Dispersive Quantization of Linear and Nonlinear Waves

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Gong Chen & —, Dispersion of discontinuous periodic waves, Proc. Roy. Soc. London A 469 (2012), 20120407.

Gong Chen & —, Numerical simulation of nonlinear dispersive quantization, Discrete Cont. Dyn. Syst. A 34 (2013), 991–1008.

Dispersion

Definition. A linear partial differential equation is called dispersive if the different Fourier modes travel unaltered but at different speeds.

Substituting

$$u(t,x) = e^{i(kx - \omega t)}$$

produces the dispersion relation

$$\omega = \omega(k), \qquad \qquad \omega, k \in \mathbb{R}$$

relating frequency ω and wave number k.

Phase velocity:
$$c_p = \frac{\omega(k)}{k}$$

Group velocity: $c_g = \frac{d\omega}{dk}$

(stationary phase)

A Simple Linear Dispersive Wave Equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3}$$

 \implies linearized Korteweg–deVries equation

 $\begin{array}{ll} \text{Dispersion relation:} & \omega = k^3 \\ \text{Phase velocity:} & c_p = \frac{\omega}{k} = k^2 \\ \text{Group velocity:} & c_g = \frac{d\omega}{dk} = 3 \, k^2 \\ \text{Thus, wave packets (and energy) move } faster (to the right) than \\ \text{the individual waves.} \end{array}$

Linear Dispersion on the Line

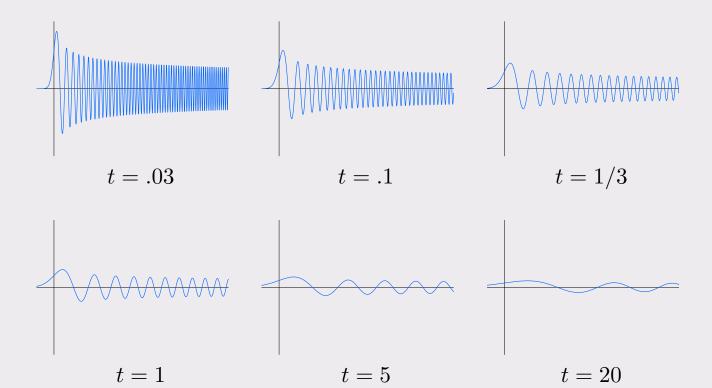
$$\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3}$$
 $u(0,x) = f(x)$

Fourier transform solution:

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k) \, e^{i \, (k \, x - k^3 \, t)} \, dk$$

Fundamental solution $u(0,x) = \delta(x)$

$$u(t,x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(kx-k^{3}t)} dk = \frac{1}{\sqrt[3]{3t}} \operatorname{Ai}\left(-\frac{x}{\sqrt[3]{3t}}\right)$$



Linear Dispersion on the Line

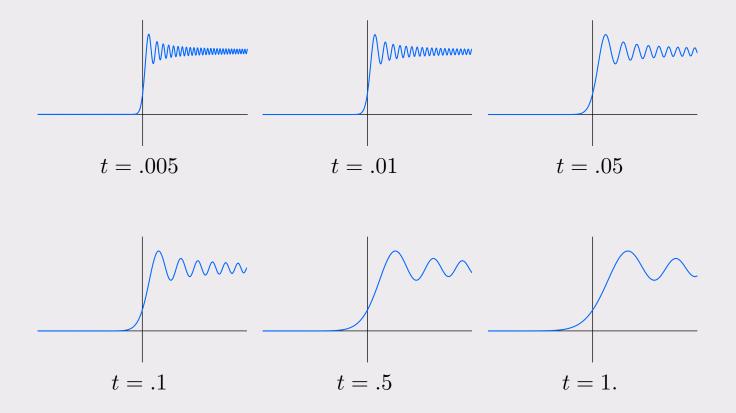
$$\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3}$$
 $u(0,x) = f(x)$

Superposition solution formula:

$$u(t,x) = \frac{1}{\sqrt[3]{3t}} \int_{-\infty}^{\infty} f(\xi) \operatorname{Ai}\left(\frac{\xi - x}{\sqrt[3]{3t}}\right) d\xi$$

Step function initial data:
$$u(0,x) = \sigma(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

 $u(t,x) = \frac{1}{3} - H\left(-\frac{x}{\sqrt[3]{3t}}\right)$
 $H(z) = \frac{z\Gamma\left(\frac{2}{3}\right)_1 F_2\left(\frac{1}{3};\frac{2}{3},\frac{4}{3};\frac{1}{9}z^3\right)}{3^{5/3}\Gamma\left(\frac{2}{3}\right)\Gamma\left(\frac{4}{3}\right)} - \frac{z^2\Gamma\left(\frac{2}{3}\right)_1 F_2\left(\frac{2}{3};\frac{4}{3},\frac{5}{3};\frac{1}{9}z^3\right)}{3^{7/3}\Gamma\left(\frac{4}{3}\right)\Gamma\left(\frac{5}{3}\right)}$
 $\implies \text{MATHEMATICA} - \text{via Meijer G functions}$



Periodic Linear Dispersion

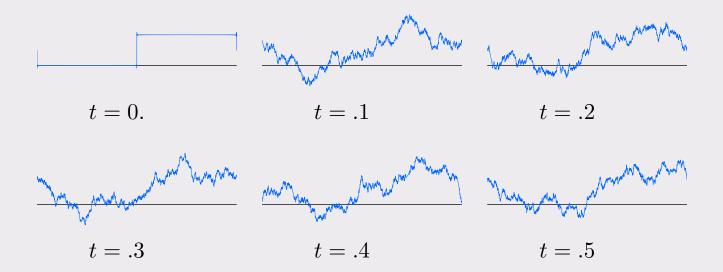
$$\frac{\partial u}{\partial t} = \frac{\partial^3 u}{\partial x^3}$$
$$u(t, -\pi) = u(t, \pi) \quad \frac{\partial u}{\partial x}(t, -\pi) = \frac{\partial u}{\partial x}(t, \pi) \quad \frac{\partial^2 u}{\partial x^2}(t, -\pi) = \frac{\partial^2 u}{\partial x^2}(t, \pi)$$

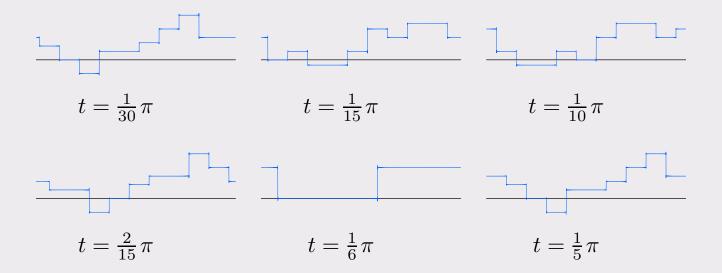
Step function initial data:

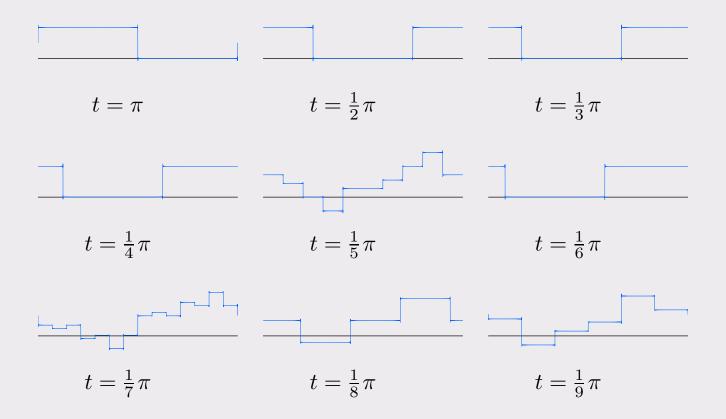
$$u(0,x) = \sigma(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

Fourier series solution formula:

$$u^{\star}(t,x) \sim \frac{1}{2} + \frac{2}{\pi} \sum_{j=0}^{\infty} \frac{\sin((2j+1)x - (2j+1)^3t)}{2j+1}$$







Theorem. At rational time $t = 2\pi p/q$, the solution $u^*(t, x)$ is constant on every subinterval $2\pi j/q < x < 2\pi (j+1)/q$. At irrational time $u^*(t, x)$ is a non-differentiable continuous function.

Lemma.

$$f(x) \sim \sum_{k=-\infty}^{\infty} c_k e^{ikx}$$

is piecewise constant on intervals $2 \, \pi \, j/q < x < 2 \, \pi \, (j+1)/q$ if and only if

 $\label{eq:ck} \hat{c}_k = \hat{c}_l, \quad k \equiv l \not\equiv 0 \mbox{ mod } q, \qquad \hat{c}_k = 0, \quad 0 \neq k \equiv 0 \mbox{ mod } q.$ where

$$\widehat{c}_k = \frac{2 \pi k c_k}{\operatorname{i} q \left(e^{-2 \operatorname{i} \pi k/q} - 1 \right)} \qquad \qquad k \not\equiv 0 \ \mathrm{mod} \ q.$$

 \implies DFT

The Fourier coefficients of the solution $u^{\star}(t, x)$ at rational time $t = 2\pi p/q$ are

$$c_k = b_k \, e^{-2\,\pi\,\mathrm{i}\,k^3\,p/q} \qquad (*)$$

where, for the step function initial data,

$$b_k = \left\{ egin{array}{ll} -{\rm i}\,/(\pi\,k), & k \ {\rm odd}, \\ 1/2, & k = 0, \\ 0, & 0 \neq k \ {\rm even}. \end{array}
ight.$$

Crucial observation:

if
$$k \equiv l \mod q$$
 then $k^3 \equiv l^3 \mod q$

which implies

$$e^{-2\pi i k^3 p/q} = e^{-2\pi i l^3 p/q}$$

and hence the Fourier coefficients (*) satisfy the condition in the Lemma. Q.E.D.

The Fundamental Solution: $F(0,x) = \delta(x)$

Theorem. At rational time $t = 2\pi p/q$, the fundamental solution F(t, x) is a linear combination of finitely many periodically extended delta functions, based at $2\pi j/q$ for integers $-\frac{1}{2}q < j \leq \frac{1}{2}q$.

Corollary. At rational time, any solution profile $u(2\pi p/q, x)$ to the periodic initial-boundary value problem is a linear combination of $\leq q$ translates of the initial data, namely $f(x + 2\pi j/q)$, and hence its value depends on only finitely many values of the initial data.

 \star The same quantization/fractalization phenomenon appears in any linearly dispersive equation with "integral polynomial" dispersion relation:

$$\omega(k) = \sum_{m=0}^{n} c_m k^m$$

where

$$c_m = \alpha \, n_m \qquad n_m \in \mathbb{Z}$$

Linear Free-Space Schrödinger Equation

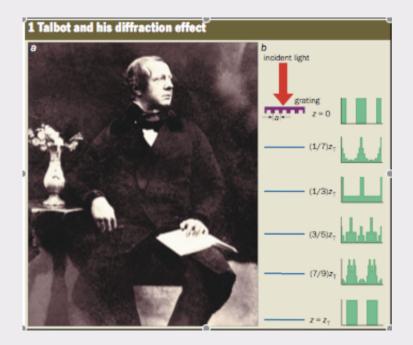
$$i \frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2}$$

The Talbot Effect

$$i \frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2}$$
$$u(t, -\pi) = u(t, \pi) \qquad \frac{\partial u}{\partial x}(t, -\pi) = \frac{\partial u}{\partial x}(t, \pi)$$

- Michael Berry, et. al.
- Bernd Thaller, Visual Quantum Mechanics
- Oskolkov
- Kapitanski, Rodnianski "Does a quantum particle know the time?"
- Michael Taylor

William Henry Fox Talbot (1800–1877)





★ Talbot's 1835 image of a latticed window in Lacock Abbey \implies oldest photographic negative in existence.

A Talbot Experiment

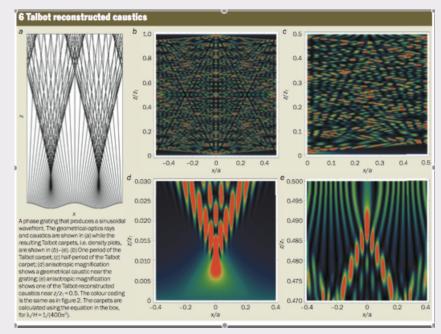
Fresnel diffraction by periodic gratings (1836):

"It was very curious to observe that though the grating was greatly out of the focus of the lens ... the appearance of the bands was perfectly distinct and well defined ... the experiments are communicated in the hope that they may prove interesting to the cultivators of optical science."

— Fox Talbot

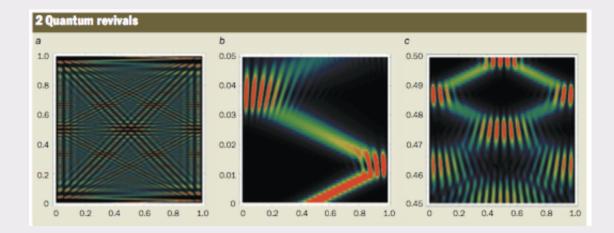
 \implies Lord Rayleigh calculates the Talbot distance (1881)

The Quantized/Fractal Talbot Effect



- Optical experiments Berry & Klein
- Diffraction of matter waves (helium atoms) Nowak et. al.

Quantum Revival



- Electrons in potassium ions Yeazell & Stroud
- Vibrations of bromine molecules

Vrakking, Villeneuve, Stolow

Periodic Linear Schrödinger Equation

$$i \frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2}$$
$$u(t, -\pi) = u(t, \pi) \qquad \frac{\partial u}{\partial x}(t, -\pi) = \frac{\partial u}{\partial x}(t, \pi)$$

Integrated fundamental solution:

$$u(t,x) = \frac{1}{2\pi} \sum_{0 \neq k = -\infty}^{\infty} \frac{e^{i(kx - k^2t)}}{k}$$

For $x/t \in \mathbb{Q}$, this is known as a Gauss sum (or, more generally, Weyl sum), of great importance in number theory $\star \star$ The Riemann Hypothesis!

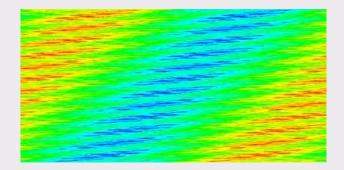
 \implies Hardy, Littlewood, Weil, I. Vinogradov, etc.

Integrated fundamental solution:

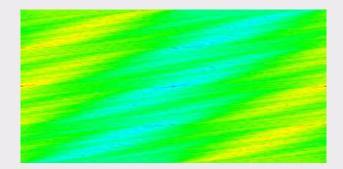
$$u(t,x) = \frac{1}{2\pi} \sum_{0 \neq k = -\infty}^{\infty} \frac{e^{i(kx-k^2t)}}{k}.$$

Theorem.

- The fundamental solution $\partial u/\partial x$ is a Jacobi theta function. At rational times $t = 2\pi p/q$, it linear combination of delta functions concentrated at rational nodes $x_j = 2\pi j/q$.
- At irrational times t, the integrated fundamental solution is a continuous but nowhere differentiable function.



Dispersive Carpet



Schrödinger Carpet

Periodic Linear Dispersion

$$\frac{\partial u}{\partial t} = L(D_x) \, u, \qquad u(t, x + 2 \, \pi) = u(t, x)$$

Dispersion relation:

$$u(t,x) = e^{i(kx-\omega t)} \implies \omega(k) = -iL(-ik)$$
 assumed real
Riemann problem: step function initial data

$$u(0,x) = \sigma(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

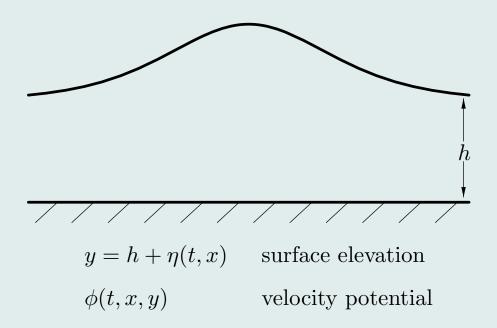
Solution:

$$u(t,x) \sim \frac{1}{2} + \frac{2}{\pi} \sum_{j=0}^{\infty} \frac{\sin[(2j+1)x - \omega(k)t]}{2j+1}.$$

 $\bigstar \bigstar \omega(-k) = -\omega(k) \text{ odd}$

Polynomial dispersion, rational $t \implies$ Weyl exponential sums

2D Water Waves

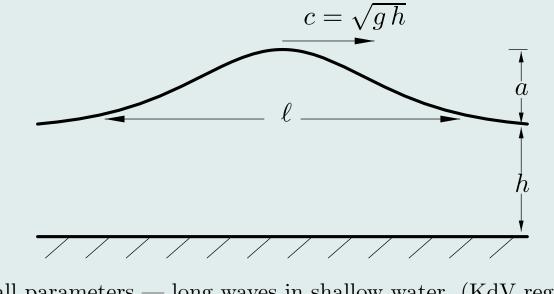


2D Water Waves

- Incompressible, irrotational fluid.
- No surface tension

$$\begin{array}{l} \phi_t + \frac{1}{2} \phi_x^2 + \frac{1}{2} \phi_y^2 + g \, \eta = 0 \\ \eta_t = \phi_y - \eta_x \phi_x \end{array} \end{array} \right\} \qquad y = h + \eta(t, x) \\ \phi_{xx} + \phi_{yy} = 0 \qquad \qquad 0 < y < h + \eta(t, x) \\ \phi_y = 0 \qquad \qquad y = 0 \end{array}$$

- Wave speed (maximum group velocity): $c = \sqrt{g h}$
- Dispersion relation: $\sqrt{g k \tanh(h k)} = c k \frac{1}{6} c h^2 k^3 + \cdots$



Small parameters — long waves in shallow water (KdV regime) $\alpha = \frac{a}{h} \qquad \beta = \frac{h^2}{\ell^2} = O(\alpha)$ Rescale:

Rescaled water wave system:

$$\begin{aligned} \phi_t + \frac{\alpha}{2} \phi_x^2 + \frac{\alpha}{2\beta} \phi_y^2 + \eta &= 0 \\ \eta_t &= \frac{1}{\beta} \phi_y - \alpha \eta_x \phi_x \end{aligned} \right\} \qquad y = 1 + \alpha \eta \\ \beta \phi_{xx} + \phi_{yy} &= 0 \qquad \qquad 0 < y < 1 + \alpha \eta \\ \phi_y &= 0 \qquad \qquad y = 0 \end{aligned}$$

Boussinesq expansion

Set

$$\psi(t,x) = \phi(t,x,0) \qquad \quad u(t,x) = \phi_x(t,x,\theta) \qquad \quad 0 \le \theta \le 1$$

Solve Laplace equation:

$$\phi(t, x, y) = \psi(t, x) - \frac{1}{2}\beta^2 y^2 \psi_{xx} + \frac{1}{4!}\beta^4 y^4 \psi_{xxxx} + \cdots$$

Plug expansion into free surface conditions: To first order

$$\psi_t + \eta + \frac{1}{2}\alpha\,\psi_x^2 - \frac{1}{2}\beta\,\psi_{xxt} = 0$$
$$\eta_t + \psi_x + \alpha\,(\eta\psi_x)_x - \frac{1}{6}\beta\,\psi_{xxxx} = 0$$

Bidirectional Boussinesq systems:

$$u_t + \eta_x + \alpha \, u \, u_x - \frac{1}{2} \,\beta \left(\theta^2 - 1\right) u_{xxt} = 0$$
$$\eta_t + u_x + \alpha \, (\eta \, u)_x - \frac{1}{6} \,\beta \left(3 \,\theta^2 - 1\right) u_{xxx} = 0$$

 $\star \star$ at $\theta = 1$ this system is integrable

 \implies Kaup, Kupershmidt

Boussinesq equation

$$u_{tt} = u_{xx} + \frac{1}{2}\alpha \, (u^2)_{xx} - \frac{1}{6}\beta \, u_{xxxx}$$

Regularized Boussinesq equation

$$u_{tt} = u_{xx} + \frac{1}{2} \alpha \, (u^2)_{xx} - \frac{1}{6} \beta \, u_{xxtt}$$

 \implies DNA dynamics (Scott)

Unidirectional waves:

$$u = \eta - \frac{1}{4} \alpha \eta^2 + \left(\frac{1}{3} - \frac{1}{2} \theta^2\right) \beta \eta_{xx} + \cdots$$

Korteweg-deVries (1895) equation:

$$\eta_t + \eta_x + \frac{3}{2} \alpha \eta \eta_x + \frac{1}{6} \beta \eta_{xxx} = 0$$

 \implies Due to Boussinesq in 1877!

Benjamin–Bona–Mahony (BBM) equation:

$$\eta_t + \eta_x + \frac{3}{2} \alpha \eta \eta_x - \frac{1}{6} \beta \eta_{xxt} = 0$$

Shallow Water Dispersion Relations

Water waves	$\pm \sqrt{k \tanh k}$
Boussinesq system	$\pm \frac{k}{\sqrt{1 + \frac{1}{3}k^2}}$
Boussinesq equation	$\pm k\sqrt{1+\frac{1}{3}k^2}$
Korteweg-deVries	$k - \frac{1}{6}k^3$
BBM	$\frac{k}{1+\frac{1}{6}k^2}$

Dispersion Asymptotics

★ The qualitative behavior of the solution to the periodic problem depends crucially on the asymptotic behavior of the dispersion relation $\omega(k)$ for large wave number $k \to \pm \infty$.

$$\omega(k) \sim k^{\alpha}$$

- $\alpha = 0$ large scale oscillations
- $0 < \alpha < 1$ dispersive oscillations
- $\alpha = 1$ traveling waves
- $1 < \alpha < 2$ oscillatory becoming fractal
- $\alpha \ge 2$ fractal/quantized

Periodic Korteweg-deVries equation

$$\frac{\partial u}{\partial t} = \alpha \, \frac{\partial^3 u}{\partial x^3} + \beta \, u \frac{\partial u}{\partial x} \qquad u(t, x + 2\ell) = u(t, x)$$

Zabusky–Kruskal (1965)

 $\alpha = 1, \qquad \beta = .000484, \qquad \ell = 1, \qquad u(0, x) = \cos \pi x.$ Lax–Levermore (1983) — small dispersion

$$\alpha \longrightarrow 0, \qquad \beta = 1.$$

Gong Chen (2011)

 $\alpha = 1, \qquad \beta = .000484, \qquad \ell = 1, \qquad u(0, x) = \sigma(x).$

Periodic Korteweg-deVries Equation

Analysis of non-smooth initial data:

Estimates, existence, well-posedness, stability, ...

- Kato
- Bourgain
- Kenig, Ponce, Vega
- Colliander, Keel, Staffilani, Takaoka, Tao
- Oskolkov
- D. Russell, B–Y Zhang
- Erdoğan, Tzirakis

Operator Splitting

$$u_t = \alpha \, u_{xxx} + \beta \, u u_x = L[\,u\,] + N[\,u\,]$$

Flow operators: $\Phi_L(t)$, $\Phi_N(t)$

Godunov scheme:

$$u_{\Delta}^{G}(t_{n}) \simeq \left(\Phi_{L}(\Delta t) \Phi_{N}(\Delta t) \right)^{n} u_{0}$$

Strang scheme:

$$u_{\Delta}^{S}(t_{n}) \simeq \left(\Phi_{N}(\frac{1}{2}\Delta t) \Phi_{L}(\Delta t) \Phi_{N}(\frac{1}{2}\Delta t) \right)^{n} u_{0}$$

Numerical implementation:

- FFT for Φ_L linearized KdV
- FFT + convolution for Φ_N conservative version of inviscid Burgers', using Backward Euler + fixed point iteration to overcome mild stiffness. Shock dynamics doesn't complicate due to small time stepping.

Convergence of Operator Splitting

★ Holden, Karlsen, Risebro and Tao prove:
 First order convergence of the Godunov scheme

$$\begin{split} u_{\Delta}^G(t_n) \simeq \big(\, \Phi_L(\Delta t) \, \Phi_N(\Delta t) \, \big)^n \, u_0 \\ \text{for initial data } u_0 \in H^s \text{ for } s \geq 5 \\ & \| \, u(t_n) - u_{\Delta}^G(t_n) \, \| \leq C \, \Delta t \end{split}$$

Second order convergence of the Strang scheme

$$\begin{split} u_{\Delta}^{S}(t_{n}) &\simeq \left(\, \Phi_{N}(\frac{1}{2}\,\Delta t \,)\,\Phi_{L}(\Delta t)\,\Phi_{N}(\frac{1}{2}\,\Delta t \,)\,\right)^{n}u_{0} \\ \text{for initial data } u_{0} \in H^{s} \text{ for } s \geq 17: \\ &\parallel u(t_{n}) - u_{\Delta}^{S}(t_{n})\,\parallel \leq C\,(\Delta t)^{2} \end{split}$$

Convergence for Rough Data?

However, subtle issues prevent us from establishing convergence of the operator splitting method for rough initial data.

- $\bullet\,$ Bourgain proves well-posedness of the periodic KdV flow in ${\rm L}^2$
- • Conservation of the L² norm establishes well-posedness in L² of the linearized flow Φ_L
- Thus, if the solution has bounded L^∞ norm, then the linearized flow is L^1 contractive
- Oskolkov proves that is the initial data is has bounded BV norm, then the resulting solution to the periodic linearized KdV equation is uniformly bounded in L^{∞}
- Unfortunately, Oskolkov's bound depends on the BV and L^{∞} norms of the initial data. Moreover, at irrational times, the solution is nowhere differentiable and has unbounded BV norm
- Also, we do not have good control of the BV norm of the nonlinear inviscid Burgers' flow Φ_N
- ????

Periodic Nonlinear Schrödinger Equation

 $\mathrm{i}\, u_t+u_{xx}+|\,u\,|^p\,u=0,\qquad x\in\mathbb{R}/\mathbb{Z},\qquad u(0,x)=g(x).$

Theorem. (Erdoğan, Tzirakis) Suppose p = 2 (the integrable case) and $g \in BV$. Then

(i) $u(t, \cdot)$ is continuous at irrational times $t \notin \mathbb{Q}$

(*ii*) $u(t, \cdot)$ is bounded with at most countably many discontinuities at rational times $t \in \mathbb{Q}$

(*iii*) When the initial data is sufficiently "rough", i.e., $g \notin \bigcup_{\epsilon > 0} H^{1/2+\epsilon}$ then, at almost all t, the real or imaginary part of the graph of $u(t, \cdot)$ has fractal (upper Minkowski) dimension $\frac{3}{2}$.

Periodic Linear Dispersive Equations

 \implies Chousionis, Erdoğan, Tzirakis

Theorem. Suppose $3 \le k \in \mathbb{Z}$ and

 $\mathrm{i}\, u_t + (-\,\mathrm{i}\,\partial_x)^k u = 0, \qquad x \in \mathbb{R}/\mathbb{Z}, \qquad u(0,x) = g(x) \in \mathrm{BV}$

(i) $u(t, \cdot)$ is continuous for almost all t

(*ii*) When $g \notin \bigcup_{\epsilon > 0} H^{1/2+\epsilon}$, then, at almost all t, the real and imaginary parts of the graph of $u(t, \cdot)$ has fractal dimension $1 + 2^{1-k} \leq D \leq 2 - 2^{1-k}$.

Theorem. For the periodic Korteweg–deVries equation

$$u_t + u_{xxx} + u \, u_x = 0, \qquad x \in \mathbb{R}/\mathbb{Z}, \qquad u(0, x) = g(x) \in \mathrm{BV}$$

(i) $u(t, \cdot)$ is continuous for almost all t

(*ii*) When $g \notin \bigcup_{\epsilon > 0} H^{1/2+\epsilon}$, then, at almost all t, the real and imaginary parts of the graph of $u(t, \cdot)$ has fractal dimension $\frac{5}{4} \leq D \leq \frac{7}{4}$.

The Vortex Filament Equation

 \implies Da Rios (1906)

Localized Induction Approximation (LIA) or binormal flow

$$\gamma_t = \gamma_s \times \gamma_{ss} = \kappa \, \mathbf{b}$$

 $\gamma(t,s) \in \mathbb{R}^3$ at time t represents the vortex filament a space curve parametrized by arc length — that moves in an incompressible fluid flow with vorticity concentrated on the filament.

Frenet frame: $\mathbf{t}, \mathbf{n}, \mathbf{b}$ — unit tangent, normal, binormal

 κ — curvature au — torsion

$$\gamma_t = \gamma_s \times \gamma_{ss}$$

Hasimoto transformation:

$$u = \kappa \exp\left(i \int \tau \, ds\right)$$

solves the integrable nonlinear Schrödinger equation:

$$\mathbf{i}\,u_t = u_{xx} + |\,u\,|^2\,u$$

de la Hoz and Vega (2013): If the initial data is a closed polygon, then at rational times the curve is a polygon, whereas at irrational times it is a fractal.

Chousionis, Erdoğan, Tzirakis (2014): further results on fractal behavior for some smooth initial data

Vortex Filament Polygons

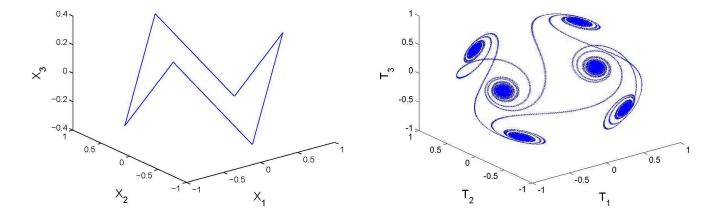


Figure 7: \mathbf{X}_{alg} and \mathbf{T}_{alg} , at $t = \frac{2\pi}{9}(\frac{1}{4} + \frac{1}{49999})$.

Vortex Filament Polygons

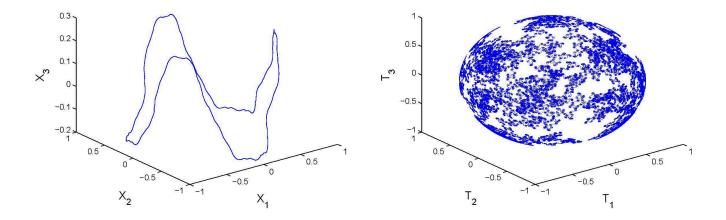


Figure 8: \mathbf{X}_{alg} and \mathbf{T}_{alg} , at $t = \frac{2\pi}{9} (\frac{1}{4} + \frac{1}{41} + \frac{1}{401}) = \frac{2\pi}{9} \cdot \frac{18209}{65764}$.

Future Directions

- General dispersion behavior
- Other boundary conditions (Fokas' Method)
- Higher space dimensions and other domains

 $(\mathrm{tori},\,\mathrm{spheres},\,\dots)$

- Dispersive nonlinear partial differential equations
- Discrete systems: Fermi–Pasta–Ulam
- Numerical solution techniques?
- Experimental verification in dispersive media?