Unitary Qubit Lattice Simulations of Multiscale Phenomena in 2D and 3D Quantum Turbulence

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

**Ubiquitous Eq. in Nonlinear Physics**

- **NONLINEAR SCHRODINGER (NLS) Eq.**
  (solitons, modulation instability ...)

- **BEC of weakly interacting dilute gas**
  - **GROSS-PITAEVSKII (GP) Eq.**

  N Bose atoms, at \( T = 0 \), can be represented by a mean-field theory for the Single Atom wave function: nonlinear term \( g |\psi|^2 \psi \) arising from the weak s-wave interactions.
\[ i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu + g |\psi(x,t)|^2 \right] \psi(x,t) \]

Madelung:
\[ \psi(x,t) = \sqrt{\rho(x,t)} \exp \left[ i\varphi(x,t)/2 \right] \]
\[ \mathbf{u}_s(x,t) = \hbar \nabla \varphi(x,t)/2 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \left( \rho \mathbf{u}_s \right) = 0 \]
\[ \rho \left( \frac{\partial \mathbf{u}_s}{\partial t} + \mathbf{u}_s \nabla \right) \mathbf{u}_s = -\nabla p + \nabla \cdot \mathbf{\Sigma} \]

\[ p = g \rho^2 \]

- **quantum vortex is topological singularity**: at the core, \( \rho \to 0 \)

- **all quantum vortices have the same strength**: vortex BEC lattice

- quantum vortex reconnection occurs even **without viscosity** (unlike classical ‘macro’ reconnection) since the quantized vortex has \( \psi \to 0 \) at the core.

- **quantum turbulence (Feynman)**: entanglement of quantized vortices
Unitary Qubit Lattice Algorithms

\[ \alpha \text{ probability amplitude for the state } |01\rangle; \quad \beta \text{ that for state } |10\rangle \]

\[ \Phi(x,t) = \begin{pmatrix} \alpha(x,t) \\ \beta(x,t) \end{pmatrix} \]

- unitary collision operator entangles locally via \( \sqrt{\text{SWAP}} \)

\[ C = \begin{pmatrix} \frac{1-i}{2} & \frac{1+i}{2} \\ \frac{1+i}{2} & \frac{1-i}{2} \end{pmatrix} \]

with \( C^2 \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix} \)

- unitary streaming operator spreads the entanglement throughout the lattice

\[ S_{\Delta x,0} \phi(x) = \begin{pmatrix} \alpha(x + \Delta x) \\ \beta(x) \end{pmatrix}, \quad S_{\Delta x,1} \phi(x) = \begin{pmatrix} \alpha(x) \\ \beta(x + \Delta x) \end{pmatrix} \]

- interleaved unitary collide-stream sequence on the qubits

\[ \hat{I}_{x,\sigma} = S_{-\Delta x,\sigma} C S_{\Delta x,\sigma} C \]

- Full Unitary Evolution Operator in 3D

\[ \hat{U}[\Omega] = \hat{I}_{x0}^2 \hat{I}_{y0}^2 \hat{I}_{z0}^2 \exp \left[ -\frac{i \varepsilon^2 \Omega(x)}{2} \right] \cdot \hat{I}_{x1}^2 \hat{I}_{y1}^0 \hat{I}_{z1}^2 \exp \left[ -\frac{i \varepsilon^2 \Omega(x)}{2} \right] \]

\[ \Phi(x,t + \Delta t) = \Phi(x,t) - i \varepsilon^2 \left[ -\sigma_x \nabla^2 + \Omega \right] \Phi(x,t) + O(\varepsilon^4) \]

- MPI - parallelization: collision operator - purely local
  streaming operator - only n.n

Mesoscopic Lattice Algorithm:

\[ \phi(x,t + \Delta t) = \hat{U}[x, \Omega] \phi(x,t) \]

diffusion ordering \( \Delta t \quad \Delta x^2 \)

complex scalar wave fn. to recover GP Eq.

\[ \psi = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \phi = \alpha + \beta \]

\[ \frac{\partial \psi(x,t)}{\partial t} = -\nabla^2 \psi(x,t) - a \left[ 1 - g \psi(x,t) \right] \psi(x,t) \]
Strong and Weak Scaling of our Unitary Qubit Algorithms - to 216K cores

**Strong Scaling**

- CRAY / Jaguarpf strong scaling - to 119982 cores
- IBM / INTREPID strong scaling - to 131072 cores

**Weak Scaling**

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<th>Grid</th>
<th>Cores</th>
<th>Wallclock</th>
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<tbody>
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<td>261.0</td>
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**Jaguarpf-CRAY XT5 (BdG)**

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**Hopper-CRAY XE6 (BdG)**

1. **Wallclock**
2. **Ideal**
Quantum Line Vortex Core Isosurfaces (n=5)
- 5 fold degenerate
- energetically more favorable to split to 5 non-deg. vortices

\[ \psi = \sqrt{\rho} \exp(i\theta) \]

\[ t = 0 \]
\[ \theta = 0 \text{ (blue)} \]
\[ \theta = 2\pi \text{ (red)} \]

\[ t = 3000 \text{ grid } 2048^3 \]
Gross-Pitaevskii Eq.

\[ i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu + g |\psi(x,t)|^2 \right] \psi(x,t) \]

- **Hamiltonian system**

\[ E_{\text{tot}} = E_{\text{quantum}}(t) + E_{\text{kinetic}}^{\text{incomp.}}(t) + E_{\text{kinetic}}^{\text{comp.}}(t) + E_{\text{int}}(t) = \text{const.} \]

- **Poincare Recurrence**
- system will, after a sufficiently long time, return arb. close its initial state.

- **Arnold Cat Map**
- the mapping is invertible, area preserving, ergodic, mixing ....

2D mapping of a unit square onto itself:

\[
\begin{pmatrix}
 x \\
 y
\end{pmatrix}
\rightarrow
\begin{pmatrix}
 2x + y \\
 2x + y
\end{pmatrix}, \text{ mod 1}
\]

**point inversion symmetry at t = 15** (pixel resolution 305x305)
Initially, no vortices ($\rho \neq 0$)

\[ \psi = \sqrt{\rho} \exp(i\theta) \]

Plots of $|\omega|$
Signature for Point-Inversion Symmetry, Poincare time

random phase i.c. (2D)

very low Internal Energy

$$E_{\text{int}} = g \int d^3x \; \rho^2$$

$$T_p / 2 = 21000 \left( \text{grid 512}^2 \right)$$

$$T_p \; L^2 \; (\text{for 2D and 3D})$$

- Effect of increasing $E_{\text{int}}$: loss of Poincare recurrence

Enstrophy is a rugged invariant for 2D incomp. N-S, but not for GP.
**Spectra in 2D and 3D Quantum Turbulence**

- **CLASSICAL TURBULENCE** (incompressible, dissipative)
  - major distinction: 2D ($E, Z$ rugged invariants) and 3D ($E$ rugged invariant) energy cascades
  - 2D: energy cascades to low $k$, enstrophy to high $k$: *like-vortices coalesce to larger vortices*.
  - 3D: energy cascades to high $k$.

- **QUANTUM TURBULENCE** (compressible, non-dissipative)
  - $Z$ not a constant of the motion in either 2D or 3D
  - energy cascades — thought to end with phonon emission for very large $k$
  - for very large $k$: vortex quantization important
  - for small $k$: bundles of quantum vortices — at large spatial scales the quantization is unimportant. Does one tend to classical turbulence?

- SGS modeling of COMPRESSIBLE CLASSICAL TURBULENCE
  - insist that the subgrid energy spectrum follow Kolmogorov $k^{-5/3}$
3D Quantum Turbulence

Total Kinetic Energy $E_{\text{KIN}}$ grid $5760^3$

**Triple Cascade Regions:**
- small $k$: Kolmogorov-like classical
- medium $k$: semi-classical regime
- large $k$: quantum vortex spectrum

$E_{\text{KIN}}(k)$ vs $k$

- $k^{-1.68}$
- $k^{-1.30}$
- $k^{-7.76}$
- $k^{-3.02}$

Visualization: 4096$^3$ grid, 512 cores 2 minutes

Vortex core isosurfaces (n=6)-zoomed-in early stages of vortex loop generation.
Grid 4960$^3$
**Spectra** \( k^{-\alpha} \), **3D QT**: \( \text{grid } 3072^3 \)

**Incompressible spectrum**

\[
\alpha = \begin{cases} 
3.4 & , 70 < k < k_\xi \\
3.0 & , k > k_\xi 
\end{cases}
\]

**Total Kinetic Energy Spectrum**

\[
\alpha = \begin{cases} 
1.66 & , 15 < k < 90 \\
8.53 & , 180 < k < 280 \\
3.04 & , 350 < k < 1000 
\end{cases}
\]
For non-degenerate linear vortices: spectra noisier and there is a loss of the incompressible $k^{-3}$ spectrum due to vortex topology changes (3D, grid $1200^3$).
2D QT: 4 vortices embedded in Gaussian BEC cloud
- winding number 2 vortices: Poincare recurrence

Quantum Kelvin-Helmholtz instability (blow-up): generation of pairs of counter-rotating vortices between neighboring vortices with the same rotation
Loss of $k^{-3}$ in 2D incompressible kinetic energy spectrum - attributable to the total loss of quantum (point) vortices

$E_{\text{incomp}} \propto k^{S_{IC}}$ for $n = 2$ vortices - no complete loss of vortices occurs, hence no spikes in the spectral exponent
Spectra - quite complex for 2D QT (different i.c’s)

Very early time evolution of the kinetic energy spectrum

(a) $t = 8K$
grid $32768^2$

(b) Triple Energy Cascade (as in 3D)
CONCLUSIONS

- unitary qubit lattice algorithm for QT (Hamiltonian) - ideally parallelized, 216k cores
- immediately encodable on a quantum computer (when available)
- Certain initial conditions yield very short Poincare recurrence times
- QT does not seem to exhibit spectral differences between 2D and 3D - most probably since enstrophy is not a constant of the motion in 2D (unlike CT)

- Kinetic energy spectrum typically exhibits 3 spectral regions: a small-k classical Kolmogorov spectrum to the very large-k quantum vortex spectrum.
Prior to this, the incompressible kinetic energy exhibits a possible quantum Kelvin wave cascade or a Saffman vorticity gradient spectrum

- Extended this GP (T = 0) system to T > 0 to give coupling between the BEC and BdG modes – still need only 2 qubits/node but the full 4-state coupling is now required.

- Extend to spin-BEC systems which will give rise to non-Abelian quantum vortex turbulence: (2s +1) BEC coupled systems. Unexplored territory.


- Eventually extend to resistive MHD, with non-trivial boundary conditions.