=1}^{N} \mathrm{Re}\big(i|v_{j+1} - v_{j-1}|^2\big)\end{aligned}$$

is zero because $|v_{j+1} - v_{j-1}|^2$ is real-valued. While the above expression vanishes for any boundary conditions, the terms

$$\begin{aligned}\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1})i\mu_1 v_j\big) &= -\frac{\mu_1}{2}\Big(\sum_{j=1}^{N} \mathrm{Re}(\bar{v}_{j+1}v_j) - \sum_{j=0}^{N-1} \mathrm{Re}(\bar{v}_{j+1}v_j)\Big) \\ &= -\frac{\mu_1}{2}\big(\mathrm{Re}(\bar{v}_N v_{N+1}) - \mathrm{Re}(\bar{v}_0 v_1)\big)\end{aligned}$$

and

$$\begin{aligned}\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1})i\partial^2 v_j\big) &= -\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\Big((\bar{v}_{j+1} - \bar{v}_{j-1})\frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2}\Big) \\ &= -\frac{1}{2\Delta x^2}\sum_{j=1}^{N} \mathrm{Re}\big((\bar{v}_{j+1} - \bar{v}_{j-1})(v_{j+1} + v_{j-1})\big) \\ &= -\frac{1}{2\Delta x^2}\sum_{j=1}^{N} \big(|v_{j+1}|^2 - |v_{j-1}|^2\big) \\ &= -\frac{1}{2\Delta x^2}\big(|v_{N+1}|^2 + |v_N|^2 - |v_1|^2 + |v_0|^2\big)\end{aligned}$$

are zero for periodic boundary conditions. There is one term left, namely

$$\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big(i(\bar{v}_{j+1} - \bar{v}_{j-1})i|v_j|^2 v_j\big) = -\frac{1}{2}\sum_{j=1}^{N} \mathrm{Re}\big((\bar{v}_{j+1} - \bar{v}_{j-1})|v_j|^2 v_j\big).$$

It is worth noting that this expression can be regarded as the Poisson bracket (see e.g. [46]) of the momentum and the nonlinear part of the Hamiltonian. In contrary to any of the other terms it cannot be reduced to its boundary terms. Hence, it does not vanish for periodic or any other boundary conditions. In fact, the group of translations, which is the symmetry that correspond to the momentum, does not act on the solutions of the nonlinear Schrödinger equation on a discrete grid.

For the sake of completeness, we briefly consider the discrete Hamiltonian

$$H(v) = \frac{\Delta x}{2} \sum_{j=1}^{N} \left(\frac{|v_{j+1} - v_j|^2}{\Delta x^2} + \frac{|v_j|^4}{2} \right).$$

The derivative takes the form

$$\langle \mathrm{d}H(v), y \rangle = \Delta x \sum_{j=1}^{N} \mathrm{Re}\Big(- \frac{\bar{v}_{j+1} - 2\bar{v}_j + \bar{v}_{j-1}}{\Delta x^2} + |v_j|^2 \bar{v}_j \Big) y_j,$$

which leads to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Big[H(v)\Big] &= \langle \mathrm{d}H(v), v_t \rangle = \langle \mathrm{d}H(v), i\partial^2 v + i|v|^2 v + i\mu_1 v + \mu_2 \partial^1 v \rangle \\ &= \frac{\mu_1}{\Delta x}\big(\mathrm{Re}(i\bar{v}_N v_{N+1}) - \mathrm{Re}(i\bar{v}_0 v_1)\big) \\ &\quad - \frac{\mu_2}{2\Delta x^2}\big(|v_{N+1}|^2 - |v_{N-1}|^2 - |v_2|^2 + |v_0|^2\big) \\ &\quad - \frac{\mu_2}{2} \sum_{j=1}^{N} \mathrm{Re}\big((\bar{v}_{j+1} - \bar{v}_{j-1})|v_j|^2 v_j\big). \end{aligned}$$

Let us summarize the time dependency of the discrete versions of mass, momentum and energy.

Proposition 4.2.1. *For the discrete mass Q_1, the discrete momentum Q_2, and the discrete energy H we obtain the identities*

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big] &= 0, \\ \frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] &= -\frac{1}{2} \sum_{j=1}^{N} \mathrm{Re}\big((\bar{v}_{j+1} - \bar{v}_{j-1})|v_j|^2 v_j\big), \\ \frac{\mathrm{d}}{\mathrm{d}t}\Big[H(v)\Big] &= -\frac{\mu_2}{2} \sum_{j=1}^{N} \mathrm{Re}\big((\bar{v}_{j+1} - \bar{v}_{j-1})|v_j|^2 v_j\big), \end{aligned}$$

where $t \mapsto (v_1, ..., v_N)$ forms a solution of the discretization of (4.1.9) via finite differences with periodic boundary conditions $v_0 = v_N$ and $v_{N+1} = v_1$.

4.2.2 Spectral Galerkin Method

The conservation of the momentum and energy can be ensured by using a spectral collocation method instead. In the following, we briefly describe this approach. For further details we refer to [26] and the references therein.

A function $\mathbf{v} \in H^1_{\text{per}}\big((x_-, x_+); \mathbb{C}\big)$ can be written as a Fourier series

$$\mathbf{v}(t,x) = \sum_{j\in\mathbb{Z}} v_j(t) e^{ijx}$$

with Fourier coefficients v_j and trigonometric functions e^{ijx}. Next, we truncate this spectral representation, namely we approximate

$$\mathbf{v}(t,x) \approx \sum_{j\in\mathcal{Z}_K} v_j(t) e^{ijx}. \tag{4.2.3}$$

Here, the index j runs over the finite set

$$\mathcal{Z}_K = \{-K, ..., K-1\} \subseteq \mathbb{Z}.$$

Differential operators and derivatives take a very simple form with respect to this representation. In particular, we have

$$\begin{aligned}\partial^1 v &= \sum_{j\in\mathcal{Z}_K} ijv_j e^{ijx},\\ \partial^2 v &= \sum_{j\in\mathcal{Z}_K} (-j^2)v_j e^{ijx},\end{aligned}$$

which can be rewritten componentwise as

$$\begin{aligned}(\partial^1 v)_j &= ijv_j,\\ (\partial^2 v)_j &= (-j^2)v_j.\end{aligned}$$

However, this does not come without a drawback. The spectral representation of the nonlinear part, which is a pointwise product in spatial coordinates, is given (see [25]) by the discrete convolution

$$\mathcal{K}(v) = \sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \bar{v}_{j_2} v_{j_3} v_{j_4} e^{ij_1 x}.$$

Consequently, its coefficients are

$$\mathcal{K}_{j_1}(v) = \sum_{\substack{j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \bar{v}_{j_2} v_{j_3} v_{j_4}.$$

In the same way as before, we check one by one the time evolution of the truncated versions of mass, momentum and energy. The spectral representation of the truncated mass functional is

$$Q_1(v) = \frac{1}{2}\sum_{j\in\mathcal{Z}_K} |v_j|^2.$$

Here, we have to remark that we leave out the proper scaling factor

$$\frac{1}{K}\frac{\pi}{x_+ - x_-}.$$

In contrary to Δx, which plays the same role in Section 4.2.1, it remains unchanged during computations and can be omitted. Differentiation of the truncated mass functional leads to

$$\langle \mathrm{d}Q_1(v), y\rangle = \sum_{j\in\mathcal{Z}_K} \mathrm{Re}(\bar{v}_j y_j).$$

Hence, the total derivative with respect to time takes the form

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_1(v)\Big] &= \langle \mathrm{d}Q_1(v), i\partial^2 v + i\mathcal{K}(v) + i\mu_1 v + \mu_2\partial^1 v\rangle \\ &= \sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big(\bar{v}_j(-ij^2 v_j + i\mathcal{K}_j(v) + i\mu_1 v_j + i\mu_2 j v_j)\big).\end{aligned}$$

For any $\lambda_j \in \mathbb{R}$ we have $\mathrm{Re}\big(i\lambda_j|v_j|^2\big) = 0$, which implies that all but one term equals zero. The remaining sum is given by

$$\sum_{j_1\in\mathcal{Z}_K} \mathrm{Re}(i\bar{v}_{j_1}\mathcal{K}_{j_1}(v)) = \sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K \\ j_1+j_2=j_3+j_4}} \mathrm{Re}(i\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}),$$

which can be seen to vanish by mapping $(j_1, j_2, j_3, j_4) \mapsto (j_3, j_4, j_1, j_2)$ since it holds

$$\mathrm{Re}(i\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}) = -\mathrm{Re}(i\bar{v}_{j_3}\bar{v}_{j_4}v_{j_1}v_{j_2}).$$

A little more involved is the analysis of the time evolution of the truncated momentum

$$Q_2(v) = \frac{1}{2}\sum_{j\in\mathcal{Z}_K} j|v_j|^2$$

with its derivative given by

$$\langle \mathrm{d}Q_2(v), y\rangle = \sum_{j\in\mathcal{Z}_K} \mathrm{Re}(j\bar{v}_j y_j).$$

For the total derivative with respect to time we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big[Q_2(v)\Big] &= \langle \mathrm{d}Q_2(v), i\partial^2 v + i\mathcal{K}(v) + i\mu_1 v + \mu_2\partial^1 v\rangle \\ &= \sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big(j\bar{v}_j(-ij^2 v_j + i\mathcal{K}_j(v) + i\mu_1 v_j + i\mu_2 j v_j)\big).\end{aligned}$$

In the same way as above, all but one term are of the form $\mathrm{Re}\big(i\lambda_j|v_j|^2\big)$ with $\lambda_j \in \mathbb{R}$. Furthermore, for the remaining term we obtain the expression

$$\begin{aligned}\sum_{j_1\in\mathcal{Z}_K} \mathrm{Re}(j_1\bar{v}_{j_1} i\mathcal{K}_{j_1}(v)) &= \sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \mathrm{Re}(ij_1\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4})\\ &= \frac{1}{2}\sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \mathrm{Re}\big(i(j_1-j_2)\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}\big)\\ &\quad - \frac{1}{2}\sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \mathrm{Re}\big(i(j_1+j_2)\bar{v}_{j_3}\bar{v}_{j_4}v_{j_1}v_{j_2}\big),\end{aligned}$$

which equals zero. Indeed, by mapping $(j_1, j_2, j_3, j_4) \mapsto (j_2, j_1, j_3, j_4)$, we get

$$\sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \mathrm{Re}\big(i(j_1-j_2)\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}\big) = 0$$

from $j_1 + j_2 = j_2 + j_1$ and $\bar{v}_{j_1}\bar{v}_{j_2} = \bar{v}_{j_2}\bar{v}_{j_1}$. Moreover, from the identity

$$\begin{aligned}\mathrm{Re}\big(i(j_1+j_2)\bar{v}_{j_3}\bar{v}_{j_4}v_{j_1}v_{j_2}\big) &= \mathrm{Re}\big(i(j_3+j_4)\bar{v}_{j_3}\bar{v}_{j_4}v_{j_1}v_{j_2}\big)\\ &= -\mathrm{Re}\big(i(j_3+j_4)\bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}\big),\end{aligned}$$

which holds due to $j_1 + j_2 = j_3 + j_4$, we conclude

$$\sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \mathrm{Re}\big(i(j_1+j_2)\bar{v}_{j_3}\bar{v}_{j_4}v_{j_1}v_{j_2}\big) = 0$$

by mapping $(j_1, j_2, j_3, j_4) \mapsto (j_3, j_4, j_1, j_2)$. The last functional we consider is the truncated energy

$$H(v) = \frac{1}{2}\sum_{j\in\mathcal{Z}_K} j^2|v_j|^2 - \frac{1}{4}\sum_{\substack{j_1,j_2,j_3,j_4\in\mathcal{Z}_K\\ j_1+j_2=j_3+j_4}} \bar{v}_{j_1}\bar{v}_{j_2}v_{j_3}v_{j_4}.$$

Differentiation of this expression leads to

$$\langle \mathrm{d}H(v), y\rangle = \sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big((j^2\bar{v}_j - \mathcal{K}_j^\star(v))y_j\big),$$

where $\mathcal{K}_j^\star(v)$ is the complex conjugate of $\mathcal{K}_j(v)$. As a consequence, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big[H(v)\Big] &= \langle \mathrm{d}H(v), i\partial^2 v + i\mathcal{K}(v) + i\mu_1 v + \mu_2\partial^1 v\rangle\\ &= \sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big((j^2\bar{v}_j - \mathcal{K}_j^\star(v))(-ij^2v_j + i\mathcal{K}_j(v) + i\mu_1 v_j + i\mu_2 j v_j)\big),\end{aligned}$$

which vanishes. Indeed, the term

$$\sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big((j^2\bar{v}_j - \mathcal{K}_j^\star(v)\big)\big(-ij^2v_j + i\mathcal{K}_j(v)\big) = -\sum_{j\in\mathcal{Z}_K} \mathrm{Re}\big(i|j^2\bar{v}_j - \mathcal{K}_j(v)|^2\big)$$

is zero because $|j^2 v_j - \mathcal{K}_j(v)|^2$ is real-valued, and the other terms already appeared in the previous computations. The following table sums up the conservation properties of the finite difference method (FDM) and the spectral Galerkin method (SGM).

	Mass	Momentum	Energy
FDM	✓		
SGM	✓	✓	✓

4.3 Split-step Fourier Method

A numerical scheme is derived by splitting the freezing equation

$$iv_t = -v_{xx} - |v|^2 v - \mu_1 v + i\mu_2 v_x$$

into a linear part

$$iv_t = -v_{xx} - \mu_1 v + i\mu_2 v_x \tag{4.3.1}$$

with its flow denoted by Φ_L^t and the remaining nonlinear part

$$iu_t = -|u|^2 u$$

with its flow given by

$$\Phi_N^t(v) = \exp(it|v|^2)v.$$

The linear problem (4.3.1) is equivalent to

$$i[\mathcal{F}u]_t(\xi, t) = (\xi^2 - \mu_1 - \mu_2\xi)[\mathcal{F}u](\xi, t)$$

in Fourier variables. This decoupled system of ordinary equations can be computed exactly. We get

$$[\mathcal{F}u](\xi, t) = e^{-i(\xi^2 - \mu_1 - \mu_2\xi)t}[\mathcal{F}u](\xi, 0)$$

for $\xi \in \mathbb{Z}$ and $t \geq 0$. Given a step size $\Delta t > 0$ we now apply the Strang splitting scheme (see [20], [35], [53], [62]), which is written as

$$\Phi_{L+N}^{\Delta t} \approx \Phi_N^{\frac{1}{2}\Delta t} \circ \Phi_L^{\Delta t} \circ \Phi_N^{\frac{1}{2}\Delta t}.$$

More precisely, the algorithm to compute a new time step reads

1. Nonlinear part with step size $\frac{\Delta t}{2}$,
2. Fourier Transform,
3. Linear part with step size Δt,
4. Inverse Fourier Transform,

5. Nonlinear part with step size $\frac{\Delta t}{2}$.

In an attempt to preserve the time efficiency of the Strang splitting, we do not solve the PDAE, but derive an explicit formula to compute μ_1 and μ_2 in each step. First of all, we differentiate at least formally the fixed phase condition with respect to t and insert $v_t = F(v) - \mathrm{d}[a(\mathbb{1})v]\mu$ and obtain

$$\mathrm{d}[a(\mathbb{1})\hat{v}]^* F(v) - \mathrm{d}[a(\mathbb{1})\hat{v}]^* \mathrm{d}[a(\mathbb{1})v]\mu = 0, \tag{4.3.2}$$

where the adjoint of $\mathrm{d}[a(\mathbb{1})v]$ with respect to the inner product $\big(\cdot,\cdot\big)_0$ is given by

$$\mathrm{d}[a(\mathbb{1})v]^\star \colon X \to \mathcal{A}^\star, \quad \langle \mathrm{d}[a(\mathbb{1})v]^\star y, \sigma\rangle = \big(\mathrm{d}[a(\mathbb{1})v]\sigma, y\big)_0.$$

If the stabilizer $G_{\hat{v}} = \{g \in G \mid a(g)\hat{v} = \hat{v}\}$ of $\hat{v}$ is trivial and v is sufficiently close to $\hat{v}$, then $\mathrm{d}[a(\mathbb{1})\hat{v}]^\star \mathrm{d}[a(\mathbb{1})v] \in L(\mathcal{A}; \mathcal{A}^\star)$ is non-singular and (4.3.2) defines a set of d linear independent equations, where d is the dimension of $\mathcal{A}$. In fact, this is a special form of Assumption 2.2.11.

By solving (4.3.2) with respect to μ, we obtain

$$\hat{\mu}(v) = \big(\mathrm{d}[a(\mathbb{1})\hat{v}]^\star \mathrm{d}[a(\mathbb{1})v]\big)^{-1} \mathrm{d}[a(\mathbb{1})\hat{v}]^\star F(v).$$

Hence, the freezing equation in the eliminated form is given by

$$v_t = F(v) - \mathrm{d}[a(\mathbb{1})v]\big(\mathrm{d}[a(\mathbb{1})\hat{v}]^\star \mathrm{d}[a(\mathbb{1})v]\big)^{-1} \mathrm{d}[a(\mathbb{1})\hat{v}]^\star F(v).$$

By choosing a smooth enough template function $\hat{v}$, the operator in (4.3.2) can be continuously expanded to a phase condition

$$\psi_{\mathrm{fix}} \colon X \times \mathcal{A} \to \mathcal{A}^\star$$

for $v \in X$ and $\mu \in \mathcal{A}$.

In our specific example resolving the fixed phase condition with respect to μ leads to

$$\hat{\mu}(v) = -\begin{bmatrix} \big(-i\hat{v}, -iv\big)_0 & \big(-i\hat{v}, -v_x\big)_0 \\ \big(-\hat{v}_x, -iv\big)_0 & \big(-\hat{v}_x, -v_x\big)_0 \end{bmatrix}^{-1} \begin{bmatrix} \big(i\hat{v}, iv_{xx} + |v|^2 v\big)_0 \\ \big(\hat{v}_x, iv_{xx} + |v|^2 v\big)_0 \end{bmatrix},$$

which continuously expands to

$$\hat{\mu}(v) = \begin{bmatrix} \big(\hat{v}, v\big)_0 & \big(i\hat{v}, v_x\big)_0 \\ \big(\hat{v}_x, iv\big)_0 & \big(\hat{v}_x, v_x\big)_0 \end{bmatrix}^{-1} \begin{bmatrix} \big(\hat{v}_x, v_x\big)_0 - \big(i\hat{v}, |v|^2 v\big)_0 \\ \big(\hat{v}_{xx}, iv_x\big)_0 - \big(\hat{v}_x, |v|^2 v\big)_0 \end{bmatrix}$$

for $\hat{v} \in H^2(\mathbb{R}; \mathbb{C})$.

Chapter 5

Numerical Computations

In Section 4.3 we have introduced a numerical scheme to solve the freezing system for the nonlinear Schrödinger equation. The main idea is to apply the Strang splitting in order to decompose the problem into two parts that are analytically (or at least more efficiently) solvable. In the following, we present numerical results, whereas the stability analysis for the fully discretized problem goes beyond the scope of this thesis. For analytical results on the geometric numerical integration of the NLS we refer to [20], the so-called backward error analysis for ordinary differential equations can be found in [34].

In addition to the NLS, we make use of the freezing method to tackle the nonlinear Klein-Gordon equation and the Korteweg-de Vries equation. In order to guarantee comparability, we stick to the Strang splitting and choose the same parameters. To be more precise, the time step size

$$\Delta t = 10^{-3}$$

and the number of Fourier nodes

$$2K = 256$$

always remain the same. After inverse Fourier transform, this results in an equidistant grid on $[x_-, x_+]$, where the upper and lower bound are given by

$$x_+ = -x_- = \frac{\pi}{0.11} \approx 28.56,$$

and the step size of this spatial grid is

$$\Delta x = \frac{1}{K}\frac{\pi}{0.11} \approx 0.223.$$

In case of the NLS, we have an explicit formula for the solution of the nonlinear part in the Strang Splitting. For the NLKG and the KdV, we make use of the implicit midpoint scheme

$$\Phi_f^{\Delta t}(v) = v + \Delta t\, f\left(\frac{v + \Phi_f^{\Delta t}(v)}{2}\right),$$

which is computed via fixed point iteration.

5.1 Nonlinear Schrödinger Equation

We consider the solitary wave solution of the NLS that is given by the parameters

$$\mu_\star = \begin{pmatrix} -1.0225 \\ 0.3 \end{pmatrix},$$

where we recall that the first component refers to the gauge transformation, whereas the second describes the velocity of the translation. These parameters solve the equation

$$\sqrt{-\left(\mu_1 + \tfrac{\mu_2^2}{4}\right)} = 1,$$

which implies that the scaling factor in (1.3.11) equals one. Hence, the profile takes the form

$$v_\star(x) = \frac{\sqrt{2}}{\cosh(x)} e^{i\,0.3\frac{x}{2}}.$$

Before we apply the freezing method, it appears expedient to have a look at the solution of the original problem, where we choose the above profile as our initial data.

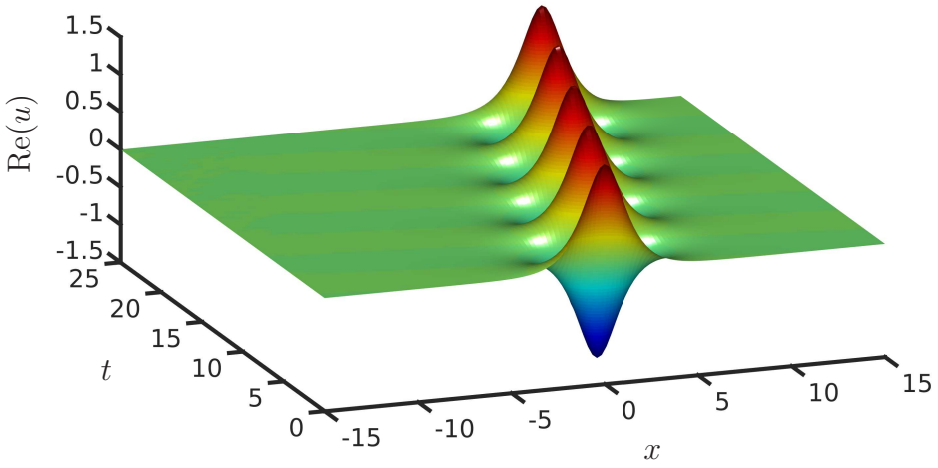


Figure 5.1.1: Solution of the original problem

The solitary wave can be understood as a consequence of the equivariance of the NLS with respect to the two-parameter group of gauge transformations and translations. As expected, we observe an oscillation and translation in our numerical approximation of the solution

$$u_\star(t,x) = e^{it} v_\star(x - 0.3t).$$

Accordingly, the imaginary part is the same as the real part, except for a constant phase shift. In the following, this is subject to change, as we apply the freezing method.

As intended, the solution of the freezing system does neither oscillate nor translate. Hence, the profile is, up to discretization and computation errors, a proper steady state.

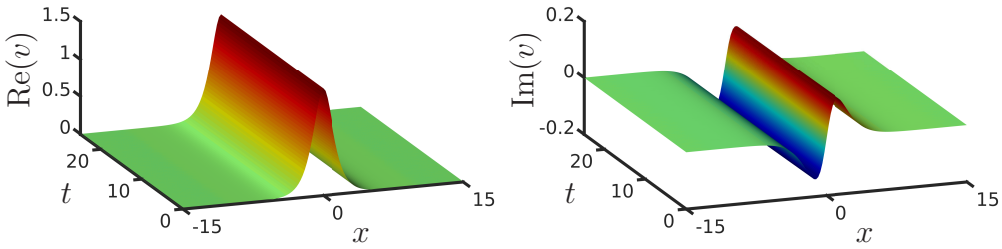


Figure 5.1.2: Solution of the freezing system

We notice that the imaginary part is of a different scale since the initial data are set up in such a way that the extreme values of the imaginary part are much smaller than the maximum of the real part. However, the imaginary part plays an important role by allowing the wave to travel. If we replace the initial data by $\frac{\sqrt{2}}{\cosh(x)}$, then no translation occurs. This is due to the fact that symmetry with respect to the y-axis is preserved by the flow of the NLS, and this symmetry is broken by the imaginary part being an odd function. Consequently, reflection of the initial data at the y-axis leads to a solitary wave that travels with the same velocity, but in the opposite direction.

Let us also have a look at the values of μ_1 and μ_2 that were obtained by our numerical computation.

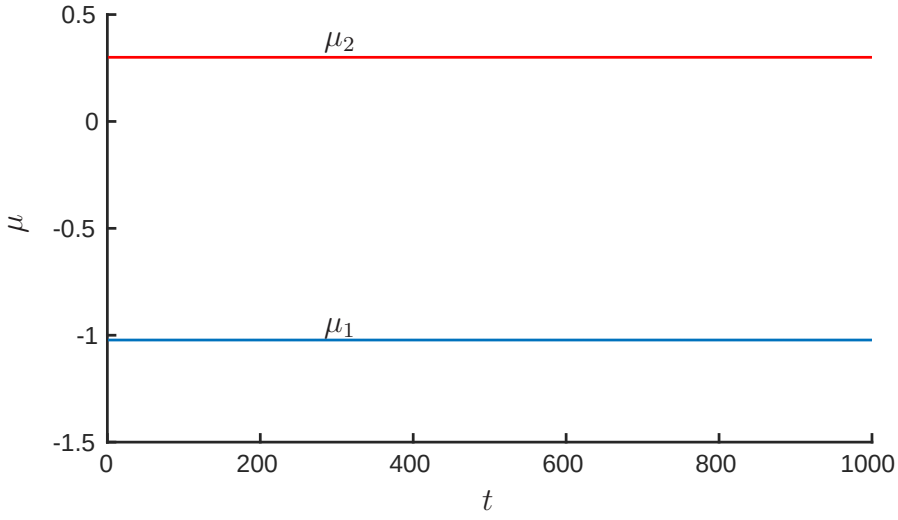


Figure 5.1.3: Frequency and Velocity

The blue line corresponds to oscillation, whereas the red line describes the velocity of translation. We have to emphasize that, as described in Section 4.3, we do not solve the PDAE system, but in each step compute μ in a preliminary calculation before we treat the linear part. While this is highly efficient, the

numerical solution does not necessarily stay on the manifold given by the phase condition, and any deviation effects the subsequent steps. Nevertheless, the values of μ_1 and μ_2 appear quite constant.

However, this is no longer true as soon as we consider perturbed initial data. The perturbation is generated by calling `rng('default')` and `rand(1,2*K)` in MATLAB. Then we multiply this vector by the perturbation factor $\frac{\varrho}{100}$ and add the result to the real part of the profile $v_\star$, which has already served as the initial data for the unperturbed problem.

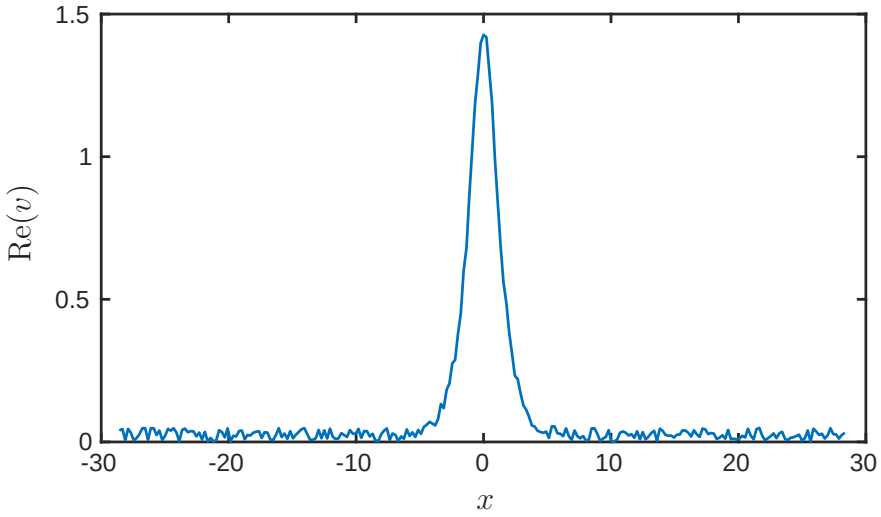


Figure 5.1.4: Perturbed initial data ($\varrho = 5$)

On the considerably large time interval $\mathcal{I} = [0, 1000]$ the profile remains in place, and in the same way, the oscillation is reduced to a negligible level.

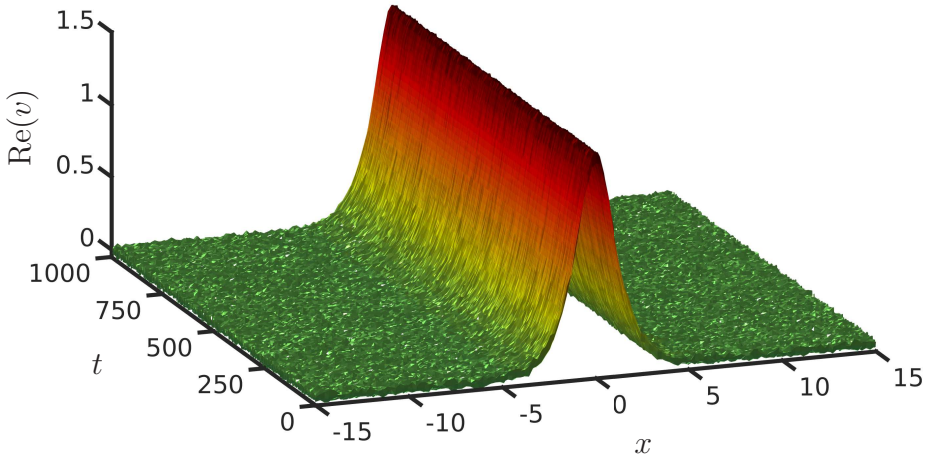


Figure 5.1.5: Solution of the perturbed problem ($\varrho = 5$)

But, in contrary to dissipative systems, perturbations do not die out. This

is due to the fact, that the linerization at the relative equilibrium has a purely imaginary spectrum. The asymptotic stability, which one can find in parabolic problems, does not occur in the Hamiltonian systems that we consider.

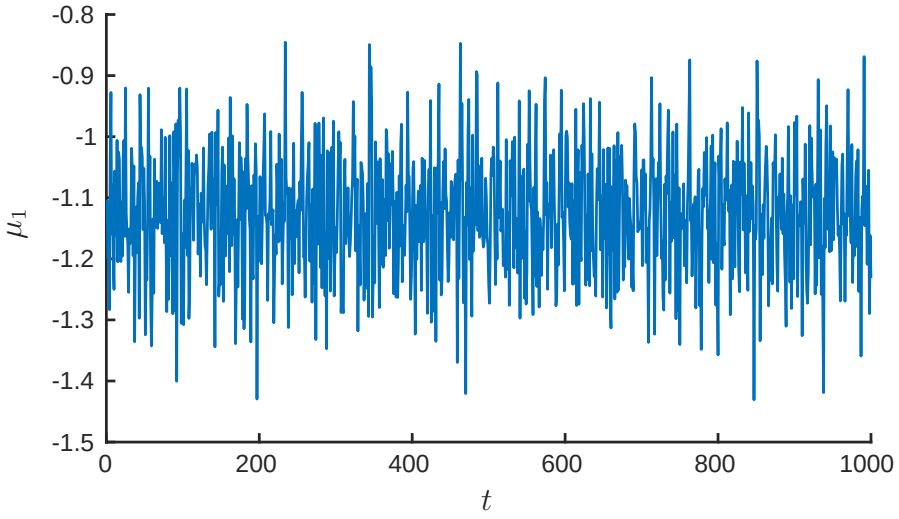


Figure 5.1.6: Frequency ($\varrho = 5$)

This has even more serious consequences for the frequency μ_1 and the velocity μ_2. Since the initial deviations never extinct, both components of μ fluctuate continuously.

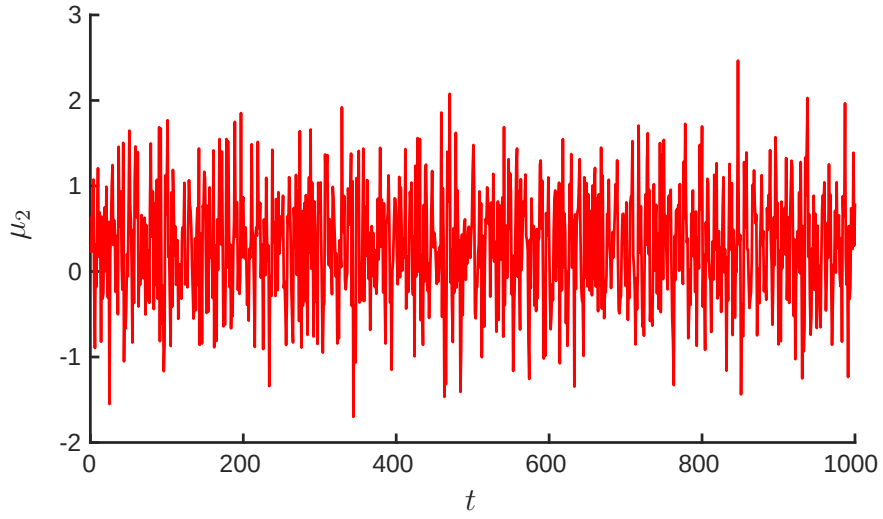


Figure 5.1.7: Velocity ($\varrho = 5$)

However, we must acknowledge that the high intensity of fluctuation is caused by the numerical scheme. Giving up the operator splitting, solving the PDAE system by the implicit midpoint scheme, and thereby complying the phase condition for all times, is highly recommended for much larger perturbations and leads to less fluctuation.

While we do not present any results for different values of $\mu_\star$, we want to remark that the oscillation tends to stabilize the profile, whereas the translation behaves to the contrary in numerical computations. We also have to mention that the choice of a perturbation with positive real numbers is completely arbitrary.

Next, we numerically analyze the stability of the relative equilibrium. What we mean by stability is that deviations for all (or at least over long) times remain small if the initial perturbation is small enough. This, of course, corresponds to our stability result in Section 2.3, even though the abstract theory does not include the impact of spatial discretization and time stepping. In order to sustain the theoretical by numerical results, we compare the deviations that occur for those initial perturbations that correspond to the parameters

$$\varrho \in \{4, 2, 1, 0.5, 0.25\}.$$

With respect to the discrete L^2-norm

$$\|v\|_{\Delta x,K,L^2} = \Delta x \sqrt{\sum_{j\in\mathcal{Z}_K} |v_j|^2},$$

where $\mathcal{Z}_K = \{-K, ..., K-1\} \subseteq \mathbb{Z}$, we compute the difference of the perturbed problem and the steady state of the unperturbed problem.

We should emphasize that we do not numerically solve the unperturbed stationary problem, but assume that the projection of the steady state of the continuous problems is close enough to the discrete steady state. The corresponding abstract result in Section 3.4 can be applied to the NLS, but only in the case of the one-parameter group of gauge transformations.

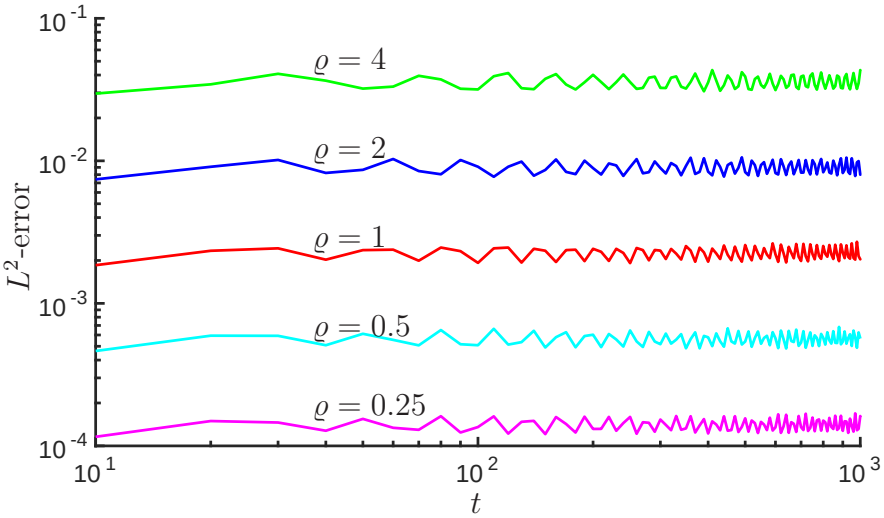


Figure 5.1.8: L^2-error

For the presentation of the results, a double logarithmic scale plot is used. We can see that for any parameter $\varrho \in \{4, 2, 1, 0.5, 0.25\}$ the L^2-error on the entire time interval $\mathcal{I} = [0, 1000]$ remains close to the initial deviation.

In addition to that, we consider the same errors in the discrete norm of the homogeneous Sobolev space $\dot{H}^1$, which is given by

$$\|u\|_{\Delta x,K,\dot{H}^1} = \Delta x \sqrt{\sum_{j\in\mathcal{Z}_K} \left|\left(\mathcal{F}^{-1}_{\Delta x,K}\, p_1 \mathcal{F}_{\Delta x,K} u\right)_j\right|^2}$$

with $p_1(\xi) = i\xi$. Here, the operations $\mathcal{F}^{-1}_{\Delta x,K}$ and $\mathcal{F}^{-1}_{\Delta x,K}$ are carried out by the fast Fourier transform in MATLAB.

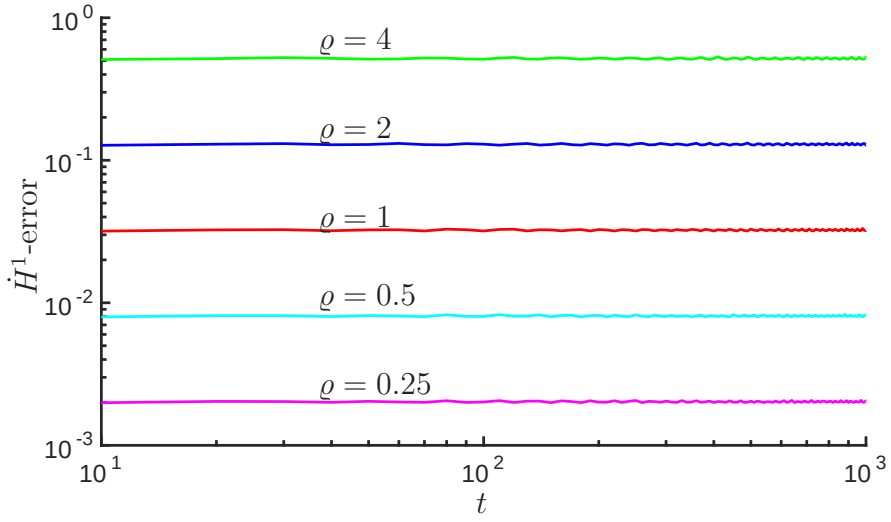


Figure 5.1.9: $\dot{H}^1$-error

As for the L^2-error, we observe a stable behavior of the profile with respect to the $\dot{H}^1$-norm. Here, we should point out that the scale on the y-axis is different.

The question arises, whether the profile remains stable for other types of perturbation. Instead of adding a global perturbation, we now locally modify the initial data.

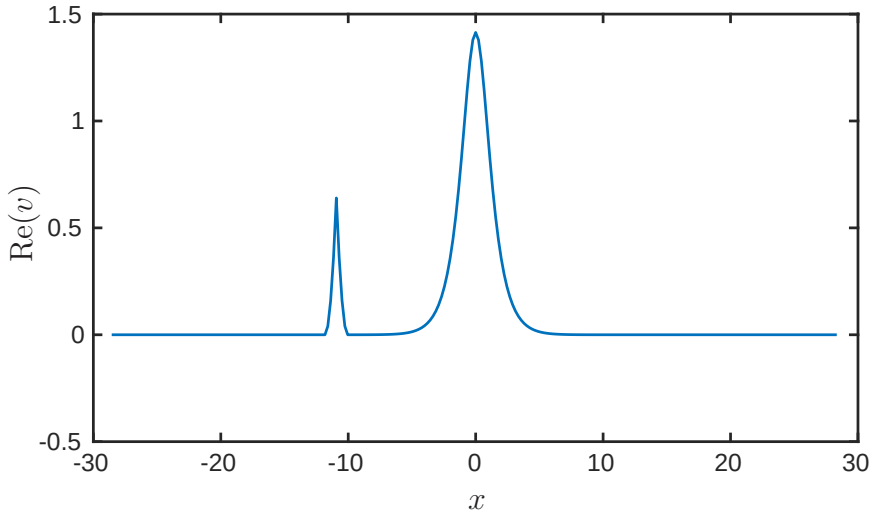


Figure 5.1.10: Local perturbation ($\ell = 4$)

We choose the peak to be roughly at -10.933 and create a perturbation based on the sequence 1, 4, 9, 16, 9, 4, 1, which we again multiply by a perturbation factor $\frac{\ell}{100}$. In particular, only an area of $\pm 4\Delta x$ around the peak is effected by the initial perturbation.

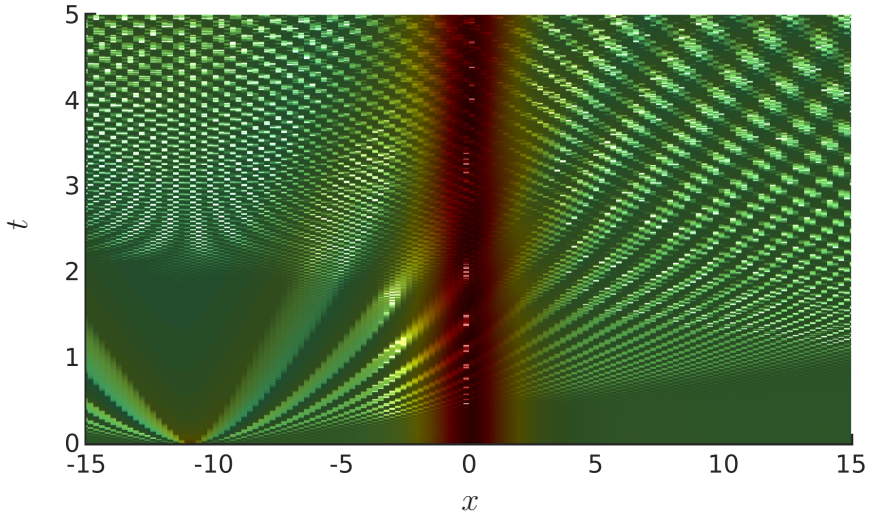


Figure 5.1.11: Time-space plot ($\ell = 4$)

In contrary to the red profile, which remains centered at $x = 0$, the freezing method hardly effects the additional peak. On the short time scale $\mathcal{I} = [0, 5]$ the top view gives us an impression of the rapid propagation of the perturbation and the interference of the wave fronts.

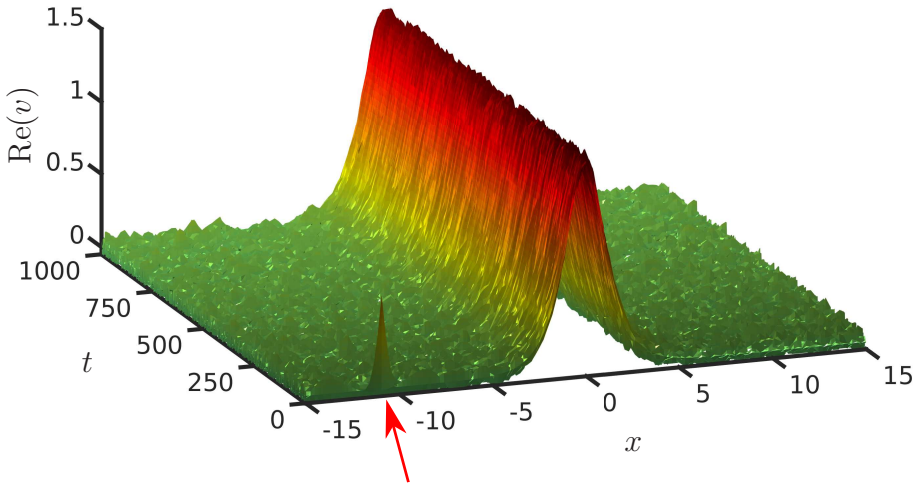


Figure 5.1.12: Solution of the locally perturbed problem ($\ell = 4$)

On the larger time scale $[0, 1000]$ the localization ceases to exist really soon. The red arrow points at the initial peak.

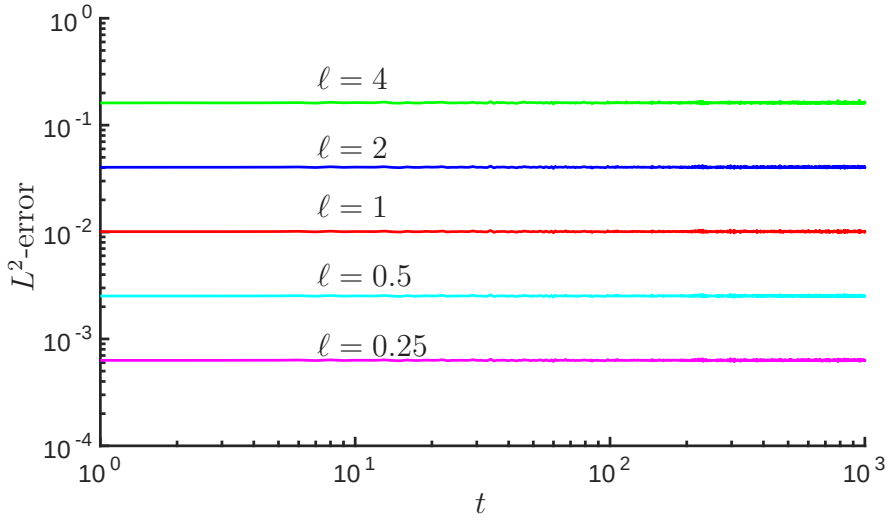


Figure 5.1.13: L^2-error - local perturbation

In the same way as before, the errors in the L^2-norm and $\dot{H}^1$-seminorm remain fairly close to the corresponding initial deviation. We should emphasize that the scale is different from the error plots for the global perturbation, and that there is no intuitive relation of ϱ and ℓ.

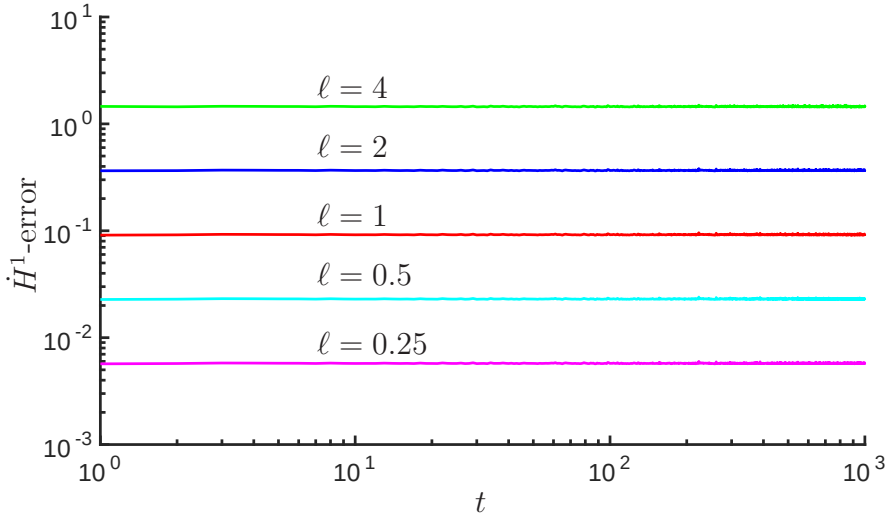


Figure 5.1.14: $\dot{H}^1$-error - local perturbation

Before we turn our focus to our next numerical example, the nonlinear Klein-Gordon equation, we first consider the NLS with another phase condition, to be more precise, the orthogonality phase condition from [6]. The basic setting is the same, in particular, the Gelfand triple

$$X \hookrightarrow X_0 = X_0^\star \hookrightarrow X^\star$$

remains unchanged. However, we require $\left\|v_t\right\|_0^2$ to be minimal at any time in-

stance. As a necessary condition this yields

$$\big(\mathrm{d}[a(\mathbb{1})v]\sigma, v_t\big)_0 = 0, \quad \sigma \in \mathcal{A},$$

and inserting the right hand side of the differential equation leads to

$$\big(\mathrm{d}[a(\mathbb{1})v]\sigma, F(v) - \mathrm{d}[a(\mathbb{1})v]\mu\big)_0 = 0, \quad \sigma \in \mathcal{A}.$$

By solving this equation with respect to μ, we obtain the implicit function

$$\hat{\mu}(v) = \big(\mathrm{d}[a(\mathbb{1})v]^\star \mathrm{d}[a(\mathbb{1})v]\big)^{-1} \mathrm{d}[a(\mathbb{1})]^\star F(v).$$

Here we recall that the adjoint of $\mathrm{d}[a(\mathbb{1})v]$ with respect to $\big(\cdot,\cdot\big)_0$ is given by

$$\mathrm{d}[a(\mathbb{1})v]^\star \colon X \to \mathcal{A}^\star, \quad \langle \mathrm{d}[a(\mathbb{1})v]^\star y, \sigma\rangle = \big(\mathrm{d}[a(\mathbb{1})v]\sigma, y\big)_0$$

for $y \in X$ and $\sigma \in \mathcal{A}$. By choosing a basis in the Lie algebra $\mathcal{A}$, the orthogonality phase condition is transformed into a system of d equations, where d is the dimension of $\mathcal{A}$.

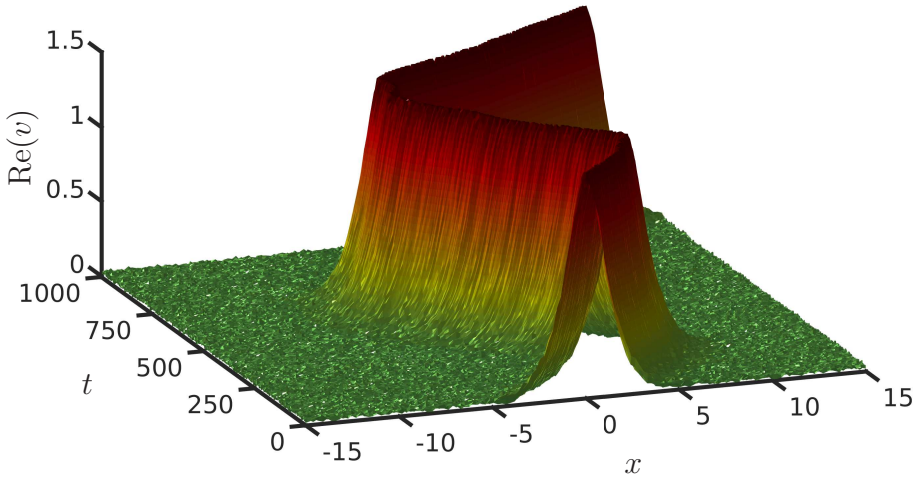


Figure 5.1.15: Orthogonality phase condition ($\varrho = 5$)

5.2 Nonlinear Klein-Gordon Equation

The NLKG, just like the NLS, possesses oscillating and traveling wave solutions, where the number of parameters depends on the dimension of the system. In case of complex-valued solutions the rotation group is only one-dimensional. Now that we consider solutions to the NLKG with images in $\mathbb{R}^3$, the rotation group is three-dimensional, which together with the translation gives us four free parameters. We select at will

$$\mu_\star = \begin{pmatrix} s_\star \\ c_\star \end{pmatrix} = \begin{pmatrix} 0.7 \\ 0.4 \\ 0.1 \\ 0.5 \end{pmatrix}.$$

By imposing the equation $S_\star \nu = s_\star \times \nu$, which we require for all $\nu \in \mathbb{R}^3$, the first three components $s_\star$ determine the rotation matrix

$$S_\star = \begin{pmatrix} 0 & -0.1 & 0.4 \\ 0.1 & 0 & -0.7 \\ -0.4 & 0.7 & 0 \end{pmatrix}.$$

The last component, which we denote by $c_\star = 0.5$, describes the velocity of the solitary wave. Compared to the previous example the deduction of the corresponding profile is much more involved. Since the NLKG is a second order evolution equation, we consider the transformation to a system of first order equations, which takes the form

$$u_t = \begin{pmatrix} u_2 \\ u_{1,xx} - u_1 + |u_1|^2 u_1 \end{pmatrix}. \tag{5.2.1}$$

In terms of the new variables (v, S, c), this system is rewritten as

$$v_t = \begin{pmatrix} v_2 - S v_1 - c v_{1,x} \\ v_{1,xx} - v_1 + |v_1|^2 v_1 - S v_2 - c v_{2,x} \end{pmatrix}.$$

As we have discussed in Section 1.3.2, the stationary problem can be reduced to the scalar equation

$$0 = (1 - c^2)\eta_{xx} + \frac{|s|^2}{1 - c^2}\eta - \eta + \eta^3,$$

the solution of which is given by

$$\eta_\star(x) = \frac{\sqrt{2\beta_\star}}{\cosh(\delta_\star x)}$$

with the two constants $\beta_\star = 1 - \dfrac{|s_\star|^2}{1 - c_\star^2}$ and $\delta_\star = \sqrt{\dfrac{\beta_\star}{1 - c_\star^2}}$. By writing

$$\xi_\star(x) = \eta_\star(x) e^{\alpha_\star x S_\star} \nu_\star$$

with $\alpha_\star = \dfrac{c_\star}{1 - c_\star^2}$, the profile takes the form

$$v_\star = \begin{pmatrix} \xi_\star \\ c_\star \xi_{\star,x} + S_\star \xi_\star \end{pmatrix}.$$

The vector $\nu_\star$ must be of unit length and orthogonal to $s_\star$, which is why we choose

$$\nu_\star = \frac{1}{\sqrt{17}} \begin{pmatrix} 0 \\ 1 \\ -4 \end{pmatrix}.$$

The solution to the original problem (5.2.1) takes the form

$$u_\star(t, x) = e^{t S_\star} v_\star(x + c_\star t),$$

and its behavior is not much different from those of the NLS. Each component of the solution is time-independent except for an oscillation and translation, which is caused by the equivariance of the NLKG.

Hence, we consider directly the solution to the freezing system with perturbed initial data. As before, we obtain a global perturbation by calling `rng('default')` and `rand(1,2*K)` in MATLAB, scale this vector by the perturbation factor $\frac{\varrho}{100}$, and add it to the first component of the exact profile.

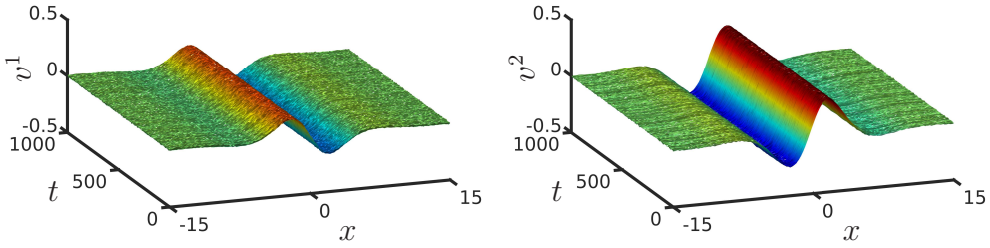


Figure 5.2.1: First and second component of the solution ($\varrho = 2$)

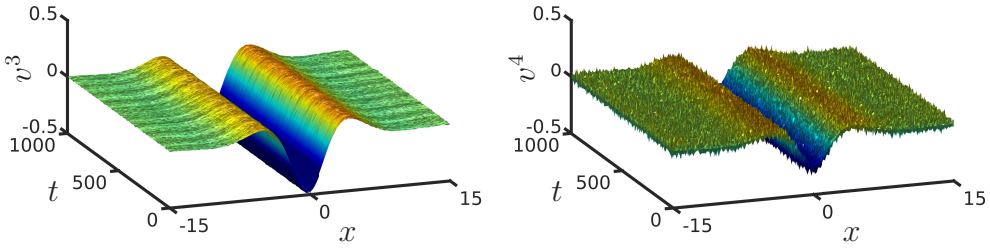


Figure 5.2.2: Third and fourth component of the solution ($\varrho = 2$)

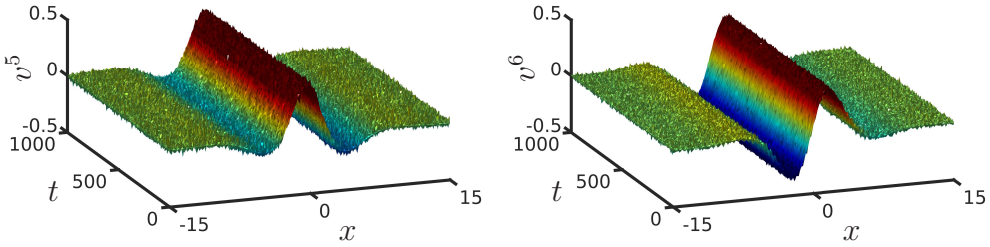


Figure 5.2.3: Fifth and sixth component of the solution ($\varrho = 2$)

On the time interval $[0, 1000]$ the solitary wave neither travels nor oscillates. But, as expected, the perturbations do not die out.

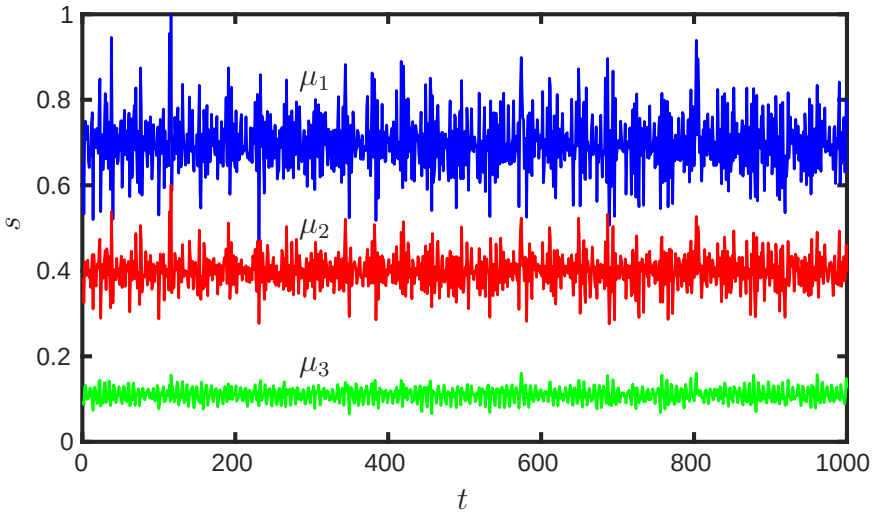


Figure 5.2.4: Frequencies ($\varrho = 2$)

The frequencies s and the velocity c fluctuate continuously, the latter with a huge margin even for the small perturbation that corresponds to $\varrho = 2$. As before, this is amplified by the numerical scheme.

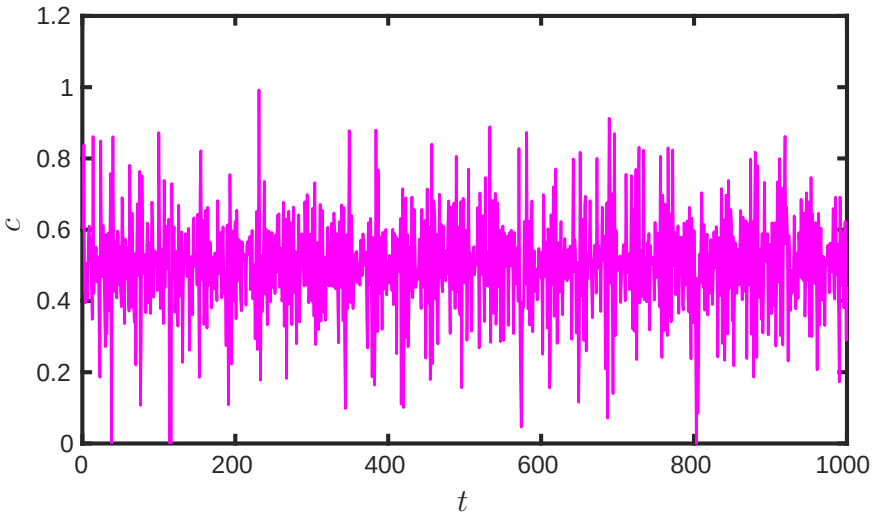


Figure 5.2.5: Velocity ($\varrho = 2$)

In order to analyze the stability of the relative equilibrium, we compute the difference of the perturbed and the unperturbed problem with respect to the discrete L^2-norm. As in the previous example, we compare the deviations that occur for initial perturbations that correspond to the parameters $\varrho \in \{4, 2, 1, 0.5, 0.25\}$. We observe a stable behavior for the small values $\varrho \in \{2, 1, 0.5, 0.25\}$, whereas for $\varrho = 4$ the linear systems to compute $\mu(t_n)$ become ill-posed after a few time-steps.

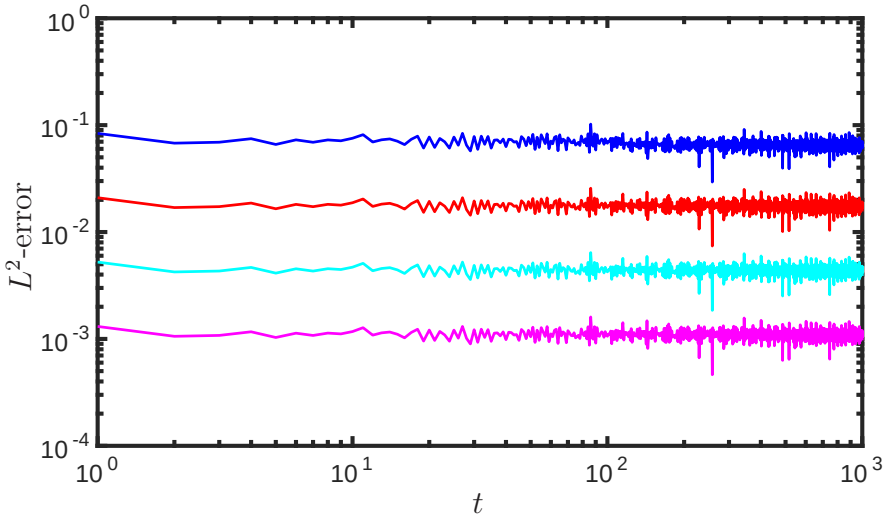


Figure 5.2.6: L^2-error

Let us remark that there is a compromise to settle this issue. Since we choose template functions of the form $\hat{v} = \begin{pmatrix} \hat{\xi} \\ 0 \end{pmatrix}$, the fixed phase condition does not depend on the nonlinearity $|v_1|^2 v_1$. Hence, it is an option to combine the Strang splitting with the PDAE formulation for the linear part of the problem and thereby reduce the fluctuation of the frequencies and of the velocity.

5.3 Korteweg-de Vries Equation

Our last numerical example is a mathematical model for surface water waves in a canal (see [42]). The Korteweg-de Vries equation (KdV)

$$u_t(t,x) = -u_{xxx}(t,x) - 6u(t,x)u_x(t,x), \quad u(0,x) = u_0(x) \tag{5.3.1}$$

can be written as an abstract evolution equation

$$u_t = F(u)$$

by setting

$$F(u) = -u_{xxx} - 6uu_x = -(u_{xx} + 3u^2)_x.$$

This function splits into two parts, the linear part $L(u) = u_{xxx}$ and the Burgers' nonlinearity $N(u) = 6uu_x$. Hence, the KdV is a nonlinear perturbation of the Airy equation

$$u_t(t,x) = -u_{xxx}(t,x).$$

We refer to [9] and [40] for the well-possedness of the inital value problem for the KdV. The main difference compared to the previous examples is the order of

the highest derivative. In order to deal with the additional derivative, a suitable symplectic form (see [46]) is given by

$$\omega(u,v) = \frac{1}{2}\int_{\mathbb{R}} \big(\mathrm{d}^{-1}u(x)v(x) - \mathrm{d}^{-1}v(x)u(x)\big)\mathrm{d}x = \big(\mathrm{d}^{-1}u, v\big)_0. \tag{5.3.2}$$

Here, the operator d^{-1} takes the form

$$\mathrm{d}^{-1}v = \mathcal{F}^{-1}\frac{1}{i\rho(\xi)}\mathcal{F}v,$$

where $\mathcal{F}$ is the Fourier transform and $\rho(\xi) = \xi$. As pointed out in [57], a suitable domain for this operator is the homogeneous Sobolev space $\dot{H}^{-\frac{1}{2}}(\mathbb{R};\mathbb{R})$, which is defined as

$$\dot{H}^s(\mathbb{R};\mathbb{R}) = \big\{v \in \mathcal{S}^\star(\mathbb{R};\mathbb{C})\colon \mathcal{F}^{-1}\dot{q}_s\mathcal{F}v \in L^2(\mathbb{R};\mathbb{C})\big\}$$

with $\dot{q}_s(\xi) = |\xi|^s$. Then d^{-1} is a bounded linear operator

$$\mathrm{d}^{-1}\colon \dot{H}^{-\frac{1}{2}}(\mathbb{R};\mathbb{R}) \to \dot{H}^{\frac{1}{2}}(\mathbb{R};\mathbb{R}),$$

and we obtain a continuous symplectic form

$$\omega\colon \dot{H}^{-\frac{1}{2}}(\mathbb{R};\mathbb{R}) \times \dot{H}^{-\frac{1}{2}}(\mathbb{R};\mathbb{R}) \to \mathbb{R}.$$

However, this homogeneous Sobolev space is not well-suited for the stability analysis of solitary waves. Without the convenience of having it fit into our abstract setting, we are forced to deal differently with the additional derivative in the linear part. Instead of the equation

$$\omega(u_t, y) = \langle \mathrm{d}H(u), y\rangle$$

for $y \in H^1(\mathbb{R};\mathbb{R})$, we rewrite the problem as

$$(u_t, y)_0 = -\langle \mathrm{d}H(u), y_x\rangle \tag{5.3.3}$$

for $y \in H^2(\mathbb{R};\mathbb{R})$. Consequently, we modify the abstract definition (1.2.11) for generalized solutions of the KdV.

Definition 5.3.1. Let $\mathcal{I} \subseteq \mathbb{R}$ be an interval. A function $u \in \mathcal{C}\big(\mathcal{I}; H^1(\mathbb{R};\mathbb{R})\big)$ is called a generalized solution of the KdV if we have

$$\int_{\mathcal{I}} \big(u(t), y\big)_0 \varphi_t(t)\mathrm{d}t = \int_{\mathcal{I}} \langle \mathrm{d}H(u(t)), y_x\rangle\varphi(t)\mathrm{d}t \tag{5.3.4}$$

for all $y \in H^2(\mathbb{R};\mathbb{R})$ and $\varphi \in \mathcal{C}_0^\infty(\mathcal{I}^\circ;\mathbb{R})$.

In the above sense, the KdV is a Hamiltonian partial differential equation, where the Hamiltonian on $H^1(\mathbb{R};\mathbb{R})$ is given by

$$H(u) = \int_{\mathbb{R}} \big(\tfrac{1}{2}u_x(x)^2 - u(x)^3\big)\mathrm{d}x. \tag{5.3.5}$$

Proposition 5.3.2. *The Hamiltonian (5.3.5) is associated with (5.3.1) in the sense that*

$$\big(F(u),v\big)_0 = \langle \mathrm{d}H(u), v_x\rangle$$

for all $u \in H^3(\mathbb{R};\mathbb{R})$ *and* $v \in H^2(\mathbb{R};\mathbb{R})$.

Proof. We start with the right hand side, the derivative of the Hamiltonian. The linear term already appeared in the previous examples. For the nonlinear term we get

$$\begin{aligned}\int_{\mathbb{R}} \big(u(x)+v(x)\big)^3\mathrm{d}x &= \int_{\mathbb{R}} u(x)^3\mathrm{d}x + \int_{\mathbb{R}} 3u(x)^2v(x)\mathrm{d}x \\ &\qquad + \int_{\mathbb{R}} \big(3u(x)+v(x)\big)v(x)^2\mathrm{d}x \\ &= \int_{\mathbb{R}} u(x)^3\mathrm{d}x + \int_{\mathbb{R}} 3u(x)^2v(x)\mathrm{d}x + \mathcal{O}\big(\|v\|_1^2\big)\end{aligned}$$

since $H^1(\mathbb{R};\mathbb{R})$ is a generalized Banach-algebra. This implies

$$H(u+v) = H(u) + \int_{\mathbb{R}} \big(u_x(x)v_x(x) - 3u(x)^2v(x)\big)\mathrm{d}x + \mathcal{O}\big(\|v\|_1^2\big),$$

whence we get

$$\langle \mathrm{d}H(u), v\rangle = \int_{\mathbb{R}} \big(u_x(x)v_x(x) - 3u(x)^2v(x)\big)\mathrm{d}x = \big(u_x, v_x\big)_0 - \big(3u^2, v\big)_0.$$

Furthermore, integration by parts yields

$$\begin{aligned}\big(F(u),v\big)_0 &= -\int_{\mathbb{R}} \big(u_{xx}(x) + 3u(x)^2\big)_x v(x)\mathrm{d}x \\ &= \int_{\mathbb{R}} \big(u_{xx}(x) + 3u(x)^2\big)v_x(x)\mathrm{d}x \\ &= -\big(u_x, v_{xx}\big)_0 + \big(3u^2, v_x\big)_0 \\ &= \langle \mathrm{d}H(u), v_x\rangle\end{aligned}$$

for all $u \in H^3(\mathbb{R};\mathbb{R})$ and $v \in H^2(\mathbb{R};\mathbb{R})$. □

The Korteweg-de Vries equation is equivariant under the action of a one-parameter translation group. This Lie group is simply $G = \mathbb{R}$ and the group action $a\colon G \to GL\big(H^1(\mathbb{R};\mathbb{R})\big)$ is given by

$$a(\gamma)v = v(\cdot - \gamma)$$

for $\gamma \in G = \mathbb{R}$. The derivative of $a(\cdot)v$ at the identity element $\mathbb{1}$ is

$$\mathrm{d}[a(\mathbb{1})v]\mu = -\mu v_x,$$

where we have $\mu \in \mathcal{A} = \mathbb{R}$. Moreover, the expression

$$B(v)\mu = \omega(\mathrm{d}([a(\mathbb{1})v])\mu, \cdot)$$

extends to a bounded linear operator $B(\cdot)\mu\colon H^1(\mathbb{R};\mathbb{R}) \to H^{-1}(\mathbb{R};\mathbb{R})$ with

$$B(v)\mu = \big(\mu v, \cdot\big)_0.$$

As in the abstract setting, we rewrite this as $\mathrm{d}Q(v)\colon \mathcal{A} \to X^\star$ satisfying

$$\langle \mathrm{d}Q(v)\mu, y\rangle = \big(\mu v, y\big)_0$$

for $y \in H^1(\mathbb{R};\mathbb{R})$.

This leads to the conserved quantity

$$Q(v)\mu = \tfrac{1}{2}\mu\|v\|_0^2.$$

Due to the symmetry under translation, the KdV possesses solitary wave solutions. As an example, the initial value

$$u_0(x) = \frac{1}{2\cosh^2\left(\frac{x}{2}\right)}$$

yields the solution

$$u_\star(t,x) = \frac{1}{2\cosh^2\left(\frac{x-t}{2}\right)}. \tag{5.3.6}$$

A one-parameter family of solitary wave solutions (see e.g. [46]) is associated with (5.3.6). As in the case of the nonlinear Schrödinger equation, we deduce these solutions by exploiting the scale invariance. If u is a solution on $\mathcal{I} = [0,T]$, then so is u^λ on $\mathcal{I}^\lambda = [0,\lambda^3 T]$, where u^λ is given by

$$u^\lambda(t,x) = \lambda^2 u(\lambda^3 t, \lambda x)$$

for $\lambda > 0$. Due to this scaling, the solution (5.3.6) is transformed into

$$u_\star(t,x) = \frac{\lambda^2}{2\cosh^2\left(\frac{\lambda}{2}(x-\lambda^2 t)\right)}. \tag{5.3.7}$$

By setting $\mu = \lambda^2$, we change the notation, such that (5.3.7) becomes

$$u_\star(t,x) = v_\star(x-\mu t) \tag{5.3.8}$$

with

$$v_\star(x) = \frac{\mu}{2\cosh^2\left(\frac{\sqrt{\mu}}{2}x\right)}.$$

The orbital stability of solitary waves for equations of Korteweg-de Vries type has been proven in [10]. We suppose that a modified version of this approach

might be used to analyze the stability of our PDAE formulation for the KdV. This, however, is work in progress.

In the following, we restrict ourselves to numerical tests of the freezing method for the KdV. An analytical approach to operator splitting for partial differential equations with Burgers' nonlinearity, such as the KdV, can be found in [37] and the references therein. In case of our freezing problem, we have a linear part

$$v_t = -v_{xxx} + i\mu_2 v_x,$$

which in Fourier variables is solved by

$$[\mathcal{F}u](\xi, t) = e^{i(\xi^3+\mu_2\xi)t}[\mathcal{F}u](\xi, 0),$$

and a remaining nonlinear part

$$v_t = -6vv_x = -3\big[v^2\big]_x$$

with its flow denoted by Φ_N^t. Then the Strang splitting reads

$$\Phi_{L+N}^{\Delta t} \approx \Phi_L^{\frac{1}{2}\Delta t} \circ \Phi_N^{\Delta t} \circ \Phi_L^{\frac{1}{2}\Delta t},$$

where Φ_L^t is the linear flow. In our computations, we make use of the exact solution for the linear part and apply the implicit midpoint scheme to approximate in Fourier variables the solution of nonlinear part, i.e., we consider the equation

$$v_t = -3i\xi\mathcal{F}\big(\mathcal{F}^{-1}(v)\big)^2.$$

As in the previous examples, we call the codes `rng('default')` and `rand(1,2*K)` in MATLAB to generate a global perturbation, which we scale by the perturbation factor $\frac{\varrho}{100}$ and add to the unperturbed initial data.

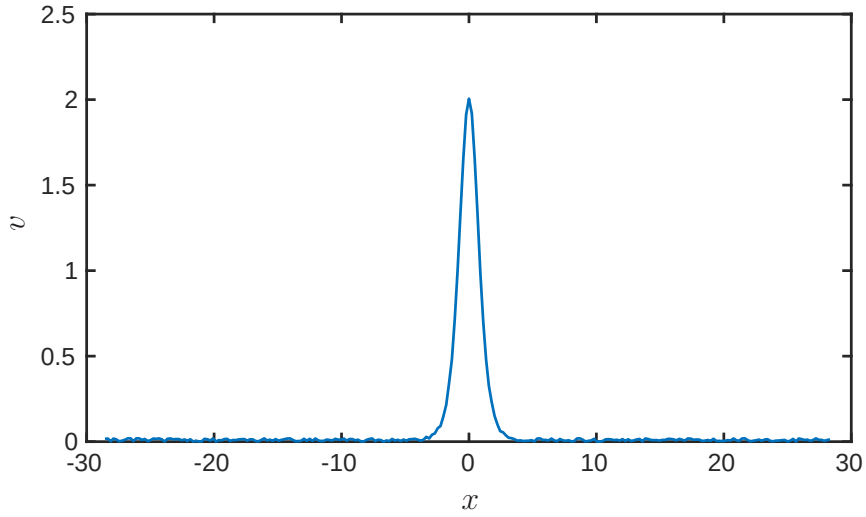


Figure 5.3.1: Perturbed initial data ($\varrho = 2$)

In contrary to the NLS and the NLKG there is no rotational symmetry involved, i.e., the solutions of the original problem travel, but do not oscillate. Thus, the freezing method only deals with the translation symmetry.

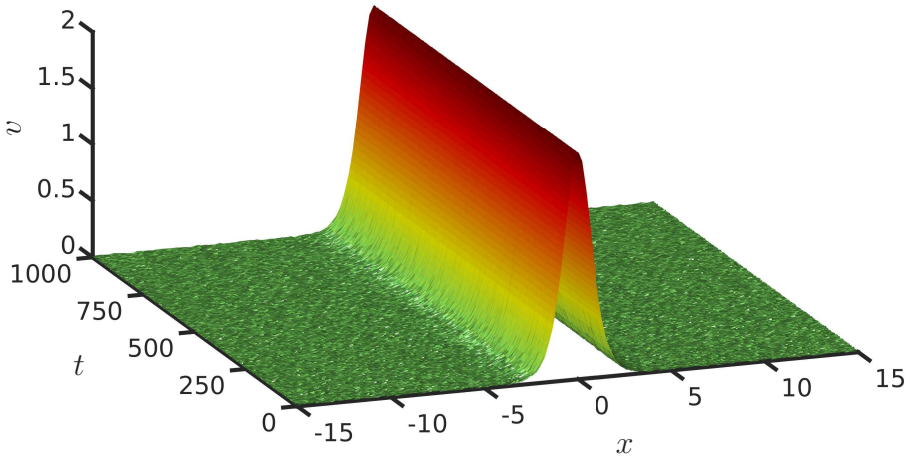


Figure 5.3.2: Solution of the perturbed problem ($\varrho = 2$)

The results are not much different from the two previous examples. For small perturbations the profile stays in place, i.e., the freezing method works as expected. But, same as before, the velocity μ is subject to a fluctuation with high intensity. As a result, for large perturbation we obtain ill-posed linear systems for $\mu(t_n)$ after some time steps.

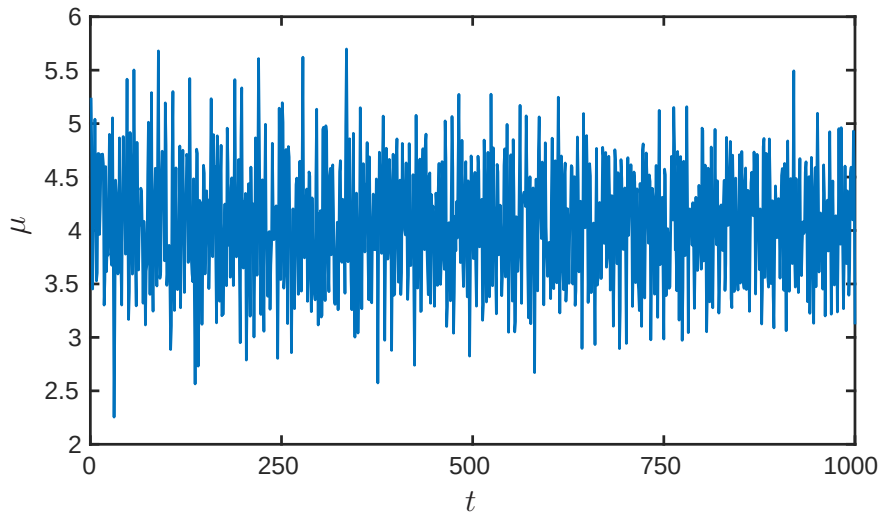


Figure 5.3.3: Velocity ($\varrho = 2$)

There is another very interesting aspect to the KdV. In [7] the freezing method for parabolic problems was extended to handle multifronts and multipulses that travel at different speeds. While this is still an open problem for Hamiltonian

systems, the collision of solitary waves and the decomposition of multi-soliton solutions have already attracted interest among mathematicians and theoretical physists (see e.g. [5]). Colliding solitary waves recover their shapes, where the only result of the collision is a phase shift, a discovery that goes back to [66]. The faster solitary wave shifts slightly forward, and the slower one is squeezed backwards. Let us numerically show the phase shift in the collision between two solitary wave solutions of the KdV equation. As our initial data we add up $v_\star(\cdot + 15)$ with $\mu = 2$ and $v_\star(\cdot + 5)$ with $\mu = 1$.

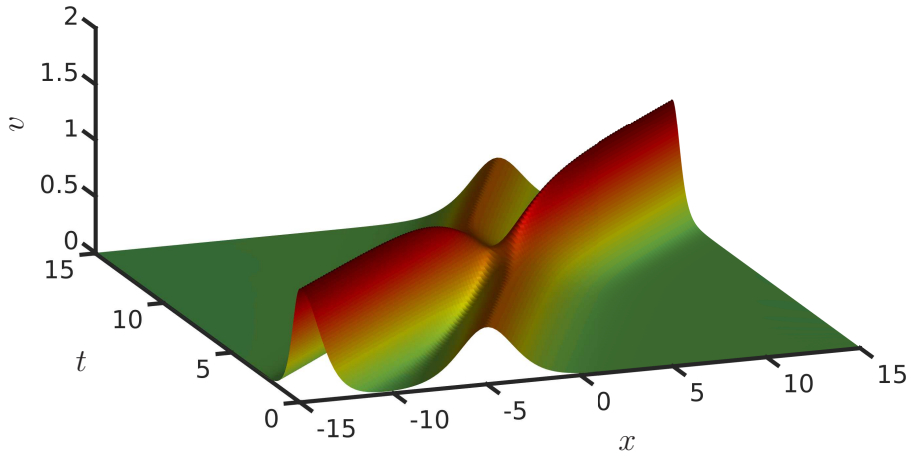


Figure 5.3.4: Phase shift in the original problem

In general, the freezing method must be modified to handle this situation in a satisfactory manner. However, we can make use of our basic approach as long as the two solitary waves differ sufficiently in size. In our specific example we choose $\mu = 4$ and add a small solitary wave centered at $x = 8$ with $\mu = 1$.

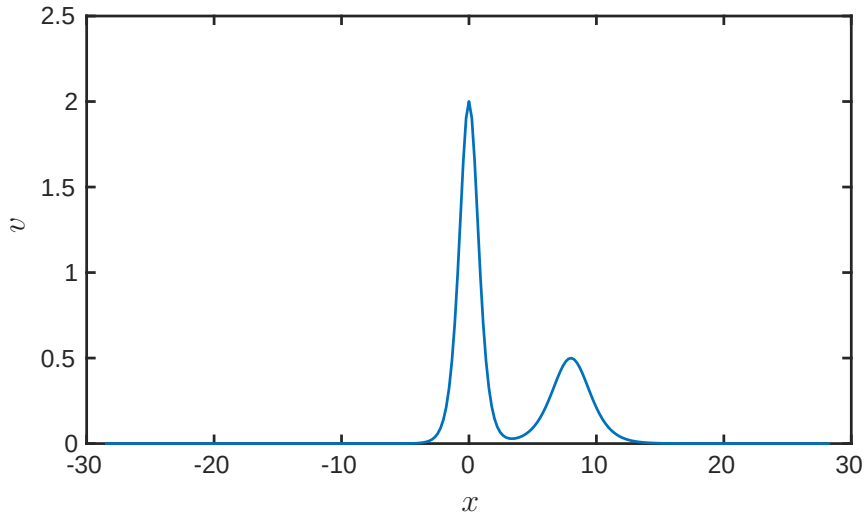


Figure 5.3.5: Initial data

Due to the periodicity of the spatial domain, the solitary waves collide several times, but regain their shapes after each collision. The interaction during the collision is very similar to the original problem, and we are rather interested in long time effects. For the sake of presentability, we have shrunk the time domain to $[0, 100]$ and selected the top view.

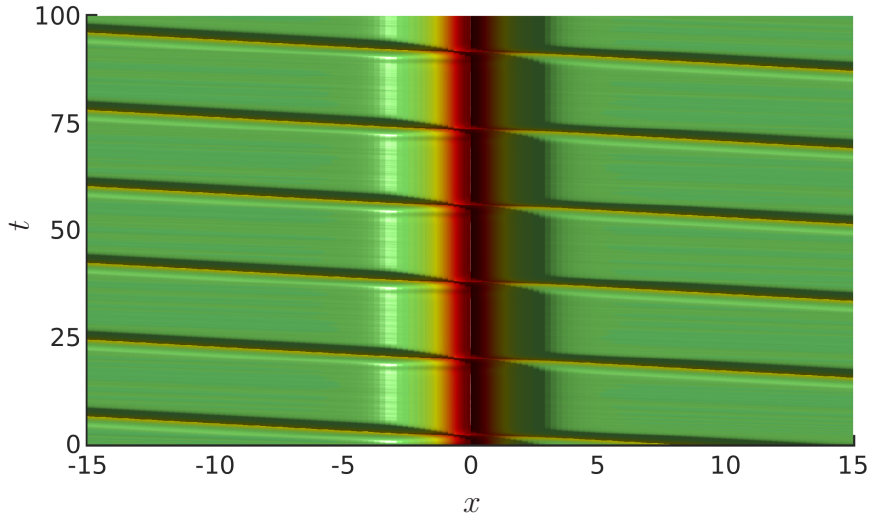


Figure 5.3.6: Fixed phase condition (time-space plot)

The small solitary wave travels with non-zero velocity, whereas the red profile, which corresponds to the large solitary wave, stays centered at $x = 0$ and no phase shift occurs.

It is quite interesting to see that at the beginning of the interaction the value of μ does not increase monotonically, but instead an adjustment occurs twice. After that, the large values of μ impede the phase shift to the right side.

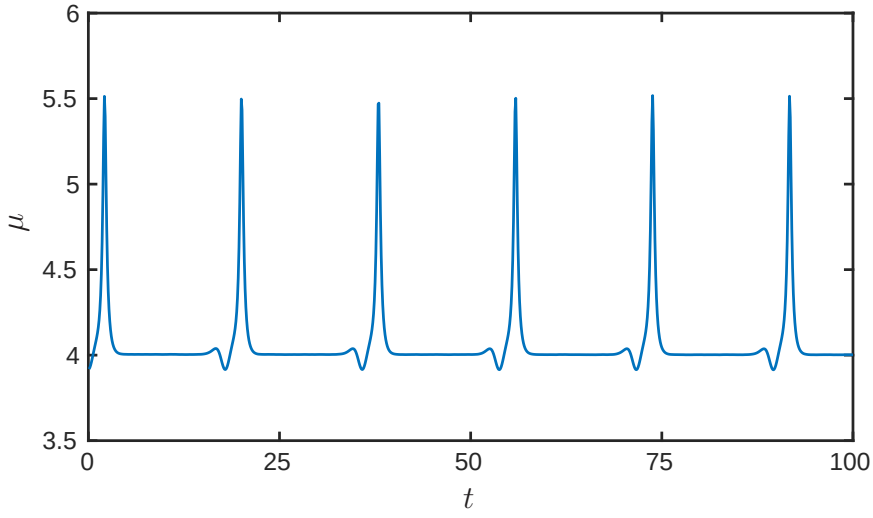


Figure 5.3.7: Fixed phase condition (velocity)

For comparison, we repeat this numerical experiment, but replace the fixed phase condition by the orthogonality phase condition, which we already applied to the NLS in Section 5.1.

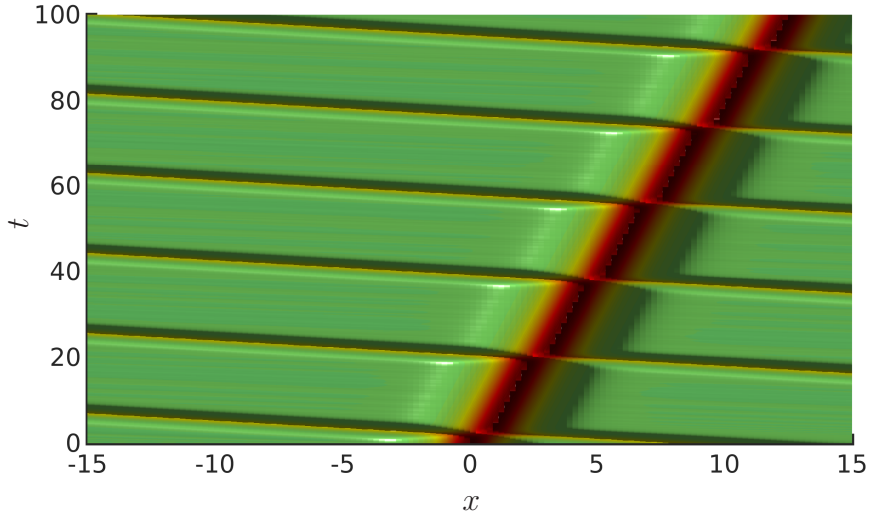


Figure 5.3.8: Orthogonality phase condition (time-space plot)

As we have seen in case of the NLS, the orthogonality phase condition is not well-suited for Hamiltonian systems. We notice that the freezing does not work as expected since the red profile moves to the right hand side. But, even more, after each collision it is subject to an additional phase shift.

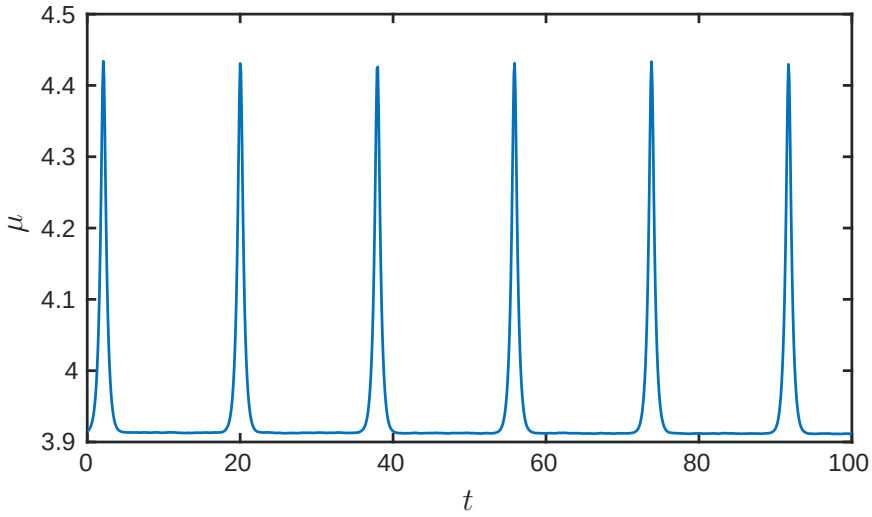


Figure 5.3.9: Orthogonality phase condition (velocity)

From the values of μ we can conclude two things. First, the values of μ during times when no interaction occurs are much lower than $\mu_\star = 4$. This results in the large solitary wave to travel to the right hand side. Second, the shape of the graph of μ during the collision is quite different from the fixed phase condition and the maximum is much lower. This is why the additional phase shift occurs.

Conclusions and Perspectives

In this thesis, we have considered the application of the freezing method to equivariant Hamiltonian systems such as the nonlinear Schrödinger equation. By adding a phase condition, the original problem was transformed into a partial differential algebraic equation, for which relative equilibria of the original problem appeared as stationary states.

In the well-known Grillakis-Shatah-Strauss setting, the freezing approach for the continuous problem turns out quite satisfactory. As shown in Chapter 2, the stationary states become stable in the sense of Lyapunov.

When it comes to the impact of spatial semi-discretization, there is still a big discrepancy between analytical and numerical results. According to our numerical results, the freezing method is far more robust than expected.

The geometric numerical integration, in first place, the challenge to construct a modified energy and obtain backward error analysis results, remains an open problem. The analysis of symplectic time discretization methods for the freezing system goes beyond the scope of this thesis and provides much room for future work.

Appendix A

Auxiliaries

A.1 Exponential Map

Given a Lie group G with Lie algebra $\mathcal{A}$, the exponential map from $\mathcal{A}$ to G is defined by $e^\sigma = \gamma(1)$, where $\gamma\colon \mathbb{R} \to G$ is the unique one-parameter subgroup of G generated by $\sigma \in \mathcal{A}$.

Proposition A.1.1. *Let G be a Lie group and let $\mathcal{A}$ be its Lie algebra.*

(a) For any $\sigma \in \mathcal{A}$, the mapping $t \mapsto e^{t\sigma}$, $t \in \mathbb{R}$ yields a one-parameter subgroup of G generated by σ.

(b) The exponential map is a smooth map from $\mathcal{A}$ to G and restricts to a diffeomorphism from some neighborhood of $0 \in \mathcal{A}$ to a neighborhood of $\mathbb{1} \in G$.

Proof. See [43] for the proof. □

A.2 Lie Group Inverse

Lemma A.2.1. *Let G be a Lie group and let $\mathfrak{f}\colon G \to G$ be the inverse mapping, i.e. $\mathfrak{f}(\gamma) = \gamma^{-1}$. Then the derivative $\mathrm{d}\mathfrak{f}(\gamma)\colon T_\gamma G \to T_{\gamma^{-1}} G$ is given by*

$$\mathrm{d}\mathfrak{f}(\gamma) = -\mathrm{d}L_{\gamma^{-1}}(\mathbb{1})\mathrm{d}R_{\gamma^{-1}}(\gamma) = -\mathrm{d}R_{\gamma^{-1}}(\mathbb{1})\mathrm{d}L_{\gamma^{-1}}(\gamma).$$

In particular, we find at unity $\mathrm{d}\mathfrak{f}(\mathbb{1})\colon \mathcal{A} \to \mathcal{A}$, $v \mapsto -v$.

Proof. We consider the equation $\mathbb{1} = \gamma\gamma^{-1}$ and apply the chain rule (see [1]) to deduce

$$0 = \mathrm{d}L_\gamma(\gamma^{-1})\mathrm{d}\mathfrak{f}(\gamma) + \mathrm{d}R_{\gamma^{-1}}(\gamma).$$

A similar application of the chain rule, namely differentiating $g = \gamma^{-1}\gamma g$ with respect to g, shows that

$$\mu = \mathrm{d}L_{\gamma^{-1}}(\gamma g)\mathrm{d}L_\gamma(g)\mu$$

for all $\mu \in T_g G$, and in particular that $\mathrm{d}L_{\gamma^{-1}}(\mathbb{1})\mathrm{d}L_\gamma(\gamma^{-1})$ is the identity mapping on $T_{\gamma^{-1}} G$. The second identity is proven in the same way by differentiating $\mathbb{1} = \gamma^{-1}\gamma$ instead. □

A.3 Implicit Functions on Banach Manifolds

Lemma A.3.1. *Let G, U, Y be Banach manifolds of class $\mathcal{C}^k$ with $1 \le k \le \infty$, $\mathfrak{U} \subseteq G \times U$ open, and $(g_0, u_0) \in \mathfrak{U}$. Provided that $F \in \mathcal{C}^k(\mathfrak{U}; Y)$ and $F(g_0, u_0) = 0$, the following statements are equivalent.*

(a) $F(\cdot, u_0)$ is a $\mathcal{C}^k$-diffeomorphism of an open neighborhood of g_0 onto an open neighborhood of 0.

(b) $F_g(g_0, u_0)$ is an isomorphism from $T_{g_0}G$ to T_0Y.

(c) There are open neighborhoods $\mathfrak{V} \subseteq \mathfrak{U}$ of (g_0, u_0) and $V \subseteq U$ of u_0 and a function $\hat{g} \in \mathcal{C}^k(V; G)$ such that $F(g, u) = 0$ and $(g, u) \in \mathfrak{V}$ if and only if $g = \hat{g}(u)$ and $u \in V$ and

$$d\hat{g}(u) = -\big[F_g(\hat{g}(u), u)\big]^{-1} F_u(\hat{g}(u), u).$$

Proof. We refer to Theorem 8.41 in [61]. □

A.4 Young's Inequality

Lemma A.4.1. *For $\varepsilon > 0$ and $E \in \mathbb{R}$ it holds the inequality*

$$\varepsilon x^2 - E(xy + y^2) \ge \tfrac{1}{2}\varepsilon x^2 - \left(E + \frac{E^2}{2\varepsilon}\right) y^2.$$

Proof. Young's inequality gives us

$$\varepsilon x^2 - 2Exy + \frac{E^2}{\varepsilon} y^2 = \left(\sqrt{\varepsilon} x - \frac{E}{\sqrt{\varepsilon}} y\right)^2 \ge 0.$$

This implies

$$\tfrac{1}{2}\varepsilon x^2 - Exy \ge -\frac{E^2}{2\varepsilon} y^2, \tag{A.4.1}$$

which, by direct computation, leads to the assertion of the lemma. □

A.5 Finite Rank Perturbations

Lemma A.5.1. *Let $\big(X, \|\cdot\|\big)$ be a Banach space with dual space $\big(X^\star, \|\cdot\|_{X^\star}\big)$ and $L\colon X \to X^\star$ a bounded linear operator. Moreover, let $V = \operatorname{span}\{v_1, ..., v_d\}$ be a finite-dimensional subspace and $v_1^\star, ..., v_d^\star$ form a dual basis, i.e., $\langle v_j^\star, v_k\rangle = \delta_{jk}$ for $j, k = 1, ..., d$ and $\langle v_j^\star, y\rangle = 0$ for all $y \in Y$, where $X = V \oplus Y$. If $\langle Ly, y\rangle \ge c\|y\|^2$ holds for all $y \in Y$, then we can find $\lambda > 0$, which only depends on $c > 0$ and $\|L\|_{X^\star \leftarrow X}$, with the following property. The perturbed operator*

$$\widetilde{L}u = Lu + \lambda \sum_{j=1}^{d} \langle v_j^\star, u\rangle v_j^\star \tag{A.5.1}$$

satisfies

$$\langle \widetilde{L}u, u\rangle \geq \widetilde{c}\,\|u\|^2$$

for all $u \in X$.

Proof. We decompose $u = v + y$ into $v \in V$ and $y \in Y$. The positivity of L on the subspace Y and $\big\|L\big\|_{X^\star \leftarrow X} \leq C$ for some $C > 0$ lead to

$$\begin{aligned}\langle Lu, u\rangle &= \langle Ly, y\rangle + \langle Ly, v\rangle + \langle Lv, y\rangle + \langle Lv, v\rangle \\ &\geq c\|y\|^2 - C(2\|y\|\|v\| + \|v\|^2) \geq m\|y\|^2 - M\|v\|^2,\end{aligned}$$

where the last step is due to Lemma A.4.1. The proof is finished by applying the squared triangle inequality

$$\|u\|^2 \leq (\|y\| + \|v\|)^2 \leq 2\|y\|^2 + 2\|v\|^2$$

to the positivity estimate

$$\langle \widetilde{L}u, u\rangle = \langle Lu, u\rangle + \lambda\|v\|^2 \geq m\|y\|^2 + (\lambda - M)\|v\|^2,$$

where we have to choose $\lambda > M = C + \dfrac{C^2}{2c}$. ∎

A.6 Lipschitz Inverse

Lemma A.6.1. *Let* $\big(X, \|\cdot\|_X\big)$ *and* $\big(Y, \|\cdot\|_Y\big)$ *be Banach spaces with* $x_0 \in X$ *and denote by* $L\colon X \to Y$ *a linear homeomorphism. If there exist positive constants* $\delta, c_1, c_2 > 0$ *and a mapping* $F\colon \overline{\mathcal{B}}_\delta(x_0) \subseteq X \to Y$ *such that*

(i) $\big\|F(x_1) - F(x_2)\big\|_Y \leq c_0\big\|x_1 - x_2\big\|_X$,

(ii) $c_0 < c_1 \leq \dfrac{1}{\big\|L^{-1}\big\|_{X \leftarrow Y}}$,

(iii) $\big\|Lx_0 + F(x_0)\big\|_Y \leq \delta(c_1 - c_0)$,

then the equation

$$(L + F)(x) = 0$$

has a unique solution $x_\star \in \overline{\mathcal{B}}_\delta(x_0)$, *and the stability estimate*

$$\big\|x_1 - x_2\big\|_X \leq \frac{1}{c_1 - c_0}\big\|(L + F)(x_1) - (L + F)(x_2)\big\|_Y$$

holds for all $x_1, x_2 \in \overline{\mathcal{B}}_\delta(x_0)$.

Proof. By defining $T(x) = -L^{-1}F(x)$, we rewrite the equation $Lx + F(x) = 0$ as an equivalent fixed point problem $T(x) = x$. From the inequality

$$\big\|T(x_1) - T(x_2)\big\|_X \leq \big\|L^{-1}\big\|_{X\leftarrow Y}\big\|F(x_1) - F(x_2)\big\|_Y \leq \frac{c_0}{c_1}\big\|x_1 - x_2\big\|_X$$

for $x_1, x_2 \in \overline{\mathcal{B}}_\delta(x_0)$ and

$$\begin{aligned}\big\|T(x_1) - x_0\big\|_X &\leq \big\|T(x_1) - T(x_0)\big\|_X + \big\|T(x_0) - x_0\big\|_X \\ &\leq \frac{c_0}{c_1}\big\|x_1 - x_0\big\|_X + \big\|L^{-1}\big\|_{X\leftarrow Y}\big\|F(x_0) + Lx_0\big\|_Y \\ &\leq \frac{c_0}{c_1}\delta + \frac{1}{c_1}\delta(c_1 - c_0) = \delta,\end{aligned}$$

we conclude that T is a contraction on the closed ball $\overline{\mathcal{B}}_\delta(x_0)$. Hence, the existence of a unique solution follows from the contraction mapping principle. Moreover, the stability estimate is a consequence of

$$\begin{aligned}\big\|x_1 - x_2\big\|_X &\leq \big\|(I - T)x_1 - (I - T)x_2\big\|_X + \big\|Tx_1 - Tx_2\big\|_X \\ &\leq \big\|L^{-1}\big\|_{X\leftarrow Y}\big\|(L + F)x_1 - (L + F)x_2\big\|_Y + \frac{c_0}{c_1}\big\|x_1 - x_2\big\|_X\end{aligned}$$

for $x_1, x_2 \in \overline{\mathcal{B}}_\delta(x_0)$. □

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