Unitary Quantum Lattice Algorithms For Classical and Quantum Turbulence - part 1

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OVERVIEW

1. **Computational journey of our research group**

2. **Lattice Boltzmann Algorithms (LBM-MHD) -**
Gordon Bell finalists 2005 (Earth Simulator)

3. **QLA for NLS, KdV - 1D. : exactly soluble - solitons**

4. **QLA for 1D MHD-Burgers : NMR Expt. -**
Burgers Eq.

5. QLA for GP/NLS for scalar BEC : quantum vortex
   - 2D and 3D Quantum Turbulence

6. QLA for Spin-2 BECs : non-Abelian vortices

7. QLA for Maxwell Equations

- **GIVEN the pde's -** what are the unitary collision-streaming sequence of operators needed to recover the pde's to 2nd order accuracy ?

Interested in time evolution of system :

- this puts great stress on adequate qubit coherence times, fidelity of gates, error corrections … for a feasible quantum computer (> 10 years…?)

- The QLA can be directly encoded onto a quantum computer

- QLA ideally parallelizes on classical supercomputers
  - tested to over 780,000 cores (*IBM Mira, Argonne)*

1. COMPUTATIONAL JOURNEY

1.1 plasma physics (nonlinear) : MHD

$\hbar = 0$

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{u}) = 0 \quad , \quad \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u}\right) = -\nabla p(\rho) + (\nabla \times \mathbf{B}) \times \mathbf{B} + \nu \nabla^2 \mathbf{u}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \eta \nabla^2 \mathbf{B} \quad , \quad \nabla \bullet \mathbf{B} = 0$$

- **Nonlinear terms — severe headache computationally**
  - Discrete mesoscopic lattice kinetic approach (LB)

$$\mathbf{x}, t \rightarrow \mathbf{x}, \vec{\xi}_j, t$$

$$\frac{\partial f_j(\mathbf{x}, t)}{\partial t} + \vec{\xi}_j \bullet \nabla f_j = -\frac{1}{\tau}\left[f_j - f_j^{eq}(\mathbf{v}, \mathbf{B})\right] \qquad Moments: \ \sum_j f_j = \rho \ , \ \sum f_j \vec{\xi}_j = \rho \mathbf{u}$$

Streaming	local collisions
Linear advection	algebraic nonlinear terms

- **one major problem with simple LB :** *some* $f_j < 0$

  [c.f., Klein-Gordon - Dirac   positive definite density]

- entropic LB : exact discrete H-fn constraint
- more exotic lattices than D2Q9 , D3Q27
- matrix collision operator (MRT)
- collisions in moment space, streaming in coord space

- LB extremely well parallelized : local collision operator, shift operator
  - our codes run on *Earth Simulator* (Japan), Gordon Bell finalists in 2005

Idea :

[ths streaming operate is already unitary]

Can one use only unitary collision operators?

→ **one has the beginnings of a QLA - since the streaming operators are already unitary**

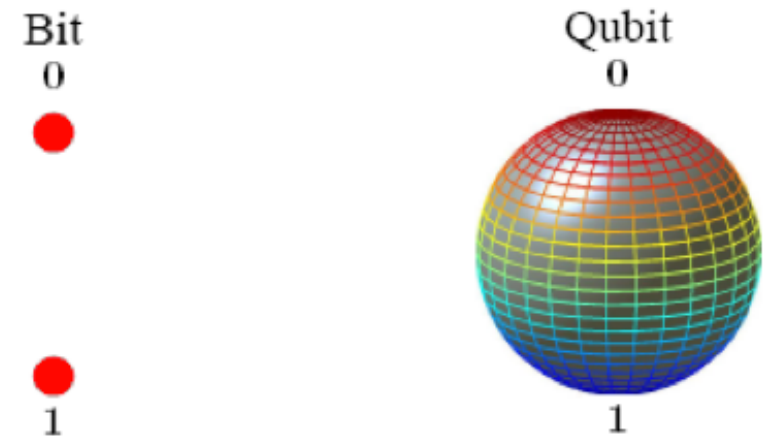
→ NLS - ubiquitous equation of nonlinear physics - integrable in 1D

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + \left[g|\psi|^2 - \mu\right]\psi$$

- water waves, rogue waves - solitons
- plasma physics, nonlinear optics (dark, bright solitons)
- ground state of BEC (mean field theory)
  [Gross-Pitaevskii equation - quantum vortices/dark solitons]

- **1D NLS — integrable:**
  - can benchmark QLA against exact analytic solutions

QUBITS and ENTANGLEMENT



1-qubit: $|q_1\rangle = \alpha_1|1\rangle + \alpha_0|0\rangle \quad , |q_2\rangle = \beta_1|1\rangle + \beta_0|0\rangle$

$$, \quad \sum_{i=0}^{1}|\alpha_i|^2 = \sum_{i=0}^{1}|\beta_i|^2 = 1$$

→ Entangled 2-qubit state: cannot be factored into a tensor product of 1-qubit states

→ Tensor Product : $|q_1\rangle \otimes |q_2\rangle \equiv |q_1 q_2\rangle = \alpha_1\beta_1|11\rangle + \alpha_1\beta_0|10\rangle + \alpha_0\beta_1|01\rangle + \alpha_0\beta_0|00\rangle$

→ Bell State : $\dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$ - - an entangled state

for this would require: $\alpha_1 = 0 \; or \; \beta_0 = 0$

↓ ↓

no $|11\rangle$ no $|00\rangle$

- **in QLA, the unitary local collision operator will entangle the on-site qubits**

QUANTUM RANDOM WALK

- walker described by

$$H_P : position\ , with\ basis\ states\ |i\rangle$$

$$H_C :\ Hilbert\ space\ for\ 2-sided\ coin\ ,\ basis\ \{|\uparrow\rangle\ ,|\downarrow\rangle\}$$

$$H_{TOT} = H_C \otimes H_P$$

2 unitary operators : *coin* *position*

→ $\hat{S}$ - streaming operator s.t $\hat{S}: |\uparrow\rangle \otimes |i\rangle \rightarrow |\uparrow\rangle \otimes |i+1\rangle$

$$\hat{S}: |\downarrow\rangle \otimes |i\rangle \rightarrow |\downarrow\rangle \otimes |i-1\rangle$$

→ $1-qubit\ Hadamard\ gate$ $\hat{H}_{HAD}(|\uparrow\rangle) = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$

$$\hat{H}_{HAD}(|\downarrow\rangle) = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}}$$

- suppose at t = 0 : spin-down at origin $|\downarrow\rangle \otimes |0\rangle$

1st time step:

$$\hat{H}_{HAD} : |\downarrow\rangle \otimes |0\rangle \rightarrow \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}} \otimes |0\rangle$$

$$\hat{S} : \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}} \otimes |0\rangle = \hat{S} : \frac{|\uparrow\rangle \otimes |0\rangle}{\sqrt{2}} - \frac{|\downarrow\rangle \otimes |0\rangle}{\sqrt{2}}$$

$$\rightarrow \frac{|\uparrow\rangle \otimes |1\rangle}{\sqrt{2}} - \frac{|\downarrow\rangle \otimes |-1\rangle}{\sqrt{2}}$$

i.e., after 1 time step, a particle at the origin $|0\rangle$, *with spin down* $|\downarrow\rangle$

has probability of $\frac{1}{2}$ of being at $|1\rangle$, $\left(\textit{with spin up}\,|\uparrow\rangle\right)$

and probability of $\frac{1}{2}$ of being at $|-1\rangle$, $\left(\textit{with spin down}\,|\downarrow\rangle\right)$

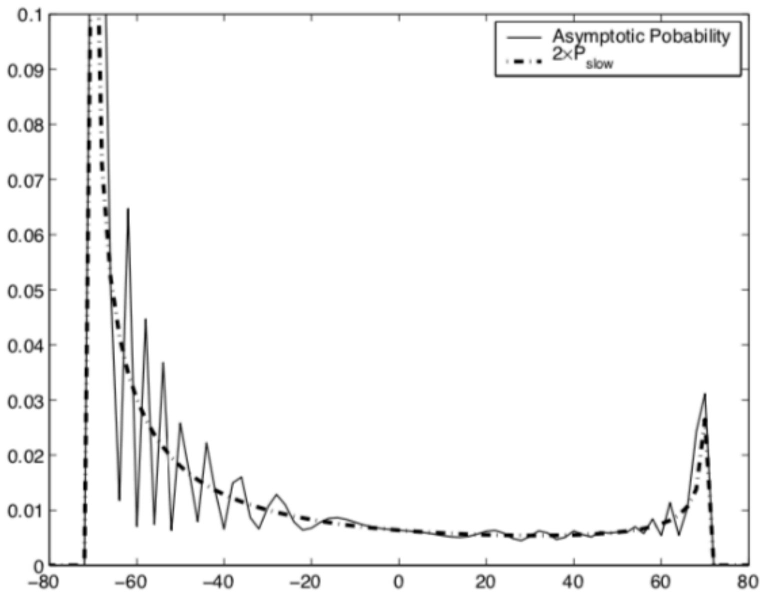
spatial location $|i\rangle \rightarrow$

time	-4	-3	-2	-1	0	1	2	3	4
0					1 (1)				
1				$\frac{1}{2}$ ($\frac{1}{2}$)		$\frac{1}{2}$ ($\frac{1}{2}$)			
2			$\frac{1}{4}$ ($\frac{1}{4}$)		$\frac{1}{2}$ ($\frac{1}{2}$)		$\frac{1}{4}$ ($\frac{1}{4}$)		
3		$\frac{1}{8}$ ($\frac{1}{8}$)		$\frac{5}{8}$ ($\frac{3}{8}$)		$\frac{1}{8}$ ($\frac{3}{8}$)		$\frac{1}{8}$ ($\frac{1}{8}$)	
4	$\frac{1}{16}$ ($\frac{1}{16}$)		$\frac{5}{8}$ ($\frac{1}{4}$)		$\frac{1}{8}$ ($\frac{3}{8}$)		$\frac{1}{8}$ ($\frac{1}{4}$)		$\frac{1}{16}$ ($\frac{1}{16}$)

I.e., asymmetry in probability after t = 3:
Probability 5/8 at x = -1 ,
Probability 1/8 at x = +1

Classically (no Hadamard gate) at t = 3 :
probability 3/8 at x = -1,
probability 3/8 at x = +1.

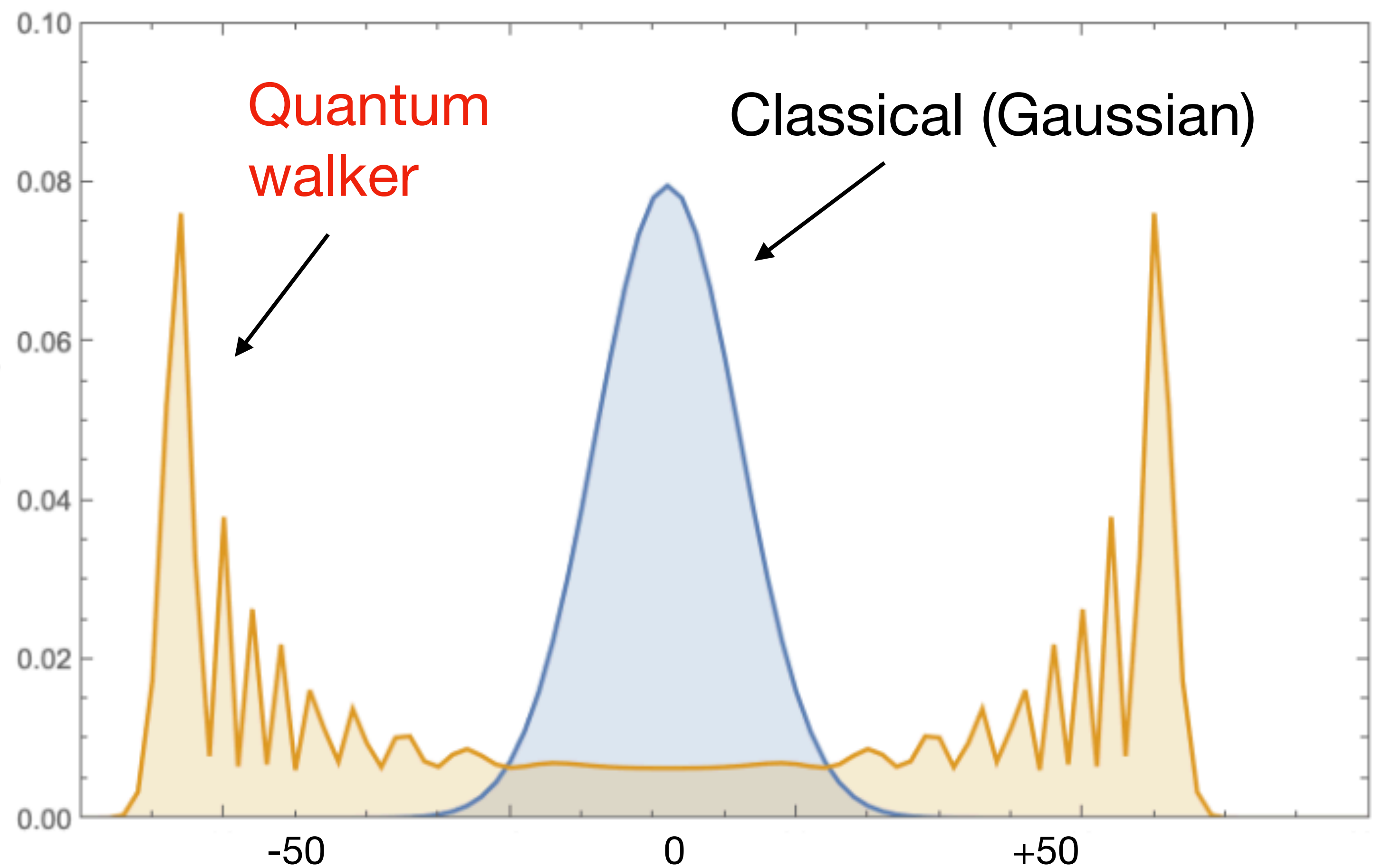
At t = 100



One can achieve results very different from those of classical physics by using quantum gates

For symmetric walker, t = 0

$$\frac{|\uparrow\rangle + i|\downarrow\rangle}{\sqrt{2}} \otimes |0\rangle$$



• now consider the effect of 2-qubit gates on 2-qubit system (qubit entanglement)

• Hilbert space 2^2

$$|0\rangle \otimes |0\rangle = |00\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |01\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad |10\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |11\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

• **Swap Gate**

$$\hat{C}_{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$|01\rangle \rightarrow |10\rangle$$
$$|10\rangle \rightarrow |01\rangle$$

• $\sqrt{\textbf{SWAP}}$ **Gate**

$$\hat{C}_{\sqrt{SWAP}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1+i}{2} & \frac{1-i}{2} & 0 \\ 0 & \frac{1-i}{2} & \frac{1+i}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

• universal gate

$$\left(\hat{C}_{\sqrt{SWAP}}\right)^4 = I$$

• #1. QLA for 1D-NLS $i\frac{\partial\psi}{\partial t}=-\frac{\partial^2\psi}{\partial x^2}+\left[g|\psi|^2-\mu\right]\psi$

- spatial lattice, 2 qubits/spatial node
- Restrict analysis to the subspace of 2x2 matrices :

→ the collision operator entangles the 2 qubits

→ the streaming operator moves this entanglement throughout the lattice

- introduce mesoscopic spinor field $\left|\phi(x,t)\right\rangle=\begin{pmatrix}\alpha(x,t)\\ \beta(x,t)\end{pmatrix}$

- interleaved sequence of non-commuting collide-stream unitary operators

$$\hat{L}_{x,\sigma}=\hat{S}_{-\delta x,\sigma}\hat{C}_{\sqrt{swap}}\hat{S}_{+\delta x,\sigma}\hat{C}_{\sqrt{swap}} \quad , \; \sigma=\alpha,\beta$$

- Unitary Evolution Operator $\hat{U}[\Omega]=\hat{L}^2_{x,\alpha}\; Exp\left[-\frac{i\varepsilon^2\Omega}{2}\right]\hat{L}^2_{x,\beta}\; Exp\left[-\frac{i\varepsilon^2\Omega}{2}\right]$

- $\left|\phi(x,t+\delta t)\right\rangle=\hat{U}[\Omega]\left|\phi(x,t)\right\rangle \longrightarrow \left|\phi(x,t+\delta t)\right\rangle=\left(1-i\varepsilon^2\left[-\hat{\sigma}_x\nabla^2+\Omega\right]\right)\left|\phi(x,t)\right\rangle+O(\varepsilon^4)$

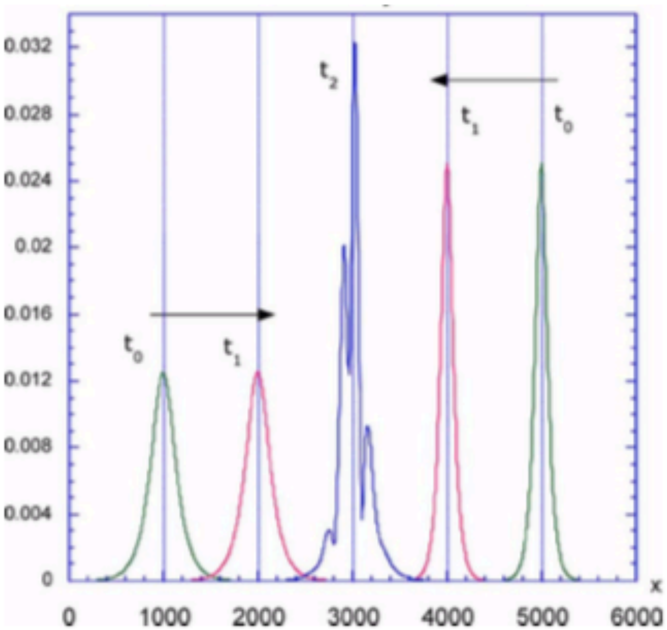
with $\delta x=O(\varepsilon)$

• #1D. QLA for 1D-NLS $\quad i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + \left[g|\psi|^2 - \mu \right]\psi$

To recover the order parameter $\psi(x,t) = \begin{pmatrix} 1 & 1 \end{pmatrix} \bullet |\phi(x,t)\rangle = \alpha(x,t) + \beta(x,t)$

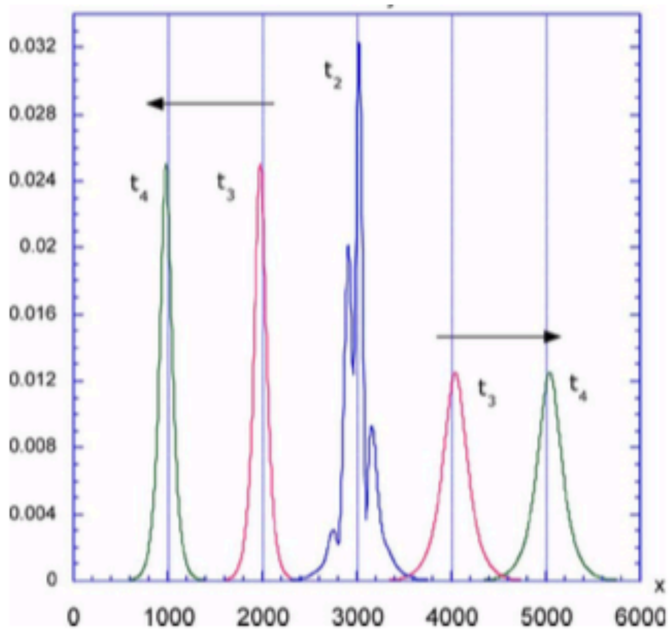
Require diffusion ordering : $\delta t = \varepsilon^2 = \delta x^2$ $\qquad$ Choose $\Omega = g|\psi|^2$

QLA: $\quad |\phi(x,t+\delta t)\rangle = \hat{L}^2_{x,\alpha}\ Exp\left[-\frac{i\varepsilon^2\Omega}{2}\right] \hat{L}^2_{x,\beta}\ Exp\left[-\frac{i\varepsilon^2\Omega}{2}\right] \ |\phi(x,t)\rangle$



(a)

pre – collision

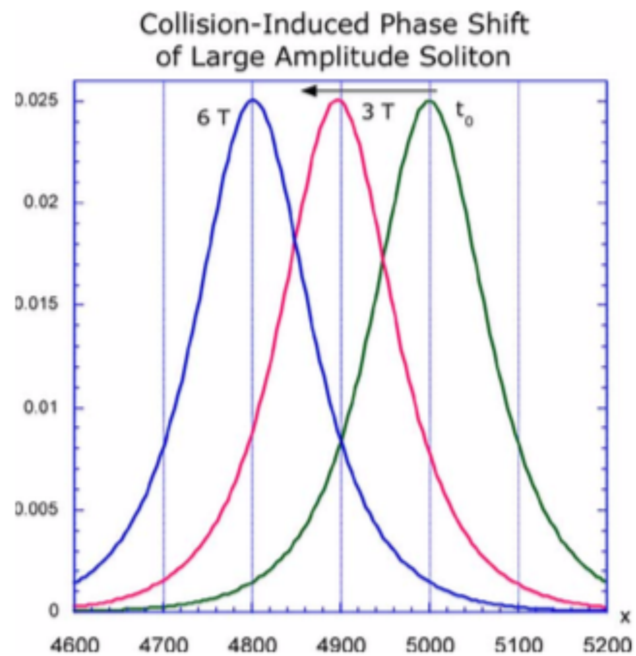


(b)

post – collision

$T = 160K$

$6T$ – 12 collisions



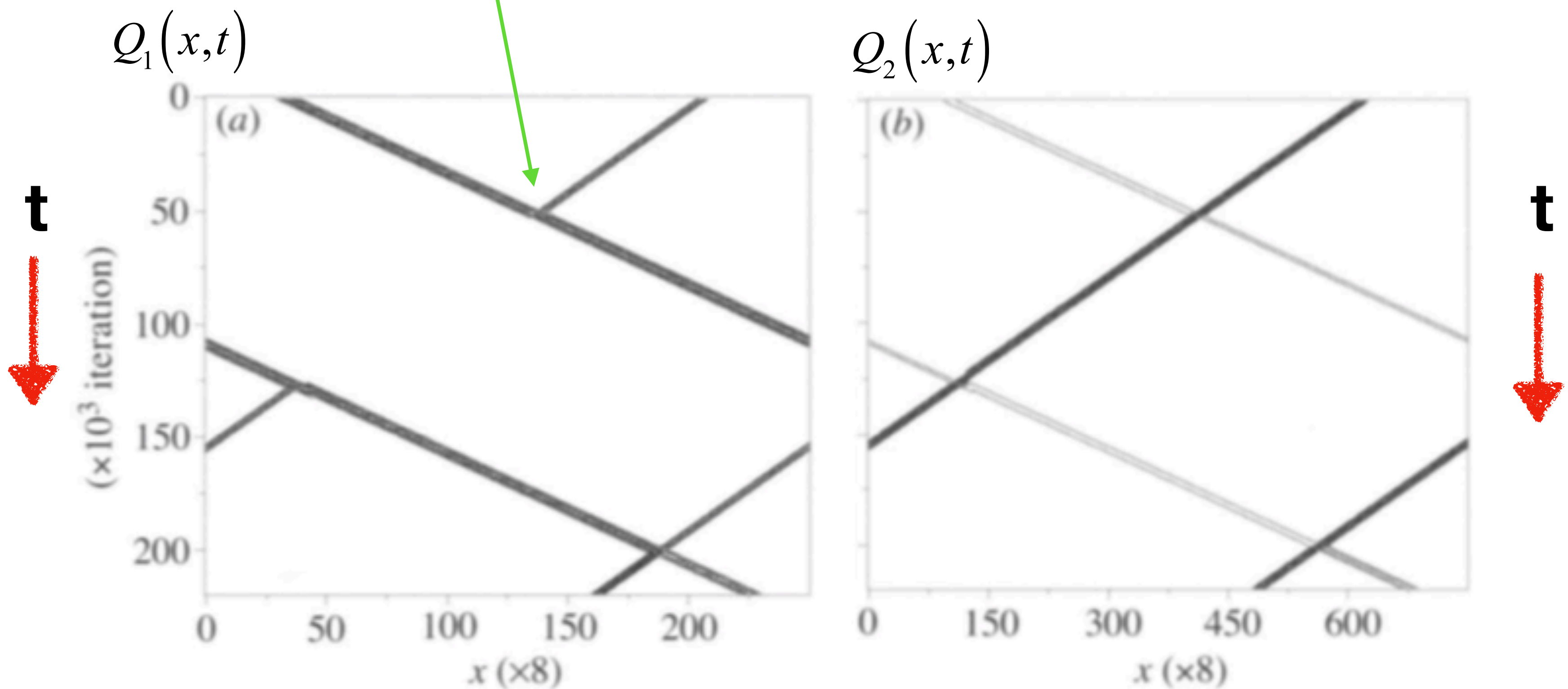
Manakov Inelastic Soliton Collision

- 2 coupled NLS : 4 qubits/lattice pt.

$$\left.\begin{aligned} i\frac{\partial Q_1}{\partial t} + \frac{\partial^2 Q_1}{\partial x^2} + 2\mu[|Q_1|^2 + B|Q_2|^2]\cdot Q_1 = 0, \\ i\frac{\partial Q_2}{\partial t} + \frac{\partial^2 Q_2}{\partial x^2} + 2\mu[|Q_2|^2 + B|Q_1|^2]\cdot Q_2 = 0, \end{aligned}\right\}$$

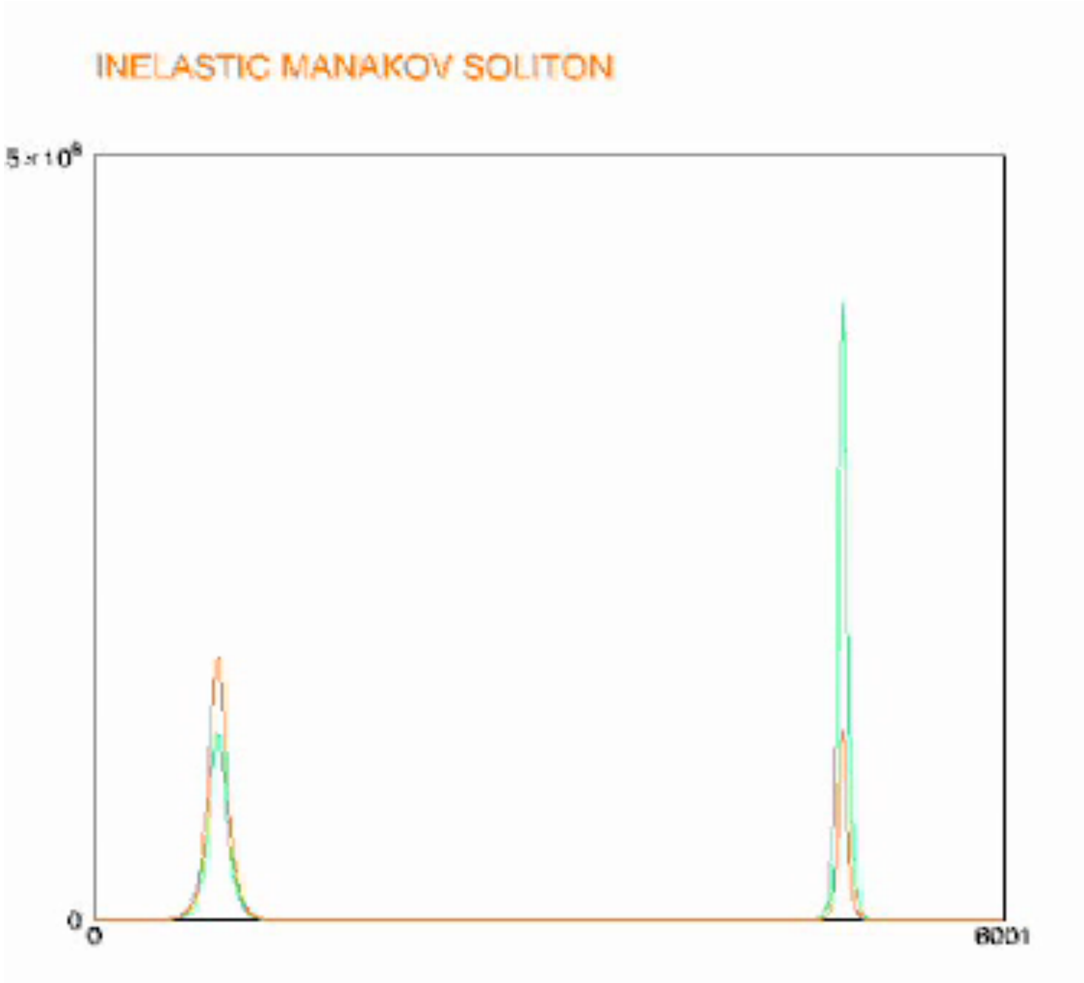
Integrable if B = 1

Inelastic Collision *for special* $Q_1(t=0)$ *and* $Q_2(t=0)$



$2-coupled\ \ NLS\ \ equations$

2 polarizations : green, brown QLA: 4 qubits/node



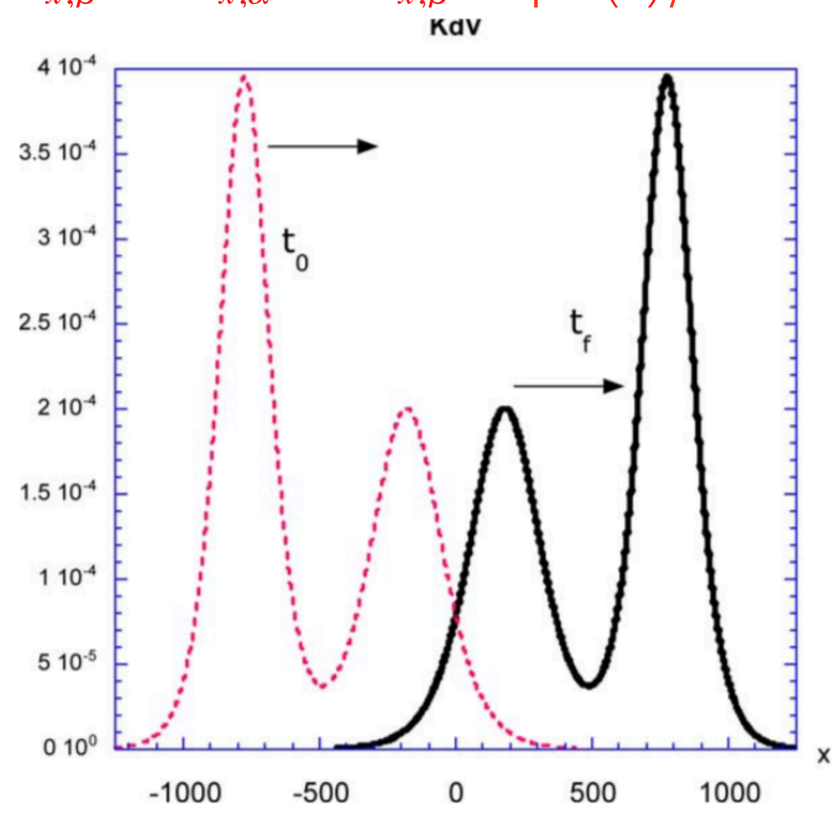
#2. KdV (waves in shallow water, Fermi-Pasta-Ulam-Tsingou)

Zabusky-Kruskal : lack of thermalization/ergodicity because of soliton collisions retaining their asymptotic profiles -- "soliton symmetry"

$$\frac{\partial \psi}{\partial t} + 6\psi \frac{\partial \psi}{\partial x} + \frac{\partial^3 \psi}{\partial x^3} = 0$$

QLA : entangle 2 qubits via $\hat{C}_{KdV} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$

$$|\psi(t+\delta t)\rangle = \hat{S}_{x,\alpha} \hat{C}^{\dagger} . \hat{S}_{-x,\beta} \hat{C} . \hat{S}_{-x,\alpha} \hat{C}^{\dagger} . \hat{S}_{x,\beta} \hat{C} . \hat{S}_{-x,\alpha} \hat{C} . \hat{S}_{x,\beta} \hat{C}^{\dagger} . \hat{S}_{x,\alpha} \hat{C} . \hat{S}_{-x,\beta} \hat{C}^{\dagger} |\psi(t)\rangle$$



- → $Now \quad \hat{C}.\hat{C}^{\dagger}.\hat{C}.\hat{C}^{\dagger} = \hat{I}$
- → Interlacing $\hat{C}$ and $\hat{C}^{\dagger}$ eliminates the $\partial^2 / \partial x^2$
- → $Scaling: \ \delta x = \varepsilon \ , \ \delta t = \varepsilon^3 \ , \ \Omega = i\varepsilon^3 \frac{\partial \psi}{\partial x}$

#3. MHD-Burgers Dissipative System - "1D Alfvenization"

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{\partial}{\partial x}\left(\frac{B^2}{2}\right) + \mu\frac{\partial^2 u}{\partial x^2} \quad , \quad \frac{\partial B}{\partial t} + \frac{\partial}{\partial x}(u\,B) = \eta\frac{\partial^2 B}{\partial x^2}$$

μ ↑ viscosity, η ↑ resistivity

$\mathbf{u} = u(x,t)\hat{\mathbf{x}}$

$\mathbf{B} = B(x,t)\hat{\mathbf{z}}$

QLA : 4 qubits/lattice point $\quad |q_i(x)\rangle = \sqrt{p_i(x)}|1\rangle + \sqrt{1-p_i(x)}|0\rangle \quad , \quad i=1...4$

[1] state preparation : Given u$(x,0)$, $B(x,0)$ $\Rightarrow p_1 = (1+u+B)/2 = p_3$

$$p_2 = (1+u-B)/2 = p_4$$

$$|\psi(x)\rangle = |q_1(x)\rangle \otimes |q_2(x)\rangle \otimes |q_3(x)\rangle \otimes |q_4(x)\rangle$$

[2] local collisional entanglement : $|\psi'(x)\rangle = \hat{C}|\psi(x)\rangle$

[3] non-unitary post-collision measurement : $p_i'(x) = \langle\psi'(x)|\hat{N}_i|\psi'(x)\rangle$

$\hat{N}_i$ = number operator for the ith qubit

[4] streaming operator : $\mathrm{p}_i(x+e_i,t+1) = p_i(x,t) + \langle\psi(x,t)|\,\hat{C}^\dagger\hat{N}_i\hat{C} - \hat{N}_i|\psi(x,t)\rangle$

Mesoscopic Repr. :

QLA for MHD-Burgers : unitary, reversible

Macroscopic Repr.

Dissipative transport coefficients $\mu, \ \eta$

$$Macrofields: \quad u(x,t) = \frac{1}{2}\sum_{i=1}^{4} p_i(x,t) \quad , \quad B(x,t) = \frac{1}{2}\left[p_1(x,t) + p_2(x,t) - p_3(x,t) - p_4(x,t) \right]$$

- **Example: 1D Burgers Eq.** $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$

- NMR Expt. : $U = e^{iH}$, $H \longrightarrow$ NMR pulses

  lattice : 16 grid points

  2 qubits/lattice site

  (use of inhomogeneous **B**)

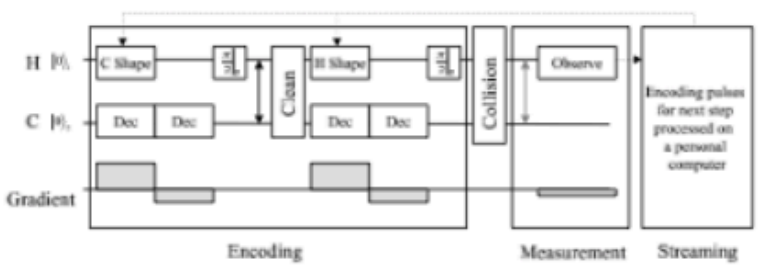
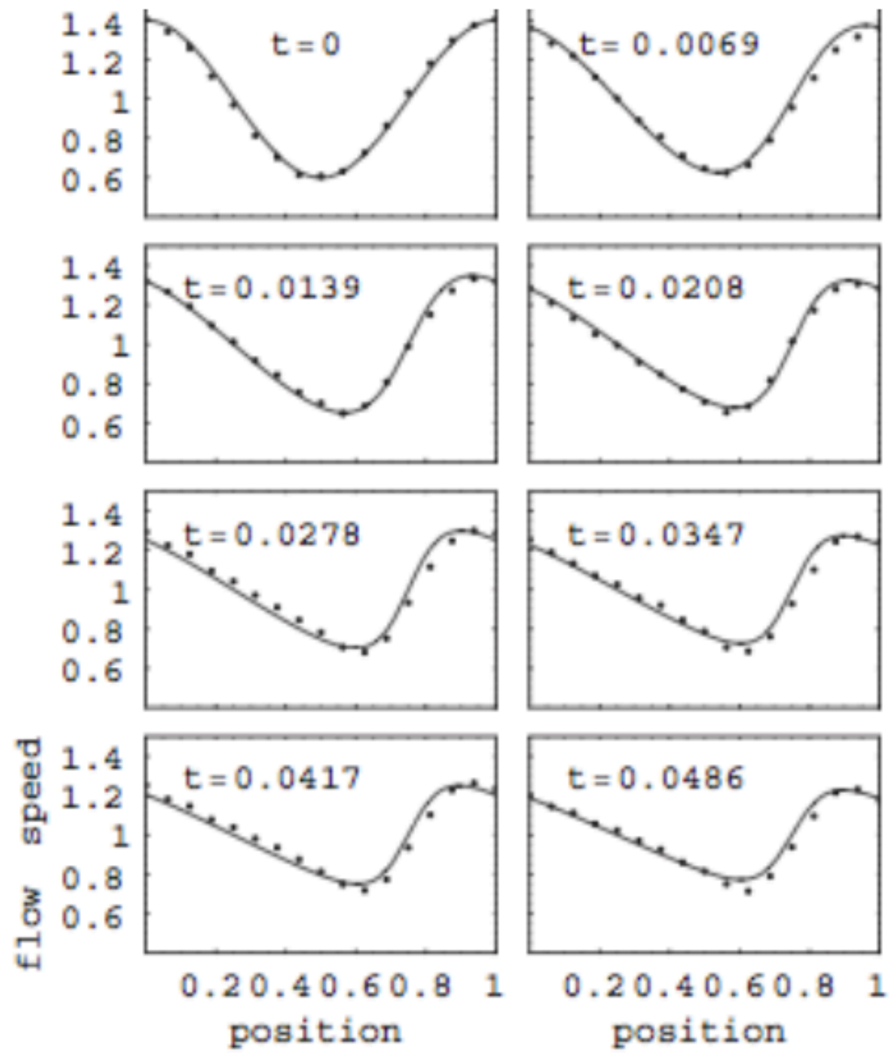


FIG. 1: QLG algorithm implemented in four steps. Three horizontal lines represent proton spin, carbon spin and fried gradients. Both starting magnetizations are encoded in proton channel first due to the high signal to noise ratio while decoupled in carbon channel to prevent interfering of scalar coupling. The collision operator is applied after the initialization. Measurements are also taken in two steps in the proton channl followed by data processing in a personal computer.



(Cory et. al., 2004)

#4. Peregrine Rogue Wave [1D NLS breather solution]

$$i\frac{\partial\psi}{\partial t} + \frac{\partial^2\psi}{\partial x^2} + |\psi|^2\psi = 0$$

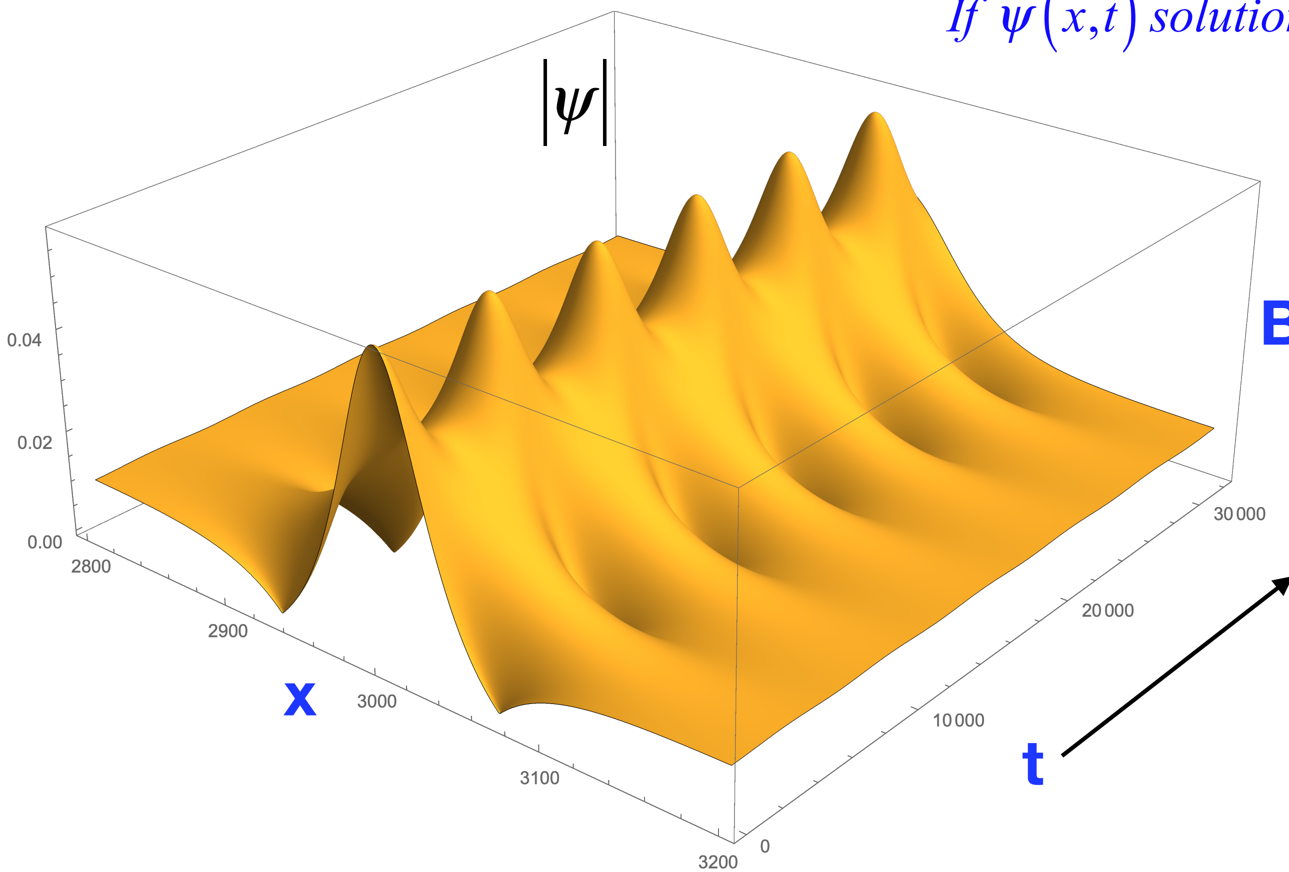
Ma t − periodic breather :

$$period = \frac{2\pi}{\Omega}$$

$$\Omega = \sinh 2\varphi\,,\ \ p = \sqrt{2}\,\sinh\varphi$$

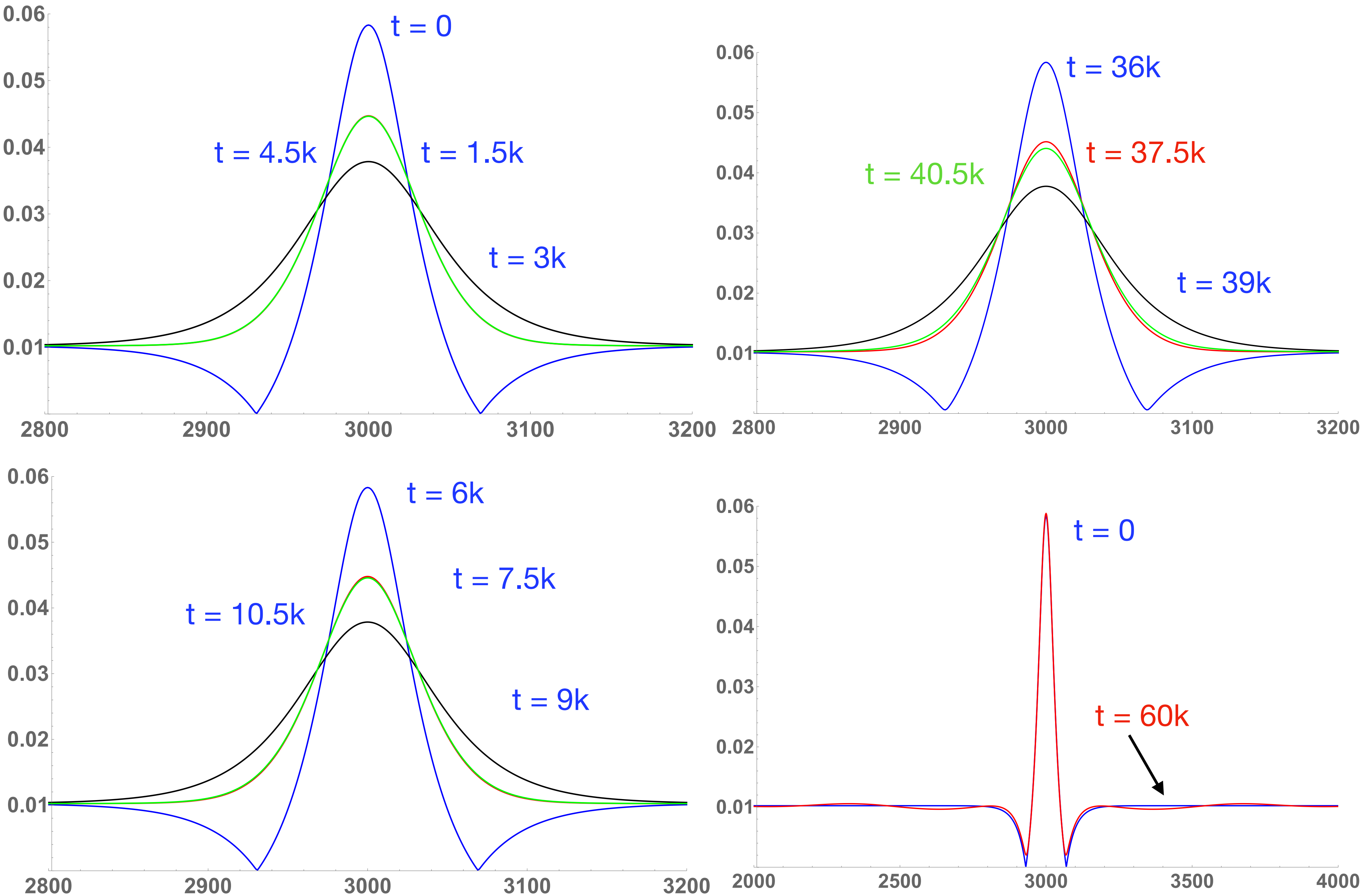
$$\psi(x,t) = e^{-it}\frac{\cos(\Omega t - 2i\varphi) - \cosh\varphi\cosh(px)}{\cos(\Omega t) - \cosh\varphi\cosh(px)}$$

If $\psi(x,t)$ *solution* $\Rightarrow \alpha\psi(\alpha x, \alpha^2 t)$ *also solution*



Breather period : t = 6k

QLA for Ma Breathers: Period = 6k



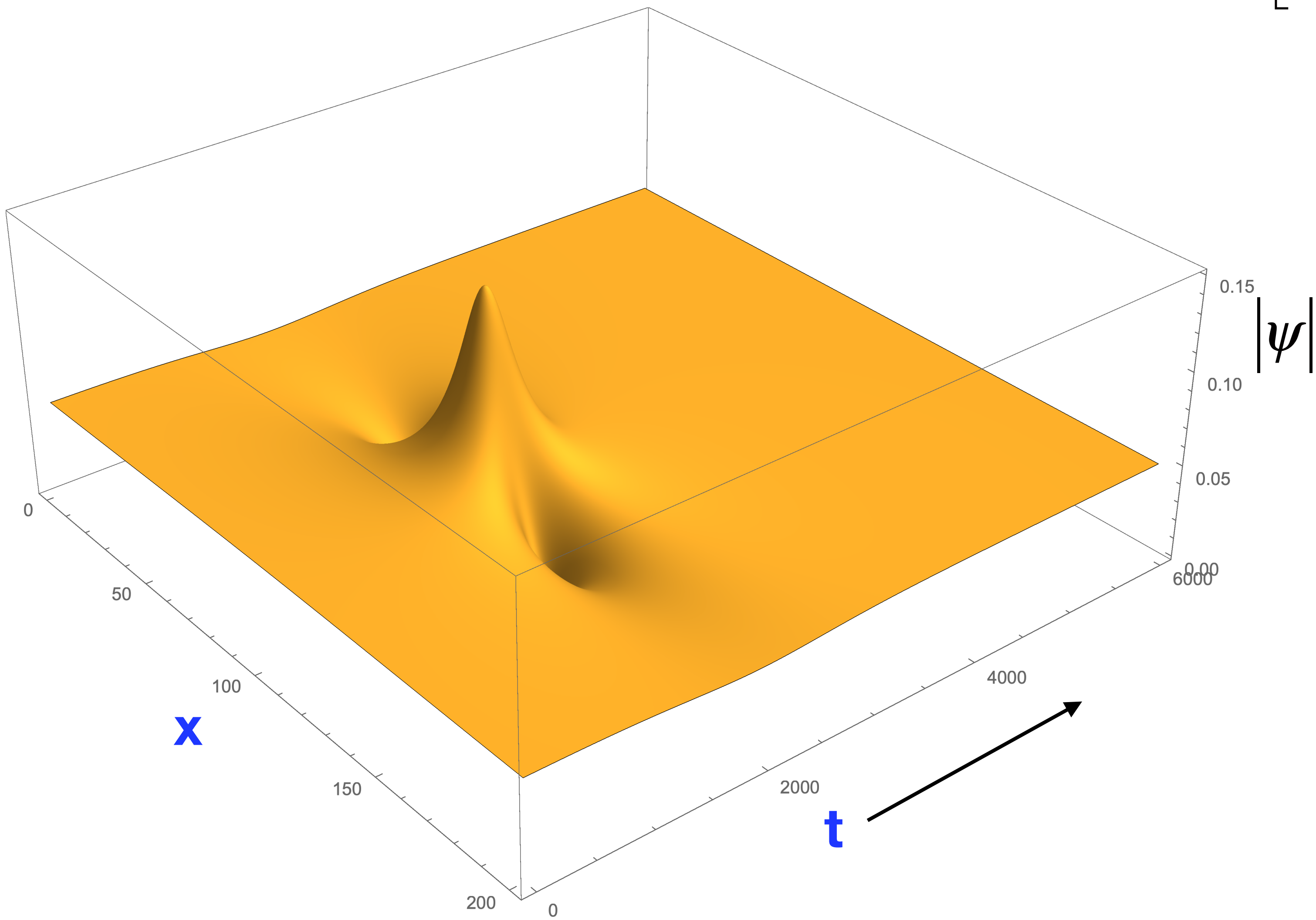
Peregrine Rogue Wave $\varphi \to 0$

$$\psi = \alpha\, e^{i\alpha^2 t'}\left[1 - \frac{4\left(1+2i\alpha^2 t'\right)}{1+2\alpha^2 x'^2 + 4\alpha^4 t'^2}\right]$$

$$x' = x - x_0 \;,\; t' = t - t_0$$

$$x_0 = 100 \;,\; t_0 = 2000,$$

$$\alpha = 0.05$$



Peregrine Rogue Wave

$$\hat{T} = -\nabla^2$$
$$\hat{V} = -|\psi|^2$$

- **FFT : streaming to all orders**

Unitary op.

$$i\frac{\partial\psi}{\partial t} = \left[\hat{T} + \hat{V}\right]\psi \quad \Rightarrow \psi\left(t+\varepsilon^2\right) = Exp\left[-i\varepsilon^2\left(\hat{T}+\hat{V}\right)\right]\psi\left(t\right)$$

- **non-commuting Operators**

(Baker-Campbell-Hausdorff)

$$\exp\left[-i\varepsilon^2\left(\hat{T}+\hat{V}\right)\right] = \exp\left[-i\varepsilon^2\hat{V}/2\right]\exp\left[-i\varepsilon^2\hat{T}\right]\exp\left[-i\varepsilon^2\hat{V}/2\right] + O\left(\varepsilon^4\right)$$

$$\psi\left(x,t+\varepsilon^2\right) = \exp\left[-i\varepsilon^2\hat{V}/2\right]\bullet\hat{\mathbf{F}}^{-1}\left[\exp\left[-i\varepsilon^2k^2\right]\bullet\hat{\mathbf{F}}\left[\exp\left[-i\varepsilon^2\hat{V}/2\right]\psi\left(x,t\right)\right]\right] + O\left(\varepsilon^4\right)$$

i.e., unitary collision step: in x-space
unitary streaming step: in k-space $e^{i\varepsilon^2\nabla^2} \rightarrow e^{-i\varepsilon^2k^2}$

QLA : unitary algorithm.

Peregrine wave is awkward because numerical noise can rapidly lead to a divergent scheme.

QLA Representation $i\frac{\partial\psi}{\partial t}+\frac{\partial^2\psi}{\partial x^2}+|\psi|^2\psi=0$

$$\psi\left(x,t+\varepsilon^2\right)=\exp\left[-i\varepsilon^2\hat{V}/2\right]\bullet\hat{\mathbf{F}}^{-1}\left[\exp\left[-i\varepsilon^2k^2\right]\bullet\hat{\mathbf{F}}\left[\exp\left[-i\varepsilon^2\hat{V}/2\right]\psi\left(x,t\right)\right]\right]+O\left(\varepsilon^4\right)$$

$$\psi\rightarrow\begin{pmatrix}q_0\\q_1\end{pmatrix}\quad,\quad\exp\left[-i\varepsilon^2\hat{V}/2\right]\rightarrow\hat{C}=\begin{pmatrix}\cos\theta & -i\sin\theta\\ -i\sin\theta & \cos\theta\end{pmatrix}$$

$$\theta=\frac{\pi}{4}-\frac{1}{2}\hat{V}\ ,\quad NLS\ \hat{V}=|\psi|^2$$

QLA-FFT : only 2 applications of Collision Operator

$$\begin{pmatrix}q_0\\q_1\end{pmatrix}_{t+\delta t}=\hat{C}\hat{\mathbf{F}}^{-1}\left[e^{-i\varepsilon^2k^2}\right]\hat{\mathbf{F}}\left[\hat{C}\begin{pmatrix}q_0\\q_1\end{pmatrix}_t\right]$$