Thermalization and Initial State-Recurrence in Discrete KdV-like Lattices

Garrett Taylor Nieddu

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THERMALIZATION AND INITIAL STATE-RECURRENCE IN DISCRETE KdV-LIKE LATTICES

by

Garrett Taylor Nieddu

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ABSTRACT

Title of Thesis: THERMALIZATION AND INITIAL STATE-RECURRENCE IN DISCRETE KDV-LIKE LATTICES

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Three discretizations of the Korteweg de-Vries equation are studied; convergence rate, initial state-recurrence, and the energy distribution of the three schemes are all considered. For each discrete scheme over 300 lattices with varying grid sizes were investigated, and the solutions were compared with other lattices from the same scheme, as well as solutions from the other two. It is found that the two schemes that are least accurate display the best recurrence at intermediate grid sizes, away from convergence. This is a notable result because the best recurrence is expected to be found in the most accurate, and converged lattices. It is also observed that there is no clear correlation between thermalization and initial state-recurrence strength.
THERMALIZATION AND INITIAL STATE-RECURRENCE IN DISCRETE KDV-LIKE LATTICEs

A THESIS

Submitted in partial fulfillment of the requirements
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GARRETT TAYLOR NIEDDU

Montclair State University
Montclair, NJ
December 2012
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1 Background

1.1 Fermi Pasta and Ulam

The study of initial-state recurrence, and by extension the study of solitons, has its genesis in what is known as the Fermi, Pasta, and Ulam problem (FPU). The Korteweg-de Vries (KdV) equation, and its discretizations, are ultimately derivative of the FPU system, and are best understood in that context.

The FPU problem, named after three scientists, Enrico Fermi, John Pasta, and Stanislaw Ulam, is concerned with the lack of thermalization found in the numerical simulations of a non-linear mass spring system; the FPU model describes such a system, a string of masses held together by non-linear springs (springs that do not follow Hooke’s law). Thermalization is the dissipation of heat or energy from a central location, throughout a cooler ambient area. It was thought that the transmission of kinetic energy among the masses in the FPU system would act like the transmission of kinetic energy between molecules, and thus like the spread of heat. In the numerical simulations of the FPU model, an initial state must be chosen; this initial state, or initial condition, was chosen in early experiments to be one period of a sine or cosine wave.

In the FPU system, a physical state may be described in terms of component sine and cosine waves, each identified by its specific amplitude and frequency. Each component wave represents a portion of the system’s state in terms of velocity. Thus, the squared amplitude of a component wave is the energy found in the corresponding frequency, or “mode”. The systems considered here are Hamiltonian systems, and thus conserve energy. Since the physical state we are describing is in terms of velocity, and the energy is proportional to velocity squared, if we know the amplitude of a component we know the proportion of total energy in that component.

Fermi Pasta and Ulam, and later Zabusky and Kruskal, use an initial condition of a single period sine or cosine wave; an initial condition that is very distinctive in Fourier, or frequency, space\cite{7, 11}. With these initial conditions, the system’s initial state can be described by the amplitude of the lowest frequency wave component. By making the initial condition distinctive in Fourier space, a return to the initial state of the system, at time greater than $t_0 = 0$, would be distinctive as well.

Given an initial condition as described, with all of its energy in the lowest Fourier mode, the energy is expected to make its way out of the low mode into progressively higher Fourier modes. Fermi, Pasta, and Ulam observed that in their simulations, instead of populating the higher modes as expected, the energy leaks up into a small
range of higher modes, and then returns to the low mode [7]. This is the phenomenon that is called initial-state recurrence, and it was first observed by Fermi, Pasta, and Ulam.

1.2 KdV

The Korteweg-de Vries (KdV) equation,

\[ u_t + uu_x + \delta^2 u_{xxx} = 0, \]  

(1)
can be derived as an asymptotic limit of the FPU model[10]. It is now known that the Korteweg-de Vries equation is found often in nature; originally studied in water waves, it is also studied in the context of optics, and acoustics. Interestingly, Zabusky and Kruskal only meant to look at a special case of the FPU model, and the continuous equation they derived was not initially recognized as the KdV equation. At the time the KdV equation was primarily associated with shallow water waves, and was not known to be a universal wave equation derivable from a large variety of physical systems[1].

Simulations of the FPU system played a key role in the development of experimental mathematics. When mathematicians of the mid-twentieth century were not able to solve the KdV(1) equation analytically, it was a natural step to use numerical simulations to gain insight into the system’s dynamics.

1.3 Zabusky and Kruskal

Zabusky and Kruskal studied the KdV(1) equation numerically, by running numerical time evolution simulations on a spatial discretization of the KdV equation,

\[ \frac{d}{dt} u_n = \frac{(u_{n-1} + u_n + u_{n+1})(u_{n-1} - u_{n+1})}{6h} + \delta^2 \frac{u_{n-2} - 2u_{n-1} + 2u_{n+1} - u_{n+2}}{2h^3}, \]  

(2)
where the discretization is made on a lattice of length \( L \), with discrete nodes evenly spaced a distance of \( h \) apart, and \( u_n = u(nh) \) for \( n \in \{1, 2, 3, \ldots N-1\} \). With the parameter values \( \delta = .022 \) and \( h = \frac{1}{64} \), they were able to see their model manifest near-recurrence of the initial state. Since, as \( h \to 0 \), the lattice has the KdV equation as its limit, it is in direct lineage to the FPU system, and the near recurrence of the single frequency cosine wave initial condition was expected. However, the observation of elastically interacting solitary waves, coined \textit{solitons}, was not expected [11].

Having observed the solitons, Zabusky and Kruskal attributed recurrence to the nature of soliton interaction[11]. The claim was that as the solitons spread apart from one another, due to periodic boundary conditions, the faster solitons would essentially “lap” the others and cause collisions. These collisions result in interaction, and when the interaction is among all the present solitons, it will cause a near-recurrence to the initial state [11].
1.4 Integrability and Solitons

The discovery of solitons, and their inelastic interaction, would inspire the development of the inverse scattering transform (IST). In the late 1960s, the inverse scattering transform was pioneered by Gardner, Greene, Kruskal and Miura, and was originally used to find solutions of the KdV equation and the non-linear Schrödinger equation[5]. In the decade that followed, Ablowitz, Kaup, Newell and Segur, and separately Lax, worked to generalize the method[5].

The inverse scattering transform is a method of expressing a non-linear evolution equation as a pair of linear operators, with a compatibility condition. Instead of studying a single non-linear problem, we consider two related linear problems. If a solution to the associated differential equation, or system of differential equations, can be constructed, that non-linear evolution equation is called integrable.

The observation of initial-state recurrence in the KdV equation has been connected to the non-linear and inelastic interaction of solitons since the 1965 Zabusky Kruskal paper [11]. The analytic soliton solutions of integrable systems are found using the IST, and to say an equation is integrable implies the existence of soliton solutions. Thus, if the initial-state recurrence is due to the soliton solutions and the way they interact with one another, it is natural to expect that an integrable discretization should show stronger recurrence.

1.5 Spatial Discretizations

Since 1965, several discretizations of the KdV equation have been investigated; some investigations have used discretizations to model the KdV(1) equation, as Zabusky and Kruskal did, while other investigations consider the discretizations themselves, including work done by Abe and Inoue[4, 11]. Numerical experimentation, on a variety of such discretizations, led A. D. Trubatch to hypothesize that it is not "closeness" to the KdV(1) equation, but rather a distinct property of the discrete systems that explains the initial-state recurrence in the discretizations[2].

Three methods of spatial discretization were identified as important to compare; (a) the Zabusky Kruskal lattice(2), where the initial state recurrence was originally seen; (b) a discretization made using inverse scattering methods, to ensure integrability of the discrete equation; and (c) the spectral discretization, the quickest and most accurate of the schemes[4]. The spectral methods relatively quick convergence allows us to see KdV equation dynamics, rather than discrete model dynamics.

1.5.1 Zabusky Kruskal Discretization

In their 1965 paper, Zabusky and Kruskal employed a finite-differencing discretization on a spatial lattice of length $L$ with $N$ discrete nodes to approximate the Korteweg-deVries equation(1). The Zabusky Kruskal(ZK) lattice(2) converges to KdV as $N \to \infty$ with error $\mathcal{O}(h^2)$ [11].

In the Zabusky Kruskal discretization(2), the spatial derivatives of the KdV(1)
1.5 Spatial Discretizations

The first derivative \( u_x \) is approximated by the central difference.

\[
\frac{du}{dx} = D_0(u),
\]

where \( D_0 \) is the central difference operator acting on a vector \( u \). The derivative at a point \( n \) is approximated by

\[
D_0(u_n) = \frac{u(n+1) - u(n-1)}{2h}.
\]

The third derivative \( u_{xxx} \) is approximated by the central difference operation being applied after both the left hand difference and the right hand difference operators are applied in sequence, so that

\[
\frac{d^3u}{dx^3} = D_0(D_+(D_-(u))).
\]

Where \( D_+ \) is the right hand difference operator acting on a vector \( u \), and \( D_- \) is the left hand difference operator, acting on a vector \( u \). The right hand derivative at a point \( n \) is approximated by

\[
D_+(u_n) = \frac{u(n+1) - u(n)}{h},
\]

and the left hand derivative at a point \( n \) is approximated by

\[
D_-(u_n) = \frac{u(n) - u(n-1)}{h}.
\]

Here we are using the slope of the secant lines to approximate the derivative \( \frac{1}{2}h \) to the left (\( D_- \)) of \( u_n \), and \( \frac{1}{2}h \) to the right (\( D_+ \)) of \( u_n \). \( D_0 \), however, is the average of \( D_- \) and \( D_+ \), and approximates the derivative at the point \( u_n \) itself.

The main point of interest is the non-linear term, \( uu_x \). One might use a number of different quantities to approximate \( u \), the most obvious being \( u \) itself. If just \( u \) is used, however, a conservation law is inadvertently broken, and the energy in the system "blows up". The correct approximation to use is a three point average,

\[
u_n = \frac{u_{n+1} + u_n + u_{n-1}}{3}.
\]

The parameters used by Zabusky and Kruskal, \( \delta = .022, \ N = 128, \ L = 2 \), resulted in initial-state recurrence[11]. The experiments run by Zabusky and Kruskal were meant to simulate the KdV(1) equation. We now know that the experiments do not represent a converged state for the model, and the dynamics displayed are not actually those of the KdV equation, but of the discrete system.

For this reason, when other groups went to verify the experiment, and used higher accuracy models that were closer to convergence, inconsistent dynamics were observed between the methods of discretization[3, 4].
1.5 Spatial Discretizations

1.5.2 Inverse Scattering Method

The integrable discretization, given as

\[
\frac{d}{dt} u_n = \left(1 + \frac{h^2 u_n}{6 \delta^2}\right) \left[ \frac{u_{n-1}(u_{n-2} - u_n)}{12h} + \frac{u_{n+1}(u_n - u_{n+2})}{12h} \right] + \frac{(u_{n-1} + 2u_n + u_{n+1})(u_{n-1} + u_{n+1})}{12h} + \delta^2 \frac{u_{n-2} - 2u_{n-1} + 2u_{n+1} - u_{n+2}}{2h^3},
\]

was developed by Herbst and Trubatch. It was found by discretizing the associated linear scattering problem, and then choosing a time-dependence so that the compatibility condition has the KdV equation as a continuum limit [6].

1.5.3 Spectral Method

In the 1979 paper by Abe and Abe, along with the 1980 paper by Abe and Inoue, several discretizations of KdV(1) were analyzed in terms of convergence and computational expense. There was a focus on the spectral method, which relies on Fourier analysis, and is of higher accuracy and quicker convergence than the ZK discretization (2), the integrable discretization (9), or any of the other discretizations studied [3, 4].

A review of Fourier methods helps make sense of the spectral method. Given a function, \( f(x, t) \), that is continuous and periodic in space, we write

\[
f(x, t) = \sum_n \hat{c}_n(t) e^{\frac{2\pi i n x}{L}},
\]

for \( n \in \mathbb{Z} \). Each \( \{\hat{c}_n\}_t \) are the complex Fourier coefficients to \( f \) at time \( t \). After re-arranging to solve for a particular \( \hat{c}_k \), and performing a single integration (over the spatial period) on the entire equation, we determine that the form for the Fourier coefficients is given by

\[
\hat{c}_k = \int_0^L f(x) e^{-\frac{2\pi i k x}{L}} dx
\]

where \( L \) is the spatial period. Considering a lattice of length \( L \), with discrete spatial nodes \( N \), and treating a sequence of ordered pairs, \((nh, f(nh))\), as a sampling of the function described above, we can use the discrete substitution \( x = nh \). Translating (12) into its discrete counter-parts produces

\[
\hat{c}_k = \frac{L}{N} \sum_n f(nh) e^{-\frac{2\pi i k nh}{L}}
\]
Since our data is real, we have the condition \( \hat{c}_k = \hat{c}^{*-k} \). So we re-write

\[
\hat{c}_k = \frac{L}{N} \sum_n f_ne^{-2\pi i kn/N}
\]

when our sum is taken symmetrically about \( n = 0 \).

The spectral discretization\(^{10}\) is the discrete spectral representation of the KdV\(^{1}\) equation, where our function \( f(x, t) = u(x, t) \) is a solution to the KdV equation, and \( \hat{u}_n \) is the \( n^{th} \) Fourier coefficient of \( u \). Notice that in Fourier space the derivative \( \frac{du}{dx} \) simplifies, from a difference quotient, to the multiplication, \( \left( \frac{i2\pi k}{L} \right) \hat{u} \). The non-linear term, however, has been turned into a convolution sum.

The convolution sum is a truncated sum, so that we are only considering relevant frequencies. For example, if there are an odd number of nodes, and \( M = \) our coefficients can be labeled from \(-M \leq \ell \leq M\), we also need for \(-M \leq k - \ell \leq M\). Together this forces \(-M + k \leq \ell \leq M\). The higher frequencies are effectively being shaved off to prevent aliasing.

Abe and Abe, as well as Abe and Inoue, ran simulations on a variety of discretizations, and found that the spectral method\(^{10}\) has the fastest convergence rate among those investigated\(^4\). In these simulations however, expected near recurrence was not found\(^{3, 4}\). Evidence suggests that the simulations run by Abe and Inoue, which had a maximum \( N \)-value of 70, had not considered the system for a large enough \( N \)-value. Both groups, Zabusky and Kruskal and Abe \textit{et.al}, studied models of a scaling and grid size that was away from convergence, and did not “act” like the KdV\(^{1}\) equation.

### 1.6 Recurrence Hypotheses

The accepted explanation for the recurrence in the Zabusky Kruskal Lattice\(^2\) is “closeness” to KdV, which is integrable as a PDE, and has soliton solutions. The implied conclusion being that stronger recurrence will be seen when:

1. the grid spacing, \( h \), gets smaller. For our discrete system, \( h = \frac{L}{N} \) where \( h \) is grid spacing, \( L \) is the length over which our lattice will span, and \( N \) is the number of evenly spaced nodes being considered;

2. more-accurate methods of discretization are used;

3. the discretization used is integrable as a system of ODEs.

Therefore, when analyzing our three schemes we expect that;

1. when \( N \), the number of discrete nodes being considered, gets large enough, the discrete models should converge. Once converged, initial-state recurrence strength should be at a maximum for the scheme. The strength of each discrete scheme’s maximum recurrence should be less than or equal to the maximum initial-state recurrence displayed by the KdV\(^{1}\) equation. For most initial
conditions there is not an analytical solution to the KdV equation. When analyzing numerical solutions that have no analytical solution to be compared to, the numerical solutions of the converged spectral scheme are used in place of an analytical solution.

2. a more accurate discretization, such as the spectral method\(^{(10)}\), should show stronger recurrence than less accurate discretizations.

3. for a given \(N\)-value, an integrable discretization's recurrence strength should be stronger than a non-integrable discretization.

2 Convergence of a Traveling Wave Solution

Each of the three schemes presented here had been developed, analyzed, and used previous to this investigation\(^{[11, 3, 4, 6]}\). The convergence and convergence rate of each scheme is well established. I independently analyzed and confirmed the convergence rate of the schemes for thoroughness, and to provide a check that the code is producing correct results. Details of the code can be found in the Appendix.

To analyze convergence, an analytic solution,

\[
u(x - ct) = 12(\delta k)^2 \text{sech}^2 (k(x - ct - x_0))\]  \hspace{1cm} (15)

was used as an initial condition for each of our schemes. This is a traveling wave solution of KdV, with speed \(c\), and with a peak initially displaced \(x_0\) units to the right of zero. The values for \(x_0\) and \(k\) were chosen to force \(u(0) = u(L) \approx 10^{-9}\), a value lower than our error tolerance, and thus effectively zero. The amount of time it should take for the traveling wave to move through one boundary and back around to the center of the length was determined.

The Error in each plot refers to the shape error in each scheme. The peak was interpolated for each time evolution \((\tilde{u}_n)\), this is the experimental value, then the analytical wave solution \((u_n)\) was superimposed over the numerical solution. The error for an \(N\)-sized lattice was calculated by taking the maximum of the difference between the actual and the experimental, over all discrete nodes, divided by the maximum of the actual and 1 at that node,

\[
E(N) = \max \left( \frac{|\tilde{u}_i - u_i|}{\max(u_i, 1)} \right) \tag{16}
\]

for \(i \in 0, 1, 2, 3, \ldots N - 1\).
Figure 1: Plot of $\ln(E)$ vs $\ln(h)$ for Zabusky Kruskal Scheme, where $E$ is the error and $h$ is $L/N$.

Figure 2: Plot of $\ln(E)$ vs $\ln(h)$ for the Integrable Scheme, where $E$ is the error and $h$ is $L/N$.

Figures 1 and 2 show plots of $\ln(E)$ vs $\ln(h)$, where $E$ is the error, and $h$ is the distance between nodes. Since it is established that the error for each scheme is approximately $E(h) = ch^2$ (for a constant $c$), we can expect that $\ln(E) = 2\ln(h) + \ln(c)$. Thus a $\ln(E)$ vs $\ln(h)$ plot should look like a line of slope 2, if our code is working properly and the error is really $O(h^2)$. In both cases we see the expected convergence rate.
3 Initial-State Recurrence

3.1 Recurrence Profiles

3.1.1 Zabusky Kruskal Discretization

The analysis of initial-state recurrence is first made on a single lattice, with a particular grid size. Since we have three equations of the form $\frac{du}{dt} = f(u, t)$, we call them evolution equations, and can use a Runge-Kutta method with variable time stepping to calculate the approximate progression of the velocity profile over time. The function $ode5r$, from the ode package in GNU Octave, was used to perform the time integration[9, 8]. The function $ode5r$ is a fifth order implicit Runge-Kutta method based on the fortran solver Radau5. Once calculated, we have a velocity profile for each time step taken, and Fourier analysis is used to measure the energy in the low mode at each time step.

The vertical axes, in Figures 4, 5, and 6, measure the proportion of total energy. On the horizontal axes is time; the height of the curve at a time corresponds to the portion of total energy in the low mode at that time. At $t = 0$, our system is just a sinewave of period $L$ (this is the low mode), and thus the magnitude of the corresponding Fourier coefficient squared is the total energy, and thus has a value for very small values of $h$ the plot goes flat, it means that the error from the spatial discretization of the scheme is insignificant compared to the error from the time integrator. Here we use a fifth-order Runge-Kutta with variable time stepping, the built in function $ode5r$, from GNU Octave’s ode package[9, 8].

For the spectral scheme, where error is given by $E(h) = k e^{ch}$ (for constants $c$ and $k$), we expect that $\ln(E) = \ln(k) + ch$. Thus the approximately linear correlation between $\ln(E)$ and $h$, shown in 3, indicates that our code is working and converging at the expected rate. You will notice that for very small values of $h$ the plot goes flat, it means that the error from the spatial discretization of the scheme is insignificant compared to the error from the time integrator. Here we use a fifth-order Runge-Kutta with variable time stepping, the built in function $ode5r$, from GNU Octave’s ode package[9, 8].

Figure 3: Plot of $\ln(E)$ vs $h$ for the Spectral Scheme, where $E$ is the error and $h$ is $L/N$. 

The analysis of initial-state recurrence is first made on a single lattice, with a particular grid size. Since we have three equations of the form $\frac{du}{dt} = f(u, t)$, we call them evolution equations, and can use a Runge-Kutta method with variable time stepping to calculate the approximate progression of the velocity profile over time. The function $ode5r$, from the ode package in GNU Octave, was used to perform the time integration[9, 8]. The function $ode5r$ is a fifth order implicit Runge-Kutta method based on the fortran solver Radau5. Once calculated, we have a velocity profile for each time step taken, and Fourier analysis is used to measure the energy in the low mode at each time step.

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3.1 Recurrence Profiles

3.1.1 Initial- State Recurrence

As time increases, the energy leaks away from the low mode, but then partially returns.

In Figure 4 it can be seen that the first several recurrences are very strong, and almost all of the system's energy returns to the low mode after \( t \approx 10 \). In total, the primary show of initial state recurrence has about twenty-two recurrences, ranging from over 90% of total energy, down to about 25% of total energy.

Each plot is only a view of one mode, for one grid size, for one scheme. More comprehensive analysis is later employed, largely to compare recurrence for a variety of \( N \)-values. The choice of this particular grid size for the Zabusky Kruskal scheme was two fold, first the recurrence seen here is about the best recurrence that we have observed in the scheme, second, this is the grid size that Zabusky Kruskal used in their classic publication[11].

3.1.2 Integrable Scheme

The analogous plot for the integrable scheme is shown in Figure 5. The primary recurrence event’s period lasts longer and consists of more recurrences than the ZK scheme’s, about thirty-two recurrences as compared with twenty-two. Over all, the recurrence events are very similar in the ZK and integrable schemes, both with approximately linear decay of the initial recurrence over time.
3.1 Recurrence Profiles

It can be seen in Figure 1 and 2, that the grid sizes used here; \( N = 128 \), which corresponds to \( \ln(h) \approx -4.16 \); and \( N = 170 \), which corresponds to \( \ln(h) \approx -4.44 \); have relatively large error from the spatial discretizations. Each scheme, the ZK scheme and the integrable scheme, converge with \( O(h^2) \). We used these values because these solutions show particularly strong initial-state recurrence, when compared to solutions of the same scheme, using other \( N \)-values.

![Figure 5: Integrable Low Mode, N=170: Energy vs Time](image)

3.1.3 Spectral Scheme

The profile in Figure 6 was chosen to show an example of the spectral scheme’s best recurrence. Although a grid size of \( N = 400 \) is chosen, any profile for \( N > 110 \) could be used, the difference is almost indiscernible after \( N \approx 100 \).

Here, the primary set consists of only about five or six recurrences, and lasts to approximately \( t = 60 \). While in the other two schemes, a recurrence of 90% of total energy was achieved more than once, it is not in the spectral scheme.

If compared to Figures 4 and 5, the spectral plot displays a weaker average recurrence strength in its first set of recurrences, and the recurrence decays at a greater rate. This is contrary to the expectation, as the spectral scheme is the most accurate of the three.
3.2 N-Independence of Recurrence Times

Each plot in Figure 7 shows a peak initial-state recurrence, with strength at least 30% of total energy, as a marker +. For any particular marker, the recurrence is found in the numerical simulations run with an N-value indicated by the marker’s horizontal position, and at a time indicated by the marker’s vertical height.

While there is no iron-clad rule that describes how much of the initial energy must return to the initial state to constitute an initial state recurrence, the Zabusky Kruskal scheme displays multiple regimes of recurrence, and this can help us decide what is useful to consider. As one set of peaks is in decline, there is another set of peaks that are growing. In Figure 4 you can see at time $\approx 220$, the two regimes meet. The strength of the recurrences about this point is approximately between 25% and 30% of total energy. If our two-dimensional plots include anything below this range, it is hard to distinguish the recurrences of one regime from the other.

For these plots, as well as those that visualize recurrence strength, we are only considering recurrences out to time $t = 120$. This allows us to see the strongest recurrences in each scheme, without making the plots too crowded.

Notice the persistence of the recurrence period between schemes, and the persistence of recurrence time across N-values. Regardless of the convergence, or of the strength of the recurrence, the period of time between peak recurrences is almost
constant. This structure allows us to consider the recurrence events, independent of the times of recurrence, more easily.

In Figure 7a we can see that the main pillar of recurrence, that happens approximately where $115 \leq N \leq 140$, is narrower than in Figure 7b, where the pillar is approximately present where $120 \leq N \leq 190$. The shape and position of this central pillar tells us which $N$-values show the “best” recurrence. A wide pillar suggests persistence of recurrence over a large range of $N$-values. Therefore, recurrences in Figures 7a and 7b, have recurrence phenomenon that disappear for very large and very small $N$-values. Since the corresponding equations, the Zabusky Kruskal equation(2) and the integrable discretization(9), converge as $N$ gets large, this is an unexpected result.

In Figure 7c, no such pillar is obviously identified. Since the spectral scheme converges so quickly, we end up with more of an “on off” switch than a gradual transition. So to the far left of the plot, where $N$ is small, there are initial-state recurrences, but with no particular pattern. This is common to each scheme, in the lower dimensional systems, presumably from the error in the spatial discretization. Then as $N$ increases, the spectral scheme converges, and the recurrences appear and remain stable throughout.

### 3.3 Recurrence Strength

#### 3.3.1 Zabusky Kruskal Discretization

By analyzing solutions of the Zabusky Kruskal discretization(2) with systematically varied grid sizes, it becomes apparent that the grid size used by Zabusky Kruskal at the time of their writing the paper was not fine enough to be a numerical simulation of the Korteweg-de Vries equation(1). This can be seen in Figure 8, where each, time-independent, point on the graph represents a recurrence that is seen in simulations run with an $N$ sized lattice, with a strength indicated by the vertical height of the point. A point on the plot, $(N, |c_1|^2)$, or (grid size, energy in the lowest Fourier mode), represents a recurrence of strength $|c_1|^2$, in a lattice with $N$ nodes. As was observed, in the recurrence time plot 7a, there are recurrences which only exist for an intermediate range of $N$-values. Here, we can now see that the recurrences right around $N = 128$ show relatively strong recurrence, as the grid size gets larger, $N \to \infty$ and so $h \to 0$, the recurrence strength gets weaker. Thus the recurrence strength gets relatively weak towards convergence. This contradicts the hypothesis that the KdV(1) equation is the source of the recurrence. If we are able to achieve our strongest recurrence at an intermediate grid size, then it suggests that the discretization itself is displaying initial-state recurrence independent of its relation to the KdV equation, its continuum limit.
3.3 Recurrence Strength

(a) ZK scheme

(b) Integrable scheme

(c) Spectral scheme

Figure 7: Each plot represents initial-state recurrence events with a ‘+’ marker. Each recurrence happens in a lattice of grid size \( N \) (horizontal axis) and at a time indicated by the marker’s vertical height. \( \text{Time} < 120 \) and peak energy \( > 30\% \)
3.3 Recurrence Strength

3.3.2 Integrable Scheme

For the integrable scheme, Figure 9 shows a very similar trend to the corresponding ZK scheme’s plot, Figure 8. To the far left, when $N$ is small, the scheme is not converged, we have a region of random recurrences, but no initial-state recurrence trend. On the far right, where $N$ is large, we see the recurrences leveling off, going towards the converged state. In both schemes we see a middle zone, for an intermediate range of $N$-values, where initial-state recurrence is relatively strong.
Figure 9: Integrable Scheme: Each marker represents a recurrence that occurs in simulations run with $N$ grid points (indicated by the marker’s horizontal position), with a strength as a proportion of the total energy (indicated by the markers vertical height). Recurrences chose for time $< 120$ and $|c_1|^2 > .25$

As is described in the caption, this plot only shows recurrences that happen for $t < 120$. Right below the main “hump” in the graph, where the strongest recurrence takes place, there is an empty area. This is because of the time restriction. If the time restraint is removed, most of the plot, up to about $|c_1| = .5$, will be filled with markers, as well as the area under the hump. The plots seen here are only meant to describe and contrast the primary recurrence events of our three schemes.

### 3.3.3 Spectral Scheme

In the ZK and integrable scheme’s solutions, we can see that for small $N$-values, the numerical solutions show no systematic or regular recurrence. For middle $N$-values, we have an intermediate zone of maximal initial-state recurrence, and then for larger $N$-values we head towards convergence. For these, the recurrence strength in terms of $N$ can be divided into three states, unconverged, maximum recurrence, and converged. In Figure 10 it can be seen that the spectral scheme shows only two basic zones: unconverged, and converged.
Figure 10: Spectral Scheme: Each marker represents a recurrence that occurs in simulations run with N grid points (indicated by the marker’s horizontal position), with a strength as a proportion of the total Energy (indicated by the markers vertical height). Time $< 120$ and $|c_1|^2 > .25$

In Figure 10, each horizontal line of markers indicates the strength of a recurrence from KdV(1). The occurrence of these horizontal lines are a result of convergence, which happens for a relatively small value of $N$ in the spectral scheme. It is important to remember that this plot is time independent, and that the proximity of two horizontal lines in the plot indicates that there are two recurrences of similar strength, and says nothing about when in time the recurrences happen.

4 Recurrence and Thermalization

4.1 Zabusky Kruskal Scheme

Figures 11a, 11b, and 11c, shows the mode on the horizontal axis, and an average energy on the vertical axis. The average energy was found for the time range $0 \leq t < 250$. In Figure 11a, a gradual shift of energy is seen. For grid size 80, when we see no systematic recurrence, the energy distribution is not too severely weighted towards the low frequency modes. As expected, the lack of recurrence corresponds to a state of increased thermalization (energy sharing among modes). For each curve we increase the grid size by 10, and by the time we are at $N = 120$, there has been a pretty drastic shift towards the lowest frequency modes. The second and third
figures show similar curves, first out to \( N = 200 \) and then out to \( N = 400 \). Notice that regardless of the strength of the recurrence, the energy distribution shows only one of two basic profiles, either “thermalized”, or “long term”.

It is clear that, for lattices with a small \( N \)-value, we have no recurrence, and a relatively high level of thermalization. Then, for a mid-range of \( N \)-values, we have a maximum recurrence, and an energy profile which is less thermalized. There is not notable difference, however, between the curves from the maximum recurrence, and the converged behavior. Thus there are two notably different types of recurrence which have effectively identical energy distributions.

If it was the case that recurrence and thermalization were exactly contradictory phenomena, then we would not expect to see this sudden switch to the long term behavior. We would expect the level of thermalization to be inversely proportional to the recurrence strength, and for the transition away from (or towards) thermalization to be as gradual as the change in recurrence strength.

4.2 Integrable Scheme

Figure 12 shows the same phenomenon in the integrable scheme(9), as is seen in the solutions of the Zabusky Kruskal discretization(2) (Figure 11). There are three distinct zones of recurrence, but only two distinct energy distributions.

Notice that when looking at the recurrence strengths over a large range of \( N \)-values, Figures 8 and 9 show that the two peaks do not occur for the same range of \( N \)-values. The correlation between the energy profile and the initial-state recurrence becomes even less clear upon a close inspection of these two cases. ZK and integrable schemes. For the ZK scheme, the energy profile reaches its converged state right before it sees a maximum recurrence; about \( N = 120 \), with a maximum recurrence at about \( N = 128 \). For the integrable scheme, we see the long term state form even sooner \( N = 100 \), although maximum recurrence is found at about \( N = 170 \).

The initial expectation is to find a direct correlation between recurrence strength and the energy profile, where a change in recurrence strength can be related to a change in the energy profile. If this was the case we would expect that the strongest recurrences would correspond to a distinct energy profile, which obviously favored the mode of recurrence. Here we have a large array of recurrence strengths, all showing the same profile.

The second expectation is that there may be a relation between the recurrence state, and the threshold for the sudden switch to the converged energy profile. Since the long term energy profile is adopted at different stages of recurrence, about maximum for ZK(2), and much earlier than that for the integrable scheme(9), there is no obvious relation between the \( N \)-value that the energy profile switches from the thermalized to converged, and the \( N \)-value that the maximum recurrence occurs.

4.3 Spectral Scheme

In the spectral scheme we see more predictable energy profiles. For small \( N \)-values, where our scheme has not converged, we see an energy distribution that is relatively
close to thermalization when compared to the converged energy distribution. At about $N = 100$, we see that the long term energy profile is adopted, and maintained throughout.

The first two schemes both have intermediate zones of maximum recurrence, while the spectral scheme does not. One might predict that there is a fundamental difference in the energy distributions of a scheme with, overall, strong initial-state recurrence, and that of a scheme with consistently weaker initial-state recurrence, although it is not seen here. The progression towards the converged profiles are, in a general way, very similar among all schemes, but do not seem to be directly related to the corresponding recurrence states in a systematic way.
4.3 Spectral Scheme  4  RECURRENCE AND THERMALIZATION

(a) Energy Distribution in ZK Scheme: Grid Sizes 80-120

(b) Energy Distribution in ZK Scheme: Grid Sizes 80-200

(c) Energy Distribution in ZK Scheme: Grid Sizes 80-400

Figure 11: Each plot shows average energy (vertical axis) versus mode (horizontal axis) in the Zabusky Kruskal scheme, to approximately time 250, where each curve represents a grid size. Only the first 30 distinct modes are shown, the average energy beyond this point is effectively zero for lattices of any grid size.
4.3 Spectral Scheme

4. RECURRENCE AND THERMALIZATION

(a) Energy Distribution in the Integrable Scheme:
Grid Sizes 60-100

(b) Energy Distribution in the Integrable Scheme:
Grid Sizes 60-220

(c) Energy Distribution in the Integrable Scheme:
Grid Sizes 60-400

Figure 12: Each plot shows average energy (vertical axis) versus mode (horizontal axis) in the integrable Scheme, to approximately time 250, where each curve represents a grid size. Only the first 30 distinct modes are shown, the average energy beyond this point is effectively zero for lattices of any grid size.
Figure 13: These graphics depict the average energy (vertical axis) versus mode (horizontal axis) in the Spectral Scheme, to approximately time 250, where each curve represents a grid size. Only the first 30 distinct modes are shown, the average energy beyond this point is effectively zero for lattices of any grid size.

5 Conclusion

Now that a more complete picture of the initial-state recurrence in the Zabusky Kruskal(2), integrable(9), and spectral(10) lattices, has been seen, it can be observed that the best initial-state recurrence does not occur in either the most accurate method, or the most converged state. In figures 8 and 9 it is clear that there is a midrange of $N$-values with the strongest associated initial state recurrence, since the model is not converged for this midrange of $N$-values, but for much larger $N$-values, the best recurrence is seen before convergence. This indicates that the initial-state recurrence that is being seen in this midrange is a characteristic of the discrete system, not the KdV(1) equation, the limit of the system.
Figure 10 shows that the spectral scheme is lacking the midrange recurrence strength spike, and over all has weaker recurrence than either the ZK scheme, 8, or the integrable scheme, 9. Since the spectral scheme is the most accurate, and shows us a converged state, this contradicts the premise that it is “closeness” to the KdV equation that causes the initial-state recurrence in the discretizations.

The energy profiles are clear; presented are examples of drastically different initial-state recurrence phenomena, with identical or near identical energy profiles. In both figures 11 and 12 we see three plots, approximately corresponding to our three states of recurrence: an unconverged zone with no systematic recurrence, an unconverged zone that shows maximum recurrence, and a zone of systematic but relatively weak recurrence. Regardless of our three tiers of recurrence we see only two basic energy profiles, the relatively thermalized profile, and the profile of convergence. Particularly we know that most of the simulations that display strong initial-state recurrence (those with a “midrange” gridsize in either the ZK scheme or integrable scheme) share an energy profile with the converged simulations (large grid sizes for the ZK scheme and the integrable scheme, and above $N \approx 100$ for the spectral scheme). While it is certainly true to say that thermalization excludes the possibility of initial-state recurrence, it seems that systems may have the same distribution of energy among modes, and show different recurrence behavior.

Appendix

Code for Octave

Zabusky Kruskal Discretization

ZK discretization’s function code

```octave
function udot = zbk(t, u, L, dta)

%KdV: u_t=-u_x-(dta^2)*u_XXX
%zbk(t,u,L,dta) is the right hand side of the ZK discretization of KdV
%GTN

%input t=[t_0 t_end] for the sake of the solver ode5r
%u is an initial condition.
%L is the length
%dta is the value for delta.

u = u(:); %make the initial conditions a column vector

[N, R] = size(u);

z = zeros(1, Q-3); %these will be used to fill out our circulant matrices
s = zeros(1, Q-5);
h = L/N; %here we define h=L/N as normal

A = [1 1 z 1]; %this is my three term average to approximate u_n
```
B = circulant(A);

C = [0 -1 z 1]; %this is the negative of the first derivative
D = circulant(C);

E = [0 2 -1 s 1 -2]; %this is the negative of the third derivative
F = circulant(E);

%udot=du/dt
udot =((B*u).*(D*u))/(6*h) +((F*u)*(dta)^2)/(2*h^3);

endfunction

ZK scheme’s code to call ode solver in Octave

function [T U] = zbkrun(grid, L, dta)
%zbkrun is a function that takes parameters
%(grid size, length, delta value) and uses ode5r
%to run time evolution simulations using function @zbk

%initial conditions
h = L/grid;
x=[0:(1/grid):(1-1/grid)];
u=sin(2*pi*x);

%run ode5r on zbk, with options opt.
opt = odeset("RelTol",le-6,"AbsTol",le-6);

[T1 U1] = ode5r(@zbk, [0 125], u, opt, L, dta);
[T2 U2] = ode5r(@zbk, [125 250], U1(end,:), opt, L, dta);
[T3 U3] = ode5r(@zbk, [250 375], U2(end,:), opt, L, dta);
[T4 U4] = ode5r(@zbk, [375 500], U3(end,:), opt, L, dta);

T = [T1;T2(2:end,:);T3(2:end,:);T4(2:end,:)];
U = [U1;U2(2:end,:);U3(2:end,:);U4(2:end,:)];

%save data
sav=sprintf("save '/raid/GTN/kdvdata/zk_data/zk_\%g\_\%g_22' T U",grid,L)
eval(sav);

endfunction

Integrable Scheme

integrable discretization’s function code
function udot = kdv_rhs_in(t,u,d,L)
    % Right-hand side of
    % KdV: u_t + u u_x + d u_xxx = 0
    % BMH integrable discretization
    % on interval length L with periodic BC
    % ADT

    % d=delta^2

    N = length(u);
    h = L/N;

    Ac = sparse(circulant([2 1 zeros(1,N-3) 1]/4));
    D1 = sparse(circulant([0 1 zeros(1,N-3) -1]/(2*h)));
    D3 = sparse(circulant([0 -2 1 zeros(1,N-5) -1 2]/(2*h^3)));
    Pl = sparse(circulant([0 1 zeros(1,N-2)]));
    Mi = sparse(circulant([zeros(1,N-1) 1]));

    c = h^2/6;

    lin = d*(D3*u); % d u_xxx (linear term)
    nonla = (2/3)*(Ac*u).*(D1*u);
    nonlb = (1/6)*(Pl+Mi)*(u.*(D1*u));
    nonl = nonla + nonlb;
    nonl2 = (c/d)*u.*(lin+nonl);
    udot = -nonl2-nonl-lin;
endfunction

integrable scheme's code to call ode solver in Octave

function [T U] = in_run(grid, L, d)
    % in_run(t, grid, d, L); t is the time interval,
    % grid is the number of grid points you want
    % your lattice to have,
    % d is delta squared, from KdV, and L is the length.

    % initial conditions
    h = L/grid;
    x=[0:(1/grid):(1-1/grid)];
    u=sin(2*pi*x);

    % run ode5r @kdv_rhs_in, the right hand side of the integrable
    % discretization, with options opt
    opt = odeset("RelTol",1e-6,"AbsTol",1e-6);
Spectral discretization's function code

function udot = kdv_rhs_sp(t,u,d,L)
    %right-hand side of the KdV equation \( u_t + u u_x + d u_{xxx} = 0 \)
    % on interval of length L with periodic BC
    % ADT & GTN

    N = length(u);
    u = u(:);
    N1 = floor((N-1)/2);
    N2 = (-N/2)*ones(rem(N,2)==0);

    v = fftshift(fft(u));  % move to Fourier space
    v = v(:);
    p = conv(v,w.*v)/N;  % \( u u_x \) (nonlinear term)
    if rem(N,2)==0
        nonl = p(N/2+1:3*N/2);  % dealiased product, assume N is even
    else
        nonl = p(N1+1:3*N1+1);
    endif
    nonl = nonl(:);

    lin = (d^2)*(w.^3).*v;  % \( d^2 u_{xxx} \) (linear term)
    lin = lin(:);

    s = -nonl-lin;
udot = ifft(ifftshift(s)); % return to physical space

% real data in => real data out
if (isreal(u));
udot = real(udot);
endfunction

spectral scheme's code to call ode solver in Octave

function [T U] = sp_run(grid, d, L)
    % sp_run(grid, d, L)
    % grid is the number of discrete nodes in lattice,
    % d is the delta value from kdv,
    % and L is the length

    % initial conditions
    h = L/grid;
x = [0: (1/grid): (1-1/grid)];
u = sin(2*pi*x);

    % run ode5r on kdv_rhs_sp, with options opt
    opt = odeset("RelTol", 1e-6, "AbsTol", 1e-6);

    [T1 U1] = ode5r(@kdv_rhs_sp, [0 100], u, opt, d, L);
    [T2 U2] = ode5r(@kdv_rhs_sp, [100 200], U1(end,:), opt, d, L);
    [T3 U3] = ode5r(@kdv_rhs_sp, [200 300], U2(end,:), opt, d, L);
    [T4 U4] = ode5r(@kdv_rhs_sp, [300 400], U3(end,:), opt, d, L);
    [T5 U5] = ode5r(@kdv_rhs_sp, [400 500], U4(end,:), opt, d, L);

    T = [T1(2:end,:); T2(2:end,:); T3(2:end,:); T4(2:end,:); T5(2:end,:)];
    U = [U1(2:end,:); U2(2:end,:); U3(2:end,:); U4(2:end,:); U5(2:end,:)];

    % save data
    sav = sprintf("save '/raid/GTN/kdvdata/sp_data/sp_%dg_2_22' T U", grid);
eval(sav);
endfunction

References

[1] Comment made to Nieddu by Trubatch, from personal communication between ADT and Robert Miura.


