Linear Dynamics of Oscillating Lattices – A Spatial Discretization of the Wave Equation*

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Abstract

This work examines solutions of a spatial discretization of the classical wave equation as a model for the linearized dynamics of an infinite system of particles indexed by and having equilibrium positions $x \in h\mathbb{Z}^n$, with each particle linked to its $2n$ nearest neighbours by harmonic springs. We numerically observe the existence of a spherical monotone wavefront corresponding to the continuum light cone, the propagation of regions of maximal displacement along the principal diagonals of the lattice, and prove the emergence of second-nearest-neighbour synchronized oscillations in long time. We prove a leading-order $t^{-n/2}$ decay law for the amplitude of oscillation of each particle. We also show that the group and phase velocities of the system are bounded above by the corresponding continuum wave speed, and determine the long-time behaviour of the local and global kinetic and potential energies.

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1 Introduction

1.1 Motivation

As Friesecke remarks in [2],

> The deep question of how energy in large un-damped Hamiltonian systems is dissipated, e.g. from low to high wavenumbers, is still poorly understood... [An] innocent looking but surprisingly rich prototype system [is] the classical infinite harmonic chain. It consists of a one-dimensional chain of particles of equal mass, linked by harmonic nearest-neighbour springs.

This work examines a generalization of the infinite harmonic chain to an n-dimensional setting. As laid out in Subsection 1.4, we have two main settings for this problem: that of a harmonic lattice, and that of a spatial (but not temporal) discretization of the classical wave equation. In some sense, we are studying the propagation of disturbances (and hence energy and information) in a certain type of spatially discrete medium.

We shall now proceed to establish the equation of study as quickly as possible, and then discuss various settings for the problem of its solution.

1.2 The Equation of Study

Let $\{e_1, \ldots, e_n\}$ be the usual Euclidean basis of $\mathbb{R}^n$. For vectors $v \in \mathbb{R}^n$, write $v^j := v \cdot e_j$ for the component of v in the e_j direction, so

$$v = (v^1, \ldots, v^n) = v^1 e_1 + \cdots + v^n e_n,$$

and $\|v\|$ is the usual Euclidean norm of v.

Let $h > 0$ and consider an infinite n-dimensional lattice $\Lambda := h\mathbb{Z}^n$. Denote the set of nearest neighbours of $x \in \Lambda$ by

$$N_1(x) := \{x \pm he_j | 1 \leq j \leq n\} \tag{1.2.1}$$

and the set of second-nearest neighbours in the $\pm e_j$ directions by

$$N_2(x) := \{x \pm 2he_j | 1 \leq j \leq n\}. \tag{1.2.2}$$

We define the set of nearest-neighbour pairs (*links*, [6]),

$$\mathrm{Lk}_1(\Lambda) := \{(x,y) | x \in \Lambda, y \in N_1(x)\}. \tag{1.2.3}$$

For a twice-differentiable function $f : \mathbb{R} \to \mathbb{R}$,

$$\frac{d^2}{dx^2} f(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}, \tag{1.2.4}$$

for small h [5]. Therefore, we make the following definition:

Definition 1.2.1. [9] For $h > 0$, the *discrete Laplacian* Δ_h acting on functions $\Lambda \to \mathbb{R}^n$ is given by

$$\Delta_h f(x) := \sum_{j=1}^{n} \frac{f(x+he_j) - 2f(x) + f(x-he_j)}{h^2}. \tag{1.2.5}$$

This is by analogy with the usual Laplacian Δ for functions with second-order partial derivatives:

$$\Delta f(x) := \sum_{j=1}^{n} \frac{\partial^2}{\partial (x^j)^2} f(x). \tag{1.2.6}$$

We shall study solutions $q : \Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}^n$ to the differential equation

$$\ddot{q}(x,t) = \omega^2 h^2 \Delta_h q(x,t), \tag{1.2.7}$$

where $\omega \geq 0$, $x \in \Lambda$, an over-dot indicates partial differentiation with respect to time, t, and the discrete Laplacian acts only on the spatial part x, ignoring t.

1.3 Initial Conditions

We shall consider stationary coherent initial conditions. Since the equation (1.2.7) is linear, any stationary initial condition can be written as a superposition of such initial conditions, and the solution will be a superposition of the solutions to those special cases. Therefore, our initial conditions will be, for some choice of initial displacement vector $q_0 \in \mathbb{R}^n$,

$$\begin{aligned} q(x,0) := q_0 \delta_{x,0} &:= \begin{cases} q_0 & \text{for } x = 0; \\ 0 & \text{otherwise;} \end{cases} \\ \dot{q}(x,0) &:= 0 \text{ for all } x \in \Lambda. \end{aligned} \tag{1.3.1}$$

Even this can be further simplified: the reader who assumes throughout that $q_0 = e_1$ will lose nothing. These are the initial conditions used by Friesecke in [2].

1.4 Possible Settings

Equation (1.2.7) arises naturally in quite a few contexts. What follows is not intended to be an exhaustive list, but should illustrate that the solution of (1.2.7) is a problem with appropriate to both pure and applied mathematics.

I. Spatial Discretization of the Wave Equation. Consider the classical continuum wave equation

$$\ddot{q}(x,t) = c^2 \Delta q(x,t) = c^2 \sum_{j=1}^{n} \frac{\partial^2}{\partial (x^j)^2} q(x,t). \tag{1.4.1}$$

Just as above, the Laplacian Δ ignores t and acts on the spatial part of q. We replace the ordinary continuous Laplacian by the discrete one and pass to the corresponding minimal domain of definition for q (that is, $\Lambda = h\mathbb{Z}^n$ instead of $\mathbb{R}^n$). (1.4.1) is the "limit" of (1.2.7) (in the sense that the R.H.S. of (1.2.7) tends to the R.H.S. of (1.4.1)) as $h \to 0$ with ωh held constant and equal to c.

II. Linearized Dynamics of a Harmonic Lattice. Consider Λ to be a lattice of mass m particles with reference positions $x \in h\mathbb{Z}^n \subset \mathbb{R}^n$. $q(x,t)$ denotes the displacement of the particle with rest position x from x at time t. Each particle is joined to its $2n$ nearest neighbours in the $\pm e_j$ directions by harmonic springs of natural length h and elasticity κ. The force on the particle $x \in \Lambda$ arising from the spring connecting x to $x + he_j$ is

$$\kappa \left(\| q(x+he_j,t) + he_j - q(x,t) \| - h \right) \frac{q(x+he_j,t) + he_j - q(x,t)}{\| q(x+he_j,t) + he_j - q(x,t) \|}.$$

However, we can linearize the system and replace this nonlinear expression with

$$\kappa \left(q(x+he_j,t) - q(x,t) \right).$$

This is an appropriate simplification for $\|q(x,t)\| \ll h$. In this linearized situation, the Newtonian equation of motion for the displacement $q(x,t)$ of the particle x is

$$
\begin{aligned}
m\ddot{q}(x,t) &= \sum_{y\in N_1(x)} \kappa\left(q(y,t)-q(x,t)\right), \\
&= \kappa \sum_{j=1}^{n} \left(q(x+he_j,t)-q(x,t)-(q(x,t)-q(x-he_j,t))\right), \\
&= \kappa \sum_{j=1}^{n} \left(q(x+he_j,t)-2q(x,t)+q(x-he_j,t)\right), \\
&= \kappa h^2 \Delta_h q(x,t).
\end{aligned}
$$

This is (1.2.7) with $\omega := \sqrt{\kappa/m}$. See Figure 1.4.1 for an illustration of this setup in dimension $n = 2$.

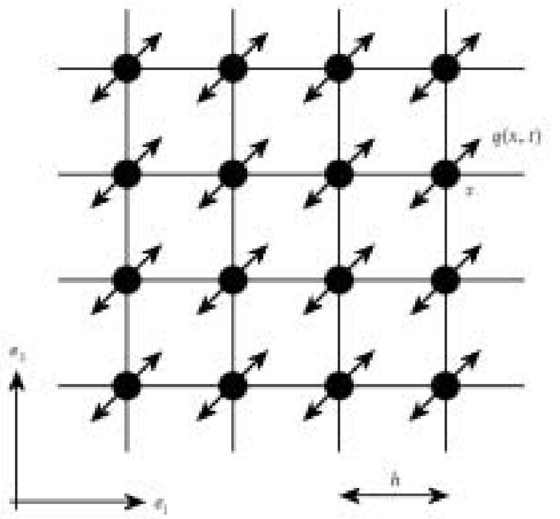

Figure 1.4.1: A 2-dimensional oscillating lattice $h\mathbb{Z}^2$.

III. Generalization of the Bessel Function J_m. The Bessel function of the first kind, $J_m : \mathbb{R} \to \mathbb{R}$ is defined by

$$J_m(\tau) := \frac{1}{2\pi}\int_{S^1} e^{i\tau\sin\theta} e^{-im\theta}\, d\theta \tag{1.4.2}$$

where $m \in \mathbb{Z}$. J_m is the solution of the ordinary differential equation

$$\tau^2 \frac{d^2}{d\tau^2} J_m(\tau) + \tau \frac{d}{d\tau} J_m(\tau) + (\tau^2 - m^2) J_m(\tau) = 0.$$

For reasons that will become clear after we review Friesecke's work in dimension $n = 1$ (Subsection 3.2) and apply spectral and Fourier methods to the problem (Section 5), we would like to generalize this notion to $\mathcal{J}_m : \mathbb{R} \to \mathbb{R}$, given by

$$\mathcal{J}_m(\tau) := \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} e^{i\tau \sqrt{\sum_{j=1}^n \sin^2 \theta^j}} e^{-im\cdot\theta} \, d\theta, \tag{1.4.3}$$

where $m \in \mathbb{Z}^n$.

The discretization of differential equations, partial and ordinary, is not a new endeavour. Difference methods have been applied in many contexts, in particular to approximately compute solutions to differential equations. From Jost [3]:

> The basic idea of the difference methods consists in replacing the given differential equation by a difference equation with step size h and trying to show that for $h \to 0$, the solutions of the difference equations converge to a solution of the differential equation.

Jost goes on to show that many of the properties of the continuous Laplacian carry over to the discrete Laplacian (e.g. the maximum principle). In considering the discretized version of the heat / diffusion equation

$$\dot{u}(x, t) = k^2 \Delta u(x, t),$$

Jost discretizes in both time and space, using the same step size in all variables. However, we have performed only a *partial* discretization of the wave equation, and this causes a considerable change in the character of the solutions.

2 Preliminary Results

2.1 The Uncoupled Situation – Simple Harmonic Motion

For future reference and comparison, it will be helpful to examine briefly the dynamics of a single particle in the lattice if all other particles are held fixed in their reference positions. For convenience, we shall consider the single mobile particle to be the particle at the origin. In dimension $n = 1$ we have

$$\begin{aligned}\ddot{q}(0,t) &= \omega^2 h^2 \Delta_h q(0,t) \\ &= \omega^2 \left(q(h,t) - 2q(0,t) + q(-h,t)\right) \\ &= -2\omega^2 q(0,t).\end{aligned}$$

It is clear that we shall obtain a similar equality for dimension n:

$$\ddot{q}(0,t) = -2n\omega^2 q(0,t) \tag{2.1.1}$$

We can readily solve this ODE as $q(0,t) = Ae^{i\sqrt{2n}\omega t} + Be^{-i\sqrt{2n}\omega t}$ for some $A, B \in \mathbb{C}^n$. At time $t = 0$:

$$\begin{aligned}q(0,0) &= A + B, \\ \dot{q}(0,0) &= i\sqrt{2n}\omega(A - B).\end{aligned}$$

Assuming a non-zero initial displacement and stationary initial conditions we see that $A = B = \frac{1}{2}q_0 \in \mathbb{R}^n$. Thus, using the identity $\cos z = \frac{1}{2}(e^{iz} + e^{-iz})$,

$$q(0,t) = q_0 \cos\left(\sqrt{2n}\omega t\right). \tag{2.1.2}$$

That is, the particle oscillates along a line through its rest position, in the direction of its initial displacement, with angular frequency $\sqrt{2n}\omega$ and amplitude $\|q_0\|$.

2.2 Symmetry and Linearity

We now use the linearity of (1.2.7) and the symmetry of the lattice Λ to simplify our system of study when we have initial conditions (1.3.1).

Definitions 2.2.1. Let $\mathrm{Isom}(\Lambda)$ denote the group of *isometries*[1] of Λ:

$$\mathrm{Isom}(\Lambda) := \{\iota : \Lambda \to \Lambda \,|\forall x, y \in \Lambda, d_\Lambda(x, y) = d_\Lambda(\iota(x), \iota(y))\}\,.$$

Let $\mathrm{Isom}_0(\Lambda) := \{\iota \in \mathrm{Isom}(\Lambda) | \iota(0) = 0\}$ be the subgroup of $\mathrm{Isom}(\Lambda)$ that fixes the origin.

$\mathrm{Isom}_0(\Lambda)$, which is isomorphic to the isometry group of the unit hypercube in n dimensions, has a nice presentation as

$$\mathrm{Isom}_0(\Lambda) \cong \left\langle \rho_1, \ldots, \rho_n \,\middle|\, \begin{array}{c} \rho_1^2 = \cdots = \rho_n^2 = 1 \\ (\rho_1\rho_2)^3 = \cdots = (\rho_{n-2}\rho_{n-1})^3 = 1 \\ (\rho_{n-1}\rho_n)^4 = 1 \end{array} \right\rangle .$$

Geometrically, the ρ_j, $1 \leq j \leq n-1$, represent reflections in coordinate hyperplanes of codimension 1 orthogonal to the basis vectors e_j; ρ_n is a reflection in a hyperplane of codimension 1 perpendicular to $e_1 + \cdots + e_n$. This is illustrated in Figure 2.2.1, for the case $n = 2$.

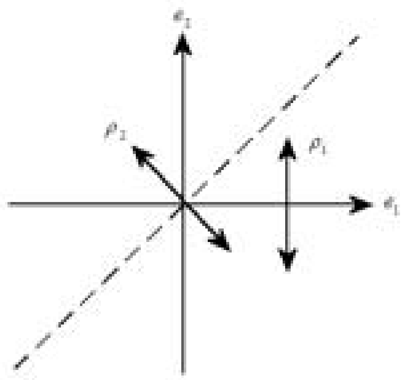

Figure 2.2.1: The reflections ρ_j generating the isometry group $\mathrm{Isom}_0(h\mathbb{Z}^2)$.

Considerations of symmetry under $\mathrm{Isom}_0(\Lambda)$ lead us to the following elementary lemma that will simplify a later proof and allow us to optimize our numerical simulation of the system:

[1]See Appendix A for an elucidation of distance and isometry on a lattice.

Lemma 2.2.2. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let $x, x' \in \Lambda$. Suppose that $x' = \iota(x)$ for some $\iota \in \mathrm{Isom}_0(\Lambda)$. Then $q(x,t) = q(x',t)$ for all times $t \geq 0$.*

Proof. Note that equation (1.2.7) can be written in the form

$$\ddot{q}(x,t) = \omega^2 \sum_{y \in N_1(x)} (q(y,t) - q(x,t)).$$

Now observe that for any $x \in \Lambda$ and $\iota \in \mathrm{Isom}(\Lambda)$, $\iota(N_1(x)) = N_1(\iota(x))$. This is certainly true for $\iota \in \mathrm{Isom}_0(\Lambda)$. Thus, if $x' = \iota(x)$, $t \geq 0$,

$$\begin{aligned}
\ddot{q}(x',t) &= \omega^2 \sum_{y' \in N_1(x')} (q(y',t) - q(x',t)) \\
&= \omega^2 \sum_{y' \in N_1(\iota(x))} (q(y',t) - q(\iota(x),t)) \\
&= \omega^2 \sum_{y' \in \iota(N_1(x))} (q(y',t) - q(\iota(x),t)) \\
&= \omega^2 \sum_{y \in N_1(x)} (q(y,t) - q(x,t)) \\
&= \ddot{q}(x,t).
\end{aligned}$$

So x and x' have the same equation of motion. It is easy to see that under initial conditions (1.3.1), $q(x,0) = q(x',0)$ and $\dot{q}(x,0) = \dot{q}(x',0)$. So $q(x,t) = q(x',t)$ for all times $t \geq 0$. □

Proposition 2.2.3. *A system evolving according to (1.2.7) satisfies*

$$q(x,t), \dot{q}(x,t) \in \mathrm{span}\{q(x,0), \dot{q}(x,0) | x \in \Lambda\}$$

for all $x \in \Lambda$ and $t \geq 0$.

Proof. This is obvious: equation (1.2.7) is linear and autonomous. □

Corollary 2.2.4. *A system evolving according to (1.2.7) with initial conditions (1.3.1) satisfies, for all $x \in \Lambda$ and $t \geq 0$, $q(x,t) = u(x,t)q_0$ for some twice-differentiable function $u : \Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}$.*

Proof. (1.3.1) $\Rightarrow \text{span}\{q(x,0), \dot{q}(x,0) | x \in \Lambda\} = \mathbb{R}q_0$. $\square$

Thus, given initial conditions (1.3.1), define $u : \Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ by

$$q(x,t) = u(x,t)q_0. \tag{2.2.1}$$

$u(x,t)$ is the normalized amplitude of displacement of particle x at time t, normalized with respect to the initial excitation q_0. Therefore, if we are in the situation of initial conditions (1.3.1), we are essentially studying solutions $u : \Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ to

$$\ddot{u}(x,t) = \omega^2 h^2 \Delta_h u(x,t)$$

for $x \in \Lambda$, $t \geq 0$, where Δ_h acts on functions $\Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ in the obvious way. The corresponding initial conditions are

$$\begin{aligned} u(x,0) &:= \delta_{x,0}, \\ \dot{u}(x,0) &:= 0. \end{aligned}$$

2.3 Energy Considerations

In this subsection we shall introduce the kinetic and elastic potential energies of the system and use them to derive a bound on $\|q(x,t)\|$ for $t > 0$ under coherent initial conditions (1.3.1).

Some elementary physical observations about the system give us a nice conserved quantity. The kinetic energy of a particle of mass m moving with velocity v is $\frac{1}{2}m\|v\|^2$. Thus, we make the following definition:

Definitions 2.3.1. The *kinetic energy* of particle $x \in \Lambda$ at time t is

$$T(x,t) := \frac{1}{2}m\|\dot{q}(x,t)\|^2.$$

For $\Omega \subseteq \Lambda$, write $T_\Omega(t) := \sum_{x\in\Omega} T(x,t)$; write $T(t)$ for $T_\Lambda(t)$.

The elastic potential energy stored in a spring of elasticity κ extended by an amount ε is $\frac{1}{2}\kappa\varepsilon^2$. Because of the linearization of the equation of motion that we have chosen, we perform a corresponding linearization of potential energy so that force = ∇ potential energy. In this setting, the elastic potential energy stored at time t in the n springs in the positive e_j directions that are attached to particle $x \in \Lambda$ is

$$\frac{\kappa}{2} \sum_{j=1}^{n} \|q(x + he_j, t) - q(x, t)\|^2.$$

Definitions 2.3.2. The *elastic potential energy* in the $2n$ springs attached to a particular particle $x \in \Lambda$ at time t shall be denoted by $V(x,t)$, with

$$\begin{aligned} V(x,t) &:= \frac{\kappa}{4} \sum_{y \in N_1(x)} \|q(y,t) - q(x,t)\|^2 \\ &= \frac{\kappa}{4} \sum_{j=1}^{n} \left(\|q(x + he_j, t) - q(x,t)\|^2 + \|q(x - he_j, t) - q(x,t)\|^2 \right). \end{aligned}$$

Define $V_\Omega(t)$ and $V(t)$ as in the kinetic energy case.

The reader will note that $V(x,t)$ is actually $\frac{1}{2}$ of the energy in the links of which x is a member; this is to avoid double counting so that we have the desirable relation

$$\begin{aligned} V(t) &= \sum_{x \in \Lambda} V(x,t) \\ &= \sum_{x \in \Lambda} \frac{\kappa}{2} \sum_{j=1}^{n} \|q(x + he_j, t) - q(x,t)\|^2 \end{aligned}$$

Definitions 2.3.3. The *total energy* of particle $x \in \Lambda$ at time t is

$$\mathcal{E}(x,t) := T(x,t) + V(x,t).$$

Define $\mathcal{E}_\Omega(t)$ and $\mathcal{E}(t)$ as before.

Definitions 2.3.4. The *Lagrangian* of particle $x \in \Lambda$ at time t is

$$\mathcal{L}(x,t) := T(x,t) - V(x,t).$$

Define $\mathcal{L}_\Omega(t)$ and $\mathcal{L}(t)$ as before.

In the situation of initial conditions (1.3.1),

$$
\begin{aligned}
V(0) &= 2V(0,0) \\
&= \frac{\kappa}{2}\sum_{j=1}^{n}\left(\|q(he_j,0)-q(0,0)\|^2 + \|q(-he_j,0)-q(0,0)\|^2\right), \\
&= \frac{\kappa}{2}2n\|q(0,0)\|^2, \\
&= n\kappa\|q_0\|^2.
\end{aligned}
$$

It is easy to see that for all t and x, $V(x,t), V(t), T(x,t)$ and $T(t) \geq 0$.

Assuming that there are no frictional, thermal etc. losses of energy, the total energy $\mathcal{E}(t) := T(t) + V(t)$ must be a conserved quantity:

$$\mathcal{E}(t) := V(t) + T(t) \equiv V(0) + T(0) =: \mathcal{E}(0). \tag{2.3.1}$$

If the initial condition is stationary, with $\dot{q}(x,0) = 0$ for all $x \in \Lambda$, as in (1.3.1), then $T(0) = 0$ and so

$$\mathcal{E}(t) := V(t) + T(t) \equiv V(0). \tag{2.3.2}$$

Proposition 2.3.5. *A system evolving according to (1.2.7) with initial conditions (1.3.1) satisfies, for all $x \in \Lambda$ and $t \geq 0$, $\|q(x,t)\| \leq \|q(0,0)\| = \|q_0\|$.*

Proof. Let $x \in \Lambda$ and $t \geq 0$ be arbitrary. Initial conditions (1.3.1) $\Rightarrow T(0) = 0$. Conservation equation (2.3.2) $\Rightarrow 0 \leq V(t), T(t) \leq V(0)$ and $V(t) = V(0)$ if and only if all particles are stationary at time t. Consider $V(x,t)$; $0 \leq V(x,t) \leq V(0,0)$ and $V(x,t)$ is maximized if all the other particles are in their equilibrium positions, since then $V(y,t) = 0$ for $y \notin N_1(x) \cup \{x\}$. So

$$V(x,t) \leq \frac{1}{2}V(t) \leq \frac{1}{2}V(0) = V(0,0).$$

If $q(y,t) = 0$ for $y \neq x$ then

$$
\begin{aligned}
V(x,t) &= \frac{\kappa}{4}\sum_{y\in N_1(x)}\|q(y,t)-q(x,t)\|^2, \\
&= \frac{\kappa}{4}\sum_{y\in N_1(x)}\|q(x,t)\|^2, \\
&= \frac{n\kappa}{2}\|q(x,t)\|^2.
\end{aligned}
$$

Since $V(0,0) = \frac{n\kappa}{2}\|q_0\|^2$ it follows that $\|q(x,t)\| \leq \|q(0,0)\| = \|q_0\|$. □

Corollary 2.3.6. *A system evolving according to (1.2.7) with initial conditions (1.3.1) satisfies, for all $x \in \Lambda$ and $t \geq 0$, $q(x,t) = u(x,t)q_0$ for some twice-differentiable function $u : \Lambda \times \mathbb{R}_{\geq 0} \to [-1,1] \subset \mathbb{R}$.*

Proof. The existence of $u : \Lambda \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ such that $q(x,t) = u(x,t)q_0$ is the statement of Corollary 2.2.4. Proposition 2.3.5 then implies that $|u(x,t)| \leq 1$. □

We also have the following easy lemma:

Lemma 2.3.7. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let $0 \leq t_0 \leq \infty$. Then the following are all equivalent:*

(i) $T(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$ *as* $t \to t_0$*;*

(ii) $V(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$ *as* $t \to t_0$*;*

(iii) $\mathcal{L}(t) \to 0$ *as* $t \to t_0$*.*

Proof. These equivalences are easy to see from the two equations $T(t) = \mathcal{E}(0) - V(t)$ and $\mathcal{L}(t) := T(t) - V(t)$. □

3 Previous Studies

We shall now briefly review the solution of the continuum wave equation in $\mathbb{R}^n$ and the results proved by Friesecke [2] in the case $\Lambda = h\mathbb{Z}$.

3.1 The Continuum Wave Equation

In this subsection we briefly review the classical wave equation in $\mathbb{R}^n$ in order that we shall be able to compare and contrast the behaviour of solutions to (1.2.7) with solutions to the continuum wave equation (1.4.1).

We seek solutions $u : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ to

$$\ddot{u}(x,t) = c^2 \Delta u(x,t).$$

We can apply the Fourier transform as in Subsection 5.1 to obtain

$$\ddot{\hat{u}}(\xi,t) = -c^2 \|\xi\|^2 \hat{u}(\xi,t),$$

which we can solve as

$$\hat{u}(\xi,t) = A(\xi)e^{ic\|\xi\|t} + B(\xi)e^{-ic\|\xi\|t}.$$

Subject to stationary initial conditions, we have that

$$\hat{u}(\xi,t) = \hat{u}(\xi,0)\cos\left(c\|\xi\|t\right).$$

An important object in the study of solutions to the wave equation is the idea of the light cone:

Definition 3.1.1. Define the *light cone* of speed $c \in \mathbb{R}$ and centre $(x_0,t_0) \in \mathbb{R}^n \times \mathbb{R}$ by

$$\mathfrak{C}_c(x_0,t_0) := \left\{ (x,t) \in \mathbb{R}^n \times \mathbb{R} \middle| \, \|x - x_0\| \le c|t - t_0| \right\}. \tag{3.1.1}$$

It is a fact that $u(x_0,t_0)$ depends only upon $u(x,t)$ for $(x,t) \in \mathfrak{C}_c(x_0,t_0)$ with $t < t_0$; in particular, $u(x_0,t_0)$ is unaffected by $u(x,t)$ for $(x,t) \in \operatorname{Ext}\mathfrak{C}_c(x_0,t_0)$ with $t < t_0$, where

$$\begin{aligned}\operatorname{Ext}\mathfrak{C}_c(x_0,t_0) &:= (\mathbb{R}^n \times \mathbb{R})\backslash\mathfrak{C}_c(x_0,t_0) \\ &= \left\{ (x,t) \in \mathbb{R}^n \times \mathbb{R} \middle| \, \|x - x_0\| > c|t - t_0| \right\}.\end{aligned}$$

(In dimension $n = 3$, something even stronger is true: $u(x_0,t_0)$ depends only upon $u(x,t)$ for

$$(x,t) \in \partial\mathfrak{C}_c(x_0,t_0) = \left\{ (x,t) \in \mathbb{R}^n \times \mathbb{R} \middle| \, \|x - x_0\| = c|t - t_0| \right\},$$

the boundary of the light cone, with $t < t_0$, and is independent of the other $u(x,t)$.)

Similarly, $u(x_0,t_0)$ influences only those $u(x,t)$ for $(x,t) \in \mathfrak{C}_c(x_0,t_0)$ with $t > t_0$, etc. Intuitively, this means that an initial excitation (e.g., a flash of light) at (x_0,t_0) is visible only to an observer at position x once a time of $\|x - x_0\|/c$ has passed after t_0.

All of this is an affirmation of the statement that the speed of light c is an absolute maximum, and that no information is transmitted through the medium via the wave equation at any speed faster than c. This will turn out to contrast starkly with the behaviour of solutions to the spatially discretized wave equation (1.2.7).

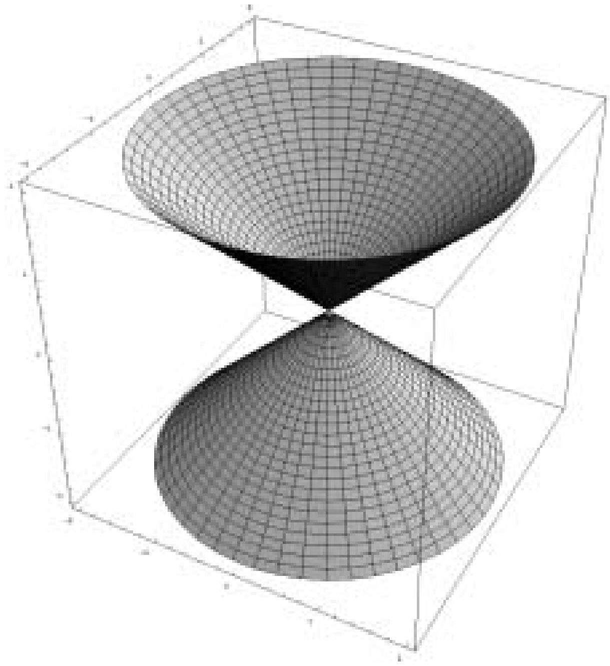

Figure 3.1.1: The boundary of the light cone, $\partial\mathfrak{C}_1(0,0) \subset \mathbb{R}^2 \times \mathbb{R}$, in the region $|t| \leq 2$.

3.2 The Case $n = 1$ – The Infinite Harmonic Chain

The case $n = 1$ has been studied by Friesecke [2]. Friesecke takes two approaches, the techniques of Green's functions and Fourier transforms, to establish the exact equation of motion

$$\begin{aligned} q(hm, t) &= J_{2m}(2t\omega), \\ &= \frac{1}{2\pi} \int_0^{2\pi} e^{i2t\omega \sin z} e^{-i2mz} \, dz, \end{aligned}$$

where J_m is the Bessel function of the first kind as defined by equation (1.4.2). Friesecke proves the following conclusions:

Proposition 3.2.1. [2] *Under the evolution equation (1.2.7) with initial data (1.3.1) with $q_0 = 1$, the particle initially excited obeys the equation*

$$\ddot{q}(0,t) + \frac{1}{t}\dot{q}(0,t) + 4\omega^2 q(0,t) = 0 \tag{3.2.1}$$

for all $t > 0$.

That is, compared to the undamped and uncoupled oscillator equation (2.1.1),

$$\ddot{q}(0,t) + 2\omega^2 q(0,t) = 0,$$

coupling to the chain induces

(i) a damping coefficient proportional to $1/t$, and

(ii) an effective hardening of the spring constant by a factor of 2.

These changes can be seen in Figure 3.2.1. For comparison, the later Figures 4.3.1 and 4.3.2 show the corresponding changes in dimensions $n = 2$ and 3.

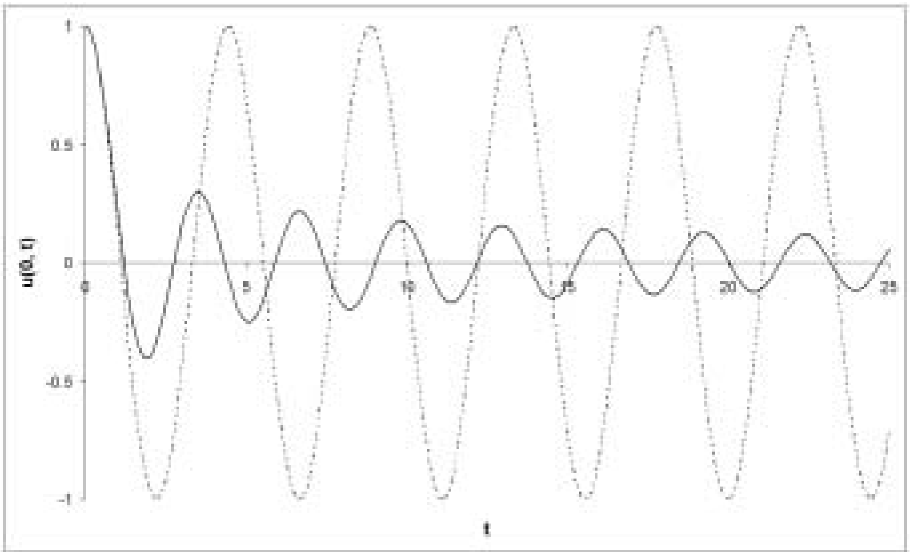

Figure 3.2.1: A plot of $u(0,t)$ for $t \in [0, 25]$ in the coupled (solid line) and uncoupled (dotted line) cases, dimension $n = 1$.

Proposition 3.2.2. [2] *Under the evolution equation (1.2.7) with initial data (1.3.1) with* $q_0 = 1$*, for all* $t > 0$*,*

(i) (Monotone wavefront) in the region $\{m \in \mathbb{Z} \| m| > \omega t\}$*, the displacements* $q(hm, t)$ *are positive and strictly decreasing with* $|m|$*;*

(ii) (Ultra-oscillatory wake) in the region $\left\{m \in \mathbb{Z} \,\middle|\, |m| \leq \frac{1}{\sqrt{2}}\omega t\right\}$*, each particle possesses a nearest neighbour with displacement of opposite sign,*

i.e. at least one of $q(hm,t)q(h(m+1),t)$ *and* $q(hm,t)q(h(m-1),t)$ *is* ≤ 0.

Sketch Proof. The proof of (i) above revolves around the following facts:

(i) the recursion identity

$$J_m(\tau) = \frac{\tau}{m}\frac{J_{m-1}(\tau) - J_{m+1}(\tau)}{2}, \tag{3.2.2}$$

(ii) for any fixed $\tau > 0$, $J_m(\tau) \to 0$ as $|m| \to \infty$;

(iii) for any fixed $\tau > 0$, $J_m(\tau) > 0$ for $|m|$ sufficiently large;

(iv) for $|m| > \tau > 0$, $J_m(\tau)$ has no positive local maximum with respect to m.

These facts together imply that for $|m| > \tau > 0$,

$$J_{|m|-1}(\tau) > J_{|m|}(\tau) > J_{|m|+1}(\tau) > J_{|m|+2}(\tau) > \cdots > 0.$$

□

Proposition 3.2.2(i) shows a fascinating change in the role of the light cone. In the continuum case, (1.4.1), we have $u(x,t) \equiv 0$ for $(x,t) \in \operatorname{Ext}\mathfrak{C}_c(0,0)$. Proposition 3.2.2, however, tells us that the displacements in $\operatorname{Ext}\mathfrak{C}_{\omega h}(0,0)$ are not zero, but instead are strictly positive!

What is the cause of this apparent collapse of the idea that the waves should travel at finite speed? The reason is simple, and is perhaps best visualized in the setting of an infinite lattice of particles joined by harmonic springs. Suppose particle $x \in \Lambda$ moves slightly; how long will it take before the particles $y \in N_1(x)$ "feel" this motion? A quick examination of (1.2.7) tells us that they "feel" it instantly: the acceleration of a particle at time t is determined the positions of its neighbours at that same time t. For this reason, small positive displacements propagate with infinite speed.

In reality, however, particles do not interact instantly. If, for instance, the particles were atomic particles interacting via the electromagnetic force, the interaction between them is carried by a photon, and photons do not travel instantly; they travel at the speed of light!

There is another *caveat* to this notion of "infinite wavespeed", in that because the particle displacements in Ext $\mathfrak{C}_{\omega h}(0,0)$ are strictly positive, there is no "contrast" in the data observed in this region. An observer fixed in space must wait until (s)he lies within the light cone to receive any contrasting (i.e., negative, with $q(x,t) < 0$) displacement data. In fact, information carried by the wave travels at most at speed $\omega h < \infty$; this assertion is justified by the arguments of Subsection 6.2.

We hope to generalize Proposition 3.2.2 to dimension n. The n-dimensional version of part (i) would assert the existence of a spherical wavefront expanding at constant finite speed, outside which $q(x,t)\cdot q(0,0) \geq 0$ and and $\|q(x,t)\|$ is strictly decreasing with increasing $\|x\|$. We will see that the n-dimensional analogue of part (ii) is somewhat less definite than the $n = 1$ case.

Proposition 3.2.3. [2] *Under the evolution equation (1.2.7) with initial data (1.3.1) with* $q_0 = 1$*,*

(i) (Synchronized binary oscillations) for each fixed $m \in \mathbb{Z}$

$$q(hm,t) = \frac{(-1)^m}{\sqrt{\pi \omega t}} \cos\left(2\omega t - \frac{\pi}{4}\right) + O(t^{-1}) \ \textit{as}\ t \to \infty;$$

(ii) (Travelling peaks) as $t \to \infty$*,*

$$q(hm,t)|_{|m|=\omega t} = \frac{\Gamma(1/3)}{2 \cdot 3^{1/6} \pi (\omega t)^{1/3}} + O(t^{-2/3}).$$

The salient point to extract from Proposition 3.2.3 is that the amplitude of oscillation of any particular particle decays like $t^{-1/2}$, but the amplitude of displacement of the wavefront travelling along the two branches of the 1-dimensional continuum light cone decays like $t^{-1/3}$. We shall try to generalize these decays laws for general $n \in \mathbb{N}$.

4 Numerical Simulation

4.1 Numerical Simulation

Recall the equation of motion (1.2.7):

$$\ddot{q}(x,t) = \omega^2 h^2 \Delta_h q(x,t).$$

We can apply the approximation formula (1.2.4) to (1.2.7) to approximate partial differentiation of q with respect to t and obtain the approximation that for small $\delta > 0$,

$$q(x,t+\delta) \approx (\delta\omega h)^2 \Delta_h q(x,t) + 2q(x,t) - q(x,t-\delta). \tag{4.1.1}$$

We can use this approximation to define an iterative procedure to simulate the dynamics of the lattice. We shall denote the displacements in this numerical model by $Q(x,t)$. Fix a small[2] $\delta > 0$ and an $\omega = \sqrt{\kappa/m} \geq 0$. The values $Q(x,t)$ are recursively defined for $t \in \delta\mathbb{N}$ by

$$Q(x,t+\delta) := (\delta\omega h)^2 \Delta_h Q(x,t) + 2Q(x,t) - Q(x,t-\delta),$$

where $Q(x,0) = Q(x,-\delta)$ are our given initial position data.

Since we cannot simulate a countably infinite collection of particles, we consider not the whole of Λ but instead a (suitably large) subset $\Lambda|_w \subset \Lambda$, $w > 0$, defined by

$$\Lambda|_w := \left\{ x = (x^1, \dots, x^n) \in \Lambda \,\middle|\, |x^j| < w \text{ for } j = 1, \dots, n \right\}.$$

Simply put, $\Lambda|_w$ is an n-dimensional cube of particles with $2\lfloor w \rfloor + 1$ particles along each side. (For the rest of this section, assume that $w \in \mathbb{N}$.)

The model (4.1.1) is, however, not a particularly good one. Its main flaw is that it is nonlinear and thus can do poorly at obeying (2.3.1) and fail to conserve the total energy in the system. A better (i.e. more conservative)

[2] δ must be small enough, for instance, to satisfy the Courant-Friedrich-Lévy condition $\delta < h/c = \omega^{-1}$, i.e. that our time step should not be longer than the time taken for the continuum wave to cross one spatial interval.

model can be obtained by considering the following system of two equations, which is equivalent to (1.2.7):

$$\begin{cases} \dot{p}(x,t) = \omega^2 h^2 \Delta_h q(x,t), \\ p(x,t) = \dot{q}(x,t). \end{cases}$$

A naïve way to turn this into a numerical program would be to consider the system in which we recursively define for $t \in \delta\mathbb{N}$

$$\begin{cases} \acute{Q}(x,t+\delta) := \acute{Q}(x,t) + \delta\omega^2 h^2 \Delta_h Q(x,t), \\ Q(x,t+\delta) := Q(x,t) + \delta\acute{Q}(x,t), \end{cases} \tag{4.1.2}$$

with initial data $Q(x,0)$ and $\acute{Q}(x,0)$. ($\acute{Q}$ takes the place of $\dot{q}$). However, we actually get an even better model if we use the system

$$\begin{cases} \acute{Q}(x,t+\delta) := \acute{Q}(x,t) + \delta\omega^2 h^2 \Delta_h Q(x,t), \\ Q(x,t+\delta) := Q(x,t) + \delta\acute{Q}(x,t+\delta). \end{cases} \tag{4.1.3}$$

Lemma 2.2.2 allows us to make a small short-cut, for we need only simulate the subset of $\Lambda|_w$ for which all particles have all coordinates ≥ 0. In the case that $x^j = 0$ we count the neighbour $x + he_j$ twice, since $x - he_j$ then lies outside the scope of our simulation. The model (4.1.3), with this symmetry short-cut, is the one used to model to short- to medium-time dynamics of the system. The program used is outlined in Subsection 4.2.

Of course, it will happen that for points x that lie on one or more "faces" of $\Lambda|_w$ that the sum $\Delta_h Q(x,t)$ makes reference to points outside $\Lambda|_w$, and hence outside our model. The points x for which this problem occurs will be those with at least one coordinate $|x^j| = w$. There are three ways of resolving this difficulty:

(i) simply define $Q(x,t) := 0$ for all t and all $x \in \Lambda \backslash (\Lambda|_w)$ i.e. fix the particles $x \in \Lambda \backslash (\Lambda|_w)$;

(ii) neglect the existence of, and all forces arising from springs connected to, particles $x \in \Lambda \backslash (\Lambda|_w)$;

(iii) consider $\Lambda|_w$ to be a discretized version of the n-torus, i.e. having opposite faces identified. That is, think of $\Lambda|_w$ as $\Lambda/\sim$, where $x \sim y$ if and only if $x - y \in wh\mathbb{Z}^n$.

These three possible resolutions correspond to three possible boundary conditions on the problem restricted to the cube $\Lambda|_w$:

(i) fixed boundary conditions;

(ii) free boundary conditions;

(iii) opposite boundary edges compatible (equal).

4.2 Outline of Simulation Program

The system (1.2.7) with initial conditions (1.3.1) has been simulated using object-oriented C++. We simulate the behaviour of the bounded subset $\Lambda|_w$ of Λ for a choice of $w > 0$.

We begin by specifying certain physical parameters: the model dimension n, the lattice spacing h, and $\omega = \sqrt{\kappa/m}$. We also specify the initial displacement q_0. We also specify certain other parameters for the simulation: the time step δ, the boundary conditions (fixed, free or periodic). We specify the length of time that the simulation will cover, the types of outputs we shall require and at what frequency.

We create a collection of w^n atom objects; this collection corresponds to

$$\{x \in \Lambda | 0 \leq hx^j < w \text{ for } j = 1, \ldots, n\}.$$

These atom objects are indexed by integers, but there are functions that allow us to freely translate between the integer label of an atom and its equilibrium position. The atom object stores the equilibrium position of the atom, its displacement and velocity at times t and $t + \delta$, and the labels of its $2n$ nearest neighbours. As indicated in the previous subsection, we use the symmetry of the problem and consider only atoms with all coordinates non-negative. Having created this collection of atoms, we apply the initial conditions.

At each time step t, we then do the obvious thing. For each particle in the simulation, we calculate the sum of forces from its nearest neighbours, and use (4.1.3) to define the position and velocity of the particle at the next time step. Once this calculation has been done for all atoms, we copy the "future" data into the space for "the present", and repeat until we have covered the desired length of time, outputting data as the simulation parameters dictate.

We have the following types of data output:

(i) Displacement and velocity data. At each time t, the program outputs to a new file (one for each time t) the equilibrium position x, the displacement $Q(x,t)$ and the velocity $\acute{Q}(x,t)$ of each particle $x \in \Lambda|_w$.

(ii) Displacement data for the unit cube. Similar to the above, but the data is displacement-only, is written to a single file, and is given only for the particles with all coordinates 0 or h. This is useful for identifying the number of asymptotic phases of the system (see Subsection 6.3).

(iii) Energy data. At each time t, the program calculates the total kinetic energy, $T(t)$, and potential energy in the system, $V(t)$. The program then outputs t, $V(t)$, $T(t)$, $V(t)+T(t)$ and the Lagrangian $T(t)-V(t)$ to a single file. The program also makes a note of the percentage error in the total energy, i.e.

$$\left(\frac{V(t)+T(t)}{V(0)+T(0)}-1\right)\times 100\%$$

as a check on the validity of the model.[3]

(iv) Wavespeed data. The location of the maximum displacement from equilibrium is identified by an exhaustive search. The location of the monotone wavefront is identified by a sequence of checks, approaching 0 from "$+\infty$" along the e_1 axis.

(v) Colour image. Colour values are assigned to each particle using the hue/saturation/luminance colour scheme. In essence, the colour assigned to a particle indicates the direction of its displacement and the brightness (luminance) of the colour the magnitude of displacement; greater luminance indicates greater displacement. A black pixel corresponds to zero displacement. [2D only.]

(vi) Greyscale image. Greyscale values $G(x,t) \in \{0,1,\ldots,255\} \subset \mathbb{Z}$ are defined by $G(x,t) := \lfloor 128(U'(x,t)+1)\rfloor$, where $U' := \mathrm{sgn}(U)\sqrt{|U|}$ and

[3] With $\delta = 0.001$, this error is typically of order 0.01% or smaller.

$U(x,t)q_0 = Q(x,t)$. Thus, a particle close to its equilibrium position will have associated to it a grey pixel; a particle with displacement very close to q_0 will have a nearly white pixel; a particle with displacement very close to $-q_0$ will have a nearly black pixel. (The transformation $U' := \mathrm{sgn}(U)\sqrt{|U|}$ has the effect of increasing the contrast of the picture.) [2D only.]

The source code for the program and a pre-compiled executable file have been included on a disk with this project report, along with a guide for the use of the program.

4.3 Observations and Hypotheses

Having implemented the model (4.1.3) in dimensions $n = 1, 2, 3$, we make some observations and hypotheses for the behaviour of the system for general n.

Our first observations concern the particle at the origin. As can be seen in Figures 4.3.1 and 4.3.2, $u(0,t)$ does not exhibit the same 'nice' oscillation and decay in dimensions $n > 1$ that it does in dimension $n = 1$ (Figure 3.2.1). This indicates to us right away that the exact dynamics of the n-dimensional system are going to be considerably more complicated than the 1-dimensional system.

As (1.2.7) is a spatial discretization of the wave equation (1.4.1), one quantity that we should be interested in is the speed of the wave's propagation. In fact, there are several phenomena whose speed of propagation we shall wish to identify. The first that we shall consider is the speed of propagation of the region of greatest displacement. In more detail:

Definitions 4.3.1. For $t \geq 0$ let $x_\star(t) \in \Lambda$ be such that

$$\|q(x_\star(t), t)\| = \max_{x \in \Lambda} \|q(x,t)\|.$$

Define the *maximum displacement wavespeed* by

$$c_\star = \limsup_{t \to \infty} \frac{\|x_\star(t)\|}{t}$$

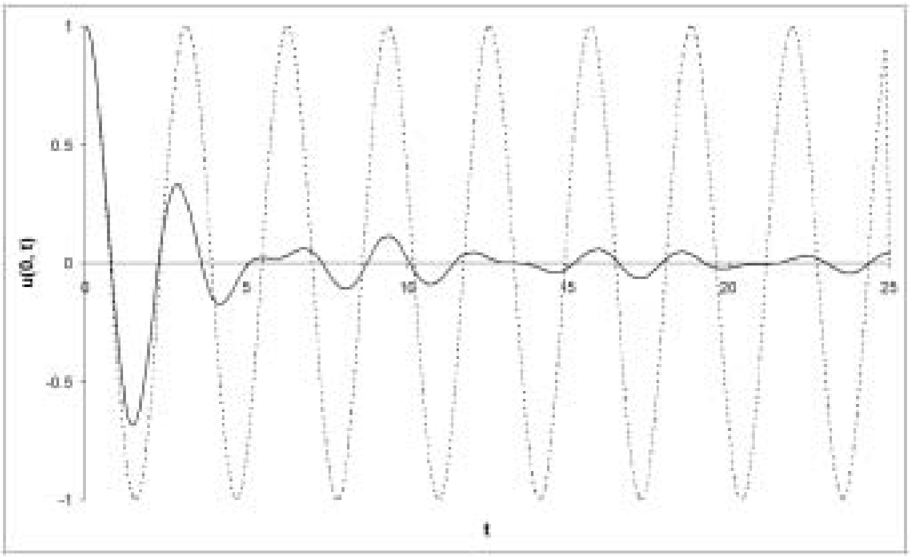

Figure 4.3.1: A plot of $u(0,t)$ for $t \in [0, 25]$ in the coupled (solid line) and uncoupled (dotted line) cases, dimension $n = 2$. Cf. Figures 3.2.1, 4.3.2.

We make the following observations based on simulations in dimensions $n = 1, 2, 3$:

Observations 4.3.2. (Diagonal Propagation of Maximal Displacement.)

(i) The wavespeed $c_\star \approx \frac{1}{\sqrt{n}}\omega h$.

(ii) The point $x_\star(t)$ *appears to move along the principal diagonals of the lattice: if* $x_\star(t) = (x_\star^1(t), \dots, x_\star^n(t))$ *then* $|x_\star^1(t)| \approx \dots \approx |x_\star^n(t)|$.

(iii) There appears to be a decay constant $d_\star \approx -\frac{n}{3}$ *such that* $\|q(x_\star(t), t)\| \sim t^{d_\star}$.

A second wavespeed that we define is $c_\bullet$, the speed of expansion of a spherical wavefront centred at the origin. Keeping Friesecke's 1-dimensional result Proposition 3.2.2(i) in mind, we define $c_\bullet$ as follows:

Definition 4.3.3. Define $c_\bullet$ to be the infimum of all non-negative constants c with the property that $\forall x \in \Lambda$ with $\|x\| > ct$, $q(x,t) \cdot q(0,0) \geq 0$ and $\|q(x,t)\|$ is decreasing with $\|x\|$.

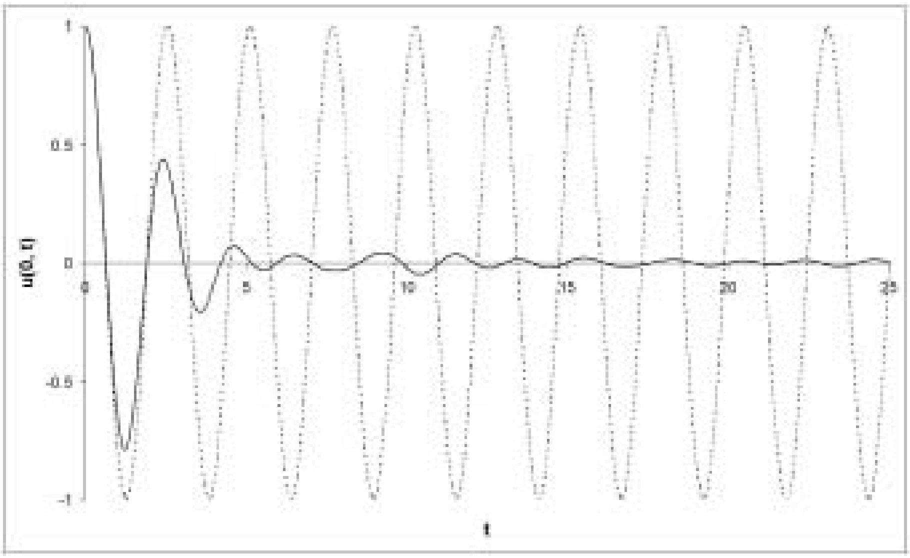

Figure 4.3.2: A plot of $u(0, t)$ for $t \in [0, 25]$ in the coupled (solid line) and uncoupled (dotted line) cases, dimension $n = 3$. Cf. Figures 3.2.1, 4.3.1.

Observations 4.3.4. (Spherical Monotone Wavefront.) *There appears to be a constant* $c_\bullet \approx \omega h$ *such that for* $t > 0$*, in the region* $\operatorname{Ext} \mathfrak{C}_{c_\bullet}(0, 0)$ *(the exterior of the continuum light cone), the displacements* $q(x, t)$ *satisfy* $q(x, t) \cdot q(0, 0) > 0$ *and* $\|q(x, t)\|$ *is strictly decreasing with increasing* $\|x\|$*.*

We also make the following observations about the long-term behaviour of the system.

Observations 4.3.5. (Oscillatory Wake.)

(i) There appears to be a constant $c_\circ$ *such that in the region* $\Lambda|_{c_\circ t}$ *each particle is synchronized with its second-nearest neighbours in the* $\pm e_j$ *directions, i.e.* $q(x, t) \approx q(y, t)$ *for* $y \in N_2(x)$*.*

(ii) There appears to be a decay constant $d_\circ \approx -\frac{n}{2}$ *such that for any* x *in this region,* $\|q(x, t)\| \sim t^{d_\circ}$*.*

Note that this is also somewhat different from the corresponding statement in dimension $n = 1$ (see Proposition 3.2.2(ii)). In that case we know not only that second-nearest neighbours become synchronized, but that nearest neighbours become anti-synchronized. As we shall see later, although the oscillations of $x \in \Lambda$ and $y \in N_1(x)$ decay at the same rate, they do not tend to a phase difference of π (exact anti-synchronization) except in dimension $n = 1$.

Observations 4.3.2 and 4.3.4 illustrate a startling difference between dimension $n = 1$ and dimensions $n > 1$. That is, in dimension $n = 1$, maximal displacement "lives on" the first monotone wavefront and the two phenomena are coincident and travel at the same speed (it is trivially true that $x_\star(t)$ moves along the 'principal diagonal' of the infinite harmonic chain $h\mathbb{Z}$, which is $h\mathbb{Z}$ itself). However, in dimensions $n > 1$, maximal displacement travels at a slower speed than the first monotone wavefront, and while the monotone wavefront is spherical, the regions of maximal displacement are concentrated about the principal diagonals of the lattice. Moreover, the speed of propagation of the monotone spherical wavefront is independent of dimension, whereas the speed of propagation of maximal displacement is strictly decreasing with dimension.

Observations 4.3.2 and 4.3.4 also show that the spatial discretization of the continuum wave equation (1.4.1) to obtain (1.2.7) causes another major departure from the character of the solution to the continuum wave equation. The solution to the wave equation in $\mathbb{R}^n$ is invariant under the isometry group $\mathrm{O}(n)$; the solutions are spherically symmetric. However, the solutions to (1.2.7) with initial conditions (1.3.1) are not spherically symmetric: they enjoy invariance only under the action of $\mathrm{Isom}_0(\Lambda) \subset \mathrm{O}(n)$. Even the first spherical monotone wavefront, a "ghostly echo" of the continuum light cone, does not have equal amplitude around its circumference. This distinction is not visible in dimension $n = 1$, for $\mathrm{Isom}_0(h\mathbb{Z}) \cong \mathrm{O}(1) \cong \{\mathrm{id}, x \mapsto -x\}$.

See Figure 4.3.3 for an illustration of some of these phenomena in dimension $n = 2$.

Let us summarize some of what we know and have hypothesized so far:

Phenomenon	Known for $n = 1$, [2]	Hypothesized for $n \in \mathbb{N}$
First spherical monotone wavefront		
Speed of travel, $c_\bullet$	ωh	ωh
Decay of amplitude	$\sim t^{-1/3}$	?
Maximal displacement		
Speed of travel, $c_\star$	ωh	$\frac{1}{\sqrt{n}}\omega h$
Decay of amplitude	$\sim t^{-1/3}$	$\sim t^{-n/3}$
Oscillatory wake		
Speed of expansion, $c_\circ$	$\frac{1}{\sqrt{2}}\omega h$	?
Decay of amplitude	$\sim t^{-1/2}$	$\sim t^{-n/2}$

At this point it may be wise to remark on the repeated occurrence of the term ωh in our wavespeeds, for instance $c_\star \approx \frac{1}{\sqrt{n}}\omega h$. After a cursory examination of the equation of motion (1.2.7) and its continuous counterpart (1.4.1) we should not be surprised to find that wavespeed depends on ωh, for, as we have previously remarked, the continuum wave equation (1.4.1) is the "limit" of (1.2.7) as $h \to 0$ with ωh held constant and equal to c. An observer outside the lattice, measuring distances and speeds with respect to the ambient space $\mathbb{R}^n$, would wish to regard ωh as being the proper wavespeed.

There is another way to see the situation. The formula $\|x_\star(t)\| = \omega h t$ in dimension $n = 1$ tells us that the peak displacement "lives on" the ωth particles from the origin in the positive and negative directions. But the particle x is $\|x\|/h$ places away from the origin, so the point $x_\star(t)$ moves at a speed of ω lattice spacings per unit time.

We make another observation concerning the behaviour of the system with respect to energy (see Figure 4.3.4):

Observations 4.3.6. (Energies) *As* $t \to 0$,

(i) $T(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$;

(ii) $V(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$;

(iii) $\mathcal{L}(t) \to 0$.

Note that, by Lemma 2.3.7, we need only prove one of these three statements in order to know that all of them are true.

5 Spectral and Fourier Methods

In this section we give two alternative approaches to the derivation of an integral form for the equation of motion of an arbitrary particle $x \in \Lambda$. In the first subsection we shall apply the Fourier transform to the equation of motion (1.2.7) and derive our integral equation by that means. In the second subsection our approach is to examine the discrete Laplacian operator Δ_h and apply the spectral theory of operators on Hilbert spaces.

5.1 Fourier Methods

Again we recall (1.2.7):

$$\begin{aligned} \ddot{q}(x,t) &= \omega^2 h^2 \Delta_h q(x,t), \\ &= \omega^2 \sum_{j=1}^{n} \left(q(x+he_j,t) - 2q(x,t) + q(x-he_j,t) \right). \end{aligned}$$

Rather than assume total familiarity with the general Fourier transform, we shall briefly review the essential facts. Essentially, the Fourier transform of a function defined on a topological group G is a function defined on the dual group $\hat{G}$, which is itself a topological group when G is Abelian.

Definition 5.1.1. [4] A *topological group* is a group with a topology on the underlying set, with respect to which the map $G \times G \to G$ given by $(x,y) \mapsto xy^{-1}$ is continuous. The *Pontrjagin dual* $\hat{G}$ of a topological group G is the set of equivalence classes of irreducible unitary representations of G.[4]

Such irreducible representations in $\hat{G}$ are one-dimensional (and hence irreducible) when G is Abelian. For some "nice" groups G, $\hat{G}$ is isomorphic to a similarly "nice" group, as in:

$$\begin{aligned} \widehat{\mathbb{R}^n} &\cong \mathbb{R}^n, \\ \widehat{\mathbb{T}^n} &\cong \mathbb{Z}^n, \\ \widehat{\mathbb{Z}^n} &\cong \mathbb{T}^n, \\ \widehat{\mathbb{Z}_m} &\cong \mathbb{Z}_m. \end{aligned}$$

[4]When G is some space, $\hat{G}$ is the space of wavenumbers of oscillations on G; physicists often use the term *Brillouin zone* for this space.

The third example is the one that interests us. The following theorem guarantees that (once some normalizations of measures are made) when we pass from G to the dual of G, and then to the dual of the dual, we end up with the same group and function as we started with:

Theorem 5.1.2. (Pontrjagin's Theorem [4].) *For an arbitrary locally compact commutative group G, the canonical mapping of G into $\hat{\hat{G}}$ is an isomorphism of topological groups. Haar measures on G and $\hat{G}$ can be normalized so that the Fourier transforms from G to $\hat{G}$ and from $\hat{G}$ to $\hat{\hat{G}} = G$ will be connected by the relations*

$$\hat{f}(\chi) = \int_G f(g)\chi(g)\, dg$$
$$f(g) = \int_{\hat{G}} \hat{f}(\chi)\overline{\chi(g)}\, d\chi$$
$$\int_G |f(g)|^2\, dg = \int_{\hat{G}} \left|\hat{f}(\chi)\right|^2\, d\chi$$

If the group G is compact and the measure dg is normalized so that $\int_G dg = 1$ then the group $\hat{G}$ is discrete and each of its points has measure 1. Conversely, if G is discrete and each of its points has measure 1, then $\hat{G}$ is compact and $\int_{\hat{G}} d\chi = 1$.

Definition 5.1.3. Let $\mathcal{H}^0$ denote *zero Hausdorff measure* on a discrete set D, defined by $\mathcal{H}^0(S) := \#S$ for $S \subseteq D$.

For us, $\Lambda = h\mathbb{Z}^n$ is indeed a discrete locally compact commutative group. The Haar measure on Λ is $\mathcal{H}^0$. The irreducible unitary representations of $h\mathbb{Z}^n$ are the functions $x \mapsto e^{i\xi\cdot x}$ for $h\xi \in \mathbb{T}^n$. Thus, the dual group $\widehat{\Lambda} := \mathrm{Hom}(\Lambda, S^1) = h^{-1}\mathbb{T}^n$, where $\mathbb{T}^n$ is the n-torus with addition modulo 2π:

$$\mathbb{T}^n := \left\{ (\xi^1, \ldots, \xi^n) \middle|\, \xi^j \in (-\pi, \pi] \subset \mathbb{R} \right\} \cong \mathrm{Hom}(\Lambda, \mathbb{C})$$

Since $\int_{h^{-1}\mathbb{T}^n} 1\; d\xi = (2\pi/h)^n$, $\widehat{\Lambda}$ has the normalized Haar measure $\left(\frac{h}{2\pi}\right)^n \mathcal{L}^n$, where $\mathcal{L}^n$ is n-dimensional Lebesgue measure. (See Figure 5.1.1.)

Theorem 5.1.4. *The Fourier transform from Λ to $\widehat{\Lambda}$ satisfies the following:*

(i) The Fourier transform of $f : \Lambda \to \mathbb{C}$ is $\hat{f} : \widehat{\Lambda} \to \mathbb{C}$ given by

$$\begin{aligned}\hat{f}(\xi) &:= \int_{\Lambda} f(x) e^{-i\xi\cdot x}\, d\mathcal{H}^0(x),\\ &= \sum_{x\in\Lambda} f(x) e^{-i\xi\cdot x}.\end{aligned}$$

(ii) The reconstruction law is

$$f(x) = \left(\frac{h}{2\pi}\right)^n \int_{\widehat{\Lambda}} \hat{f}(\xi) e^{i\xi\cdot x}\, d\xi.$$

(iii) The Plancherel equality:

$$\sum_{x\in\Lambda} |f(x)|^2 = \left(\frac{h}{2\pi}\right)^n \int_{\widehat{\Lambda}} \left|\hat{f}(\xi)\right|^2\, d\xi. \tag{5.1.1}$$

(iv) The translation property that if $(T_y f)(x) := f(x+y)$ for $y \in \Lambda$, then

$$\widehat{T_y f}(\xi) = e^{i\xi\cdot y} \hat{f}(\xi). \tag{5.1.2}$$

(v) The convolution properties

$$\begin{aligned}\widehat{f * g}(\xi) &= \hat{f}(\xi)\hat{g}(\xi),\\ \widehat{fg}(\xi) &= \left(\frac{h}{2\pi}\right)^n \left(\hat{f} * \hat{g}\right)(\xi).\end{aligned}$$

Proof. (i), (ii) and (iii) follow from Theorem 5.1.2. In particular, (i) implies that the operation $f \mapsto \hat{f}$ is linear. As for (iv):

$$\begin{aligned}\widehat{T_y f}(\xi) &= \sum_{x\in\Lambda} f(x+y) e^{-i\xi\cdot x}\\ &= \sum_{z\in\Lambda} f(z) e^{-i\xi\cdot(z-y)}\\ &= e^{i\xi\cdot y} \sum_{z\in\Lambda} f(z) e^{-i\xi\cdot z}\\ &= e^{i\xi\cdot y} \hat{f}(\xi)\end{aligned}$$

(v) is included for interest and left as an exercise; it shall not be needed in this work. $\square$

We are interested in the partial Fourier transform in x, which we shall denote $q \mapsto \hat{q}$ just as before, given by

$$\begin{aligned}\hat{q}(\xi, t) &:= \int_\Lambda q(x,t) e^{-i\xi\cdot x}\, d\mathcal{H}^0(x), \\ &= \sum_{x\in\Lambda} q(x,t)e^{-i\xi\cdot x}.\end{aligned}$$

for $\xi \in \widehat{\Lambda}$. When integrating a vector quantity like $q(x,t)$, we integrate component-wise in the natural way. It is easy to see that the operation $q \mapsto \hat{q}$ commutes with the operation $q \mapsto \dot{q}$. Thus

$$\begin{aligned}\ddot{\hat{q}}(\xi,t) &= \sum_{x\in\Lambda} \omega^2 \sum_{j=1}^{n} \left(q(x+he_j,t) - 2q(x,t) + q(x-he_j,t)\right) e^{-i\xi\cdot x}, \\ &= \omega^2 \sum_{j=1}^{n} \sum_{x\in\Lambda} \left(q(x+he_j,t) - 2q(x,t) + q(x-he_j,t)\right) e^{-i\xi\cdot x},\end{aligned}$$

which, by equation (5.1.2) in Theorem 5.1.4,

$$\begin{aligned}&= \omega^2 \sum_{j=1}^{n} \left(e^{i\xi\cdot(he_j)} - 2 + e^{i\xi\cdot(-he_j)}\right) \hat{q}(x,t), \\ &= \omega^2 \sum_{j=1}^{n} \left(e^{ih\xi^j} - 2 + e^{-ih\xi^j}\right) \hat{q}(x,t).\end{aligned}$$

Hence, by the identity $\sin z = \frac{1}{2i}(e^{iz} - e^{-iz})$,

$$\ddot{\hat{q}}(\xi,t) = -4\omega^2 \left(\sum_{j=1}^{n} \sin^2 \frac{h\xi^j}{2}\right) \hat{q}(\xi,t). \tag{5.1.3}$$

If we define the function $\psi : \widehat{\Lambda} \to \mathbb{R}$ by

$$\psi(\xi) := \sqrt{\sum_{j=1}^{n} \sin^2 \frac{h\xi^j}{2}} \tag{5.1.4}$$

then we can write down the solution to the differential equation (5.1.3) as

$$\hat{q}(\xi,t) = A(\xi)e^{i2\omega\psi(\xi)t} + B(\xi)e^{-i2\omega\psi(\xi)t}. \tag{5.1.5}$$

Note that ψ is a bounded function: $0 \le \psi(\xi) \le \sqrt{n}$.

At time $t = 0$, $\hat{q}(\xi,0) = A(\xi) + B(\xi)$ and $\dot{\hat{q}}(\xi,0) = i2\omega\psi(\xi)(A(\xi) - B(\xi))$. Under initial conditions (1.3.1), $\dot{q}(x,0) \equiv 0$, so

$$\dot{\hat{q}}(\xi,0) = \hat{\dot{q}}(\xi,0) = \sum_{x\in\Lambda} 0e^{-i\xi\cdot x} = 0.$$

As for $\hat{q}(\xi,0)$:

$$\begin{aligned}\hat{q}(\xi,0) &= \sum_{x\in\Lambda} q(x,0)e^{-i\xi\cdot x},\\ &= q(0,0)e^{-i\xi\cdot 0},\\ &= q_0.\end{aligned}$$

Since $\psi(\xi)$ is not always zero, we see that $A(\xi) \equiv B(\xi) \equiv q_0/2$. Hence

$$\hat{q}(\xi,t) = \frac{q_0}{2}e^{i2\omega\psi(\xi)t} + \frac{q_0}{2}e^{-i2\omega\psi(\xi)t}, \tag{5.1.6}$$

i.e. $\hat{q}(\xi,t) = q_0\cos(2\omega\psi(\xi)t)$. Thus, applying the inverse Fourier transform yields

$$\begin{aligned}q(x,t) &= \left(\frac{h}{2\pi}\right)^n \int_{\widehat{\Lambda}} \left(\frac{q_0}{2}e^{i2\omega\psi(\xi)t} + \frac{q_0}{2}e^{-i2\omega\psi(\xi)t}\right) e^{i\xi\cdot x}\, d\xi,\\ &= \frac{q_0h^n}{2(2\pi)^n}\int_{\widehat{\Lambda}} e^{i(2\omega\psi(\xi)t+\xi\cdot x)} + e^{i(-2\omega\psi(\xi)t+\xi\cdot x)}\, d\xi.\end{aligned}$$

If we define, for $x \in \Lambda$ and $t > 0$,

$$\begin{aligned}\phi^+_{x,t}(\xi) &:= 2\omega\psi(\xi) + (\xi\cdot x)/t,\\ \phi^-_{x,t}(\xi) &:= -2\omega\psi(\xi) + (\xi\cdot x)/t,\end{aligned} \tag{5.1.7}$$

then for $t > 0$ we can re-write the above as

$$q(x,t) = \frac{q_0h^n}{2(2\pi)^n}\int_{\widehat{\Lambda}} e^{i\phi^+_{x,t}(\xi)t} + e^{i\phi^-_{x,t}(\xi)t}\, d\xi. \tag{5.1.8}$$

Another convenient expression of this equality is

$$q(x,t) = \frac{q_0 h^n}{(2\pi)^n} \int_{\widehat{\Lambda}} \cos\left(2\omega\psi(\xi)t\right) e^{i\xi\cdot x}\, d\xi. \tag{5.1.9}$$

If the reader wishes to check the validity of the above formulae, a quick partial verification can be made by showing that one recovers the initial conditions (1.3.1) when one sets $t = 0$.

5.2 Spectral Methods

There is another way to derive the integral equations at the end of the previous subsection, namely by the methods of the spectral theory of Hilbert space operators. The actual derivation is not hard, but would occupy several pages. Therefore, we shall only sketch the argument.

We first restrict our attention to the Hilbert space

$$\ell^2(\Lambda) := \left\{ f : \Lambda \to \mathbb{C} \;\middle|\; \|f\|_{\ell^2}^2 = \sum_{x\in\Lambda} |f(x)|^2 < \infty \right\}$$

equipped with the inner product $\langle f, g\rangle := \sum_{x\in\Lambda} f(x)\overline{g(x)}$ that induces the norm $\|\cdot\|_{\ell^2}$ by $\|f\|_{\ell^2} := \sqrt{\langle f, f\rangle}$. We then note that the discrete Laplacian $\Delta_h : \ell^2(\Lambda) \to \ell^2(\Lambda)$ is a bounded linear operator (it has operator norm $\|\Delta_h\| \le \frac{\sqrt{6n}}{h^2}$). Δ_h is also self-adjoint, i.e. $\Delta_h = \Delta_h^*$, where $\Delta_h^* : \ell^2(\Lambda) \to \ell^2(\Lambda)$ is the unique operator such that for all $f, g \in \ell^2(\Lambda)$,

$$\langle \Delta_h f, g\rangle = \langle f, \Delta_h^* g\rangle.$$

It then follows from the result usually known as the Spectral Theorem that there is a unitary operator $\mathcal{F} : \ell^2(\Lambda) \to \ell^2(\Lambda)$ such that $\mathcal{F}\circ\mathcal{F}^* = \mathcal{F}^*\circ\mathcal{F} = \mathrm{id}$ and $\mathcal{F}\circ\Delta_h\circ\mathcal{F}^*$ is diagonal. This operator $\mathcal{F}$ is none other than the Fourier transform, which is why we obtain the same integral equation as before.

6 Main Results

6.1 Preliminary Results

In this subsection we shall establish the spatial decay of the amplitude of oscillation at any fixed time $t \ge 0$. We shall need the Riemann-Lebesgue Lemma, which we recall here:

Lemma 6.1.1. (Riemann-Lebesgue [1].) *Let*

$$f_t \in L^1(\mathbb{T}^n) := \left\{ f : \mathbb{T}^n \to \mathbb{C} \,\middle|\, \|f\|_{L^1} := \int_{\mathbb{T}^n} |f(\xi)| \, d\xi < \infty \right\}.$$

Then

$$\int_{\mathbb{T}^n} f(\xi) e^{i\xi \cdot x} \, d\xi \to 0$$

as $\|x\| \to \infty$*, with* $x \in \mathbb{Z}^n$*. That is, the Fourier coefficients of an* L^1 *function decay to* 0 *as the indices of the coefficients increase to* ∞*.*

The conclusion of the Riemann-Lebesgue Lemma also holds if we replace $e^{i\xi \cdot x}$ by any trigonometric expression such as $\sin(\xi \cdot x)$ or $\cos(\xi \cdot x)$, since these are linear combinations of complex exponentials.

Note also that $f : \mathbb{T}^n \to \mathbb{C}$ bounded $\Rightarrow f \in L^1(\mathbb{T}^n)$ since

$$\|f\|_{L^1} \le \sup_{\xi \in \mathbb{T}^n} |f(\xi)| \int_{\mathbb{T}^n} 1 \, d\xi = (2\pi)^n \sup_{\xi \in \mathbb{T}^n} |f(\xi)|.$$

Proposition 6.1.2. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let* $t \ge 0$*. Then* $\|q(x,t)\| \to 0$ *as* $\|x\| \to \infty$*.*

Proof. Consider Equation (5.1.9). For any $t \ge 0$, the function $f_t(\xi) := \cos(2\omega\psi(\xi)t)$ satisfies $f_t \in L^1\left(\widehat{\Lambda}\right)$, since f_t is bounded. Also,

$$\|q(x,t)\| = \|q_0\| \left(\frac{h}{2\pi}\right)^n \left| \int_{\widehat{\Lambda}} f_t(\xi) e^{i\xi \cdot x} \, d\xi \right|,$$

so Proposition 6.1.2 follows by the Riemann-Lebesgue Lemma. □

Proposition 6.1.2 confirms our intuition that at any given time the amplitude of disturbance dies away to nothing as we move further from the source. It is vitally important to note, however, that Proposition 6.1.2 only tells us about the large-$\|x\|$ behaviour of $q(x,t)$ for fixed t. It does not tell us anything about the large-t behaviour of a given fixed $x \in \Lambda$, nor does it tell us anything about any wavefronts or maxima of displacement.

6.2 Group and Phase Velocities

When examining wave phenomena, there are two velocities of propagation that are usually considered, namely the *group velocity* and the *phase velocity*. Intuitively speaking, the phase velocity is a measure of the velocity of oscillation of the individual particles that constitute the medium through which the wave propagates. The group velocity, on the other hand, is a measure of the velocity with which information or energy carried by the wave propagates – it is the velocity of "the wave itself" as opposed to the medium in which the wave travels.

To formalize these notions, at least in one dimension, suppose we have a wave equation of the form

$$\frac{\partial^2}{\partial t^2}u(x,t) = c_2^2\frac{\partial^2}{\partial x^2}u(x,t) + c_4^2\frac{\partial^4}{\partial x^4}u(x,t) + \dots,$$

with $u : \mathbb{R}\times\mathbb{R}\to\mathbb{R}$ differentiable of the appropriate order. We can apply the usual Fourier transform

$$\hat{u}(\xi,t) = \int_{\mathbb{R}} f(x,t)e^{-i\xi x}\,dx$$

to get an equation of the form

$$\ddot{\hat{u}}(\xi,t) = -\left(c_2^2\xi^2 - c_4^2\xi^4 + \dots\right)\hat{u}(\xi,t)$$

and thus that

$$\hat{u}(\xi,t) = A(\xi)e^{i\sqrt{(c_2^2\xi^2 - c_4^2\xi^4+\dots)}t} + B(\xi)e^{-i\sqrt{(c_2^2\xi^2 - c_4^2\xi^4+\dots)}t},$$

for some $A(\xi)$, $B(\xi)$ depending on our initial data. When we take the inverse Fourier transform we get a linear combination of expressions of the form

$$\int_{\mathbb{R}} C(\xi)e^{ir(\xi)t}e^{i\xi x}\,d\xi = \int_{\mathbb{R}} C(\xi)e^{i\xi(x+\frac{r(\xi)}{\xi}t)}\,d\xi.$$

It is the term $x + \frac{r(\xi)}{\xi}t$ in the exponent that interests us. In the case of the continuum wave equation (1.4.1) we have $r(\xi) = c\xi$, and the group and phase velocities are both c for all wavenumbers ξ. In general, in dimension $n = 1$:

Definition 6.2.1. Let $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ be a solution to a wave equation of the form $\ddot{u} =$ some linear constant-coefficient spatial difference or differential expression in u. Suppose that $\hat{u}(\xi, t)$ is a linear sum of terms of the form $e^{\pm i r(\xi) t}$. Define the *phase velocity* $v_p(\xi)$ and *group velocity* $v_g(\xi)$ at wavenumber ξ by

$$\begin{aligned} v_p(\xi) &:= \frac{r(\xi)}{\xi}, \\ v_g(\xi) &:= \frac{\partial}{\partial \xi} r(\xi), \end{aligned}$$

and set

$$\begin{aligned} v_p &:= \sup_{\xi} |v_p(\xi)|, \\ v_g &:= \sup_{\xi} |v_g(\xi)|. \end{aligned}$$

In our case, $r(\xi) = 2\omega\psi(\xi)$, where ψ is as defined in equation (5.1.4). In dimension $n = 1$, therefore, we have

$$\begin{aligned} v_p(\xi) &= \frac{2\omega\psi(\xi)}{\xi}, \\ &= \frac{2\omega}{\xi} \sin \frac{h\xi}{2}, \end{aligned}$$

which is well-defined for wavenumbers $\xi \neq 0$. By l'Hôpital's rule, as $\xi \to 0$, $v_p(\xi) \to \omega h$; indeed, $v_p := \sup_\xi |v_p(\xi)| = \omega h$. As for group velocity

$$\begin{aligned} v_g(\xi) &= \frac{\partial}{\partial \xi} 2\omega\psi(\xi) \\ &= 2\omega \frac{h}{2} \cos \frac{h\xi}{2} \\ &= \omega h \cos \frac{h\xi}{2} \end{aligned}$$

In particular, $v_g = \omega h$, which justifies our earlier assertion that although the exterior of the continuum light cone $\mathfrak{C}_{\omega h}(0, 0)$ does not enjoy zero displacement, no actual information is transmitted faster than speed ωh.

We can easily generalize the notions of group and phase velocities to a wave in n dimensions:

Definition 6.2.2. Let $u : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ be a solution to a wave equation of the form $\ddot{u} =$ some linear constant-coefficient spatial difference or differential expression in u. Suppose that $\hat{u}(\xi, t)$ is a linear sum of terms of the form $e^{\pm ir(\xi)t}$. Define the *group velocity* by

$$\begin{aligned} v_g(\xi) &:= \nabla r(\xi) = \left(\frac{\partial}{\partial \xi^1} r(\xi), \ldots, \frac{\partial}{\partial \xi^n} r(\xi) \right), \\ v_g &:= \sup_\xi \|v_g(\xi)\|. \end{aligned}$$

Define the *phase velocity* by

$$\begin{aligned} v_p(\xi) &:= \frac{r(\xi)}{\|\xi\|}, \\ v_p &:= \sup_\xi |v_p(\xi)|. \end{aligned}$$

Theorem 6.2.3. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1). Then*

(i) the group velocity satisfies $v_g = \omega h$; and

(ii) the phase velocity satisfies $v_p = \omega h$.

Proof. (i) We calculate:

$$\begin{aligned} \frac{\partial}{\partial \xi^k} \psi(\xi) &= \frac{1}{2} \frac{1}{\psi(\xi)} 2 \frac{h}{2} \sin \frac{h\xi^k}{2} \cos \frac{h\xi^k}{2} \\ &= \frac{h}{4\psi(\xi)} \sin h\xi^k, \end{aligned}$$

thus

$$\nabla \psi(\xi) = \frac{h}{4\psi(\xi)} \left(\sin h\xi^1, \ldots, \sin h\xi^n \right). \tag{6.2.1}$$

Thus, we can say that in dimension n,

$$v_g(\xi) = \frac{\omega h}{2\psi(\xi)} \left(\sin h\xi^1, \ldots, \sin h\xi^n \right).$$

For $1 \le j \le n$, let $\zeta \in [0,1]^n$ be given by $\zeta^j := \sin \frac{h\xi^j}{2}$. It follows that $1 - (\zeta^j)^2 = \cos^2 \frac{h\xi^j}{2}$ and thus that $\sin h\xi^j = 4(\zeta^j)^2(1 - (\zeta^j)^2)$. Let

$$G(\zeta) := \sqrt{\frac{\sum_{j=1}^n (\zeta^j)^2 (1 - (\zeta^j)^2)}{\sum_{j=1}^n (\zeta^j)^2}}.$$

Then $\|v_g(\xi)\| = \omega h G(\zeta)$. We now show that $G(\zeta) \in [0,1]$ for $\zeta \in [0,1]^n$.

It is easy to see that $G(\zeta) \geq 0$ for all $\zeta \in [0,1]^n$ since $(\zeta^j)^2$ and $1-(\zeta^j)^2 \in [0,1]$. The lower bound $G(\zeta) = 0$ is attained by $\zeta = (1,1,\dots,1)$. Similarly, for each j, $(\zeta^j)^2(1-(\zeta^j)^2) \leq (\zeta^j)^2$, and so $G(\zeta) \leq 1$. Indeed, $G(\zeta) \to 1$ as $\zeta \to 0$. Thus $v_g = \omega h$.

(ii) $v_p(\xi) = \frac{2\omega\psi(\xi)}{\|\xi\|}$ and so

$$|v_p(\xi)|^2 = 4\omega^2 \frac{\sum_{j=1}^n \sin^2 \frac{h\xi^j}{2}}{\sum_{j=1}^n (\xi^j)^2}$$

For $\theta \in \mathbb{R}$, $|\sin\theta| \leq |\theta|$, so $\sin^2\theta \leq \theta^2$. Thus $\sum_{j=1}^n \sin^2 \frac{h\xi^j}{2} \leq \frac{h^2}{4} \sum_{j=1}^n (\xi^j)^2$. So $|v_p(\xi)| \leq \omega h$, and $|v_p(\xi)| \to \omega h$ as $\xi \to 0$, so $v_p = \omega h$. □

Theorem 6.2.3(i) makes rigorous the statement that the wave caused by the initial excitation at $0 \in \Lambda$ travels at speed $\omega h < \infty$. Note that ωh in equation (1.2.7) corresponds to c in equation (1.4.1), and so we have shown that at least some of the properties of the continuum case have passed over to the spatially discrete situation. In the case of the continuum wave equation, though, $\|v_g(\xi)\| = |v_p(\xi)| = c$ for all wavenumbers ξ. Here, however, we have an infinite collection of group and phase velocities, albeit one bounded in norm by $\omega h = c$.

6.3 Asymptotic Behaviour

The integral in (5.1.8) will be difficult to evaluate exactly to give an equation of motion for each particle. However, there are methods that will enable us to evaluate the integral for large t and thus determine the long-term dynamics of the system. The method of stationary phase (see Appendix B) tells us that the large-t behaviour of

$$\int_{\widehat{\Lambda}} e^{i\phi^{\pm}_{x,t}(\xi)t} \, d\xi$$

is dominated by the points of *stationary phase*, i.e. those ξ with $\nabla\phi^{\pm}_{x,t}(\xi) = 0$. For brevity hereafter, define the sets of points of stationary phase $S^{\pm}(x,t)$ by

$$S^{\pm}(x,t) := \left\{ \xi \in \widehat{\Lambda} \,\middle|\, \nabla\phi^{\pm}_{x,t}(\xi) = 0 \right\}.$$

Recall equation (6.2.1):

$$\nabla\psi(\xi) = \frac{h}{4\psi(\xi)}\left(\sin h\xi^1, \ldots, \sin h\xi^n\right)$$

Observe that $\nabla\psi(\xi) = 0 \Leftrightarrow$ for all j, $\xi^j \in \frac{\pi}{h}\mathbb{Z}$ and $\xi^j \notin \frac{2\pi}{h}\mathbb{Z}$ for some j. Thus,

$$\begin{aligned}\nabla\phi^{\pm}_{x,t}(\xi) &= \left(\pm 2\omega\frac{\partial}{\partial\xi^j}\psi(\xi) + \frac{\partial}{\partial\xi^j}\left(\frac{\xi\cdot x}{t}\right)\right)_{j=1}^{n}, \\ &= \pm 2\omega\nabla\psi(\xi) + x/t, \\ &= \pm\frac{\omega h}{2\psi(\xi)}\left(\sin h\xi^1, \ldots, \sin h\xi^n\right) + \frac{x}{t}.\end{aligned}$$

From here, we can compute the matrix of second-order partial derivatives:

$$\begin{aligned}D^2\phi^{\pm}_{x,t}(\xi) &= \left(\frac{\partial^2}{\partial\xi^k\partial\xi^\ell}\phi^{\pm}_{x,t}(\xi)\right)_{k,\ell=1}^{n} \\ &= \pm\frac{\omega h}{2\psi(\xi)}\left(h\delta_{k\ell}\cos h\xi^k \mp \frac{\omega h}{\psi(\xi)^2}\sin h\xi^k \sin h\xi^\ell\right)_{k,\ell=1}^{n}\end{aligned}$$

Hence

$$\begin{aligned}\xi \in S^{\pm}(x,t) &\Leftrightarrow \frac{\omega h}{2\psi(\xi)}\left(\sin h\xi^j\right)_{j=1}^{n} = \mp\frac{x}{t}, \\ &\Leftrightarrow \text{for } j = 1, \ldots, n,\ \sin h\xi^j = \mp\frac{2x^j\psi(\xi)}{\omega h t}.\end{aligned}$$

Fix $x \in \Lambda$ and let $\xi_s \in S^{\pm}(x,t)$. First, we examine the asymptotic position of ξ_s in $\widehat{\Lambda}$ as $t \to \infty$. Since ψ is bounded, $|2x^j\psi(\xi_s)/\omega h t| \to 0$ as $t \to \infty$, and so each $h\xi_s^j \to 0$ or $\pi \in S^1$. Not all the $h\xi_s^j$ can tend to zero, for then $\psi(\xi_s) \to 0$, which would contradict the assumption that $\nabla\phi^{\pm}_{x,t}(\xi_s) \equiv 0$ as $t \to \infty$. We draw three elementary conclusions:

(i) first, $2h\xi_s \to 0$ in $\mathbb{T}^n$ (remember that $2\pi \equiv 0$ in the circle group S^1);

(ii) secondly, $\lim_{t\to\infty}\psi(\xi_s) \in \left\{1, \sqrt{2}, \ldots, \sqrt{n}\right\}$;

(iii) thirdly,

$$D^2\phi^{\pm}_{x,t}(\xi_s) \to \pm\frac{\omega h^2}{2\psi(\xi_s)}\begin{pmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_n \end{pmatrix}$$

for $a_1, \dots, a_n \in \{-1, 1\}$ not all 1, since $a_j = \cos h\xi_s^j$ and not all $h\xi_s^j$ tend to 0.

Let $M(\xi_s) := \#\{1 \le j \le n | h\xi_s^j \to \pi\}$. Then $1 \le M(\xi_s) \le n$, $\psi(\xi_s) \to \sqrt{M(\xi_s)}$, and

$$(-1)^{M(\xi_s)} = \begin{vmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_n \end{vmatrix} = \prod_{j=1}^{n} a_j,$$

so

$$\det D^2\phi^{\pm}_{x,t}(\xi_s) \to (-1)^{M(\xi_s)}\left(\pm\frac{\omega h^2}{2\sqrt{M(\xi_s)}}\right)^n \ne 0.$$

Therefore, for sufficiently large t, the second derivative has full rank; the point of stationary phase is a *non-degenerate* critical point of $\phi^{\pm}_{x,t}$.

Thus, applying formula (B.1): to leading order,

$$\int_{\widehat{\Lambda}} e^{i\phi^{\pm}_{x,t}(\xi)t}\, d\xi \sim \sum_{\xi_s \in S^{\pm}(x,t)} e^{i\phi^{\pm}_{x,t}(\xi_s)t}\sqrt{\frac{(\pi i)^n}{t^n \det D^2\phi^{\pm}_{x,t}(\xi_s)}}. \tag{6.3.1}$$

We are now in a position to prove a weak version of Observation 4.3.5:

Proposition 6.3.1. (Oscillatory Wake.) *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let $x \in \Lambda$. Then, as $t \to \infty$,*

(i) $\|q(x,t)\| \lesssim t^{-n/2}$, i.e. decays at least as fast, if not faster than, $t^{-n/2}$;

(ii) $\|\dot{q}(x,t)\| \lesssim t^{-n/2}$;

(iii) for all $y \in N_2(x)$, the oscillations of x and y are asymptotically in phase and of the same amplitude.

Proof. (i) By inspection of equations (5.1.8) and (6.3.1) we see that (our approximation to) $q(x,t)$ is a sum of contributions of magnitude

$$\frac{\|q_0\|}{2(2\pi)^n}\left|\frac{\pi i\psi(\xi_s)}{t\omega h^2}\right|^{n/2} = \frac{\|q_0\|}{2}\left(\frac{\psi(\xi_s)}{4t\omega h^2}\right)^{n/2},$$

with $0 < \psi(\xi_s) \leq \sqrt{n}$. In particular, these contributions are of magnitude $t^{-n/2}$ (to leading order). It is possible that some of these contributions will cancel out, but this can only decrease the leading-order contribution to $\|q(x,t)\|$. Thus $\|q(x,t)\| \lesssim t^{-n/2}$.

(ii) Although we cannot differentiate the asymptotic expansion for $q(x,t)$ term-by-term, we can form an asymptotic expansion for $\dot{q}(x,t)$ from the inverse Fourier integral

$$\dot{q}(x,t) = -2\omega q_0\left(\frac{h}{2\pi}\right)^n \int_{\widehat{\Lambda}} \psi(\xi)\sin\left(2\omega\psi(\xi)t\right) e^{i\xi\cdot x}\, d\xi$$

This integral has exactly the same points of stationary phase as before, and they are again non-degenerate. We can apply formula (B.1) again to get another sum of terms of order $t^{-n/2}$, again possibly with cancellation. Thus $\|\dot{q}(x,t)\| \lesssim t^{-n/2}$.

(iii) Let $y \in N_2(x)$, $y = x + 2he_j$, say. As $t \to \infty$, both $|2x^j\psi(\xi_s)/\omega ht|$ and $|2y^j\psi(\xi_s)/\omega ht| \to 0$ uniformly for all j, so the elements of $S^{\pm}(x,t)$ can be made arbitrarily close to the corresponding elements of $S^{\pm}(y,t)$; in essence, we sum over the same set of stationary phase points for both x and y. Thus $q(x,t)$ and $q(y,t)$ receive asymptotically equal contributions that are possibly of different phases.

Consider the contributions to $q(x,t)$ and $q(y,t)$ coming from any particular point of stationary phase $\xi_s \in S^{\pm}(x,t)$ and examine the phase terms. The phase of the contribution to $q(x,t)$ is simply $\pm 2\omega\psi(\xi_s)t + \xi_s \cdot x$. The phase of the corresponding contribution to $q(y,t)$ is

$$\begin{aligned}\pm 2\omega\psi(\xi_s)t + \xi_s\cdot y &= \pm 2\omega\psi(\xi_s)t + \xi_s\cdot x + \xi_s\cdot 2he_j,\\ &= \pm 2\omega\psi(\xi_s)t + \xi_s\cdot x + 2h\xi_s^j,\end{aligned}$$

but $2h\xi_s^j \to 0 \in S^1$ as $t \to \infty$. Thus each contribution to $q(x,t)$ and $q(y,t)$ tends towards being in phase and of the same amplitude; thus, the oscillations of x and y are asymptotically in phase and of the same amplitude. □

Note that the statement of Proposition 6.3.1 that the oscillations of x and y are asymptotically in phase and of the same amplitude is far stronger than the statement that $\|q(x,t) - q(y,t)\| \to 0$ as $t \to \infty$, which is guaranteed by the $\lesssim t^{-n/2}$ decay law.

Proposition 6.3.1 goes some way towards establishing the long-time dynamics of any individual particle well inside the continuum light cone (the amplitude of its oscillation decays as $t^{-n/2}$), as well as telling us something about its relationship to its neighbours (each particle (asymptotically) oscillates in phase with its second-nearest neighbours). The obvious question is, what is the relationship between the (asymptotic) phase of oscillation of x and that of $x + h\alpha$, where $\alpha = (\alpha^1, \dots, \alpha^n) \in \{0,1\}^n \backslash \{(0,\dots,0)\}$?

In dimension $n = 1$, we know the answer: $\alpha = 1$ and the particle $x + h\alpha$ (asymptotically) oscillates out of phase with x. This is essentially because when $n = 1$, it is guaranteed that $h\xi_s \to \pi \in \mathbb{T}^1 = S^1$ as $t \to \infty$. However, it is not that case that $h\xi_s \to (\pi,\dots,\pi) \in \mathbb{T}^n$ for general n, and this complicates the situation somewhat. Instead of $q(x+h\alpha,t)$ picking up contributions that are (asymptotically) all out of phase with the corresponding contributions to $q(x,t)$, we instead have a mixture, some terms in phase and some out of phase depending on whether $h\xi_s^j \to 0$ or π.

Definitions 6.3.2. Define an equivalence relation $\simeq$ on Λ by $x \simeq y$ if and only if $q(x,t)$ and $q(y,t)$ are asymptotically in phase and of the same amplitude as $t \to \infty$. Define $p(n) \in \mathbb{N}$ to be the number of equivalence classes of $\simeq$ in Λ.

Intuitively, this is just a formalization of the notion that the oscillations of x and y are "the same in long time". We already know, by Proposition 6.3.1(ii), that

$$y \in N_2(x) \Rightarrow x \simeq y. \tag{6.3.2}$$

Is this implication an equivalence? Lemma 2.2.2 tells us that in dimension $n \geq 2$ it is not: consider, for example, the two particles $he_1, he_2 \in h\mathbb{Z}^2$. How many equivalence classes does $\simeq$ actually have? In other words, how many distinct phases $p(n)$ do we see emerge? Numerically, we observe that

- $p(1) = 2$: the equivalence classes are $[0]$ and $[h]$;
- $p(2) = 3$: the equivalence classes are $[(0,0)]$, $[(0,h)]$ and $[(h,h)]$;
- $p(3) = 3$: the equivalence classes are $[(0,0,0)] = [(h,h,0)]$, $[(h,0,0)]$ and $[(h,h,h)]$.

Proposition 6.3.3. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1). The number of of distinct asymptotic phases $p(n)$ satisfies $2 \le p(n) \le n+1$.*

Proof. Implication (6.3.2) makes it sufficient to determine how many distinct phases emerge among the 2^n particles in the cube

$$C := \{x \in \Lambda | x^j = 0 \text{ or } h \text{ for } 1 \le j \le n\},$$

so we can start from the initial rough bound $1 \le p(n) \le 2^n$. Lemma 2.2.2 implies that $x \simeq \iota(x)$ for all $\iota \in \mathrm{Isom}_0(\Lambda)$. There are $n+1$ orbits in C under the action of $\mathrm{Isom}_0(\Lambda)$, since $x, y \in C$ are in the same orbit if and only if

$$\#\{1 \le j \le n | x^j = h\} = \#\{1 \le j \le n | y^j = h\}. \qquad (6.3.3)$$

If $x, y \in C$ satisfy (6.3.3) then $x \simeq y$. Thus $p(n) \le n+1$.

We now show that no particle can asymptotically oscillate in phase with a nearest neighbour: i.e., $y \in N_1(x) \Rightarrow x \not\simeq y$. As in the proof of Proposition 6.3.1(iii), we consider the contributions to the oscillations of x and y at time t. For x:

$$\pm 2\omega\psi(\xi_s)t + \xi_s \cdot x,$$

and for y:

$$\begin{aligned} \pm 2\omega\psi(\xi_s)t + \xi_s \cdot y &= \pm 2\omega\psi(\xi_s)t + \xi_s \cdot x + \xi_s \cdot h e_j, \\ &= \pm 2\omega\psi(\xi_s)t + \xi_s \cdot x + h\xi_s^j. \end{aligned}$$

The difference in phases is $h\xi_s^j$, which we know to be non-zero for at least one j. So $y \in N_1(x) \Rightarrow x \not\simeq y$, and hence $p(n) \ge 2$. $\square$

It is important to note that, just as subsets of a topological space can be open, closed or neither, it is not that case that $x \not\simeq y \Rightarrow x$ and y are asymptotically π out of phase. If this were the case, we would have $p(n) = 2$ for all n, which we know to be false. Incidentally, the curious observation that $p(3) = 3$ renders false the promising hypothesis that $p(n) = n+1$.

6.4 Equipartition and Distribution of Energy

In this situation of initial conditions (1.3.1), as we have already established the initial distribution of energy is highly asymmetric: $V(0) = n\kappa\|q_0\|^2$ and $T(0) = 0$. We ask, how does this distribution evolve in time?

We first show that in the limit as $t \to \infty$, $T(t)$ and $V(t)$ are asymptotically equal and each is half the total energy of the system, as in Observation 4.3.6. This is just as in the continuum case (see, for example, [8]).

Proposition 6.4.1. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1). Then there is an equipartition of energy as $t \to \infty$. That is, as $t \to \infty$,*

(i) $T(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$;

(ii) $V(t) \to \frac{1}{2}\mathcal{E}(0) = \frac{1}{2}V(0)$;

(iii) $\mathcal{L}(t) \to 0$.

Proof. By Lemma 2.3.7, we need only prove statement (iii). We have the following formula for $\mathcal{L}(t) := T(t) - V(t)$:

$$\mathcal{L}(t) = \frac{1}{2}\sum_{x\in\Lambda}\left(m\|\dot{q}(x,t)\|^2 - \frac{\kappa}{2}\sum_{y\in N_1(x)}\|q(y,t) - q(x,t)\|^2\right) \tag{6.4.1}$$

We can easily differentiate equation (5.1.6) to obtain

$$\begin{aligned}\hat{\dot{q}}(\xi,t) &= \frac{2i\omega q_0\psi(\xi)}{2}e^{i2\omega\psi(\xi)t} - \frac{2i\omega q_0\psi(\xi)}{2}e^{-i2\omega\psi(\xi)t} \\ &= -2\omega q_0\psi(\xi)\sin\left(2\omega\psi(\xi)t\right)\end{aligned}$$

The Plancherel equality (5.1.1) from Theorem 5.1.4 then implies that

$$\begin{aligned}\sum_{x\in\Lambda}\|\dot{q}(x,t)\|^2 &= \left(\frac{h}{2\pi}\right)^n \int_{\widehat{\Lambda}} \left\|\hat{\dot{q}}(\xi,t)\right\|^2 \, d\xi \\ &= \frac{4\omega^2\|q_0\|^2 h^n}{(2\pi)^n}\int_{\widehat{\Lambda}} \psi(\xi)^2 \sin^2\left(2\omega\psi(\xi)t\right) \, d\xi\end{aligned}$$

We can consider the potential term arising from one of the $2n$ springs attached to x. By the linearity of the Fourier transform, (5.1.1) and (5.1.2):

$$\begin{aligned}\sum_{x\in\Lambda}\|q(x+he_j,t)-q(x,t)\|^2 &= \left(\frac{h}{2\pi}\right)^n\int_{\widehat{\Lambda}}\left|e^{ih\xi^j}-1\right|^2\|\hat{q}(\xi,t)\|^2\,d\xi\\ &= \frac{\|q_0\|^2h^n}{(2\pi)^n}\int_{\widehat{\Lambda}}\left|e^{ih\xi^j}-1\right|^2\cos^2\left(2\omega\psi(\xi)t\right)\,d\xi\end{aligned}$$

Note that

$$\begin{aligned}\left|e^{ih\xi^j}-1\right|^2 &= \left|e^{2ih\xi^j}-2e^{2ih\xi^j}+1\right|\\ &= \left|e^{ih\xi^j}\right|\left|e^{ih\xi^j}-2+e^{-ih\xi^j}\right|\\ &= 4\sin^2\frac{h\xi^j}{2}\end{aligned}$$

We now substitute into (6.4.1) to obtain

$$\begin{aligned}\mathcal{L}(t) &= \frac{\|q_0\|^2h^n}{2(2\pi)^n}\int_{\widehat{\Lambda}}\left\{\begin{matrix}4\omega^2m\psi(\xi)^2\sin^2\left(2\omega\psi(\xi)t\right)\\ -\frac{\kappa}{2}8\psi(\xi)^2\cos^2\left(2\omega\psi(\xi)t\right)\end{matrix}\right\}\,d\xi\\ &= -\frac{2\kappa\|q_0\|^2h^n}{(2\pi)^n}\int_{\widehat{\Lambda}}\psi(\xi)^2\cos\left(4\omega\psi(\xi)t\right)\,d\xi\\ &\to 0 \text{ as } t\to\infty\end{aligned}$$

by the Riemann-Lebesgue Lemma, since ψ is bounded, hence L^1. □

We also have the following corollary of Proposition 6.3.1:

Corollary 6.4.2. *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let $\Omega\subset\Lambda$ be any bounded subset of Λ. Then $V_\Omega(t)$, $T_\Omega(t)$, $\mathcal{E}_\Omega(t)$ and $\mathcal{L}_\Omega(t)\to 0$ as $t\to\infty$.*

Proof. Since $\Lambda\subset\mathbb{R}^n$ is a discrete space, $\Omega\subseteq\Lambda$ is bounded $\Leftrightarrow$ Ω is finite. Thus, it suffices to prove the statement for $\Omega=\{x\}$, a singleton set, since a finite sum of functions of t that tend to 0 as $t\to\infty$ has the same property. Fix $x\in\Lambda$.

Proposition 6.3.1(i) implies that for all $y\in\Lambda$, $q(y,t)\to 0$ as $t\to\infty$, so certainly $\|q(y,t)-q(x,t)\|\to 0$ for all $y\in N_1(x)$. Since $V(x,t)$ is a finite sum of such terms, $V(x,t)\to 0$ as $t\to\infty$. Similarly, by Proposition

6.3.1(ii), $\|\dot{q}(x,t)\| \to 0$ as $t \to \infty$. So $T(x,t) \to 0$ as $t \to \infty$. Since $V(x,t)$ and $T(x,t) \to 0$, it easily follows that $\mathcal{E}(x,t)$ and $\mathcal{L}(x,t) \to 0$ as $t \to \infty$. $\square$

Putting together Proposition 6.4.1 and Corollary 6.4.2 we have thus proved

Theorem 6.4.3. (Asymptotic Distribution of Energy.) *Consider a system evolving according to (1.2.7) with initial conditions (1.3.1) and let $\Omega \subset \Lambda$ be bounded. Then as $t \to \infty$,*

$$\begin{array}{ll} T_\Omega(t) \to 0, & T(t) \to \frac{1}{2}\mathcal{E}(0), \\ V_\Omega(t) \to 0, & V(t) \to \frac{1}{2}\mathcal{E}(0), \\ \mathcal{E}_\Omega(t) \to 0, & \mathcal{E}(t) \equiv \mathcal{E}(0), \\ \mathcal{L}_\Omega(t) \to 0, & \mathcal{L}(t) \to 0. \end{array}$$

Physically, Theorem 6.4.3 tells us that the wave transports all energy, kinetic and potential, through and away from any bounded region in Λ, and that the global distribution of kinetic and potential energy is asymptotically in balance – the system is, in some sense, "oscillating as much as it has been perturbed from equilibrium".

7 Final Remarks

7.1 Conclusions

To conclude, we have seen that the spatially discretized wave equation with stationary coherent initial conditions is essentially 1-dimensional in its solutions (Corollary 2.3.6). We have established the long-term behaviour of any given particle $x \in \Lambda$, and its synchronization with second-nearest neighbours (Proposition 6.3.1). In Proposition 6.3.3 we established a bound on the number of phases that emerge in long time. We have determined the long-term behaviour of both the local and the global energy distributions (Theorem 6.4.3). We have seen that, despite the apparent disintegration of the continuum light cone, the group and phase velocities remain bounded by the corresponding continuum wavespeed (Theorem 6.2.3).

Numerically, we have observed these phenomena and many more: in particular, we have observed a monotone wavefront essentially coincident with the boundary of the continuum light cone. We have also observed that maximal displacement propogates along the principal diagonals of the lattice at the continuum wavespeed $/\sqrt{n}$ and that its amplitude decays as $t^{-n/3}$.

7.2 Suggestions for Further Research

One would hope that the various observations made about wavefront phenomena can be put on a more sound mathematical basis. For instance:

(i) Is it possible to generalize the recursion relation (3.2.2) and other facts used in the proof of Proposition 3.2.2 to the function $\mathcal{J}_m$ and thus establish the existence of the monotone spherical wavefront in dimension n?

(ii) Can the method of stationary phase be applied to find the location, speed of travel and decay of amplitude of maximum displacement, a method that does work quite easily in dimension $n = 1$?

(iii) Can we obtain a precise estimate for the shape and speed of expansion of the region within which the N_2-synchronization applies, along the lines of Proposition 3.2.2(ii)?

(iv) Are there precise formulae or large-n asymptotics for the number $p(n)$? Even more strongly, is there a precise relationship between the equilibrium position $x \in \Lambda$ and the asymptotic phase of $q(x, t)$?

Appendices

A Distance on a Lattice

At first sight it may seem odd that the wavespeeds in Observations 4.3.2 and 4.3.4 differ by a factor of $\frac{1}{\sqrt{n}}$. One way of explaining this is that we are incorrectly measuring distance in the lattice Λ. We have the usual Euclidean notion of distance that is appropriate to the ambient space $\mathbb{R}^n$:

$$d_{\mathbb{R}^n}(x,y) := \|x-y\| = \sqrt{\sum_{j=1}^{n} |x^j - y^j|^2}.$$

However, the correct distance to use on the lattice is the so-called "taxicab metric":

$$d_\Lambda(x,y) := \sum_{j=1}^{n} |x^j - y^j|. \tag{A.1}$$

The two metrics $d_{\mathbb{R}^n}$ and d_Λ are topologically equivalent: for all $x, y \in \mathbb{R}^n$,

$$d_{\mathbb{R}^n}(x,y) \le d_\Lambda(x,y) \le \sqrt{n} d_{\mathbb{R}^n}(x,y).$$

The lower bound is attained precisely when $x-y$ is a scalar multiple of some e_j; the upper bound is attained precisely when $x-y$ is a scalar multiple of $\pm e_1 \pm \cdots \pm e_n$ for some choice of signs. Thus, the two metrics are equal only in dimension $n = 1$.

Recall that a particle exhibiting maximum displacement from its equilibrium position at time t, $x_\star(t)$, travels at a speed of $\frac{1}{\sqrt{n}}\omega h$ when observed with respect to the ambient space, in the sense that

$$d_{\mathbb{R}^n}(0, x_\star(t)) = \|x_\star(t)\| \approx \frac{\omega h t}{\sqrt{n}}.$$

Points $x_\star(t)$ also "live on" the principal diagonals of Λ:

$$|x_\star^1(t)| = \cdots = |x_\star^n(t)| \approx \frac{\omega h t}{n}.$$

Thus $d_\Lambda(0, x_\star(t)) \approx \omega h t$: from the point of view of an observer intrinsic to the lattice, the points of maximum displacement move at speed ωh regardless of dimension.

B The Method of Stationary Phase

The method of stationary phase can be found in much literature. A rigorous treatment can be found in [7]. What follows is intended only to give the general idea of the method and how it applies to this situation.

We wish to study so-called *oscillatory integrals* of the form

$$I(t) = \int_{\mathbb{R}^n} F(x) e^{if(x)t}\, dx,$$

in particular how they behave for large t. We assume that f varies rapidly in x compared to F. The idea is that for large t most of the contribution to the integral occurs near points x_0 where $\nabla f(x_0) = 0$, since the rapid variation of f elsewhere leads to contributions "cancelling out".

The method of stationary phase expands the phase function in the exponent as a Taylor series [9]:

$$\begin{aligned} f(x) &= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{j=1}^{n} (x^j - x_0^j) \frac{\partial}{\partial x'^j} \right)^k f(x') \Bigg|_{x'=x_0} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \left((x - x_0) \cdot \nabla_{x'} \right)^k f(x') \Bigg|_{x'=x_0} \end{aligned}$$

In particular, for x near x_0,

$$f(x) \approx f(x_0) + \nabla f(x_0) \cdot (x - x_0) + \frac{1}{2} \left(D^2 f(x_0)(x - x_0) \right) \cdot (x - x_0) + O(\|x - x_0\|^3).$$

Writing

$$A := D^2 f(x_0) = \begin{pmatrix} \frac{\partial^2}{\partial x^1 \partial x^1} f(x) & \cdots & \frac{\partial^2}{\partial x^1 \partial x^n} f(x) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial x^n \partial x^1} f(x) & \cdots & \frac{\partial^2}{\partial x^n \partial x^n} f(x) \end{pmatrix} \Bigg|_{x=x_0}$$

and neglecting terms of order 3 and above[5], we have

$$f(x) \approx f(x_0) + (A(x - x_0)) \cdot (x - x_0),$$

[5] The assumption that we can neglect terms of order 3 and above is a nontrivial one, and requires some proof that we omit here. The order 3 term will obviously be important if, for instance, $D^2 f(x_0)$ does not have full rank.

and thus, making a linear change of variables $y = x - x_0$,

$$I(t) \approx F(x_0)e^{if(x_0)t} \int_{\mathbb{R}^n} e^{i(Ay)\cdot yt} \, dy.$$

Since mixed partial derivatives commute, the matrix A is symmetric, and so can be diagonalized. Let U be an orthogonal ($U^\intercal U = UU^\intercal = I$) $n \times n$ matrix so that $U^\intercal AU = \tilde{A}$, where $\tilde{A}$ is diagonal:

$$\tilde{A} = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_n \end{pmatrix},$$

where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of $\tilde{A}$ (and also those of A). We now make a second change of variables, $z = U^\intercal y$:

$$\begin{aligned} \int_{\mathbb{R}^n} e^{i(Ay)\cdot yt} \, dy &= \int_{\mathbb{R}^n} e^{i(AUz)\cdot(Uz)t} \, d(Uz) \\ &= \int_{\mathbb{R}^n} e^{i(\tilde{A}z)\cdot zt} \, dz \end{aligned}$$

($d(Uz) = dz$ since U is orthogonal and so preserves the volume element in $\mathbb{R}^n$.)

$$\begin{aligned} &= \int_{\mathbb{R}^n} e^{i(\lambda_1(z^1)^2+\dots+\lambda_n(z^n)^2)t} \, d(z^1, \dots, z^n) \\ &= \prod_{j=1}^n \int_{\mathbb{R}} e^{i\lambda_j(z^j)^2 t} \, dz^j \\ &= \prod_{j=1}^n \sqrt{\frac{\pi i}{\lambda_j t}} \end{aligned}$$

by the standard result that $\int_{\mathbb{R}} e^{-s^2} \, ds = \sqrt{\pi}$,

$$\begin{aligned} &= \sqrt{\frac{(\pi i)^n}{t^n \det \tilde{A}}} \\ &= \sqrt{\frac{(\pi i)^n}{t^n \det A}} \end{aligned}$$

since U is orthogonal, so $\det \tilde{A} = \det A$.

Thus, for large t, we have that to leading order, as $t \to \infty$,

$$I(t) \sim F(x_0)e^{if(x_0)t}\sqrt{\frac{(\pi i)^n}{t^n \det D^2 f(x_0)}}. \tag{B.1}$$

When we apply this method to our problem F is the constant function taking the value of the initial displacement vector of the particle at the origin, and f is one the phase functions $\phi^{\pm}_{x,t}$. Also, we apply the method to an integral over $h^{-1}\mathbb{T}^n$ rather than $\mathbb{R}^n$; for large t, however, the same asymptotics apply.

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The program simulating the system was written in object-oriented C++ and compiled using Microsoft$^{(R)}$ Visual C++$^{(R)}$ 6.0.

Figure 3.1.1 was generated using Wolfram$^{(R)}$ Mathematica$^{(R)}$ 5.0.

This document was typeset in LaTeX2e and compiled using MiKTeX 2.2.

References

[1] Friesecke, G. Lectures for *MA433 Fourier Analysis*. University of Warwick, 2003.

[2] Friesecke, G. Dynamics of the Infinite Harmonic Chain: Conversion of Coherent Initial Data into Synchronized Binary Oscillations. 2003.

[3] Jost, J. *Partielle Differentialgleichungen.* Springer-Verlag, Heidelberg, 1998. English edition: *Partial Differential Equations.* Springer-Verlag, New York, 2002.

[4] Kirillov, A.A. *Elementy Teorii Predstavleniĭ.* Nauka, Moscow, 1972. English translation: *Elements of the Theory of Representations.* Trans. Hewitt, E. Springer-Verlag. 1975.

[5] Nelson, D. (ed.) *The Penguin Dictionary of Mathematics*, 3rd Edition. Penguin, 2003.

[6] Rugh, H.H. Lyapunov Bounds for Lattice Gauge Dynamics. *Commun. Math. Phys.* **200**, 487–494, 1999.

[7] Stein, E.M. *Harmonic Analysis: Real-variable Methods, Orthogonality, and Oscillatory Integrals.* Princeton University Press, 1993.

[8] Strichartz, R.S. *A Guide to Distribution Theory and Fourier Transforms.* CRC Press, 1993.

[9] Weisstein, E.W. *MathWorld – A Wolfram Web Resource.* http://mathworld.wolfram.com. Wolfram Research / CRC Press LLC, 1999–2004.

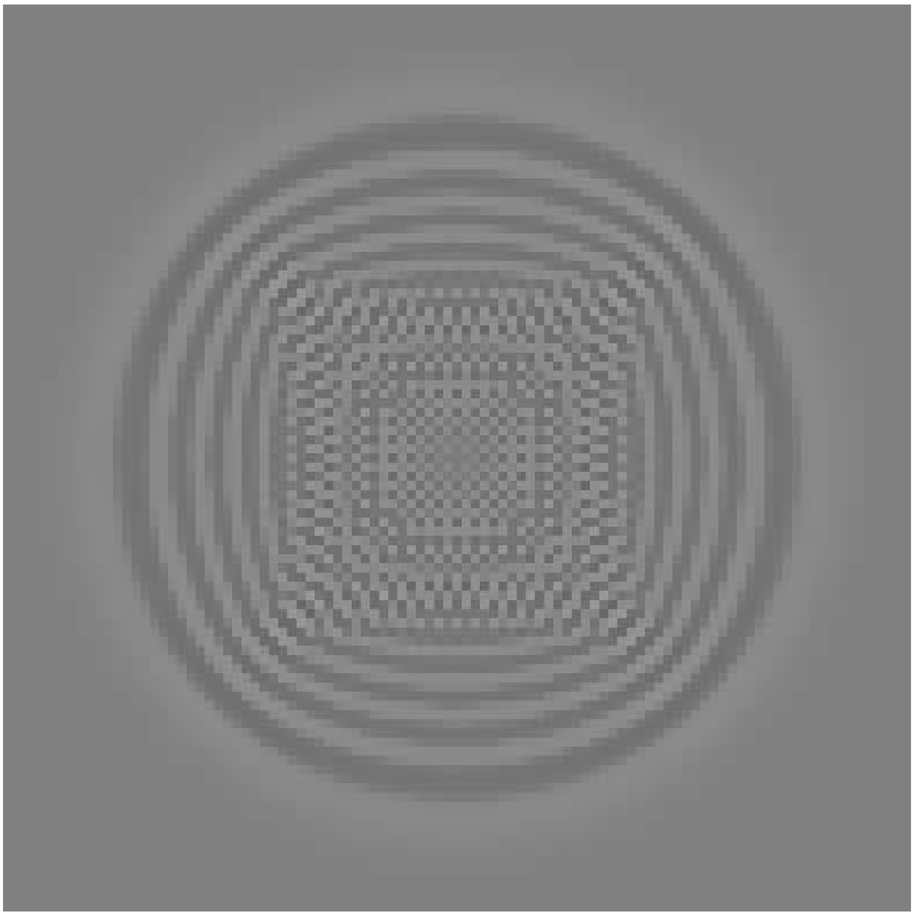

Figure 4.3.3: A plot of $u(x,t)$ at $t = 40$ in dimension $n = 2$, $|x^1|, |x^2| < 50h$. Greyscale values $G(x,t)$ are assigned as in Subsection 4.2. The spherical monotone wavefront, the concentration of maximal displacement along the principal diagonals of the lattice, and the beginnings of synchronization of second-nearest neighbours are all visible.

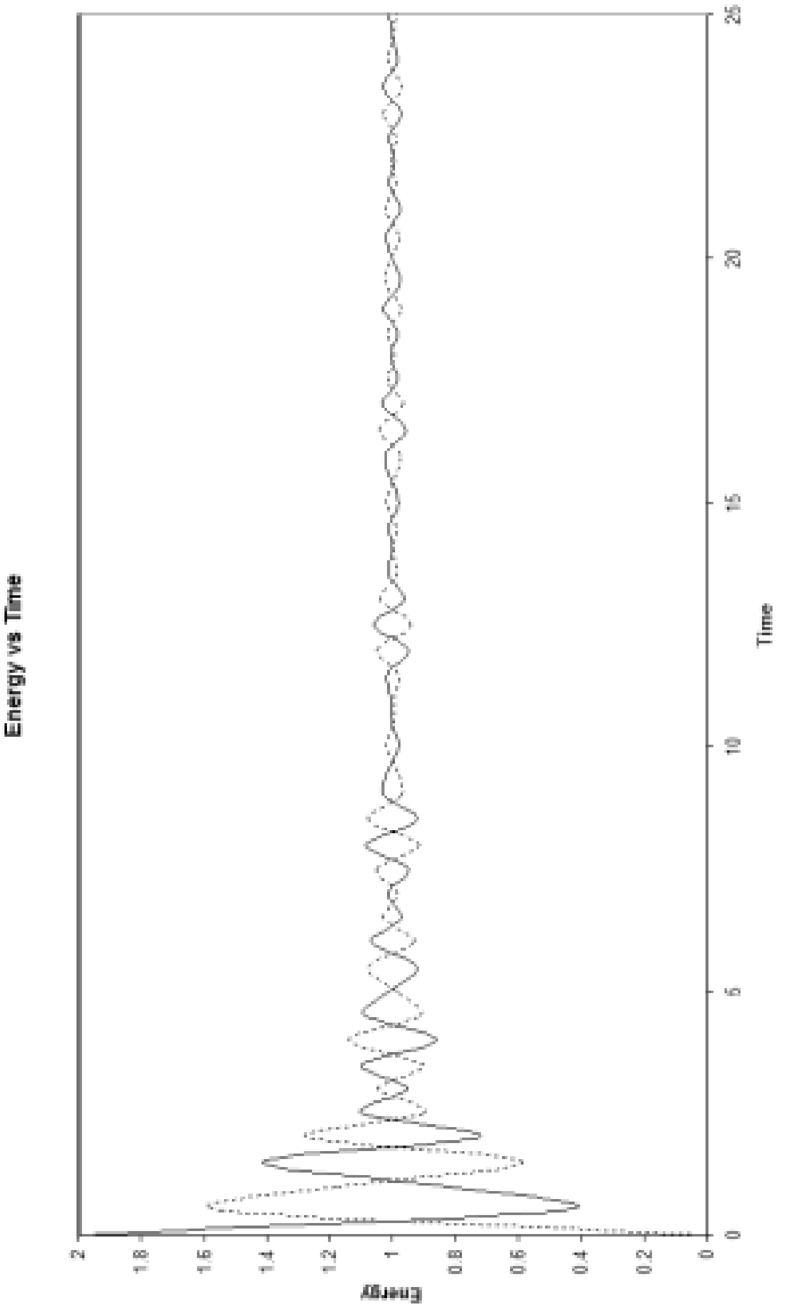

Figure 4.3.4: A plot of $T(t)$ (dotted line), $V(t)$ (solid line) and $\mathcal{E}(t)$ (heavy line) for $t \in [0, 25]$, with $n = 2$, $m = \kappa = 1$, $q_0 = e_1$.

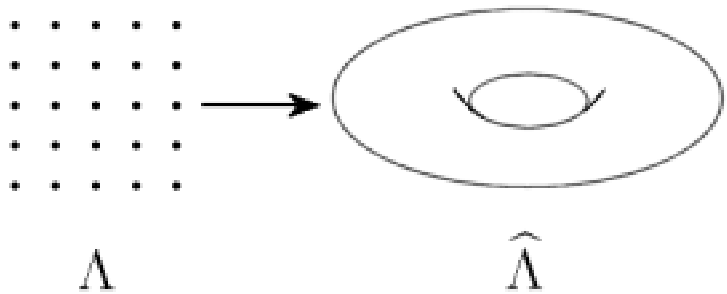

Figure 5.1.1: The lattice $\Lambda = h\mathbb{Z}^n$ and its Pontrjagin dual $\widehat{\Lambda} = h^{-1}\mathbb{T}^n$.