Lecture 5. The Gross-Pitaevskii model

- A. Scott, "Nonlinear Science" (Sec. 3.3)
- R. Ricca, "The hydrodynamics of the Gross-Pitaevskii equation" (Sec. 1, 2, 5, 8, 10)

The wave equation has solutions

$$\phi(x,t) = A\, e^{i(kx-\omega t)}, \quad \omega(k) = ck.$$

A general solution is an integral over Fourier components

$$\Phi(x,t) = \int F(k)\, e^{i[kx-\omega(k)t]}\, dk$$

where $F(k)$ are amplitudes depending on the initial condition.

Dispersion relation

A wave function has wave solutions with angular frequency ω and wave number k with

$$\omega = \omega(k).$$

Quadratic dispersion

Consider a localized wave form with main frequency ω_0 and dispersion, for ω close to ω_0,

$$\omega = \omega_0 + b_1(k - k_0) + b_2(k - k_0)^2 + \dots.$$

The wave form is

$$\Phi(x,t) = e^{i(k_0 x - \omega_0 t)} \int F(k)\, e^{i[(k-k_0)x - b_1(k-k_0)t - b_2(k-k_0)^2 t]}\, dk$$

where $e^{i(k_0 x - \omega_0 t)}$ is a *carrier wave*.
We are interested in the *envelope wave*

$$\phi(x,t) = \int F(\kappa + k_0)\, e^{i(\kappa x - b_1 \kappa t - b_2 \kappa^2 t)}\, d\kappa, \qquad \kappa = k - k_0.$$

Note that

$$\frac{\partial \phi}{\partial t} = \int -i(b_1\kappa + b_2\kappa^2) F(\kappa + k_0)\, e^{i(\kappa x - b_1 \kappa t - b_2 \kappa^2 t)}\, d\kappa = -b_1 \frac{\partial \phi}{\partial x} + i b_2 \frac{\partial^2 \phi}{\partial x^2}.$$

Second order in space, first order in time

Thus, ϕ satisfies the linear equation

$$i\left(\frac{\partial\phi}{\partial t} + b_1\frac{\partial\phi}{\partial x}\right) + b_2\frac{\partial^2\phi}{\partial x^2} = 0.$$

This is a wave equation with dispersion relation

$$\omega = b_1\kappa + b_2\kappa^2.$$

Exercise

Assume

$$\phi(x,t) = u(x,t)e^{i(rx-st)}$$

to find that (choose appropriate r, s)

$$u_t + b_2 u_{xx} = 0.$$

The Schrödinger equation

Matter at the microscopic scale is governed by the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V(\boldsymbol{r})\Psi$$

where $V(\boldsymbol{r})$ is a function depending on space (potential).

- m is the mass of a particle.
- $\hbar$ has dimensions of action (energy $\cdot$ time).

This is a type of wave equation.

Exercise (Constant potential)

(a) Show that, in one space dimension with V a constant potential, it admits solutions of the form $\Psi(x,t) = e^{i(x-vt)}$ *where* v *is constant. (b) Apply a transformation and eliminate the last term (in the case of constant V).*

Rationalisation

Example

Define normalised time and space variables and give the normalised form of the above Schrödinger equation. In one space dimension, this is

$$i\frac{\partial \Psi}{\partial \tau} = -\frac{\partial^2 \Psi}{\partial x^2} + \Psi$$

where x, τ are dimensionless variables.

Lecture 5b. Total number of particles

The total probability of finding a particle, or the total number of particles, is conserved

$$N = \int \Psi \Psi^* \, d^3x = \int |\Psi|^2 \, d^3x$$

where Ψ^* is the complex conjugate of $\Psi \in \mathbb{C}$.

$$\begin{aligned} \frac{d}{dt} \int \Psi \Psi^* \, dx &= \int \Psi^* \frac{d\Psi}{dt} + \Psi \frac{d\Psi^*}{dt} = \dots \\ &= i\frac{\hbar}{2m} \int (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) \, d\boldsymbol{S} = 0 \end{aligned}$$

where we assume that the field Ψ is constant at spatial infinity $[\nabla \Psi(x \to \pm\infty) = 0]$.

Ψ has dimensions $1/L^{3/2}$ where L is length.

The nonlinear Schrödinger equation

Assume that the potential is made by the atoms themselves

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + g|\Psi|^2\Psi$$

This model applies to

- The collective motion of atoms in superfluids
- Trapped photons which are strongly interacting
- Quasiparticles in semiconductors
- ...

Stationary states

Simple solutions of the equation are crucial in order to understand the qualitative behaviour of all its solutions and, consequently, the behaviour of the system that it models.

Stationary states

We assume the simple time dependence

$$\Psi(\boldsymbol{x}, t) = e^{-i\frac{\mu}{\hbar}t}\psi(\boldsymbol{x})$$

and obtain the eigenvalue problem

$$\mu\psi = -\frac{\hbar^2}{2m}\Delta\psi + g|\psi|^2\psi$$

A constant solution is $|\psi|^2 = \mu/g \equiv \rho$.

Rationalization of the nonlinear Schrödinger equation

Dimensionless form

Make the substitution $\Psi(\boldsymbol{x},t) = e^{-i\frac{\mu}{\hbar}t}\psi(\boldsymbol{x},t)$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + g|\psi|^2\psi - \mu\psi$$

Apply the transformations

$$\boldsymbol{x} \to \frac{\hbar}{(2m\mu)^{1/2}}\boldsymbol{x}, \qquad t \to \frac{\hbar}{2\mu}t, \qquad \psi \to \rho^{1/2}\psi$$

and obtain the dimensionless form

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta\psi + \frac{1}{2}(|\psi|^2 - 1)\psi$$

For all localized solutions of this equation $|\psi| \to 1$ as $|\boldsymbol{x}| \to \infty$.

Atoms confined in a potential

A harmonic potential

$$V(x,y,z) = \frac{1}{2} m\omega^2 r^2, \qquad r^2 = x^2 + y^2 + z^2.$$

The Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi + \frac{1}{2} m\omega^2 r^2 \psi - \mu\psi.$$

We make the transformations

$$\boldsymbol{x} \to \sqrt{\frac{\hbar}{m\omega}}\, \boldsymbol{x}, \qquad t \to \frac{t}{\omega}, \qquad \mu \to \hbar\omega\, \mu$$

and obtain the dimensionless form

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2} \Delta\psi + \frac{1}{2} r^2 \psi - \mu\psi.$$

We assume a nonlinear model with a harmonic potential.

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \frac{1}{2}m\omega^2 r^2\psi + G|\psi|^2\psi - \mu\psi.$$

We make the transformations

$$\boldsymbol{x} \to \alpha\,\boldsymbol{x}, \quad t \to \frac{t}{\omega}, \quad \mu \to \hbar\omega\,\mu, \quad \text{where } \alpha = \sqrt{\frac{\hbar}{m\omega}}$$

and we notice that we may rationalize ψ by

$$\psi \to \frac{\psi}{\alpha^{3/2}}.$$

Thus we obtain the dimensionless form

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta\psi + \frac{1}{2}r^2\psi + g|\psi|^2\psi - \mu\psi, \qquad g = \frac{G}{\hbar\omega\,\alpha^3} = \frac{Gm}{\hbar^2\omega\alpha}.$$

Lecture 5c. Hamiltonian formulation for continuous systems

The variational derivative

We have seen that, for a functional $F = \int \mathcal{F}(x, y, y_x)dx$, the functional derivative is

$$\frac{\delta F}{\delta y} = \frac{\partial \mathcal{F}}{\partial y} - \frac{d}{dx}\left(\frac{\partial \mathcal{F}}{\partial y_x}\right)$$

Hamilton's equations

Consider a pair of conjugate variables $\phi(x), \pi(x)$ and an energy functional $E = \int \mathcal{E}(\phi, \pi)dx$, then

$$\dot{\phi} = \frac{\delta E}{\delta \pi}, \qquad \dot{\pi} = -\frac{\delta E}{\partial \phi}.$$

Hamiltonian for the Nonlinear Schrödinger equation

Define the Hamiltonian functional

$$E = \frac{1}{2} \int \left[|\nabla\psi|^2 - |\psi|^2 + \frac{1}{2}|\psi|^4 \right] d^3x$$
$$= \frac{1}{2} \int \left[\nabla\psi\nabla\psi^* - \psi\psi^* + \frac{1}{2}(\psi\psi^*)^2 \right] d^3x.$$

The Nonlinear Schrödinger equation as a Hamiltonian system

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta\psi + \frac{1}{2}(|\psi|^2 - 1)\psi \Rightarrow i\dot{\psi} = \frac{\delta E}{\delta\psi^*}$$

We can prove that the energy functional is conserved.

We have to show that

$$\frac{dE}{dt} = \ldots = 0.$$

Example (Conjugate variables)

Identify the pair of conjugate variables for the Gross-Pitaevskii model.

Focusing and defocusing NLS

A more general version of the NLS is

$$i\dot{\psi} = -\frac{1}{2}\psi'' \pm \frac{1}{2}|\psi|^2\psi$$

where the dot denotes time derivative and the prime denotes space derivative.

- The equation with the (+) sign is called the *defocusing* NLS.
- The equation with the (-) sign is called the *focusing* NLS.

Localized solution of the defocusing NLS in one space dimension

The static NLS in one dimension

We assume $\psi = \psi(x)$ satisfying the normalized equation

$$\psi'' + (1 - |\psi|^2)\psi = 0.$$

We are searching for solutions such that $\psi(x) \to \pm 1$ as $x \to \pm\infty$ (localized solutions).

Exercise (Static soliton in NLS)

Integrate the static NLS. The solution is of the form

$$\psi(x) = \tanh(cx)$$

where c is a constant (determine the constant).

Traveling solution of the defocusing NLS

The NLS in one dimension

We have $\psi = \psi(x,t)$ satisfying

$$i\dot{\psi} = -\frac{1}{2}\psi'' + \frac{1}{2}(|\psi|^2 - 1)\psi$$

where the dot denotes time derivative and the prime denotes space differentiation.

We are searching for solutions such that $|\psi(x,t)| \to 1$ as $x \to \pm\infty$ (localized solutions).

The traveling wave ansatz

We assume $\psi(x,t) = \psi(\xi)$ with $\xi = x - vt$ satisfying

$$\frac{1}{2}\psi'' - iv\psi' - \frac{1}{2}(|\psi|^2 - 1)\psi = 0$$

where the prime denotes differentiation with respect to ξ.

Exercise

Find traveling wave solutions of the NLS in the form

$$\psi(\xi) = ic_1 + c_2 \tanh(c_3 \xi).$$

We have

$$\psi(x,t) = i\sin\theta - \cos\theta\, \tanh\left[\frac{\cos\theta}{2}(x + \sin\theta\, t)\right], \quad 0 \le \theta < 2\pi.$$

Localized solution of the focusing NLS in one space dimension

The static NLS in one dimension

Let $\psi = \psi(x,t)$ satisfying the equation

$$i\dot{\psi} = -\frac{1}{2}\psi'' - \frac{1}{2}|\psi|^2\psi.$$

Assume

$$\psi(x,t) = e^{i\frac{\mu}{2}t}u(x)$$

where u satisfies

$$u'' + (|u|^2 - \mu)u = 0.$$

Exercise (Static soliton in NLS)

The solution is of the form

$$\psi(x) = \sqrt{2}\alpha\, e^{i\frac{\alpha^2}{2}t}\,\mathrm{sech}(\alpha x)$$

where α is an arbitrary parameter.

Traveling solution of the focusing NLS

Exercise (A transformation)

Show that if $\psi(x,t)$ is a solution of the focusing NLS then a traveling solution is

$$\exp\left[i\frac{v_e}{2}\left(x-\frac{v_e}{2}t\right)\right]\psi(x-v_e t,t)$$

where v_e is a constant (a velocity).

Since $\psi \in \mathbb{C}$ we may write

$$\psi(x, y) = \rho(x, y)\, e^{i\Theta(x,y)}$$

where ρ is the modulus and Θ the argument of the complex variable.

Sometimes, it is convenient to work in polar coordinates (r, θ) and look for functions $\rho = \rho(r)$. We need the Laplacian in polar coordinates

$$\Delta\psi = \frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}$$

Vortex solutions

Let us assume the form

$$\psi(r,\theta) = \rho(r)\, e^{i\theta}.$$

The function $\rho(r)$ satisfies

$$\Delta\psi + (1 - |\psi|^2)\psi = 0 \Rightarrow \rho'' + \frac{\rho'}{r} - \frac{\rho}{r^2} + \rho(1-\rho^2) = 0.$$

The boundary condition at spatial infinity has to be

$$\rho(r) \to 1, \qquad \text{as } r \to \infty.$$

At the origin, we must have

$$\rho(r=0) = 0,$$

since, if $\rho(0) \neq 0$ then ψ would be multivalued.

Flow velocity

The continuity equation is

$$\frac{\partial}{\partial t}(\psi\psi^*) + i\frac{\hbar}{2m}\boldsymbol{\nabla}(\psi\boldsymbol{\nabla}\psi^* - \psi^*\boldsymbol{\nabla}\psi) = 0.$$

The density is

$$n = \psi\psi^*.$$

The flow velocity $\boldsymbol{v}$ is identified from

$$n\boldsymbol{v} = i\frac{\hbar}{2m}(\psi\boldsymbol{\nabla}\psi^* - \psi^*\boldsymbol{\nabla}\psi).$$

In one space dimension

$$v = \frac{\hbar}{m}\partial_x\Theta \qquad \text{or} \quad \boldsymbol{v} = \boldsymbol{\nabla}\Theta \quad \text{(3D, dimensionless)}$$