Quantum Lattice Gas Algorithm for Quantum Turbulence and Vortex Reconnection in the Gross-Pitaevskii Equation

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Abstract
The ground state wave function for a Bose Einstein condensate is well described by the Gross-Pitaevskii equation. A Type-II quantum algorithm is devised that is ideally parallelized even on a classical computer. Only 2 qubits are required per spatial node. With unitary local collisions, streaming of entangled states and a spatially inhomogeneous unitary gauge rotation one recovers the Gross-Pitaevskii equation. Quantum vortex reconnection is simulated – even without any viscosity or resistivity (which are needed in classical vortex reconnection).

1. Introduction
Turbulence is a crucial problem with profound ramifications from basic physics to detailed engineering design that remains as one of the greatest unsolved problems in classical physics. Turbulence simulations on supercomputers are playing a critical role in our understanding of classical turbulence. However direct numerical simulations (DNS) are restricted to Reynolds numbers \(\text{Re} \ll 10^5\) since the number of grid nodes required scales as \(\text{Re}^{9/4}\). The complexities of classical turbulence are further compounded by the inability to accurately define a classical “eddy” \([1]\). This creates some ambiguity in the phenomenology of the inertial cascade and the self-similarity in the dynamics of the smaller eddies which leads to the Kolmogorov \(k^{-5/3}\) inertial energy spectrum \([1]\). Actually, an instantaneous snapshot of the turbulence would show many vortices of different length scales co-existing, complicating the simple cascade argument. Moreover, it is now known from experimental data \([1]\) that classical turbulence exhibits intermittency – an effect unexplainable by the simple Kolomogorov theory. The non-Gaussian velocity probability distribution exhibits long tails, indicative of violent rare events and possible fractal behavior.

In the early 1950’s, experiments \([2]\) on superfluid helium \((^4\text{He})\) examined the physics of quantized vortices. In contrast to classical eddies, a quantized vortex in a quantum fluid is a well defined stable topological defect/soliton: the vorticity vanishes everywhere in a simply-connected region, with the circulation quantized. The hydrodynamics of this quantum fluid is typically treated by a two-fluid Landau model: an inviscid superfluid with a viscous normal fluid. Experimental studies on superfluid turbulence first focused on the physics of thermal counterflow – i.e., when the normal fluid flow is driven in the opposite direction to the superfluid flow. When this relative flow velocity exceeds a critical value, the superfluid dissipates. Feynman \([3]\) argued that this represented a superfluid turbulent state with tangled quantized vortices. However,
this superfluid turbulence cannot be directly related to classical turbulence since there is no classical counterpart to the thermal quantum counterflow. This then led to superfluid experiments without thermal counterflows, and these experiments showed consistency with the Kolmogorov formalism and energy spectrum. This similarity between classical and superfluid turbulence was explained by mutual friction between the coupling of the superfluid and normal fluid, leading to a ‘conventional fluid’ [4]. This then led to experiments at even lower temperatures where the effects of the normal fluid become negligible. For these systems a macroscopic number of Bose particles (e.g., in $^{4}$He) occupy the ground state. The dynamics of this BEC state can be described by the Gross-Pitaevskii (GP) equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu + g |\Psi(x,t)|^2 \right] \Psi(x,t) \quad (1)$$

[In the case of $^{3}$He, $m$ is the mass of the BCS condensation of a Cooper pair of atoms]. $\Psi$ is the macroscopic wave function, $\mu$ the chemical potential, and $g$ is the coupling constant. Under the Madelung transform

$$\Psi(x,t) = \sqrt{\rho(x,t)} \exp \left[ i\phi(x,t) / 2 \right] \quad (2)$$

the GP Eq. (1) is transformed into an (inviscid) compressible Euler equation with an augmented quantum pressure [2], where $\rho$ is the condensate density, and the superfluid velocity $v_s(x,t) = \hbar \nabla \phi(x,t) / m$. In a simply connected domain, $\nabla \times v_s = 0$, while in multi-connected volume (around a singular core) there is quantization of circulation $\oint v_s \cdot d\ell = n \left( 2\pi \hbar / m \right)$, $n$ integer. Free vortex lines, of width given by the healing length $\xi = \hbar / \sqrt{2mg\rho}$, can exist in the bulk of the superfluid provided that the line has a central core at which $\Psi \to 0$. At these very low temperatures, quantum turbulence can only arise through the existence of quantized vortex lines which are entangled. Typically this entanglement is not strictly random, but locally polarized so as to produce velocity fields on scales much larger than the inter-vortex line spacing [6]. It is this local polarization that permits flows on a wide range of length scales – analogous to classical turbulence. The quantized vortices can decay only by (a) emission of sound waves through vortex reconnection [7], or (b) Kolmogorov inertial cascade till one reaches elementary excitations on the order of the healing length.

A fundamental difference between quantum turbulence and the classical (incompressible) Kolmogorov turbulence is that the quantum vortices flow in a compressible medium. The quantized vortices contribute to the incompressible kinetic energy $E_{kin}^i$, while the excitations at wavelengths $<\xi$ contribute to the compressible part of the kinetic energy $E_{kin}^c$. Because the superfluid is inviscid, total energy is conserved. The quantum vortex reconnections can occur even without viscosity because, unlike classical reconnection, the quantized vortex has density $\rho \to 0$.

In this paper we will examine quantum vortex reconnection using a Type-II quantum algorithm requiring only the entanglement and streaming of 2 qubits/spatial node on the 3D lattice. The unitary quantum evolution, represented by quantum logic gates, ensures a computational stable algorithm. The evolution operator governing the
time development of the ground state wave function for the GP equation can be cast as a local 3-step interleaved algorithm on the 2 qubits at each spatial node: (a) a local unitary entanglement of the 2 qubits at each node, (b) unitary streaming of the entangled qubits to nearby lattice sites, and (c) an inhomogeneous unitary gauge operator for particle-field interactions.

Previous computational methods to solve the GP equation are the vortex-filament [10] and spectral decomposition algorithms [8]. Our quantum lattice gas algorithm not only offers an alternate method that scales ideally on classical computers but it is very suited for implementation on Type-II quantum computers [9].

2. Energy Conservation in the Gross-Pitaevskii Equation

At the quantum vortex core, the wave function $\psi = 0$ so that the Madelung transformation is singular. To determine evolution "fluid" equations valid even at the vortex core, Nore et. al. [8] use the Noether theorem on the invariance of the $\psi^4$ - action functional

$$\mathcal{Z} = 2 \int dt \int d^3x \left[ \frac{i}{2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) + \left( \nabla |\psi|^2 - |\psi|^2 + \frac{1}{2} |\psi|^4 \right) \right]$$

(3)

The energy conservation equation arises from the time invariance of Eq. (3). One can then decompose the total energy

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{qu}} + E_{\text{int}}$$

(4)

where

$$E_{\text{kin}} = \frac{1}{4} \int d^3x \left( \sqrt{\rho} \, \mathbf{v} \right)^2 = \frac{1}{4} \int d^3x \left( \frac{\psi^* \nabla \psi - \psi \nabla \psi^*}{|\psi|} \right)^2,$$

$$E_{\text{qu}} = \frac{1}{4} \int d^3x \left( \nabla \sqrt{\rho} \right)^2 = \frac{1}{4} \int d^3x (\nabla |\psi|)^2,$$

and

$$E_{\text{int}} = \frac{1}{2} \int d^3x \left( -\rho + \frac{1}{2} \rho^2 \right) \Rightarrow E_{\text{int}} = \frac{1}{2} \int d^3x \, |\psi|^4$$

(5)

on removing the normalization

$$\int d^3x \, \rho = \int d^3x \, |\psi|^2 = \text{const.}$$

(6)

from the interaction energy term.

3. Quantum Algorithm for the Gross-Pitaevskii Equation

Consider a 2-spinor field

$$\phi(x,t) = \begin{pmatrix} \alpha(x,t) \\ \beta(x,t) \end{pmatrix}$$

(7)

where $\alpha$ and $\beta$ are complex amplitudes. The $\sqrt{\text{SWAP}}$ quantum operator $C$

$$C = \begin{pmatrix} 1-i & 1+i \\ 2 & 2 \\ 1+i & 1-i \\ 2 & 2 \end{pmatrix}$$

(8)
acts locally at each spatial position \( x \), and entangles each pair of spinor amplitudes: \( C\phi \).

Since

\[
\begin{pmatrix} 1 \\ 1 \end{pmatrix} = C \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\]

the complex scalar density

\[
\psi = (1 1). \phi = \alpha + \beta
\]

is conserved by the collision operator \( C \). Thus the probability \( |\phi|^2 \) is also locally conserved. Local equilibrium is achieved when the amplitudes are equal: \( \alpha = \beta \). This local equilibrium is broken when one of these spinor components undergoes (unitary) streaming to \( x + \Delta x \). To conserve probability, we thus introduce complementary displacements of the spinor components. In particular, we consider the two unitary streaming operators on the 2-spinor:

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

We now consider an interleaved sequence of quantum collision \( C \) and streaming \( S_{\Delta x,\sigma} \) operators and their adjoints on the 2-spinor so that not only is the total density \( \int d^3x \phi(x) \), and in turn the total probability \( \int d^3x \left| a(x) \right|^2 + \left| b(x) \right|^2 \), is conserved but that we are close to the identity operator. An example of such interleaved collide-stream sequence on the spinor component \( \sigma \):

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

The full evolution operator for 3D spatial dynamics takes the form

\[
\hat{U}[\Omega] = \hat{I}_{x,0}^2 \hat{I}_{y,1}^2 \hat{I}_{z,0}^2 \exp \left[ -i\epsilon^2 \Omega(x) \right] \hat{I}_{z,1}^2 \hat{I}_{y,1}^2 \hat{I}_{x,0}^2 \exp \left[ -i\epsilon^2 \Omega(x) \right]
\]

where \( \epsilon \) is a small parameter and \( \Omega \) is either a local state reduction (for Type-II quantum computers) or an external potential (for Type-I quantum computers). To recover the GP equation we will need to choose \( \Omega \) to be a local state reduction. The evolution operator \( \hat{U}[\Omega] \) is spatially dependent only through the local state reduction \( \Omega \):

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

On performing Taylor expansions in \( \epsilon \ll 1 \), we obtain the following quantum lattice gas equation

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

where \( \sigma_x \) is the standard \( x \)-component Pauli matrix. Under diffusion scaling \( |\Delta x|^2 = \Delta t = \epsilon^2 \) and with the local state reduction

\[
\Omega = |\psi|^2 - 1
\]

and taking the density moment, Eq. (9), of Eq. (14), we obtain the GP equation

\[
i\frac{\partial \psi}{\partial t} = -\nabla^2 \psi + \left( |\psi|^2 - 1 \right) \psi + O(\epsilon^2)
\]
4. Numerical Simulation of Vortex Reconnection Dynamics in BEC

Here we present some simulations of quantum vortex reconnection and where we see the emission of Kelvin waves that propagate along the vortex tubes well before reconnection occurs. This reconnection [11, 12] occurs even in the absence of viscosity and resistivity because for the quantized vortices the density vanishes at the vortex core. In the standard filament and spectral decomposition algorithms, one enforces the boundary condition $|\psi| \to 1$ as $|x| \to \infty$. However, in our quantum lattice algorithm the local state reduction $\Omega = O(e^2)$, so we look for solutions of the scaled GP equation

$$i \frac{\partial \psi}{\partial t} = -\nabla^2 \psi + \left( |\psi|^2 - a_\infty \right) \psi \quad \text{with} \quad |\psi| \to \sqrt{a_\infty} \quad \text{as} \quad |x| \to \infty$$

(17)

A straight line vortex solution to Eq. (17) can be found following the Pade asymptotic representation introduced by Berloff [13] for the solution of Eq. (1). Indeed, using cylindrical coordinates a simple vortex tube (parallel to the z-axis) can be found for Eq. (17) in the form

$$\psi(r, \varphi, z, 0) = R(r) \exp(i\varphi)$$

with

$$R(r) = \sqrt{ \frac{r^2(a_1 + a_\infty b_2 r^2)}{1 + b_1 r^2 + b_2 r^4}}$$

(18)

On performing asymptotic expansion, one finds

$$a_1 = \frac{11}{32} a_\infty^2, \quad b_1 = \frac{a_\infty}{3}, \quad b_2 = \frac{a_1}{12}$$

(19)

We first present some of our quantum vortex simulations on a 260$^3$-spatial grid assuming initial conditions of 3 vortex tubes, each respectively parallel to the x-, y- and z-axes (Fig. 1) and symmetrically located in the first octant of the cube. To enforce periodicity, one must use mirror vortices throughout the other seven octants [8, 11]. In the figures below, we just show the vortex isosurfaces in this first octant.
In our quantum lattice simulation we find the density normalization and total energy are well conserved (density to 8 digits, energy to 5 digits). The time evolution of the kinetic, quantum and the non-constant part of the interaction energy, Eq. (5), are shown in Fig. 2.
The time evolution of the kinetic and quantum energies, Eq. (5) for the 3-vortex initial condition. The non-constant part of the interaction energy is a factor of 1000 below that of $E_{\text{kin}}$ and $E_{\text{qu}}$.

After 80 time steps, Fig. 3, one sees the Kelvin wave giving a helical twist to the vortex tubes – and even close to the vortex one sees the Kelvin wave effect.
(c) $t = 320$

(d) $t = 360$

(e) $t = 600$
Fig. 3  The time evolution of two isosurfaces of $|\psi(x,t)|$ for the initial 3-quantum vortex problem, with initial conditions shown in Fig. 1. The two isosurfaces shown at each time snapshot are for (i) close to the vortex core (isosurface on the right) and an (ii) outer isosurface (on the left). The times shown are: (a) $t = 80$, (b) $t = 200$, (c) $t = 320$, (d) $t = 360$, (e) $t = 600$, (f) $t = 1000$, (g) $t = 2000$, (h) $t = 3000$. Kelvin waves can be seen to propagate along the vortex tubes even by time $t = 80$. By $t = 320$, vortex reconnection is just about to occur in the outer isosurface, but the core isosurfaces are not near reconnection. All the quantum vortices are reconnected at $t = 360$, with subsequent breakup at later times.

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References