**Università degli Studi di Verona**

DIPARTIMENTO DI INFORMATICA
Corso di Laurea in Matematica Applicata

Tesi di laurea triennale

# First steps in the study of a theory of vortex reconnections in quantum fluids

Candidato:
**Ruben Franchetto**
**Matricola VR492502**

Relatore:
**Prof. Nicola Sansonetto**

**Anno Accademico 2023-2024**

# Contents

# Introduction

Quantum fluids are a state of matter observed when a particular system of particles is cooled to extremely low temperatures, close to absolute zero, and whose properties cannot be explained by classical theories.

The first quantum fluid observed was Helium-4 (the Helium isotope with two neutrons) cooled to a temperature below $2.17K$ [15], where it goes through a phase transition into a different liquid state, called Helium II.
Helium II shows the following unusual properties:

- lack of viscosity,
- fluid creep: Helium II spontaneously moves up and out its container,
- fountain effect: Helium II can produce a permanent fountain when heated.

Another characteristic of quantum fluids is the presence of quantized vortices: the fluid can only circulate around whirlpools of fixed size and the amount of circulation can only take discrete values [14].

The behavior of Helium II and of other quantum fluids was predicted by the theory of **Bose-Einstein condensates** (BEC), independently developed in 1924 by Satyendra Nath Bose [18] and Albert Einstein [1]. The main insight behind the theory is that as the temperature gets closer to absolute zero, particles start to occupy the same quantum state of minimum energy. This behavior is observed in the so-called boson particles (like photons and Helium-4 atoms), that are quantum particles of integer spin. However this fact indirectly also applies to fermions (like electrons, protons and neutrons) which, because of the Pauli exclusion principle, cannot occupy the same quantum state, but at low temperatures can bind together in bosonic multiplets called "Cooper pairs" [12], that behave as true bosons.

In the first part of this paper we will explain the Gross-Pitaevskii Equation (GPE), a nonlinear Schrödinger equation which models the dynamics of Bose-Einstein condensates. After a quick introduction to the mathematical theory of quantum mechanics based on [16], we will derive the GPE from the effective interaction potential [4] and the Hartree approximation [7], then we will put in evidence some interesting analogies between this equation and the classical Euler equations of fluid dynamics [5].

In the second part we will outline the properties of quantum vortices, following the ideas in [5], and study a simple model of vortex reconnection [20], using a local approximation and a power series analytical solution of the GPE.

Chapter 1

# The Gross-Pitaevskii equation

## 1.1 Introduction to Quantum Mechanics

We will denote the complex conjugate of a complex number $z$ with $z^*$.

**Definition.** *Let $V$ be a complex vector space. A **Hermitian inner product** $\langle \cdot, \cdot \rangle$ on $V$ is a map $V \times V \to \mathbb{C}$ with the following properties:*

*i. Conjugate symmetry: $\langle \boldsymbol{v}, \boldsymbol{w} \rangle = \langle \boldsymbol{w}, \boldsymbol{v} \rangle^*$ for $\boldsymbol{v}, \boldsymbol{w} \in V$.*

*ii. Right linearity: $\langle \boldsymbol{u}, \alpha\boldsymbol{v} + \beta\boldsymbol{w} \rangle = \alpha\langle \boldsymbol{u}, \boldsymbol{v} \rangle + \beta\langle \boldsymbol{u}, \boldsymbol{w} \rangle$ for $\alpha, \beta \in \mathbb{C}$ and $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in V$.*

*iii. Positive definiteness: if $\boldsymbol{v} \in V$ is not zero then $\langle \boldsymbol{v}, \boldsymbol{v} \rangle > 0$.*

*With $\langle \cdot, \cdot \rangle$ we can equip $V$ with*

*i. a norm $\| \cdot \|$, defined by $\|\boldsymbol{v}\| = \langle \boldsymbol{v}, \boldsymbol{v} \rangle^{\frac{1}{2}}$,*

*ii. a metric $d$, defined by $d(\boldsymbol{u}, \boldsymbol{v}) = \|\boldsymbol{u} - \boldsymbol{v}\|$,*

*iii. a dual $\boldsymbol{v}^*$ of each vector $\boldsymbol{v} \in V$, defined by $\boldsymbol{v}^* : V \to \mathbb{C}$, $\boldsymbol{w} \mapsto \langle \boldsymbol{v}, \boldsymbol{w} \rangle$*

From conjugate symmetry we can easily prove additional properties: non-degeneracy for the right argument, and left anti-linearity:

$$\forall \alpha, \beta \in \mathbb{C} \ \langle \alpha\boldsymbol{u} + \beta\boldsymbol{v}, \boldsymbol{w} \rangle = \alpha^* \langle \boldsymbol{u}, \boldsymbol{w} \rangle + \beta^* \langle \boldsymbol{v}, \boldsymbol{w} \rangle$$

**Definition.** *Let $L$ be a linear operator on a complex vector space $V$. The adjoint of $L$ is the linear operator $L^* : V \to V$ such that*

$$\forall \boldsymbol{v} \in V \ \langle L\boldsymbol{v}, \boldsymbol{w} \rangle = \langle \boldsymbol{v}, L^*\boldsymbol{w} \rangle.$$

*If $L = L^*$ we call $L$ self-adjoint, if instead $L^* = -L$ we call $L$ skew-adjoint.*

We are most interested in self-adjoint operators because of the Spectral Theorem:

**Theorem.** *Let $L$ be a self-adjoint linear operator on a vector space $V$, then the following properties hold:*

*i. The eigenvalues of $L$ are real numbers.*

*ii. There exists an orthonormal basis of $V$ composed of eigenvectors of $L$.*

**Definition.** *Let $V$ be a complex vector space with a Hermitian inner product $\langle \cdot, \cdot \rangle$. We call $V$ metrically complete when every Cauchy sequence of elements of $V$ converges to a vector in $V$. A space with such properties is called a **Hilbert space**.*

We now list the axioms of the Dirac-Von Neumann mathematical formulation of quantum mechanics:

**Axiom 1.** *The state of a quantum mechanical system is given by a non-zero vector $\Psi$ of a Hilbert space $\mathcal{H}$.*

**Axiom 2.** *The observables (results of a measurement) of a quantum mechanical system are self-adjoint linear operators on $\mathcal{H}$.*

**Axiom 3.** *There is a distinguished observable, the Hamiltonian $\widehat{H}$, which measures the system's energy. The time evolution of states $\Psi(\boldsymbol{r}, t) \in \mathcal{H}$ is given by the Shrödinger equation:*

$$i\hbar\partial_t \Psi = \widehat{H}\Psi,$$

*where $\hbar$ is the reduced Plank constant (Plank's constant divided by $2\pi$) and it is experimentally measured to be around* $1.055 \times 10^{-34}\text{Joule} \cdot \text{seconds}$.

When describing the position of a particle in three dimensional space the usual choice for $\mathcal{H}$ is $L^2(\mathbb{R}^3, \mathbb{C})$, where $L^2(X)$ indicates the space of square-integrable functions of the function space $X$. In this case we call $\Psi$ a wavefunction of the system, and our inner product becomes $\langle \Psi, \Phi \rangle = \int \Psi^* \Phi dV$. As explained in more detail in Section 1.3, every eigenvector of the Hamiltonian represents a stable configuration of the system whose energy is the associated eigenvalue. For this reason we also require the Hamiltonian $\widehat{H}$ to have eigenvalues bounded from below, as this ensures the existence of a stable minimum energy state.

This mathematical framework is then physically interpreted by the following phenomenological principles:

**Principle 1.** *States for which the value of an observable can be characterized by a well-defined number are the states that are eigenvectors for the corresponding self-adjoint operator. The value of the observable in such a state will be a real number, the associated eigenvalue of the state (as guaranteed by the spectral theorem).*

**Principle 2 (Born rule).** *Given an observable $\hat{O}$ and two unit-norm states $\Psi_1$ and $\Psi_2$ that are eigenvectors of $\hat{O}$ with respectively distinct eigenvalues $\lambda_1$ and $\lambda_2$, the linear combination state $c_1\Psi_1 + c_2\Psi_2$ will not have a well-defined value for the observable $\hat{O}$. If one attempts to measure this observable, one will get either $\lambda_1$ or $\lambda_2$, with respective probabilities*

$$\mathcal{P}\big(\hat{O}\Psi = \lambda_1\big) = |c_1|^2 \,/(|c_1|^2 + |c_2|^2)$$

*and*

$$\mathcal{P}\big(\hat{O}\Psi = \lambda_2\big) = |c_2|^2 \,/(|c_1|^2 + |c_2|^2)$$

.

Following the Born rule we can also calculate the value of expectation of a measurement:

**Definition.** *We call a wavefunction $\Psi$ normalized when $\|\Psi\|^2 = 1$.*

**Definition.** *Let $\hat{O}$ be an observable with a numerable set of eigenvalue-eigenvector pairs $\{(\lambda_k, \Psi_k)\}_{k\in\mathbb{N}}$, with each $\Psi_k$ normalized, and $\Psi = \sum_{k\in\mathbb{N}} c_k\Psi_k$ be a wavefunction. The value of expectation $\overline{O}$ of the observable $\hat{O}$ for the wavefunction $\Psi$ is*

$$\overline{O}\Psi := \sum_{k\in\mathbb{N}} \mathcal{P}\big(\hat{O}\Psi = \lambda_k\big)\lambda_k = \frac{\sum_{k\in\mathbb{N}} |c_k|^2 \ \lambda_k}{\|\Psi\|^2}.$$

**Theorem.** *Let $\hat{O}$ be an observable with a numerable set of eigenvalue-eigenvector pairs $\{(\lambda_k, \Psi_k)\}_{k\in\mathbb{N}}$, with each $\Psi_k$ normalized, and $\Psi$ be a normalized wavefunction, then*

$$\overline{O}\Psi := \int \Psi^* \hat{O} \Psi dV.$$

*Proof.* From the Spectral Theorem we know that $\{\Psi_k\}_{k\in\mathbb{N}}$ is a set of orthonormal eigenvectors of $\hat{O}$ that form a system of generators of $\mathcal{H}$. We can decompose $\Psi$ on the basis of eigenvectors, $\Psi = \sum_{k=1}^{\infty} c_k \Psi_k$, with $\sum_{k\in\mathbb{N}} |c_k|^2 = 1$ and write

$$\begin{aligned}
\int \Psi^* \hat{O} \Psi dV &= \int \left( \sum_{k=0}^{\infty} c_k^* \Psi_k^* \right) \left( \sum_{k=0}^{\infty} \lambda_k c_k \Psi_k \right) dV \\
&= \int \sum_{j,k=0}^{\infty} \lambda_k c_j^* c_k \Psi_j^* \Psi_k dV \\
&= \sum_{j,k=0}^{\infty} \lambda_k c_j^* c_k \int \Psi_j^* \Psi_k dV \\
&= \sum_{j,k=0}^{\infty} \lambda_k c_j^* c_k \delta_{jk} \\
&= \sum_{k=0}^{\infty} |c_k|^2 \ \lambda_k = \overline{O}\Psi.
\end{aligned}$$

□

If $\hat{O}$ has a continuous spectrum $S$, we instead write (a bit informally) $\Psi = \int_{\sigma(\hat{O})} c(\lambda)\Psi_\lambda d\lambda$, where $\sigma\big(\hat{O}\big)$ is the spectrum of $\hat{O}$, $\lambda$ is an eigenvalue of the spectrum and $\Psi_\lambda$ is the eigenvector of $\lambda$ (see e.g. [11] page 15).
The orthonormality of eigenvectors here can be expressed by the Dirac delta:

$$\int \Psi_\lambda^* \Psi_\mu dV = \delta(\lambda - \mu) \quad \text{for } \lambda, \mu \in \sigma\big(\hat{O}\big).$$

Note that this identity implies that in this case the eigenvectors are not square-integrable, meaning that they lie outside our Hilbert space and are not to be considered a proper physical state but a "state density". The wavefunction being normalized implies

$$\int_{\sigma(\hat{O})} |c(\lambda)|^2 \ d\lambda = 1.$$

The expected value is calculated with the same steps, using integrals instead:

$$\int \Psi^* \hat{O} \Psi dV = \int \left( \int_{\sigma(\widehat{O})} c^*(\lambda) \Psi^*_\lambda d\lambda \right) \left( \int_{\sigma(\widehat{O})} \lambda c(\lambda) \Psi_\lambda d\lambda \right) dV$$
$$= \int_{\sigma(\widehat{O})} \lambda \ |c(\lambda)|^2 \ d\lambda = \overline{O}.$$

For a more rigorous understanding of the difference between discrete and continuous spectra see appendix A.

## 1.2 The free particle

In the matter-wave theory developed by de Broglie in 1924 [3], particles are described by waves. The momentum $\boldsymbol{p}$ carried by a particle is related to its wavelength $\lambda$ by the relation $|\boldsymbol{p}|\lambda = 2\pi\hbar$, and its kinetic energy is instead related to its frequency $\omega$ with $K = \hbar\omega$.

For a planar wave of unitary amplitude $\Psi(\boldsymbol{r}, t) = \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))$, where $\boldsymbol{k}$ is the wave vector, $\omega$ is the angular frequency and $\cdot$ is the Euclidean dot product. The wavelength $\lambda$ can be calculated with $\lambda = \frac{2\pi}{|\boldsymbol{k}|}$, therefore $\boldsymbol{p} = \hbar\boldsymbol{k}$. A more general formula can be derived by observing that

$$\nabla \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)) = i\boldsymbol{k} \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))$$
$$\Rightarrow -i\hbar\nabla \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)) = \boldsymbol{p} \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)),$$

therefore the momentum operator can be read as $\hat{P} = -i\hbar\nabla$, whose eigenvectors are wavefunctions and eigenvalues are momentum measurements. The same can be done for the frequency:

$$\partial_t \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)) = -i\omega \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))$$
$$\Rightarrow i\hbar\partial_t \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)) = K \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)),$$

therefore, with the same logic, the kinetic energy operator is $\widehat{K} = i\hbar\partial_t$. From these and the formula for kinetic energy $K = \frac{|\boldsymbol{p}|^2}{2m}$ we can derive Schrödinger's equation for a free particle:

$$\Delta(\exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))) = - \ |\boldsymbol{k}|^2 \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))$$
$$\Rightarrow -\frac{\hbar^2}{2m}\Delta(\exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))) = K \exp(i(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t))$$
$$\Rightarrow i\hbar\partial_t \Psi = -\frac{\hbar^2}{2m}\Delta\Psi.$$

We introduce the potential energy operator $\hat{V}$, whose eigenvalues are potential energy measurements, to model conservative forces acting on particles. Similarly to classical mechanics the Hamiltonian operator is defined as the sum of the kinetic and potential energy operators:

$$\widehat{H} = \widehat{K} + \hat{V} = -\frac{\hbar^2}{2m}\Delta + \hat{V}.$$

## 1.3 Time-independent solutions

States in which the energy has definite values are called *stationary states* of a system ([11], page 28). From Principle 1 of 1.1 we see that there must exist eigenfunctions $\Psi_s$ of the Hamiltonian operator such that:

$$\widehat{H}\Psi_s = E\Psi_s,$$

where $E$ is a non-negative real number. For $\Psi_s$ the Schrödinger equation becomes

$$i\hbar\partial_t\Psi_s = E\Psi_s, \tag{1}$$

In this case we call $\Psi_s$ a **stationary state.**

**Theorem.** *The solution of the Cauchy problem*

$$\begin{cases} i\hbar\partial_t\Psi = E\Psi, E \in \mathbb{R} \\ \Psi(\boldsymbol{r}, 0) = \Psi_0(\boldsymbol{r}) \end{cases}$$

*where* $\Psi_0$ *is a stationary state satisfying* $\widehat{H}\Psi_0 = E\Psi_0$*, is*

$$\Psi(\boldsymbol{r}, t) = \exp\left(\frac{-iEt}{\hbar}\right)\Psi_0(\boldsymbol{r})$$

*Proof.* The problem can be solved by separating the set of variables. We suppose

$$\Psi(\boldsymbol{r}, t) = f(t)\psi(\boldsymbol{r}),$$

where $f$ is a function of time and $\psi$ is a function of space. In the points where $\psi = 0$ we can easily see $\Psi = 0$ at all times, and elsewhere we can expand Equation 1:

$$\begin{aligned} i\hbar\partial_t(f(t)\psi(\boldsymbol{r})) &= Ef(t)\psi(\boldsymbol{r}), \\ \Rightarrow i\hbar\psi(\boldsymbol{r})f'(t) &= Ef(t)\psi(\boldsymbol{r}) \\ \Rightarrow f'(t) &= \frac{E}{i\hbar}f(t), \end{aligned}$$

which is solved by

$$f(t) = k\exp\left(\frac{-iEt}{\hbar}\right), k \in \mathbb{C}.$$

Substituting back we obtain

$$\Psi(\boldsymbol{r}, t) = \exp\left(\frac{-iEt}{\hbar}\right)\tilde{\psi}(\boldsymbol{r}),$$

where $\tilde{\psi} = k\psi$. Imposing the initial condition we get $\tilde{\psi} = \Psi_0$. □

The phase of a stationary state changes linearly with time, but position probability densities, calculated as $|\Psi(\boldsymbol{r})|^2$, are time-independent.

## 1.4 Particle interactions in Bose-Einstein condensates

Since Bose-Einstein condensates are extremely diluted, the three and higher number body interactions can be ignored, and only two-body interactions are taken into account in the model.

To avoid having to calculate short-range correlations between atoms in detail, it is convenient to introduce the concept of an effective interaction. This describes interactions among long wavelength, low frequency degrees of freedom of a system when coupling of these degrees of freedom via interactions with those at shorter wavelengths has been taken into account.
The effective interaction potential of two particles is

$$U_0\delta(\boldsymbol{r}-\boldsymbol{r}'),$$

where $\delta$ is Dirac's delta and $\boldsymbol{r}$, $\boldsymbol{r}'$ are the particles' positions. Given the scattering length $a$, wich is the characteristic length of the effective interaction and is measured experimentally, we can calculate the effective interaction coefficient $U_0$ with

$$U_0 = \frac{4\pi\hbar^2 a}{m}.$$

See [4] chapter 5 for a detailed derivation of the effective interaction for Bose-Einstein condensates.

## 1.5 Derivation of the Gross-Pitaevskii equation

In a Bose-Einstein condensate, all bosons share the same single-particle state $\phi(\boldsymbol{r})$. Therefore, applying the Hartree approximation (see appendix B) we suppose each of the $N$ particles to be independent and write the N-particle wavefunction $\psi$ as:

$$\psi(\boldsymbol{r}_1,...,\boldsymbol{r}_N) = \prod_{i=1}^{N}\phi(\boldsymbol{r}_i).$$

Taking into account only effective interactions we obtain the Hamiltonian for the $i$-th particle:

$$\widehat{H}_i = \widehat{K} + V(\boldsymbol{r}_i) + U_0\sum_{j<i}\delta(\boldsymbol{r}_i-\boldsymbol{r}_j),$$

the average energy of the $i$-th particle is:

$$\begin{aligned}E(\phi_i) &= \int \phi(\boldsymbol{r}_i)^*\left[\frac{-\hbar^2}{2m}\Delta + V(\boldsymbol{r}_i) + U_0\sum_{j<i}\phi(\boldsymbol{r}_j)^*\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\phi(\boldsymbol{r}_j)\right]\phi(\boldsymbol{r}_i)dV_i \\ &= \int\left[\frac{\hbar^2}{2m}|\nabla\phi(\boldsymbol{r}_i)|^2 + V(\boldsymbol{r}_i)|\phi(\boldsymbol{r}_i)|^2 + U_0\sum_{j<i}|\phi(\boldsymbol{r}_i)|^4\right]dV_i,\end{aligned}$$

where we used the following identity:

$$\int \big(\phi(\boldsymbol{r}_i)\phi(\boldsymbol{r}_j)\big)^* \delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\phi(\boldsymbol{r}_i)\phi(\boldsymbol{r}_j) dV_i = \int \phi(\boldsymbol{r}_i)\phi(\boldsymbol{r}_i)^* \phi(\boldsymbol{r}_i)\phi(\boldsymbol{r}_i)^* dV_i$$
$$= \int |\phi(\boldsymbol{r}_i)|^4 \, dV_i,$$

as the Dirac delta lets us substitute variables, and the next equality for kinetic energy:

**Theorem.** *Let $D \subset \mathbb{R}^3$ be a compact subset with a piecewise smooth boundary $\partial D$, and $\phi \in L^2(D, \mathbb{C}) \cap C^1(D, \mathbb{C})$ a wavefunction for a closed physical system, then*

$$E_{\text{kin}}(\phi) = -\frac{\hbar^2}{2m} \int \phi(\boldsymbol{r})^* \Delta\phi(\boldsymbol{r}) dV = \frac{\hbar^2}{2m} \int |\nabla\phi(\boldsymbol{r})|^2 \, dV.$$

*Proof.*

$$\phi^*\Delta\phi + |\nabla\phi|^2 = \phi^*\Delta\phi + \nabla(\phi^*) \cdot \nabla(\phi) = \nabla \cdot (\phi^* \nabla\phi)$$
$$\Rightarrow \int_D [\phi^*\Delta\phi + |\nabla\phi|^2] dV = \int_D \nabla \cdot (\phi^*\nabla\phi) dV = \oint_{\partial D} \phi^* \nabla\phi \cdot \hat{\boldsymbol{n}} dS,$$

where for the last equality we used the divergence theorem to integrate along the domain boundary, with $\hat{\boldsymbol{n}}$ being the normal versor of the boundary and $dS$ the area element. Up to dimensional constants this is the average momentum flow through the domain's boundary, which is by definition zero for closed systems. Therefore we can write

$$\int_D [\phi^*\Delta\phi + |\nabla\phi|^2] dV = 0$$
$$\Rightarrow -\int_D \phi^*\Delta\phi dV = \int_D |\nabla\phi|^2 \, dV$$

□

In a BEC we can assume all particles are at a minimum energy state, therefore we can use the calculus of variations to find the wavefunction $\phi_0$ that minimizes the total average energy. The average energy of the whole system is the sum of every particle's average energy:

$$E(\phi_0) = N \int \left[ \frac{\hbar^2}{2m} |\nabla\phi_0(\boldsymbol{r})|^2 + V(\boldsymbol{r})|\phi_0(\boldsymbol{r})|^2 + U_0 \frac{N-1}{2} |\phi_0(\boldsymbol{r})|^4 \right] dV.$$

It's useful to introduce the wavefunction of the condensed state, defined as

$$\Psi(\boldsymbol{r}) = \sqrt{N}\phi_0(\boldsymbol{r}).$$

For $N \gg 1$ we can apply the approximation $N(N-1) \approx N^2$ and rewrite the average energy as

$$E(\Psi) = \int \left[ \frac{\hbar^2}{2m} |\nabla \Psi(\boldsymbol{r})|^2 + V(\boldsymbol{r}) |\Psi(\boldsymbol{r})|^2 + \frac{U_0}{2} |\Psi(\boldsymbol{r})|^4 \right] dV.$$

The three terms of the sum are respectively the kinetic, the potential and the internal energy densities. $\Psi$ is normalized with $\int |\Psi(\boldsymbol{r})|^2 \, dV = N$.
We can find the wavefunction with minimum average energy with the method of Lagrange multipliers:

**Theorem.** *Let $\mathcal{N} = \left\{ \Psi : \mathbb{R}^3 \to \mathbb{C}, \int |\Psi(\boldsymbol{r})|^2 \, dV = N \right\}$ be the space of $N$-normalized wavefunctions, then $\Psi_0 = \operatorname{argmin}_{\Psi \in \mathcal{N}} E(\Psi)$ solves the time independent equation*

$$\left[ \widehat{K} + V + U_0 |\Psi_0|^2 \right] \Psi_0 = \mu \Psi_0$$

*with $\mu \in \mathbb{R}$.*

*Proof.* This proof is rather informal, with many technical details omitted (e.g. about the existence of a minimum). We define the energy density of the GPE as

$$\mathcal{E}(\boldsymbol{r}, \Psi) = \frac{\hbar^2}{2m} \Psi^*(\boldsymbol{r}) \Delta \Psi(\boldsymbol{r}) + \Psi^*(\boldsymbol{r}) V(\boldsymbol{r}) \Psi(\boldsymbol{r}) + \Psi^*(\boldsymbol{r})^2 \frac{U_0}{2} \Psi(\boldsymbol{r})^2,$$

so that $\mathcal{E}(\Psi) = \int D(\boldsymbol{r}, \Psi) dV$. Since $\Psi_0$ is at the energy minimum it solves the problem

$$\begin{cases} \delta E(\Psi) = 0 \\ \int \Psi^* \Psi dV = N \end{cases}.$$

Using the method of Lagrange multipliers we write

$$\delta \left( E(\Psi_0) - \mu \int \Psi_0^* \Psi_0 dV \right) = 0$$

$$\Rightarrow \delta \int [\mathcal{E}(\boldsymbol{r}, \Psi_0) - \mu \Psi_0^* \Psi] dV = 0$$

where $\mu$ is the Lagrange multiplier, and since we can let $\Psi_0$ and $\Psi_0^*$ vary independently ([11] page 58) we take the variational derivative w.r.t to $\Psi_0^*$ to obtain

$$\int \partial_{\Psi^*} [\mathcal{E}(\boldsymbol{r}, \Psi) - \mu \Psi_0^* \Psi_0 dV] \delta \Psi^* dV = 0$$

$$\Rightarrow \partial_{\Psi^*} \mathcal{E}(\boldsymbol{r}, \Psi) = \partial_{\Psi^*} (\mu \Psi^* \Psi)$$

$$\Rightarrow \frac{\hbar^2}{2m} \Delta \Psi(\boldsymbol{r}) + V(\boldsymbol{r}) \Psi(\boldsymbol{r}) + \Psi^*(\boldsymbol{r}) U_0 \Psi(\boldsymbol{r})^2 = \mu \Psi(\boldsymbol{r})$$

$$\Rightarrow \left[ \frac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) + U_0 \, |\Psi(\boldsymbol{r})|^2 \right] \Psi(\boldsymbol{r}) = \mu \Psi(\boldsymbol{r})$$

□

Therefore the Hamiltonian operator of the GPE is

$$\widehat{H} = \widehat{K} + V + U_0 |\Psi|^2.$$

In the literature the Lagrange multiplier $\mu$ is called the *chemical potential* (e.g. see [4]).

## 1.6 Conservation of energy

Following [13] we now calculate the time derivative of the energy of the system. In the previous chapter we've shown that the total average energy for a wavefunction $\Psi$ on a spatial domain $D$ is

$$\begin{aligned} E(t) &= \int_D \left[ \frac{\hbar^2}{2m} |\nabla \Psi|^2 + V|\Psi|^2 + \frac{U_0}{2}|\Psi|^4 \right] dV \\ &= \int_D \left[ \frac{\hbar^2}{2m} (\nabla \Psi)^* \cdot \nabla \Psi + V \Psi^* \Psi + \frac{U_0}{2} (\Psi^* \Psi)^2 \right] dV. \end{aligned}$$

**Theorem.** *The time derivative of the energy on a bounded domain $D$ is*

$$E'(t) = \frac{\hbar^2}{m} \operatorname{Im} \left( \int_{\partial D} (V + U_0|\Psi|^2) \Psi^* \nabla \Psi - \frac{\hbar^2}{2m} \int_{\partial D} \Delta \Psi^* \nabla \Psi \cdot \hat{\boldsymbol{n}} dS \right).$$

*Proof.*

$$\begin{aligned} E'(t) = \int_D \Bigg[ & \frac{\hbar^2}{2m} (\partial_t (\nabla \Psi)^* \cdot \nabla \Psi + (\nabla \Psi)^* \cdot \partial_t (\nabla \Psi)) \\ & + (V + U_0|\Psi|^2)(\partial_t (\Psi^*) \Psi + \Psi^* \partial_t (\Psi)) \Bigg] dV \\ = 2\mathrm{Re} & \left( \int_D \left[ \frac{\hbar^2}{2m} \nabla \Psi \cdot \partial_t \nabla \Psi^* + (V + U_0|\Psi|^2) \Psi \partial_t \Psi^* \right] dV \right) \\ = 2\mathrm{Re} & \left( \int_D \left[ \frac{\hbar^2}{2m} (\nabla \cdot (\partial_t \Psi^* \nabla \Psi) - \partial_t \Psi^* \Delta \Psi) + (V + U_0|\Psi|^2) \Psi \partial_t \Psi^* \right] dV \right) \\ = 2\mathrm{Re} & \left( \frac{\hbar^2}{2m} \int_{\partial D} \partial_t \Psi^* \nabla \Psi \cdot \hat{\boldsymbol{n}} dS + \int_D \left[ -\frac{\hbar^2}{2m} \Delta \Psi + V \Psi + U_0 |\Psi|^2 \, \Psi \right] \partial_t \Psi^* dV \right). \end{aligned}$$

In the last equality we applied the Divergence Theorem, where $\partial D$ is the boundary of the domain, $\hat{\boldsymbol{n}}$ is the normal versor of the boundary and $dS$ is the surface element of the boundary. In the second integral we recognize the right-hand side of the GPE and substitute the left-hand side:

$$
\begin{aligned}
E'(t) &= 2\mathrm{Re}\left(\frac{\hbar^2}{2m}\int_{\partial D}\partial_t\Psi^*\nabla\Psi\cdot\hat{\boldsymbol{n}}dS + \int_D i\partial_t\Psi\partial_t\Psi^* dV\right) \\
&= 2\mathrm{Re}\left(\frac{\hbar^2}{2m}\int_{\partial D}\partial_t\Psi^*\nabla\Psi\cdot\hat{\boldsymbol{n}}dS + \cancel{\int_D i\,|\partial_t\Psi|^2 dV}\right) \\
&= \frac{\hbar^2}{m}\,\mathrm{Re}\left(\int_{\partial D}\partial_t\Psi^*\nabla\Psi\cdot\hat{\boldsymbol{n}}dS\right).
\end{aligned}
$$

Now we do the inverse and substitute $\partial_t\Psi$ with the right-hand side of the GPE divided by $i$:

$$
\begin{aligned}
E'(t) &= \frac{\hbar^2}{m}\,\mathrm{Re}\left(\int_{\partial D} -i\left[-\frac{\hbar^2}{2m}\Delta\Psi^* + V\Psi^* + U_0\,|\Psi|^2\Psi^*\right]\nabla\Psi\cdot\hat{\boldsymbol{n}}dS\right) \\
&= \frac{\hbar^2}{m}\,\mathrm{Im}\left(\int_{\partial D}(V+U_0|\Psi|^2)\Psi^*\nabla\Psi - \frac{\hbar^2}{2m}\int_{\partial D}\Delta\Psi^*\nabla\Psi\cdot\hat{\boldsymbol{n}}dS\right).
\end{aligned}
$$

□

A sufficient condition for the conservation of energy is $\nabla\Psi$ being zero on the boundary or tangent to the boundary.

## 1.7 Fluid dynamics interpretation of the GPE

**Definition.** *Let $\Psi(\boldsymbol{r},t) = \sqrt{n(\boldsymbol{r},t)}\exp(iS(\boldsymbol{r},t))$ be a wavefunction expressed in polar form, with $n$ and $S$ real valued functions. We define:*

*i. the number density field $n$ of the wavefunction, $n(\boldsymbol{r},t) = |\Psi(\boldsymbol{r},t)|^2$*
*ii. the mass density field $\rho$ of the wavefunction, $\rho(\boldsymbol{r},t) = m|\Psi(\boldsymbol{r},t)|^2 = mn(\boldsymbol{r},t)$*
*iii. the velocity field $v$ of the wavefunction, $\boldsymbol{v}(\boldsymbol{r},t) = \frac{\hbar}{m}\nabla S(\boldsymbol{r},t)$*

**Theorem.** *The GPE can be reformulated using number density and velocity, leading us to the equations*

$$
\begin{cases}
\partial_t n + \nabla\cdot(n\boldsymbol{v}) = 0 \\
m\partial_t\boldsymbol{v} + \nabla\left(\frac{1}{2}m|\boldsymbol{v}|^2 + U_0 n - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}} + V\right) = 0
\end{cases}
$$

*Proof.* The proof of this theorem is straightforward albeit laborious: we only need to expand each derivative in the GPE and separate the real and imaginary parts.

First we expand the Laplacian:

$$\begin{aligned}
\Delta \exp(iS) &= \nabla \cdot (i \exp(iS) \nabla S) \\
&= i(\exp(iS)\Delta S + \nabla \exp(iS) \cdot \nabla S) \\
&= \exp(iS)(i\Delta S - |\nabla S|^2) \\
\Rightarrow \Delta \Psi &= \Delta\big(\sqrt{n} \exp(iS)\big) \\
&= \sqrt{n}\Delta \exp(iS) + \exp(iS)\Delta\sqrt{n} + 2\nabla \exp(iS) \cdot \nabla\sqrt{n} \\
&= \exp(iS)\left(\sqrt{n}(i\Delta S - |\nabla S|^2) + \Delta\sqrt{n} + \frac{i}{\sqrt{n}}\nabla S \cdot \nabla n\right),
\end{aligned}$$

then the time derivative:

$$\begin{aligned}
\partial_t \Psi &= \partial_t\big(\sqrt{n} \exp(iS)\big) \\
&= \sqrt{n}\partial_t \exp(iS) + \exp(iS)\partial_t\sqrt{n} \\
&= \exp(iS)\left(\frac{1}{2\sqrt{n}}\partial_t n + i\sqrt{n}\partial_t S\right).
\end{aligned}$$

Plugging everything in the GPE we get

$$\begin{aligned}
\hbar\left(\frac{i}{2\sqrt{n}}\partial_t n - \sqrt{n}\partial_t S\right) = -\frac{h^2}{2m}&\left(\sqrt{n}(i\Delta S - |\nabla S|^2) + \Delta\sqrt{n} + \frac{i}{\sqrt{n}}\nabla S \cdot \nabla n\right) \\
&+ V\sqrt{n} + U_0 n^{\frac{3}{2}},
\end{aligned}$$

and by taking the imaginary part we obtain

$$\begin{aligned}
\frac{\hbar}{2\sqrt{n}}\partial_t n &= -\frac{\hbar^2}{2m}\left(\sqrt{n}\Delta S + \frac{1}{\sqrt{n}}\nabla S \cdot \nabla n\right) \\
\Rightarrow \partial_t n &= -\frac{\hbar}{m}\nabla \cdot (n \nabla S) \\
\Rightarrow \partial_t n + \nabla \cdot (n\boldsymbol{v}) &= 0,
\end{aligned}$$

which is the first of our equations. If instead we take the real part we obtain

$$\begin{aligned}
-\hbar\sqrt{n}\partial_t S &= \frac{\hbar^2}{2m}(\sqrt{n}|\nabla S|^2 - \Delta\sqrt{n}) + V\sqrt{n} + U_0 n^{\frac{3}{2}} \\
\Rightarrow \hbar\partial_t S &= -\left(\frac{\hbar^2}{2m}\left(|\nabla S|^2 - \frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + V + U_0 n\right),
\end{aligned}$$

finally on both sides we take the gradient and rearrange some dimensional constants:

$$\begin{aligned}
m\partial_t\left(\frac{h}{m}\nabla S\right) &= -\nabla\left(\frac{m}{2}\left|\frac{h}{m}\nabla S\right|^2 - \frac{h^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}} + V + U_0 n\right) \\
\Rightarrow m\partial_t \boldsymbol{v} &= -\nabla\left(\frac{1}{2}m|\boldsymbol{v}|^2 + V + U_0 n - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)
\end{aligned}$$

□

Now we can compare the obtained equations with the classical Euler equations for a barotropic, non-viscous, irrotational fluid in a conservative force field ([19] page 38):

| Gross-Pitaevskii | Euler |
|---|---|
| $\begin{cases} \partial_t n + \nabla \cdot (n\boldsymbol{v}) = 0 \\ m\partial_t \boldsymbol{v} + \nabla\Big(\frac{1}{2}m\lvert\boldsymbol{v}\rvert^2 + U_0 n - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}} + V\Big) = 0 \end{cases}$ | $\begin{cases} \partial_t \rho + \nabla \cdot (\rho\boldsymbol{u}) = 0 \\ \partial_t \boldsymbol{u} + \nabla\big(\frac{1}{2}\ \lvert\boldsymbol{u}\rvert^2 + P + U\big) = 0 \end{cases}$ |

where $\rho$ is the fluid density, $\boldsymbol{u}$ is the fluid velocity, $P$ is the thermodynamic potential and $U$ is the potential of conservative forces acting on the fluid. We can interpret $U_0 n$ to be a classical pressure potential and $-\frac{\hbar^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}}$ to be a quantum pressure potential, also known as Bohm quantum potential [6]. We can also rewrite the average kinetic energy $E_{\text{kin}}$ in terms of these fields:

**Theorem.** *A quantum fluid described by a wavefunction having density $n$ and velocity $\boldsymbol{v}$ has the following kinetic energy:*

$$K = \int \left[ \frac{\hbar^2}{2m}\ \lvert\nabla\sqrt{n}\rvert^2 + \frac{\rho}{2}\ \lvert\boldsymbol{v}\rvert^2 \right] d\boldsymbol{r}$$

*Proof.* By expanding the absolute value squared of the gradient of the wavefunction we obtain

$$\begin{aligned} \lvert\nabla\Psi\rvert^2 &= \lvert\nabla(\sqrt{n}\exp(iS)\rvert^2 \\ &= \lvert\exp(iS)\nabla\sqrt{n} + \sqrt{n}\nabla(\exp(iS))\rvert^2 \\ &= \lvert\exp(iS)\big(\nabla\sqrt{n} + i\sqrt{n}\nabla S\big)\rvert^2 \\ &= \lvert\nabla\sqrt{n}\rvert^2 + n\ \lvert\nabla S\rvert^2 \\ &= \lvert\nabla\sqrt{n}\rvert^2 + \frac{m^2 n}{\hbar^2}\ \lvert\boldsymbol{v}\rvert^2 \end{aligned}$$

Therefore the kinetic energy can be rewritten as

$$K = \frac{\hbar^2}{2m}\int \lvert\nabla\phi(\boldsymbol{r})\rvert^2\ dV = \int \left[ \frac{\hbar^2}{2m}\ \lvert\nabla\sqrt{n}\rvert^2 + \frac{mn}{2}\ \lvert\boldsymbol{v}\rvert^2 \right] d\boldsymbol{r}$$

□

The first term in the integral is the zero point energy, while the second term is the "classical" kinetic energy given by fluid motion.
Note that the field $n\boldsymbol{v} = \frac{\hbar}{m}n\nabla S$ is also called the *probability current density* $\boldsymbol{i}$ of the wavefunction ([11] page 55), and it is usually defined as

$$\boldsymbol{J} = \frac{1}{2m}\big(\Psi\hat{P}^*\Psi^* + \Psi^*\hat{P}\Psi\big),$$

where $\hat{P} = -i\hbar\nabla$ is the momentum operator.

**Theorem.** *Let* $\Psi(\boldsymbol{r},t)=\sqrt{n(\boldsymbol{r},t)}\exp(iS(\boldsymbol{r},t))$ *be a wavefunction,* $n(\boldsymbol{r},t)=|\Psi(\boldsymbol{r},t)|^2$ *its number density, and* $\boldsymbol{v}(\boldsymbol{r},t)=\frac{\hbar}{m}\nabla S(\boldsymbol{r},t)$ *its velocity, then*

$$n\boldsymbol{v}=\frac{1}{2m}\big(\Psi\hat{P}^*\Psi^*+\Psi^*\hat{P}\Psi\big)$$

*Proof.*

$$\begin{aligned}\frac{1}{2m}\big(\Psi\hat{P}^*\Psi^*+\Psi^*\hat{P}\Psi\big)&=\frac{1}{2m}\big(\sqrt{n}\exp(iS)i\hbar\nabla\big(\sqrt{n}\exp(-iS)\big)\\&\quad+\sqrt{n}\exp(-iS)(-i)\hbar\nabla\big(\sqrt{n}\exp(iS)\big)\big)\\&=\frac{i\hbar\sqrt{n}}{2m}\big(\nabla\sqrt{n}-i\sqrt{n}\nabla S-\nabla\sqrt{n}-i\sqrt{n}\nabla S\big)\\&=\frac{\hbar}{m}n\nabla S=n\boldsymbol{v}\end{aligned}$$

□

Chapter 2

# Quantum vortices

**Definition.** *Let $\Psi \in L^2(\mathbb{R}^3, \mathbb{C})$ be a wavefunction describing a quantum fluid. A **quantum vortex** $K$ is a connected subset of $\mathbb{R}^3$, with nontrivial fundamental group, where $\Psi(K) = \{0\}$.*

This definition, unusual for classsical fluid mechanics, will be justified in the following sections.

## 2.1 Circulation of quantum fluids

The circulation $\Gamma$ of a BEC around a closed, simple and oriented path $C$ is defined, as usual in fluid dynamics, as the line integral of the velocity field around $C$ ([5] section 5.2):

$$\Gamma_C(\boldsymbol{v}) = \oint_C \boldsymbol{v} \cdot d\boldsymbol{l} = \frac{\hbar}{m} \oint_C \nabla S \cdot d\boldsymbol{l}$$

where $\boldsymbol{v} = \frac{\hbar}{m}\nabla S$, $S$ is the phase of the BEC and $d\boldsymbol{l}$ is the line element of the curve. Being S the phase of the wavefuntion, $\Gamma_C$ represents the total phase variation around the closed path, and it can only take discrete values $2\pi q, q \in \mathbb{Z}$. We define the quantity $\kappa = \frac{2\pi\hbar}{m}$ as the **quantum of circulation**, so that the circulation can be written as

$$\Gamma_C(\boldsymbol{v}) = \frac{\hbar}{m} \oint_C \nabla S \cdot d\boldsymbol{l} = \frac{\kappa}{2\pi} 2\pi q = \kappa q.$$

This setup is clearly different from the classical case, where the circulation can take arbitrary real values.

## 2.2 Properties of of quantum vortices

Since $S$ is a scalar field, Poincaré's lemma ([17] Theorem 7.4.14) ensures that for $\oint_C \nabla S \cdot d\boldsymbol{l}$ to not be zero the domain of $S$ cannot be simply connected ($\nabla S \cdot d\boldsymbol{l}$ is a closed form, and if the domain of integration were simply connected it would also be exact). Therefore there must be a singularity in the $S$ field, spanning the boundary of the system or forming a loop, caused by the vanishing of the wavefunction (the complex value zero has undefined phase). This is analogous to Helmholtz's Second Theorem for vortex lines in classical fluid dynamics ([19] chapter 5). We can also prove a theorem analogous to Helmholtz's First Theorem:

**Theorem.** *Let $C_1$ and $C_2$ be two closed and simple paths with the same orientation. both winding once around a single vortex line $K$, $\boldsymbol{v} = \frac{\hbar}{m}\nabla S$ where $S$ is the phase of the BEC, then*

$$\Gamma_{C_1}(\boldsymbol{v}) = \Gamma_{C_2}(\boldsymbol{v}).$$

*Proof.*

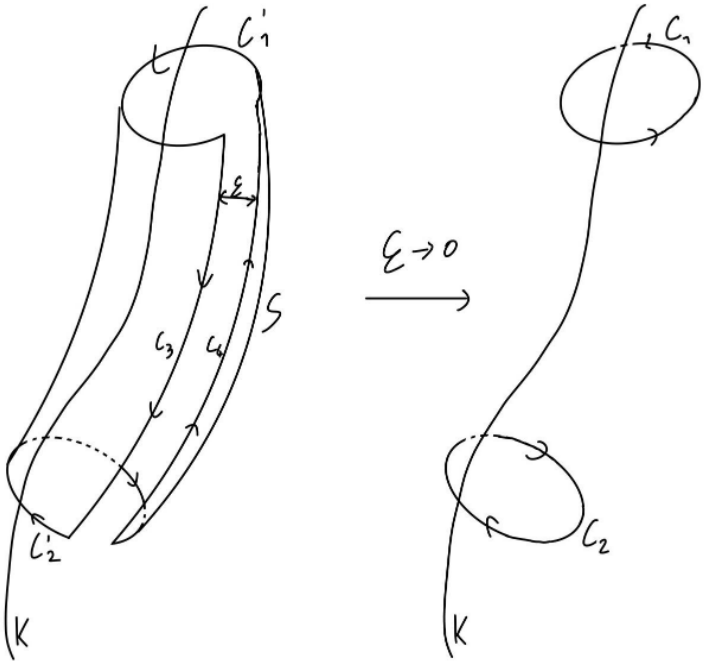



FIGURE 1. Illustration of the proof.

We start with a surface $S$ wrapping around the vortex $K$, having boundary $\partial S$ composed of the union of the curves $C_1', C_2', C_3, C_4$. The curves $C_1'$ and $C_2'$ overlap $C_1$ and $C_2$ except for complementary curves of length $\varepsilon$, and without loss of generality we suppose $C_2'$ is oriented opposite of $C_2$. From Poincaré's lemma we know that the circulation around the boundary $\partial S$ must be 0, as the vortex doesn't intersect with the surface. By taking the limit $\varepsilon \to 0$ the curves $C_3$ and $C_4$ overlap and the phase variations along $C_3$ and $C_4$ tend to opposite values and cancel out. We are left with the phase variations along $C_1'$ and $C_2'$, which also must be opposite to obtain a vanishing circulation. By reversing the orientation of $C_2'$ we complete the proof. □

Kelvin's circulation Theorem for classical fluids states that the circulation around a material (i.e. transported by the fluid flow) closed line is constant in time. This also holds for quantum fluids [2], therefore quantum vortices in ideal conditions persist indefinitely.

# Chapter 3
# Reconnections of quantum vortices

A vortex reconnection happens when two or more vortex lines cross each other. Nazarenko and West analyze the event with a local approximation, building a power series solution. This approach is well suited to the problem because the wavefunction vanishes at the reconnection point and by continuity stays close to zero around it, making the nonlinear $|\Psi|^2$ term of the GPE negligible. We then prove the following properties about vortex reconnections:

i. the process is free from singularities,
ii. around the vortex reconnection the vortex lines are anti-parallel (parallel but carrying opposite circulation values),
iii. the distance between vortex lines changes proportionally to $|t|^{\frac{1}{2}}$, with $t = 0$ being the reconnection time.

We then develop a power series solution to the full nonlinear problem.

## 3.1 Local analysis

We start with an adimensional GPE instance [20]:

$$i\partial_t \Psi + \Delta\Psi + (1 - |\Psi|^2)\Psi = 0.$$

The $(1 - |\Psi|^2)\Psi$ term can be explained by considering a uniform potential $V = -1$. This physically corresponds to a system where at infinity the fluid is saturated, with normalized density 1, and inside of which regions with non saturated fluid (our vortices) can move.

**Theorem.** *Consider a wavefunction $\Psi$ solving the GPE, with $\Psi(\mathbf{0}, 0) = 0$, then $\Phi(\boldsymbol{r}, t) = \Psi(\boldsymbol{r}, t)e^{-it}$ solves the free particle Schrödinger equation $i\partial_t\Phi + \Delta\Phi = 0$ for $\boldsymbol{r} = 0$ and $t = 0$.*

*Proof.* By linearizing the GPE at the origin we can ignore the $|\Psi|^2$ term, and by applying the change of variable $\Phi(\boldsymbol{r}, t) = \Psi(\boldsymbol{r}, t)e^{-it}$ we can simplify even further:

$$\begin{aligned} i\partial_t(\Phi e^{it}) + \Delta(\Phi e^{it}) + \Phi e^{it} &= -\Phi e^{it} + ie^{it}\partial_t\Phi + e^{it}\Delta\Phi + \Phi e^{it} \\ &= e^{it}(i\partial_t\Phi + \Delta\Phi). \end{aligned}$$

□

The new variable introduces a uniform phase shift that doesn't modify the velocity of the wavefunction. We set up as initial condition a wavefunction with two vortices intersecting at the origin $\boldsymbol{r} = 0, t = 0$:

$$\begin{cases} \Psi_0(\boldsymbol{r}) \coloneqq \Psi(\boldsymbol{r}, 0) \\ \mathrm{Re}(\Psi_0) = z \\ \mathrm{Im}(\Psi_0) = az + bx^2 - cy^2 \\ a, b, c \in \mathbb{R} \setminus \{0\} \end{cases},$$

with $\boldsymbol{r} \coloneqq (x, y, z)$. We neglect that $\Psi_0$ may diverge at infinity, because we're only interested in its evolution in a neighborhood of the origin. Solving $\Psi_0 = 0$ gives us

$$\begin{cases} z = 0 \\ y = \pm\left(\frac{b}{c}\right)^{\frac{1}{2}} x \end{cases},$$

that means that the vortices are two lines on the $xy$ plane, intersecting at the origin.

**Theorem.** *The position of the vortices in a quantum fluid described by the wave-function $\Psi$ that solves the Cauchy problem*

$$\begin{cases} i\partial_t \Psi + \Delta\Psi + (1 - |\Psi|^2)\Psi = 0 \\ \Psi(\boldsymbol{r}, 0) = \Psi_0(\boldsymbol{r}) \\ a, b, c \in \mathbb{R} \setminus \{0\} \end{cases}$$

*is locally approximated, when close to the origin and for small time steps $t$, by the equations*

$$\begin{cases} z = 2(b - c)t \\ bx^2 - cy^2 + 2a(b - c)t = 0 \end{cases}.$$

*Proof.* The linearization around the origin is applicable here since $\Psi_0(0) = 0$. The uniform phase shift doesn't modify the position of the vortices, therefore we can consider instead the free particle Schrödinger equation. Considering only small time shifts, either positive or negative, we compute the system's evolution. First for the real part:

$$\begin{aligned} \mathrm{Re}(\Phi(\boldsymbol{r}, t)) &= \mathrm{Re}(\Psi_0(\boldsymbol{r}) + \partial_t(\Phi(\boldsymbol{r}, 0))t) \\ &= \mathrm{Re}(\Psi_0(\boldsymbol{r})) + \mathrm{Re}(i\Delta\Phi_0(\boldsymbol{r}))t \\ &= \mathrm{Re}(\Psi_0(\boldsymbol{r})) - \Delta(\mathrm{Im}(\Psi_0(\boldsymbol{r})))t \\ &= z + 2(c - b)t, \end{aligned}$$

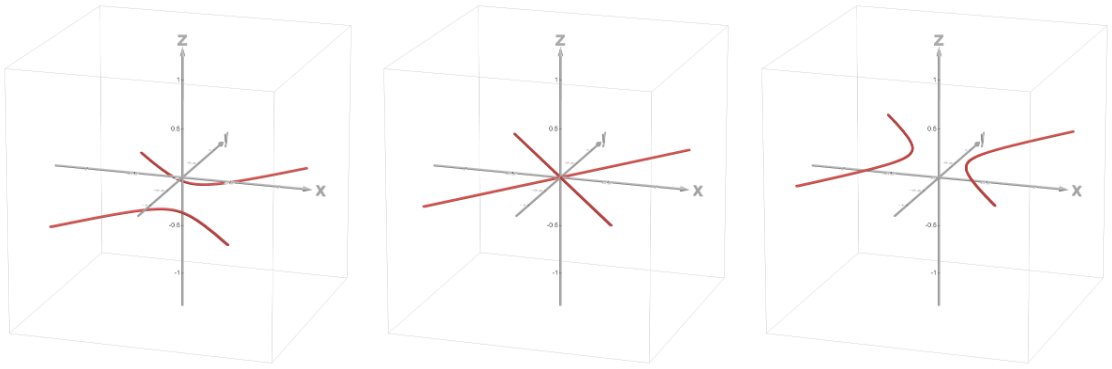
and similarly for the imaginary part:

$$\begin{aligned} \mathrm{Im}(\Phi(\boldsymbol{r}, t)) &= \mathrm{Im}(\Psi_0(\boldsymbol{r})) + \Delta(\mathrm{Re}(\Psi_0(\boldsymbol{r})))t \\ &= az + bx^2 - cy^2. \end{aligned}$$

We again solve $\Phi(\boldsymbol{r}, t) = 0$ to figure out where the vortices are going:

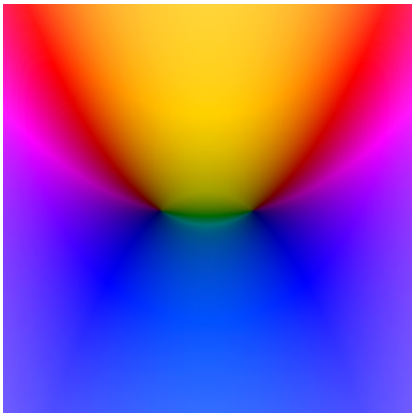
$$\begin{cases} z = 2(b - c)t \\ bx^2 - cy^2 + 2a(b - c)t = 0 \end{cases}$$

□




$t = -0.1$ $t = 0$ $t = 0.1$

**Fig. 1-3.** Motion of the vortex cores for the solution with $a = -1, b = 2, c = 1$.



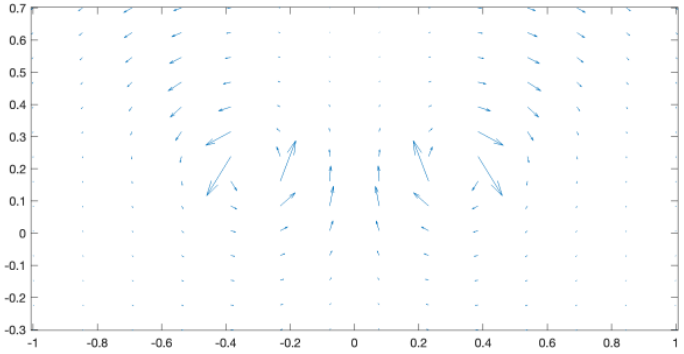



**Fig. 4.** Vertical section of the wavefunction at $t = 0.1$ with domain coloring [21], where the black spots are low density areas where the vortices are located.

**Fig. 5.** Same vertical section with a quiver plot of the velocity field (derived in 3.2).

We see now that the vortices are two separate hyperbolas for $t < 0$, come into contact forming two intersecting lines at $t = 0$ and move away from each other as hyperbolas for $t > 0$. More precisely, the vortices sweep horizontal sections of the saddle $z = bx^2 - cy^2$. We note that that solutions before and after the reconnection are related by the symmetry $t \to -t, z \to -z, x \to y, y \to x$ which shows that the vortices don't just bounce away but also "switch halves" with each other.

## 3.2 Properties of vortex reconnections

It's evident that the local solution is smooth. This is an important difference between the theoretical behavior of quantum and classical vortices, as singularities form during vortex reconnections described by the Euler equations.

**Theorem.** *Let $\Psi(\boldsymbol{r}, t)$ be a wavefunction. If $\Psi(\boldsymbol{r}, t) \neq 0$ then the velocity field $\boldsymbol{v}$ is*

$$\boldsymbol{v}(\boldsymbol{r},t) = \mathrm{Im}\left(\frac{\nabla\Psi(\boldsymbol{r},t)}{\Psi(\boldsymbol{r},t)}\right).$$

*Proof.* Let $\Psi = \sqrt{n}\exp(iS)$. We can compute the velocity field $\nabla S$ with the following identities:

$$\begin{aligned}\log(\Psi) &= \frac{1}{2}\log(n) + i(S + 2\pi k), k \in \mathbb{Z}\\ \Rightarrow \nabla(\log(\Psi)) &= \frac{\nabla\Psi}{\Psi} = \frac{\nabla n}{2n} + i\nabla S\\ \Rightarrow \mathrm{Im}\left(\frac{\nabla\Psi}{\Psi}\right) &= \nabla S = \boldsymbol{v}.\end{aligned}$$

□

Applying this to our solution we get

$$\begin{aligned}\boldsymbol{v}(x,y,z,t) &= \mathrm{Im}\left(\frac{1}{z + 2(c-b)t + i(az + bx^2 - cy^2)}\begin{pmatrix}2ibx\\ -2icy\\ 1+ia\end{pmatrix}\right)\\ \Rightarrow \boldsymbol{v}(0,0,0,t) &= \frac{a}{2(c-b)t}\begin{pmatrix}0\\0\\1\end{pmatrix}.\end{aligned}$$

If the vortex pair were in a parallel configuration we would have a vanishing velocity in the midpoint, but this is not the case, therefore the vortices are anti-parallel.
We can measure the distance between approaching vortices by solving the system

$$\begin{cases}\Phi = 0\\ y = 0\\ t < 0\\ b > c\end{cases},$$

obtaining

$$\begin{aligned}bx^2 + 2(b-c)t &= 0\\ \Rightarrow x = \pm\sqrt{\frac{2(c-b)}{b}t} &\propto \sqrt{|t|}.\end{aligned}$$

This square root law has been confirmed by experimental results [9].

## 3.3 Nonlinear solutions

We now develop a solution to the full nonlinear problem using a power series. We assume $x, y, z \sim \varepsilon$, $t \sim \varepsilon^3$ and $t_0 = 0$. Our objective is a solution $\Psi = \sum_{n=1}^{\infty}\Psi^{(n)}$, where $\Psi^{(n)} \sim \varepsilon^n$.
From the order of magnitude relations we obtain $\partial_t \sim \varepsilon^{-3}$ and $\Delta \sim \varepsilon^{-2}$, from which we can compute the orders of magnitude of each term of the GPE:

$$i\partial_t \Psi^{(m)} \sim \varepsilon^{m-3},$$

$$\Delta \Psi^{(n)} \sim \varepsilon^{n-2},$$

and

$$\left[|\Psi|^2\ \Psi\right]^{(p)} := \sum_{i,j=0?}^{p} \Psi^{*(i)} \Psi^{(j)} \Psi^{(p-i-j)} \sim \varepsilon^p.$$

Matching the orders of magnitude in the GPE and integrating along time we obtain

$$\Psi^{(n+1)} = \Psi_0^{(n+1)} + i \int_0^t \left[ \Delta \Psi^{(n)} + \Psi^{(n-2)} - \left[|\Psi|^2\ \Psi\right]^{(n-2)} \right] dt$$

where $\Psi_0^{(n)}$ are the terms of the series expansion of the initial condition.

## 3.4 Theory interlude: the Cauchy–Kovalevskaya Theorem

We introduce some notation: let $\alpha = (\alpha_1, ..., \alpha_n)$ be a multi-index, with $|\alpha| = \sum_{i=0}^{n} \alpha_i$ and $\partial_x^\alpha = \prod_{i=1}^{n} \left( \frac{\partial}{\partial x_i} \right)^{\alpha_i}$. A nonlinear Cauchy problem on $\mathbb{R}^n$ is defined as

$$\begin{cases} \partial_t^k u = G\left( \boldsymbol{x}, t, \left( \partial_x^\alpha \partial_t^j u \right)_{|\alpha|+j \le k, j<k} \right) \\ \partial_t^j u(\boldsymbol{x}, 0) = \phi_j(\boldsymbol{x}) \end{cases},$$

where $0 \le j < k$ and $\phi_0, ..., \phi_{k-1} : A \to \mathbb{R}$, with $A$ being a neighborhood of the origin.

**Theorem.** *If $G, \phi_0, ..., \phi_{k-1}$ are analytic near the origin, there is a neighborhood of the origin on which the Cauchy problem has a unique analytic solution.*

If we can find an analytic initial condition the Cauchy-Kovalevskaya Theorem ensures a non-zero convergence radius for the power series solution of the GPE. See [8] chapter 1 for a complete description and proof of this theorem.

## 3.5 Developing an initial condition

We calculate a series expansion for a simple line vortex placed on the z-axis solving the time-independent GPE $\Delta\Psi_0 + (1 - |\Psi_0|^2)\Psi_0 = 0$. We start with a wavefunction in cylindrical coordinates
$\Psi_0(r, \theta, z) = A(r)e^{i\theta}$ which when plugged in the GPE gives us

$$\begin{aligned} \Delta\left(Ae^{i\theta}\right) + (1 - A^2)Ae^{i\theta} &= 0 \\ \Rightarrow e^{i\theta}\Delta A + A\Delta\left(e^{i\theta}\right) + \cancel{2\nabla A \cdot \nabla\theta} + (1 - A^2)Ae^{i\theta} &= 0 \\ \Rightarrow e^{i\theta}(\Delta A + \cancel{iA\Delta\theta} - A|\nabla\theta|^2 + (1 - A^2)A) &= 0 \\ \Rightarrow \Delta A - A|\nabla\theta|^2 + A - A^3 &= 0. \end{aligned}$$

We also use the identities

$$\Delta A(r) = \frac{1}{r}\partial_r(r\partial_r A(r)),$$

$$|\nabla\theta|^2 = (\partial_x\theta)^2 + \big(\partial_y\theta\big)^2 = \frac{y^2+x^2}{r^4} = \frac{1}{r^2},$$

to further simplify:

$$\frac{1}{r}\partial_r(r\partial_r A(r)) + \frac{A}{r^2} + A - A^3 = 0.$$

We are looking for a recurrence relation for the coefficients of the power series expansion of A:

$$A = \sum_{n=1}^{\infty} A^{(n)} = \sum_{n=1}^{\infty} a_n r^n$$

By applying the same order of magnitude relations as in 5.3 we obtain

$$\frac{1}{r}\partial_r\big(r\partial_r A^{(n)}\big) = n^2 a_n r^{n-2} \sim \varepsilon^{n-2},$$

$$\frac{A^{(n)}}{r^2} = a_n r^{n-2} \sim \varepsilon^{n-2}.$$

By matching orders of magnitude we obtain

$$(n^2+1)a_n + a_{n-2} - \sum_{i,j=1}^{i+j<n} a_i a_j a_{n-i-j} = 0.$$

Since $a_0 = 0$ we have $a_{2n} = 0$ for all natural $n$, therefore we can write

$$\Psi_0(r,\theta,z) = g(r)re^{i\theta} = (x+iy)g(x^2+y^2),$$

with

$$g(r^2) = \sum_{n=0}^{\infty} a_{2n+1}\big(r^2\big)^n.$$

To model a vortex reconnection we rotate and translate two power series at a distance $2d$ and angle $2\alpha$ from each other and then we take their product as our initial condition. First we rotate both vortices in the xy-plane with the axis permutation $x \to y, y \to z, z \to x$. We move one vortex at a distance $d$ with the translation $z \to z - d$. Finally we rotate it with $x \to x\cos(\alpha) - y\sin(\alpha), y \to y\cos(\alpha) + x\sin(\alpha)$. On the other vortex we apply the opposite transformations: $-d$ translation and $-\alpha$ rotation along the z-axis. We end up with the following initial condition, with free parameters $\alpha$ and $d$:

$$\begin{cases} \Psi_0 = \Psi_1\Psi_2 \\ \Psi_1(x,y,z) = (y\cos(\alpha) + x\sin(\alpha) + i(z-d))g\Big((y\cos(\alpha) + x\sin(\alpha))^2 + (z-d)^2\Big). \\ \Psi_2(x,y,z) = (y\cos(\alpha) - x\sin(\alpha) + i(z+d))g\Big((y\cos(\alpha) - x\sin(\alpha))^2 + (z+d)^2\Big) \end{cases}$$

## Appendix A

# Linear operators in infinite-dimensional vector spaces

All finite-dimensional complex vector spaces are Hilbert spaces ([22] page 77), but we must check that completeness holds in the case of infinite dimensions. The case of $L^2(\mathbb{R}^3 \to \mathbb{C})$ is a special case of $L^p(\mu)$, where $\mu$ is a positive measure on an arbitrary measure space $X$, $1 \leq p \leq \infty$ and the elements of the space are functions $f : X \to \mathbb{C}$ such that $\left(\int_X |f|^p \, d\mu\right)^{\frac{1}{p}} < \infty$. All of these spaces are complete ([22] page 67).

We now turn our attention to the properties of observables in infinite-dimensional Hilbert spaces.

**Definition.** *Let $L$ be a self-adjoint linear operator on a Hilbert space $\mathcal{H}$ and $B_1 = \{x \in \mathcal{H}, \|x\| \leq 1\}$ the unit ball of $\mathcal{H}$, we call $L$ **compact** when the closure of the image of $B_1$ through $L$ is compact.*

**Definition.** *We define the **spectrum** $\sigma(L)$ of $L$ as the set $\sigma(L) \coloneqq \{\lambda \in \mathbb{C} \mid L - \lambda I$ is not bijective$\}$. We call an element $\lambda \in \sigma(L)$ **eigenvalue** of $L$ when $\mathrm{Ker}(L - \lambda I) \neq \{0\}$.*

Note that in the infinite-dimensional, not self-adjoint case not every element of the spectrum is an eigenvalue ([10] page 163). One can prove that the spectrum of a compact operator is a discrete and compact subset of $\mathbb{C}$ ([22] theorem 4.25), and that the spectral theorem holds in the same formulation, except for the possible need for a countably infinite base.

We can generalize the spectral theorem even further:

**Definition.** *We call $L \in \mathcal{H}$ **bounded** when it admits a finite operator norm $\|L\| \coloneqq \sup\{\|Lx\|, x \in \mathcal{H}, \|x\| < 1\}$.*

**Definition.** *We call $L \in \mathcal{H}$ **normal** if $TT^* = T^*T$.*

**Definition.** *We call $L \in \mathcal{H}$ a **projection** if $L^2 = L$.*

Since the spectrum of a bounded operator can be continuous we must move to an "integral" formulation of the spectral theorem:

**Definition.** *Let $\mathcal{M}$ be a $\sigma$-algebra on a set $\omega$ and $\mathcal{B}(\mathcal{H})$ the set of all bounded operators on $\mathcal{H}$, we call **resolution of the identity** a map $E : \mathcal{M} \to \mathcal{B}(\mathcal{H})$ with the following properties:*

*i. $E(\emptyset) = 0, E(\omega) = I$.*
*ii. Each $E(\omega)$ is a self-adjoint projection.*
*iii. $E(\omega' \cap \omega'') = E(\omega')E(\omega'')$.*
*iv. If $\omega' \cap \omega'' = \emptyset$ then $E(\omega' \cup \omega'') = E(\omega') + E(\omega'')$.*
*v. For every $x, y \in \mathcal{H}$, the function $E_{x,y} : \mathcal{M} \to \mathbb{C}, E_{x,y}(\omega) = \langle E(\omega)x, y\rangle$ is a complex measure on $\mathcal{M}$*

**Theorem.** *If $L \in \mathcal{H}$ is bounded and normal, then there exists a unique resolution of the identity $E$ on the Borel subsets of $\sigma(T)$ which satisfies*

$$L = \int_{\sigma(L)} \lambda dE(\lambda)$$

See [22] chapter 12 for more details.

## Appendix B
# The Hartree Approximation

The Hartree approximation, or Hartree product, is an approximation method for the $N$-body Schrödinger equation introduced in [7].
Let us consider a system of $N$ bosons. When isolated, each boson $i$ is described by a wavefunction $\psi_i \in L^2(\mathbb{R}^3, \mathbb{C})$, that solves the 1-body Schrödinger equation. The Hartree approximation consists in computing the wavefunction of the whole system as the product of each individual wavefunction:

$$\Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_N) = \prod_{i=1}^{N} \psi_i(\boldsymbol{r}_i),$$

where each $\boldsymbol{r}_i \in \mathbb{R}^3$ determines the position of the $i$-th particle. When viewed through the Born rule stated in 1.1, this approximation is equivalent to assuming every boson to be independent from the others, as any measurement of the system will be a combination of measurements of individual wavefunctions, with a probability equal to the product of individual probabilities.
We underline that the Hartree approximation is not applicable to fermions, as the resulting wavefunction is symmetric to a permutation of the position of the particles, while because of the Pauli exclusion principle the wavefunction of a system of fermions must be antisymmetric under permutation of positions, i.e.:

$$\Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_N) = \mathrm{sgn}(\sigma)\Psi\Big(\boldsymbol{r}_{\sigma(i)}, ..., \boldsymbol{r}_{\sigma(N)}\Big)$$

for any $N$-permutation $\sigma$ (see [11] Chapter IX for more details).

# References


[1] A. Einstein, "Quantentheorie des einatomigen idealen Gases," *Sitzungsberichte der Preussischen Akademie der Wissenschaften*, 1925.

[2] A. Belloni and R. L. Ricca, "On the zero helicity condition for quantum vortex defects," *Journal of Fluid Mechanics*, 2008.

[3] L. de Broglie, "Waves and quanta," *Nature*, vol. 112, 1923.

[4] C.J.Pethick and H.Smith, *Bose-Einstein Condensation in Dilute Gases*. 2008.

[5] Carlo F. Barenghi and Nick G. Parker, *A Primer on Quantum Fluids*. 2016.

[6] D. Bohm, "A Suggested Interpretation of the Quantum Theory in Terms of "Hidden Variables"," *Physical Review*, vol. 85, 1952.

[7] D. R. Hartree, *The Calculation of Atomic Structures*. 1957.

[8] G. B. Folland, *Introduction to Partial Differential Equations*, 2nd ed. 1995.

[9] G. P. Bewley, M. S. Paoletti, and K. R. Sreenivasan, "Characterization of reconnecting vortices in superfluid helium," *PNAS*, 2008.

[10] Haim Brezis, *Functional Analysis, Sobolev Spaces and Partial Differential Equations*. 2010.

[11] L. D. Landau and L. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 2nd ed. 1965.

[12] Leon N. Cooper, "Bound electron pairs in a degenerate Fermi gas," *Physical Review*, vol. 104, 1956.

[13] M. Caliari and S. Zuccher, "A Fast Time Splitting Finite Difference Approach to Gross–Pitaevskii Equations," *Communications in Computational Physics*, vol. 29, 2021.

[14] O. Gessner and A. F. Vilesov, "Imaging Quantum Vortices in Superfluid Helium Droplets," *Annual Review of Physical Chemistry*, vol. 70, 2019.

[15] P. Kapitza, "Viscosity of Liquid Helium Below the λ-Point," *Nature*, vol. 141, 1938.

[16] Peter Woit, *Quantum Theory, Groups and Representations*. 2017.

[17] Ralph Abraham, Jerrold E. Marsden, and Tudor Ratiu, *Manifolds, Tensor Analysis, and Applications*, 3rd ed. 2002.

[18] S. N. Bose, "Plancks Gesetz und Lichtquantenhypothese," *Zeitschrift für Physik*, vol. 26, 1924.

[19] S. Zuccher, *Note di Fluidodinamica*. 2024.

[20] S. Nazarenko and R. West, "Analytical solution for nonlinear Schrödinger vortex reconnection," *title of Low Temperature Physics*, vol. 132, 2003.

[21] Samuel J. Li, "Complex Function Plotter." [Online]. Available: `https://samuelj.li/complex-function-plotter/`

[22] W. Rudin, *Real and Complex Analysis*, 3rd ed. 1987.



Department of Mathematics, University of Verona