Solitons in Bose-Einstein condensates

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A. HEUCHAMPS

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Introduction

The idea of Bose-Einstein condensation dates back from the mid-1920s, when a Bengali scientist, S. N. Bose, derived a new way to get the blackbody radiation law proposed by M. Planck in 1900. The originality of Bose's work was in the way of counting the repartition of the photons emitted by the body, which he considered to be undistinguishable particles, among the different discrete energy levels of the system. Even though it was a ground-breaking discovery that would lead to a whole new physics, the importance of his work was underestimated at the time, and Bose could not get his work published. As a last attempt to reach publication in a scientific review, he contacted A. Einstein, which personally translated Bose's article and got it published in a prominent German revue.

Einstein contribution went further than just helping a quite unknown physicist to get his work published. Indeed, in 1924 and 1925, he extended Bose's work to take into account the mass of the particles. Such an extension let to a curious behaviour: under a given temperature, a macroscopic amount of particles would populate the lowest-energy state of the system. The condensation phenomenon was discovered.

While a whole new class of physics had been discovered, it was not directly understood by the physicists community, and the mechanisms leading to the condensation phenomenon were not directly understood, as is well expressed by Einstein's statement[25]

> "The difference between Boltzmann and Bose-Einstein statistics expresses indirectly a certain hypothesis on a mutual influence of the molecules which for the time being is of a quite mysterious nature."

Later on, it would be understood that the mysterious influence between particles mentioned by Einstein arises from the fact that the Hilbert space in which the particles' wavefunctions are defined had to be entirely symmetric with respect to particles permutations (which is nowadays known as the *symmetry postulate*). This requirement that the wavefunctions have to verify lie at the core of statistical quantum mechanics and is responsible, among other things, for the process of stimulated emission[10].

Since the temperature at which the condensation takes places, derived by Einstein, is very low, the Bose-Einstein condensation phenomenon was long considered to be nothing more than a theoretical curiosity. It is only in 1938 that F. London suggested that the superfluidity of ^{4}He was a manifestation of Bose-Einstein condensation[22], which brought, for the first time, the idea that a quantum phenomenon (*i.e.* the Bose-Einstein condensation) could manifest itself on a macroscopic size. Later on, other intriguing phenomena such as superconductivity or LASERs would be described as a kind of condensation, highlighting the fact that quantum mechanical effects could be observed on macroscopic scales.

The first experimental realisations of Bose-Einstein condensation were realized in very dilute alkali gases. More specifically, the first BEC were realized with ^{87}Rb[3], ^{7}Li[6], and ^{23}Na[12] in

1995, and became possible because the trapping and cooling techniques needed to reach the ultralow temperature required for the BEC realization, had been dramatically improved since Einstein's seminal paper in 1925, and those realisation led to the physics Nobel prize in 2001.

Besides the very low temperature required to reach the condensate state, another requirement has to be fulfilled: the gas has to be very dilute. This requirement comes from the fact that at such low temperatures as what is required to observe a condensate, a gaseous state could not exist: indeed, the system would rather exhibit a phase transition to the liquid, or solid, state. Such a phase transition is mainly due to recombinations and three-body collisions, which become quite seldom if the gas is sufficiently diluted. Because of the scarcity of such three-body recombinations, the gaseous state can be obtained over quite long timescales: the system is said to be in a metastable equilibrium. Another interesting point is that, at such low temperatures as what is needed to reach the condensate, the pairwise interactions between the particles of the gas can all be taken into account through a single parameter, called the *scattering length* of the atom.

In fact, the presence of interactions between particles blur a bit the idea of condensate with respect to what was first imagined. Indeed, in the case of a non-interacting gas, all the constitutive particles occupy the fundamental energy state at 0 K. If interactions are taken into account, all the particles do not occupy that state, even at the absolute 0. However, for a sufficiently low temperature, the fraction of particles not in the condensate (the so-called uncondensed particles) is small, and the system can be described by a single wavefunction.

Because the fraction of uncondensed particles is small, the gas can be described thanks to the Hartree ansatz (which considers that all the particles occupy the same state), which leads to an evolution equation for the wavefunction of the function known as the *Gross-Pitaevskii* equation, which is a particular form of the more general *Nonlinear Schrödinger equation*. That nonlinear equation is an universal equation used to model the time-evolution of complex envelope-fields in nonlinear dispersive media. In particular, the Nonlinear Schrödinger equation is used to compute the time-evolution of light pulses in optical fibres, or the evolution of optical *solitons* in Kerr-like media. The fact that the system can be described by the Gross-Pitaevskii equation (which is an effective mean-field theory) considerably simplifies the problem, since the results provided by that approximation are in very good agreement with experiments, which means that the full many-body Schrödinger equation has not necessarily to be fully solved.

Even though the Gross-Pitaevskii equation has been presented in the particular context of Bose-Einstein condensation, its range of applications is broader. Indeed, a similar equation appears in other fields of physics, such as nonlinear optics (through a certain form of Nonlinear Schrödinger equation), in biology, or even plasma physics. This highlights the fact that research on Bose-Einstein condensates is in fact quite general, and spans over multiple fields of nowadays physics.

Because of its nonlinear aspect, the GPE can give rise to peculiar behaviours of the solutions, one of which being the solitons. Such solitonic solutions have the counter-intuitive to travel in space without distortion, as opposed to regular waves (thing of water waves at the surface of a lake). In fact, such a behaviour is not specific to solitons, it only characterizes solitary waves. In order for a solitary wave to be called a soliton, it should also exhibit the property to come undistorted from a collision with another soliton. The first observation of solitonic waves dates back to 1885, when a Scottish scientist (John S. Russell) observed that a boat dragged in a narrow canal gave rise to a wave that travelled for miles without distortion, as is emphasized by Russel's saying

> "I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the

prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation."

Solitons can be of two different kinds: indeed, they can be either dark/grey or bright. The first ones are characterized by a zero density (for dark) or a density dip (for grey) at a given point, hence the name (a dark soliton can be associated to a "hole" in the density). At the point of minimum density, the phase also exhibit a sharp jump as its exhibit a tanh profile (which flattens when the speed of the soliton increases). In opposition to those dark/grey solitons, are the bright solitons, which are characterized by a maximum in the density. Such structures are well known in the community of people concerned with nonlinear optics, but it is only recently that those structures were observed in Bose-Einstein condensates, since the first observation of bright solitons in BECs dates back from 2002 [34, 19].

Those solitons are solutions to the Gross-Pitaevskii equation. Their type (dark/bright) depends upon the sign of the interactions between the atoms: repulsive interactions means a positive scattering length, and lead to dark solitons, whereas a negative scattering length means attractive interactions, which leads to bright solitons. An interesting point with Bose-Einstein condensates is that the interactions between atoms can be tuned thanks to a process called *Feshbach resonance*, and allow thus to study both types of solitons.

Even though the interactions between atoms can be tuned as desired in a Bose-Einstein condensate, the case of bright solitons has to be treated carefully, since the dimensionality of the system shows to be crucial. Indeed, in three dimensions, a condensate of atoms interacting attractively is not stable, and collapses. In lower dimensions, the picture is different: in two dimensions, a gas consisting of atoms interacting attractively can exist if the number of atoms in the condensate does not exceed a critical value. In one dimension, bright solitons can appear. Such gases in reduced dimensions can be realized experimentally if the confining potential along one or two spatial dimensions is much bigger than the others.

In order to explore the link between Bose-Einstein condensation and solitons, the work is organized as follow

- In chapter one, the Bose-Einstein condensation phenomenon in 3D is discussed. After having briefly introduced some concepts and notations of second quantisation, the case of ideal gas condensation is discussed. It will be shown that even in that most simple case, the effect of a confining potential brings some mathematical difficulties. From there, the concepts are extended to interacting gases. It will be shown that the effect of interactions drastically modifies the behaviour of the gas, even in the case where there is no confining potential, as was already noted here above.

- In chapter two, the effect of dimensionality reduction will be briefly discussed. Such a reduction is made possible by the fact that the confining potential can be made very asymmetric, leading to quasi-1D and 2D configurations. Even if there is no condensation possible above strictly 0 K (Hohenberg theorem), an interesting effect can nevertheless take place: a sharp transition to a quasi-condensed case. Such a transition is known as

the Berezinski-Kosterlitz-Thoules transition, the system manifests superfluid properties. Other interesting effects can take place, such as the Josephson effect, or even a transition to another regime, where the gas of bosons behaves like a gas of fermions. This particular regime is called the Tonks-Girardeau regime, but will not be discussed in the following.

- In chapter three, the problematic of solitons will be addressed. After having introduced the concept of solitary wave and soliton, the case of dark and bright solitons will be discussed separately. For the dark soliton, an analytic study will be performed, and lead to the conclusion that the center-of-mass of such a soliton can be interpreted as a classical particle. For the bright soliton, a numerical study is performed. In particular, it will be shown that a spectral method for the time discretization, coupled with a finite difference scheme for the spatial discretization of the Gross-Pitaevskii does not lead to a solution that fits the analytical one, because of the interaction term.

Bose-Einstein condensation in 3D

Introduction

In this chapter, the basics about Bose-Einstein condensation in three dimensions will be reviewed. Starting from general considerations regarding the condensation phenomenon, the concepts will be applied to more precise cases, such as the ideal Bose gas, with and without confinement, or to the case of an interacting gas described by a mean field theory.

1.1 The ideal Bose gas

As a gas of non-interacting bosonic particles at thermal equilibrium is considered, the system as to be coupled with an external reservoir, which function is to ensure thermalization. In that case, the gas is described, in the grand-canonical ensemble, by the equilibrium N-body density matrix

$$\hat{\rho} = \frac{1}{\mathcal{Y}} \exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right], \tag{1.1}$$

with $\beta = \frac{1}{k_B T}$ the thermal energy contained in the system (k_B being the Boltzmann constant and T the temperature of the system), $\hat{H}$ the Hamiltonian of the system, μ the chemical potential, and $\hat{N}$ the operator giving the number of particles in the system. The prefactor $\mathcal{Y}$ ensure the normalization of the density matrix $\mathrm{Tr}\left(\hat{\rho}\right) = 1$, hence

$$\mathcal{Y} = \mathrm{Tr}\left\{\exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right]\right\}.$$

Depending on whether the gas is free or trapped, the Hamiltonian takes different forms, namely (using the second quantization formalism)

$$\hat{H} = \int \hat{\Psi}^{\dagger}\left(\boldsymbol{r}, t\right)\left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2\right]\hat{\Psi}\left(\boldsymbol{r}, t\right)\mathrm{d}\boldsymbol{r}, \qquad \text{(free ideal gas)} \tag{1.2a}$$

$$\hat{H} = \int \hat{\Psi}^{\dagger}\left(\boldsymbol{r}, t\right)\left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + V_{\mathrm{trap}}\left(\boldsymbol{r}\right)\right]\hat{\Psi}\left(\boldsymbol{r}, t\right)\mathrm{d}\boldsymbol{r}, \qquad \text{(trapped ideal gas)} \tag{1.2b}$$

The point with the density matrix is that encodes all the information about the system: thanks to that operator, all the thermodynamic quantities (such as the mean energy of the system, the specific heat, etc.) can be computed.

Another interesting (if not crucial) point about the density matrix, is that it gives an information on whether a condensate can be realized in a certain state or not. Indeed, according

to [26], a Bose-Einstein condensate is realized in the state corresponding to a macroscopically big[1] eigenvalue of the one-body density matrix, given by

$$\hat{\rho}^{(1)} = N \operatorname{Tr}_{2,\ldots,N} [\hat{\rho}].$$

Choosing a base in which that operator is diagonal, it can be rewritten under the form

$$\hat{\rho}^{(1)} = \sum_k n_k |\phi_k\rangle\langle\phi_k|, \tag{1.3}$$

where the n_k's are the different eigenvalues and the $|\phi_k\rangle$ the corresponding eigenstates. That operator can also be used to encode information about the system, such as its density or coherence. Indeed, by using a space representation of the one-body density matrix, given by

$$\rho(\boldsymbol{r}, \boldsymbol{r}', t) = \langle \boldsymbol{r}' | \hat{\rho}^{(1)} | \boldsymbol{r} \rangle = \left\langle \hat{\Psi}^\dagger(\boldsymbol{r}, t) \hat{\Psi}(\boldsymbol{r}', t) \right\rangle, \tag{1.4}$$

or a momentum representation (linked to the previous one through a Fourier transform), insight on the influence of a particle located at $\boldsymbol{r}$ on another particle located at $\boldsymbol{r}'$ can be found. Moreover, the relation appearing in (1.4) is very general, in the sense that it applies to any kind of system, independent of the statistics at play, and even in out-of-equilibrium situation.

At this point, it is interesting to emphasize that the diagonal terms of the density matrix obey to the normalization condition $\int \rho(\boldsymbol{r}, t)\, \mathrm{d}\boldsymbol{r} = N$, and that the information on the coherence given by the out-of-diagonal terms is crucial when it comes to matter waves.

1.2   The field operator

In all the previous discussion, the field operator $\hat{\Psi}(\boldsymbol{r})$ has been used, and it is thus time to introduce it in a more formal way. Using the same basis as in (1.3) that diagonalizes the one-body density matrix, the creation and destruction field operators $\hat{\Psi}^\dagger(\boldsymbol{r})$ and $\hat{\Psi}(\boldsymbol{r})$ take the form

$$\hat{\Psi}^\dagger(\boldsymbol{r}) = \sum_k \hat{a}_k^\dagger \phi_k^*(\boldsymbol{r}) \quad \text{and} \quad \hat{\Psi}(\boldsymbol{r}) = \sum_k \hat{a}_k \phi_k(\boldsymbol{r}),$$

where $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators, defined through the relations

$$\hat{a}_k |n_0, n_1, \ldots, n_k, \ldots\rangle = \sqrt{n_k + 1} |n_0, n_1, \ldots, n_k + 1, \ldots\rangle$$
$$\hat{a}_k^\dagger |n_0, n_1, \ldots, n_k, \ldots\rangle = \sqrt{n_k} |n_0, n_1, \ldots, n_k - 1, \ldots\rangle,$$

where n_k is the occupation number of the single-particle state $|\phi_k\rangle$, and verifying the commutation relations

$$\left[\hat{a}_k, \hat{a}_{k'}^\dagger\right] = \delta_{k,k'}, \quad [\hat{a}_k, \hat{a}_{k'}] = \left[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\right] = 0 \quad \forall \, k, k'. \tag{1.5}$$

Combining the definition of the field operators with the expression (1.4), and using the relation $n_k = \left\langle \hat{a}_k^\dagger \hat{a}_k \right\rangle$, the space representation of the one-body density matrix takes the form

$$\rho(\boldsymbol{r}, \boldsymbol{r}') = \sum_k n_k \phi_k^*(\boldsymbol{r}) \phi_k(\boldsymbol{r}').$$

Assuming only the state $|\phi_0\rangle$ is macroscopically populated, with a population n_0, this last representation can be conveniently rewritten under the form

$$\rho(\boldsymbol{r}, \boldsymbol{r}') = n_0 \phi_0^*(\boldsymbol{r}) \phi_0(\boldsymbol{r}') + \sum_{k \neq 0} n_k \phi_k^*(\boldsymbol{r}) \phi_k(\boldsymbol{r}'),$$

---

[1]Macroscopically big has to be understood as *being of the order of N, i.e.* $\mathcal{O}(N)$

highlighting the fact that a Bose-Einstein condensate is realized in that state. The field operator associated to that last expression writes

$$\hat{\Psi}\left(\boldsymbol{r}\right) = \hat{a}_0 \phi_0\left(\boldsymbol{r}\right) + \sum_{k \neq 0} \hat{a}_k \phi_k\left(\boldsymbol{r}\right).$$

An attentive reader has probably noted that up to now, the discussed field operators do not have a time dependence, as opposed to the field operators appearing in eqs. (1.2a) and (1.2b). This comes from the generalization of the Bogoliubov approximation, consisting in writing the field operators as the combination of a classical field and a perturbation, *i.e.*

$$\hat{\Psi}\left(\boldsymbol{r}, t\right) = \Psi_0\left(\boldsymbol{r}, t\right) \hat{\mathbb{I}} + \delta\hat{\Psi}\left(\boldsymbol{r}, t\right),$$

with $\Psi_0\left(\boldsymbol{r}, t\right) = \left\langle \hat{\Psi}\left(\boldsymbol{r}, t\right) \right\rangle$ and $\delta\hat{\Psi}\left(\boldsymbol{r}, t\right)$ represents the non-condensed part of the system. In the case of a dilute ultracold gas (for a temperature reaching 0 K), that last part can be neglected, and the field operator acts exactly as a classical field[2]. It has to be noted that the replacement of the condensate fraction by a classical *c*-number is valid only in the case of a big number of particles, *i.e.* $N \gg 1$.

1.3 Derivation of thermodynamic properties

It was previously stated that the density matrix, defined in (1.1), encodes all the information about the considered system. In the following, that statement will be proved to be correct by computing some of the thermodynamic properties of the gas.

1.3.1 Occupation number

The first quantity to compute is the occupation number of an energy level. Even though its detailed expression is different for a free gas or a trapped one, its general expression stays the same, and will be shown to read

$$n_{\vec{l}} = \frac{1}{\exp\left[\beta\left(\epsilon_{\vec{l}} - \mu\right)\right] - 1}, \tag{1.6}$$

with $\epsilon_{\vec{l}}$ the energy level corresponding to the set of quantum numbers $\vec{l} = (l_x, l_y, l_z)$, and where the other quantities have the same meaning as previously.

Choosing a base in which the Hamiltonian $\hat{H}$ is diagonal and using the relation $\hat{N} = \sum_k \hat{a}_k^\dagger \hat{a}_k$, the different terms appearing in the expression of the density matrix take the form

- the numerator is written under the form

$$\exp\left[-\beta\left(\hat{H} - \mu\hat{N}\right)\right] = \exp\left[-\beta \sum_{k=0}^{+\infty}\left(\epsilon_k \hat{a}_k^\dagger \hat{a}_k - \mu \hat{a}_k^\dagger \hat{a}_k\right)\right]$$

$$= \prod_{k=0}^{+\infty} \exp\left[-\beta\left(\epsilon_k - \mu\right) \underbrace{\hat{a}_k^\dagger \hat{a}_k}_{\hat{n}_k}\right]$$

---

[2]Neglecting the non-condensed part of the gas is equivalent to the classical limit in quantum electrodynamics, where the quantum fields are replaced by the classical electric and magnetic fields.

- the denominator is written under the form

$$\text{Tr}\left\{\exp\left[-\beta\left(\hat{H}-\mu\hat{N}\right)\right]\right\} = \sum_{n_0,n_1,\ldots} \langle n_0,n_1,\ldots|\exp\left[-\beta\left(\hat{H}-\mu\hat{N}\right)\right]|n_0,n_1,\ldots\rangle$$

$$= \sum_{n_0,n_1,\ldots}\prod_{k=0}^{+\infty}\exp\left[-\beta\left(\epsilon_k-\mu\right)\underbrace{\hat{a}_k^\dagger\hat{a}_k}_{\hat{n}_k}\right]\langle n_0,n_1,\ldots|n_0,n_1,\ldots\rangle.$$

In the last expression, after the permutation of the series and the product, a geometric progression is recognized. Gathering the results together, and evaluating $\langle\hat{\rho}\rangle = \langle n_0,n_1,\ldots|\hat{\rho}|n_0',n_1',\ldots\rangle$ yields

$$\langle\hat{\rho}\rangle = \prod_{k=0}^{+\infty}\frac{1}{\mathcal{Y}_k}\exp\left[-\beta\left(\epsilon_k-\mu\right)n_k\right]\delta_{n_k n_{k'}},\quad \mathcal{Y}_k{}^3 = \frac{1}{1-\exp\left[-\beta\left(\epsilon_k-\mu\right)\right]}.$$

Continuing from there, the mean value of the occupation number can be computed thanks to the expression $\overline{\langle\hat{n}_k\rangle} = \text{Tr}\left[\hat{\rho}\hat{a}_k^\dagger\hat{a}_k\right]$. Combining the expression of the density matrix expressed in the eigenbasis of the Hamiltonian with the invariance of the trace to a cyclic permutation of its arguments and the relation

$$\hat{a}_k^\dagger\hat{a}_k\hat{\rho} = -\frac{1}{\beta\mathcal{Y}_k}\frac{\partial}{\partial\epsilon_k}\exp\left[-\beta\left(\epsilon_k-\mu\right)\hat{a}_k^\dagger\hat{a}_k\right]\prod_{k'\neq k}\exp\left[-\beta\left(\epsilon_{k'}-\mu\right)\hat{a}_k^\dagger\hat{a}_k\right],$$

the sought statistical mean value of the occupation number of the energy level $\epsilon_{\vec{k}}$, given by $\overline{\langle\hat{n}_k\rangle} = \sum_{n_0,n_1,\ldots}\langle n_0,n_1,\ldots|\hat{a}_k^\dagger\hat{a}_k\hat{\rho}|n_0,n_1,\ldots\rangle$ can finally be computed

$$\overline{\langle\hat{n}_k\rangle} = \sum_{n_0,n_1,\ldots}\langle n_0,n_1,\ldots|\hat{a}_k^\dagger\hat{a}_k\hat{\rho}|n_0,n_1,\ldots\rangle$$

$$= -\frac{1}{\beta\mathcal{Y}_k}\frac{\partial}{\partial\epsilon_k}\mathcal{Y}_k = \frac{1}{\beta}\frac{\partial}{\partial\epsilon_k}\ln\left(\frac{1}{\mathcal{Y}_k}\right)$$

$$\stackrel{\epsilon_k\geq\mu}{=}\frac{1}{\beta}\frac{\partial}{\partial\epsilon_k}\ln\left[1-e^{-\beta(\epsilon_k-\mu)}\right]$$

$$= \frac{1}{\exp\left[\beta\left(\epsilon_k-\mu\right)\right]-1}$$

It should be noted that in the previous derivations, the splitting of the mean value of the density operator $\langle\hat{\rho}\rangle$ into a product of different, independent, components highlights the fact that the eigenstates of the Hamiltonian can be seen as independent systems, all connected to the same reservoir.

1.3.2   Mean number of particles in the system

After having derived the occupation number of the different energy levels in the system, the number of particles contained in that system can be computed. By definition, that quantity is given by

$$\overline{\left\langle\hat{N}\right\rangle} = \sum_{\vec{l}}\frac{1}{\exp\left[\beta\left(\epsilon_{\vec{l}}-\mu\right)\right]-1}. \tag{1.7}$$

Since the expression for the energy $\epsilon_{\vec{l}}$ depends on whether the gas is free or not, those cases have to be treated separately.

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[3]The expression of such a "partial" partition function is valid only if $|\exp\left[-\beta\left(\epsilon_k-\mu\right)\right]| < 1 \Leftrightarrow \epsilon_k > \mu\ \forall k$

The free gas

It is well known that the energy of a free perfect gas is purely kinetic, which means

$$\epsilon_{\vec{l}} = \frac{\|\vec{P}\|^2}{2m}, \quad \vec{P} = \frac{2\pi\hbar}{L}\vec{l}.$$

Inserting that expression for the energy in the statistical mean value of the number of particles in the system given by the relation (1.7) yields a complicated expression to compute analytically. However, if the computations are made on an infinite volume, the successive terms in the series do not change drastically from one to the other (since $\|\vec{k}\|^2 \propto 1/L^2$, and $L \to +\infty$), and the series can be replaced by a Riemann integral.

Changing the integration domain of the Riemann integral from $\mathrm{d}\vec{l}$ to $\mathrm{d}\vec{P}$, the mean number of particles present in the system is given by

$$\overline{\left\langle \hat{N} \right\rangle} = \frac{V}{(2\pi\hbar)^3} \int \frac{\mathrm{d}\vec{P}}{\exp\left[\beta\left(\frac{\|\vec{P}\|^2}{2m} - \mu\right)\right] - 1}.$$

To proceed further in the computations, it can be noted that the integrand is a geometric series, provided that $\mu < \epsilon_{\vec{0}}$ (which is in good agreement with physical intuition since the occupation levels (1.6) cannot be negative). If the condition is fulfilled, the integrand can be replaced by $\sum_{l=1}^{+\infty} \exp\left[-\beta l\left(\frac{\|\vec{P}\|^2}{2m} - \mu\right)\right]$, and the integration would finally give

$$\overline{\left\langle \hat{N} \right\rangle} = \frac{V}{(2\pi\hbar)^3} \sum_{l=1}^{+\infty} \left(\frac{2\pi m}{\beta l}\right)^{3/2} \exp\left(l\beta\mu\right).$$

Introducing the thermal de Broglie wavelength $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$, dividing by the volume (to get an intensive quantity that is not affected by the limit $V \to +\infty$), and using the definition of the Bose function

$$g_p(z) = \frac{1}{\Gamma(p)} \int_0^{+\infty} \frac{x^{p-1}}{z^{-1}e^x - 1}\mathrm{d}x = \sum_{l=1}^{+\infty} \frac{z^l}{l^p},$$

the mean density of the free ideal gas is given by $\overline{\langle \hat{n} \rangle} = \frac{g_{3/2}\left(e^{\beta\mu}\right)}{\lambda_T^3}$.

A legit question to ask is under which temperature the condensate begins to form. To find that expression, the total number of particles in the system is written

$$\overline{\left\langle \hat{N} \right\rangle} = \overline{\left\langle \hat{N}_0 \right\rangle} + \overline{\left\langle \hat{N}' \right\rangle},$$

with $\overline{\left\langle \hat{N}' \right\rangle}$ the non-condensed particles, given by $\overline{\left\langle \hat{N}' \right\rangle} = \sum_{\vec{l} \neq \vec{0}} \frac{1}{\exp\left[\beta(\epsilon_{\vec{l}} - \mu) - 1\right]}$. As the condensate is reached for $\mu \to \epsilon_{\vec{0}} = 0$, the number of non-condensed particles is bounded by a non-infinite value $\overline{\left\langle \hat{N}'_{\max} \right\rangle}$, found by imposing that μ reaches its maximum value (*i.e.* $\mu = 0$ in this case).

The critical temperature above which no particles are in the condensate can then be found by noting that, in that case, $N = N'_{\max}$, which leads to

$$\overline{\left\langle \hat{N} \right\rangle} = \frac{V}{(2\pi\hbar)^3} \sum_{l=1}^{+\infty} \left(\frac{2\pi m}{\beta l}\right)^{3/2} = \zeta(3/2)\frac{V}{\lambda_{T_c}^3}, \tag{1.8}$$

which can be inverted to give the expression of the critical temperature T_c, given in this case by $T_c = \frac{2\pi\hbar^2}{mk_B}\left[\frac{n}{\zeta(3/2)}\right]^{1/3}$. Another information can be extracted from relation (1.8): when $T = T_c$, the mean distance between the atoms is of the order of the thermal de Broglie wavelength, which corresponds to the entrance in the quantum degenerate regime, where the wavefunctions of the atoms begin to overlap.

The trapped gas

For a gas trapped by an harmonic-like potential of the form $V_{\text{trap}} = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$, the different energy levels are given by

$$\epsilon_{\vec{l}} = \left(l_x + \frac{1}{2}\right)\hbar\omega_x + \left(l_y + \frac{1}{2}\right)\hbar\omega_y + \left(l_z + \frac{1}{2}\right)\hbar\omega_z.$$

The same approach as that used in the case of the free gas can be used to determine the number of particles in the system. However, another path will be followed here, which has the advantage to give a first order correction to that number of particles. For convenience, a new chemical potential $\tilde{\mu}$, including the zero point energy, is defined, $i.e.$ $\tilde{\mu} = \mu - \frac{\hbar}{2}\left(\omega_x + \omega_y + \omega_z\right)$, which leads to the expression

$$n_{\vec{l}} = \frac{1}{\exp\left[\beta\hbar\left(l_x\omega_x + l_y\omega_y + l_z\omega_z\right) - \tilde{\mu}\right] - 1}$$
$$= \frac{1}{\frac{1}{z}\exp\left[\beta\hbar\left(l_x\omega_x + l_y\omega_y + l_z\omega_z\right)\right] - 1}, \quad \text{with } z = \exp\left(\beta\tilde{\mu}\right).$$

The number of particles not in the ground state, N', is bounded from above by the quantity N'_{max}, yielding the inequality

$$\underbrace{\sum_{\vec{l}\neq\vec{0}}\left\{\frac{1}{z}\exp\left[\beta\hbar\left(l_x\omega_x + l_y\omega_y + l_z\omega_z\right)\right] - 1\right\}^{-1}}_{N'} < \underbrace{\sum_{\vec{l}\neq 0}\left\{\exp\left[\beta\hbar\left(l_x\omega_x + l_y\omega_y + l_z\omega_z\right)\right] - 1\right\}^{-1}}_{N'_{\text{max}}},$$

where, for the upper bound, z has been put equal to 1 since the sum excludes the state $\vec{l} = \vec{0}$. The upper bound N'_{max} can be evaluated more formally by writing

$$N'_{\text{max}} = \sum_{\vec{l}\neq\vec{0}}\left[\exp\left(\beta\hbar\sum_{\alpha\in\{x,y,z\}}l_\alpha\omega_\alpha\right) - 1\right]^{-1}$$
$$= \sum_{l_x\neq 0}\sum_{l_y\neq 0}\sum_{l_z\neq 0}\sum_{k=1}^{+\infty}\exp\left(k\beta\hbar l_x\omega_x\right)\exp\left(k\beta\hbar l_y\omega_y\right)\exp\left(k\beta\hbar l_z\omega_z\right).$$

In this last expression, by permuting the series over k with those over the different l's, N'_{max} can be re-expressed as

$$N'_{\text{max}} = \sum_{k=1}^{+\infty}\frac{1}{1 - \exp\left(-k\beta\hbar\omega_x\right)}\frac{1}{1 - \exp\left(-k\beta\hbar\omega_y\right)}\frac{1}{1 - \exp\left(-k\beta\hbar\omega_z\right)}. \qquad (1.9)$$

Such an expression can not be easily computed. However, it can be simplified if the different arguments of the different exponentials are small, which amounts to considering the semiclassical description of the excited states. Combining that approximation with

$$1 = o\left[\frac{1}{1 - \exp\left(-x\right)}\right] \qquad\qquad (x \to 0)$$

$$\frac{1}{1 - \exp\left(-x\right)} \sim \frac{1}{x\left(1 - \frac{x}{2}\right)} \qquad\qquad (x \to 0)$$

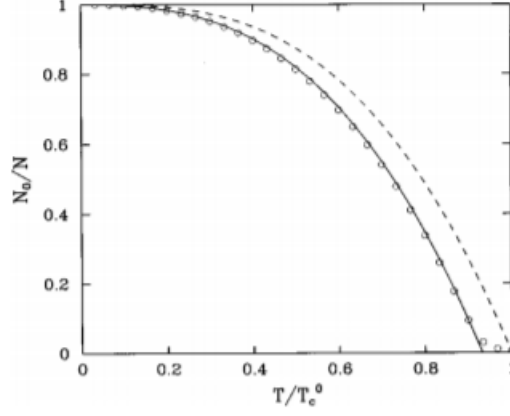$$(1 + ax)^n \sim 1 + nax \qquad\qquad (x \to 0),$$

Figure 1.1 – Condensed fraction as a function of temperature for an ideal trapped gas. The circles correspond to an exact computation with $N=1000$ in a spherically symmetric trap ($\omega_x = \omega_y = \omega_z$). The dashed and solid lines correspond to relations (1.10a) and (1.10b), respectively. Image from [9].

the expression appearing in (1.9) can be written under the form

$$N'_{\max} = \left(\frac{k_B T}{\hbar}\right)^3 \frac{1}{\omega_x \omega_y \omega_z} \sum_{k=1}^{+\infty} \frac{1}{k^3}\left(1 + \frac{k\beta\hbar\omega_x}{2}\right)\left(1 + \frac{k\beta\hbar\omega_y}{2}\right)\left(1 + \frac{k\beta\hbar\omega_z}{2}\right).$$

Keeping only the first two orders of that approximation, $N'_{\max}$ takes the form

$$N'_{\max} = \frac{1}{\omega_x \omega_y \omega_z}\left(\frac{k_B T}{\hbar}\right)^3 \zeta(3) \qquad\qquad\qquad \text{(at first order)}$$

$$N'_{\max} = \frac{1}{\omega_x \omega_y \omega_z}\left(\frac{k_B T}{\hbar}\right)^3 \zeta(3) + \frac{\omega_x + \omega_y + \omega_z}{2\omega_x \omega_y \omega_z}\left(\frac{k_B T}{\hbar}\right)^2 \zeta(2), \qquad \text{(at second order)}$$

and the condensed fraction can be computed, and is given by [9]

$$\frac{N_0}{N} \approx \frac{N - N'_{\max}}{N} = 1 - \left(\frac{T}{T_c^0}\right)^3 \qquad\qquad\qquad\qquad \text{(at first order)}$$

$$\tag{1.10a}$$

$$\frac{N_0}{N} \approx \frac{N - N'_{\max}}{N} = 1 - \left(\frac{T}{T_c^0}\right)^3 - \frac{\zeta(2)}{2}\frac{\omega_x + \omega_y + \omega_z}{\sqrt[3]{\omega_x \omega_y \omega_z \zeta^2(3)}}\left(\frac{T}{T_c^0}\right)^2 \frac{1}{\sqrt[3]{N}}, \qquad \text{(at second order)}$$

$$\tag{1.10b}$$

with T_c^0 the critical temperature above which no particles are in the condensate. Figure 1.1 shows the condensed fraction as a function of temperature for both the cases of the thermodynamic limit (1.10a) and the finite size case (1.10b), and compare them with the result of an exact quantum calculation. It can be seen that the first order correction allows to fit very well the result of the exact quantum calculations, except near $T = T_c^0$, where the interactions between the particles can no longer be neglected. Moreover, it is seen that the interactions reduce the critical temperature with respect to what is expected in the case of a perfect gas. Such interactions, which in fact play a crucial role in the behaviour of the system, will be considered and discussed later on in this text.

1.3.3 Energy and specific heat

After having found the occupation number of the energy levels and the temperature dependence of the condensed fraction, the next quantities to compute are the energy contained in the system,

as well as the specific heat of the gas. Those quantities are given by

$$\overline{\left\langle \hat{H} \right\rangle} = \sum_{\vec{l}} \frac{\epsilon_{\vec{l}}}{\exp\left[\beta\left(\epsilon_{\vec{l}} - \mu\right)\right] - 1} \quad \text{and} \quad c_V = \frac{1}{N} \frac{\partial}{\partial T} \overline{\left\langle \hat{H} \right\rangle}\Bigg|_{N,V}.$$

From those definitions, it is obvious that the case of the free gas gas and that of the trapped gas have to be treated separately. Moreover, the cases $T < T_c^0$ and $T > T_c^0$ should also be treated separately, since below the critical temperature, some particles are in the condensed state.

The free gas

Using the same semiclassical approximation as previously, the expression of the mean energy can be rewritten under an integral form as

$$\overline{\left\langle \hat{H} \right\rangle} = \frac{V}{(2\pi\hbar)^3} \int \frac{\|\vec{P}\|^2/2m}{\exp\left[\beta\left(\frac{\|\vec{P}\|^2}{2m} - \mu\right)\right] - 1} d\vec{P},$$

which can, once more, be rewritten as a geometric series. Permuting the series with the integral, the mean energy contained in the system is given by the expression

$$\overline{\left\langle \hat{H} \right\rangle} = \begin{cases} \frac{3}{2} k_B T \frac{V}{\lambda_T^3} g_{5/2}\left(e^{\beta\mu}\right) & (T > T_c^0) \\ \frac{3}{2} k_B T \frac{V}{\lambda_T^3} \zeta\left(5/2\right) & (T < T_c^0) \end{cases}$$

where the last result can be obtained by letting the chemical potential reach the lowest energy level of the system (which is 0 in the case of a free gas). To get the specific heat from those relations, the relation

$$\frac{d g_p\left(z\right)}{dz} = \frac{1}{z} g_{p-1}\left(z\right)$$

can be used, leading to the expression [32]

$$c_V = k_B \begin{cases} \frac{15v}{4} \frac{g_{5/2}\left(e^{\beta\mu}\right)}{\lambda_T^3} - \frac{9}{4} \frac{g_{3/2}\left(e^{\beta\mu}\right)}{g_{1/2}\left(e^{\beta\mu}\right)} & (T > T_c^0) \\ \frac{15v}{4} \frac{\zeta(5/2)}{\lambda_T^3} & (T < T_c^0) \end{cases}$$

where v is the volume by particle, *i.e.* $v = V/N$.

The trapped gas

By using the same manipulations, but with the correct energy spectrum, the mean energy and specific heat of the system read

$$\overline{\left\langle \hat{H} \right\rangle} = \begin{cases} N\frac{\hbar}{2}\left(\omega_x + \omega_y + \omega_z\right) + 3\frac{k_B T}{\omega_x \omega_y \omega_z}\left(\frac{k_B T}{\hbar}\right)^3 g_4\left(e^{\beta\tilde{\mu}}\right) & (T > T_c^0) \\ N\frac{\hbar}{2}\left(\omega_x + \omega_y + \omega_z\right) + 3\frac{k_B T}{\omega_x \omega_y \omega_z}\left(\frac{k_B T}{\hbar}\right)^3 \zeta\left(4\right) & (T < T_c^0) \end{cases}$$

$$c_V = \begin{cases} 12 k_B \frac{g_4\left(e^{\beta\tilde{\mu}}\right)}{g_3\left(e^{\beta\tilde{\mu}}\right)} - 9 k_B \frac{g_3\left(e^{\beta\tilde{\mu}}\right)}{g_2\left(e^{\beta\tilde{\mu}}\right)} & (T > T_c^0) \\ 12 k_B \frac{\zeta(4)}{\zeta(3)}\left(\frac{T}{T_c^0}\right)^3 & (T < T_c^0) \end{cases}$$

1.4 The interacting Bose gas

Up to now, only the perfect gas has been considered. However, it is only a rather poor approximation of reality, since all particles interact. Those interactions are fundamental since the collisions (i) ensure thermalization of the trapped atomic sample, (ii) they determine the shape and dynamics of the condensate, and (iii) they limit the achievable spatial density in the gas.

1.4.1 Scattering theory: brief reminders

Since the considered gas is very dilute, the collision processes are assumed to involve only pairs of particles. If those particles have masses m_1 and m_2 and interact via the potential $V(\boldsymbol{r}_1 - \boldsymbol{r}_2)$, the Hamiltonian of the system is

$$\hat{H} = \frac{\hat{\boldsymbol{p}}_1^2}{2m_1} + \frac{\hat{\boldsymbol{p}}_2^2}{2m_2} + V(\boldsymbol{r}_1 - \boldsymbol{r}_2).$$

It is common practice to transform such a 2-body problem into a problem involving the centre-of-mass coordinates and the relative coordinates between the two particles. Writing

$$\begin{cases} \hat{\boldsymbol{R}}_G = \frac{m_1\hat{\boldsymbol{r}}_1 + m_2\hat{\boldsymbol{r}}_2}{m_1+m_2} \\ \hat{\boldsymbol{P}}_G = \hat{\boldsymbol{p}}_1 + \hat{\boldsymbol{p}}_2 \end{cases} \quad \text{and} \quad \begin{cases} \hat{\boldsymbol{r}} = \hat{\boldsymbol{r}}_1 - \hat{\boldsymbol{r}}_2 \\ \hat{\boldsymbol{p}} = \frac{m_2\hat{\boldsymbol{p}}_1 - m_1\hat{\boldsymbol{p}}_2}{m_1+m_2} \end{cases}$$

the Hamiltonian takes the new form

$$\hat{H} = \frac{\hat{\boldsymbol{P}}_G^2}{2M} + \frac{\hat{\boldsymbol{p}}^2}{2\mu} + V(\hat{\boldsymbol{r}}),$$

with $M = m_1 + m_2$ and $\mu = \frac{m_1 m_2}{m_1+m_2}$. In this new formulation, the centre-of-mass moves as a free particle of mass M, while the "relative" particle moves as a fictional particle with reduced mass μ in the potential $V(\hat{\boldsymbol{r}})$.

To find out the scattering properties of the potential $V(\hat{\boldsymbol{r}})$, the eigenstates of the relative Hamiltonian have to be found, *i.e.* the problem

$$\left[\frac{\hat{\boldsymbol{p}}^2}{2\mu} + V(\hat{\boldsymbol{r}})\right] \psi_{\boldsymbol{k}}(\boldsymbol{r}) = E_k \psi_{\boldsymbol{k}}(\boldsymbol{r})$$

has to be solved for a given[4] energy $E_k = \frac{\hbar^2 k^2}{2\mu}$, and for a potential that is assumed to go to zero sufficiently fast for $\|\boldsymbol{r}\| \to +\infty$. By further assuming a situation in which $\|\boldsymbol{r}\| \gg b$, b being the range of the potential, the scattering amplitude can be written as the superposition of the incoming wave and the scattered wave, which reads

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) \sim \exp(i\boldsymbol{k} \cdot \boldsymbol{r}) + f(k, \boldsymbol{n}, \boldsymbol{n}') \frac{\exp(ikr)}{r}, \quad (\|\boldsymbol{r}\| \to +\infty) \tag{1.11}$$

where $\boldsymbol{n} = \frac{\boldsymbol{k}}{k}$ is the incoming direction of the wave with momentum $\hbar\boldsymbol{k}$, $\boldsymbol{n}' = \frac{\boldsymbol{r}}{r}$ is the direction of the outgoing wave, and where $f(k, \boldsymbol{n}, \boldsymbol{n}')$ is the scattering amplitude. That result comes from the fact that the previous problem can be rewritten under the form

$$(\nabla^2 + k^2)\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{2\mu}{\hbar^2} V(\boldsymbol{r})\psi_{\boldsymbol{k}}(\boldsymbol{r})$$

$$= \frac{2\mu}{\hbar^2} \int V(\boldsymbol{r}')\psi_{\boldsymbol{k}}(\boldsymbol{r}')\delta(\boldsymbol{r} - \boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'.$$

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[4]It can be noted that the problem is the inverse of what is done in introductory quantum mechanics courses, in which the eigenstates are known and the energy is sought.

The fundamental solution to that equation is given by an outgoing spherical wave [11], *i.e.*
$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = -\frac{1}{4\pi}\frac{\exp(ikr)}{r}$, which yields the total expression of the sought $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ to be given by

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{\mu}{2\pi\hbar^2}\int\frac{\exp(ik\|\boldsymbol{r}-\boldsymbol{r}'\|)}{\|\boldsymbol{r}-\boldsymbol{r}'\|}V(\boldsymbol{r}')\psi_{\boldsymbol{k}}(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'.$$

If the potential has a finite range b, the expression $\|\boldsymbol{r}-\boldsymbol{r}'\|$ can be Taylor expanded to give

$$\|\boldsymbol{r}-\boldsymbol{r}'\| \approx \|\boldsymbol{r}\| - \frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{\|\boldsymbol{r}\|} + \mathcal{O}\left(\frac{1}{\|\boldsymbol{r}\|}\right), \quad (\|\boldsymbol{r}'\|\to 0).$$

This expansion allows to identify the scattering amplitude $f(k,\boldsymbol{n},\boldsymbol{n}')$ to the expression

$$f(k,\boldsymbol{n},\boldsymbol{n}') = -\frac{\mu}{2\pi\hbar^2}\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{r}')V(\boldsymbol{r}')\psi_{\boldsymbol{k}}(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}', \quad \text{with } \boldsymbol{k}' = k\boldsymbol{n}'.$$

This equality shows that the scattering problem is implicit, since it relates the value of $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ far from the scattering region to the value of that function inside the region where the scattering is important. However, it can be simplified if the scattering state is developed at first order in V, yielding

$$f(k,\boldsymbol{n},\boldsymbol{n}') = -\frac{\mu}{2\pi\hbar^2}\int\exp[-i\boldsymbol{k}'(\boldsymbol{r}'-\boldsymbol{r})]V(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'.$$

This expression is known as the Born approximation and shows that the scattering amplitude is simply the spatial Fourier transform of the scattering potential. Once the scattering amplitude has been computed, other quantities, such as the differential and total cross-sections, can be computed. Those quantities are given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(k,\boldsymbol{n},\boldsymbol{n}')|^2 \quad \text{and} \quad \sigma(k,\boldsymbol{n}) = \int|f(k,\boldsymbol{n},\boldsymbol{n}')|^2\,\mathrm{d}n', \tag{1.12}$$

respectively, and give access to the number of particles emitted per unit time and unit incident flux within the solid angle $\mathrm{d}\Omega$ (for the differential cross-section), and to the total area of the incoming beam that is scattered, and can be seen as how the particles perceive the potential (for the total cross-section).

Since the gas in which those interactions take place is very cold, and thus the involved energies are small, the scattering process can be considered as being isotropic (at least if the potential decreases fast enough at infinity), which means that the scattering amplitude is independent of $\boldsymbol{n}$ and $\boldsymbol{n}'$, and the asymptotic expression of the Hamiltonian eigenstate takes the form

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) \sim \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + f(k)\frac{\exp(ikr)}{r}. \tag{1.13}$$

In order to proceed further and get the exact expression of $\psi_{\boldsymbol{k}}(\boldsymbol{r})$, the full 3D Schrödinger equation should be solved, which is a quite tedious task. However, with suited assumptions on the potential, further computations can be made.

1.4.2 Radial potential

By considering that the scattering potential is purely radial, *i.e.* of the form $V(\boldsymbol{r}) = V(r)$, it is clear that the symmetry of the problem require the scattering amplitude to be only a function of the angle made between the directions of the incoming and the scattered waves ($\boldsymbol{n}\cdot\boldsymbol{n}' = \cos(\theta)$), so that the scattering amplitude is written $f(k,\boldsymbol{n},\boldsymbol{n}') = f(k,\theta)$.

The radial symmetry of the problem involving the existence of a common base to the operators $\hat{H}$, $\hat{\boldsymbol{L}}_z$ and $\hat{\boldsymbol{L}}^2$, the general solution to the (time-independent) Schrödinger equation can be written

$$\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right) = \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} c_{lm} \frac{u_l\left(r\right)}{r} Y_l^m\left(\theta, \varphi\right) \tag{1.14}$$

with θ and φ the polar and azimuthal angles around the $z-$axis, and $Y_l^m\left(\theta, \varphi\right)$ the spherical hamonics verifying

$$\begin{cases} \hat{\boldsymbol{L}}^2 Y_l^m\left(\theta, \varphi\right) = l\left(l+1\right) \hbar^2 Y_l^m\left(\theta, \varphi\right) & l = 0, 1, 2, \dots \\ \hat{L}_z Y_l^m\left(\theta, \varphi\right) = m\hbar Y_l^m\left(\theta, \varphi\right) & m = -l, -l+1, \dots, l-1, l \end{cases}$$

Injecting relation (1.14) into the general 3D Schrödinger equation yields the 1D radial Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu} \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l\left(l+1\right) \hbar^2}{2\mu r^2} + V\left(r\right) \right] u_l\left(r\right) = E u_l\left(r\right), \quad l = 0, 1, 2, \dots$$

The solution of that equation, if no potential is considered, is expressed as a spherical Bessel function, and behaves as $\sin\left(kr - l\frac{\pi}{2}\right)$ at large distances, whereas the solution to the full equation takes the form, for a potential that tends towards 0 sufficiently fast enough, of a linear combination of complex exponentials. The results thus read

$$u_l^{\text{free}}\left(r\right) = \sqrt{\frac{2k^2}{\pi}} r j_l\left(kr\right) \xrightarrow{kr \gg 1} \sqrt{\frac{2}{\pi}} \sin\left(kr - l\frac{\pi}{2}\right) \qquad \text{(free solution)}$$

$$u_l\left(r\right) = A_l \exp\left(ikr\right) + B_l \exp\left(-ikr\right) = C_l \sin\left(kr + \tilde{\delta}_l\right) \qquad \text{(complete solution)}$$

with $\delta_l = \tilde{\delta}_l + l\frac{\pi}{2}$ the phase shift between the two solutions caused by the scattering potential, which of course depends on the energy, i.e. $\delta_l = \delta_l\left(k\right)$. The crucial point about those phase shifts is that they are enough to fully describe the scattering amplitude. Indeed, by using Rayleigh's decomposition of the exponential

$$\exp\left(ikz\right) = \sum_{l=0}^{+\infty} i^l\left(2l+1\right) j_l\left(kr\right) P_l\left(\cos\theta\right)$$

$$\overset{kr \gg 1}{\approx} \frac{1}{kr} \sum_{l=0}^{+\infty} i^l\left(2l+1\right) \sin\left(kr - l\frac{\pi}{2}\right) P_l\left(\cos\theta\right),$$

and the decomposition of $\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right)$ on the Legendre polynomial basis $\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right) = \sum_{l=0}^{+\infty} \sqrt{\frac{2l+1}{4\pi}} \frac{u_l(r)}{r} P_l\left(\cos\theta\right)$, the asymptotic expression for the scattering amplitude is

$$\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right) = \sum_{l=0}^{+\infty} e^{il\pi/2} e^{i\delta_l} \frac{c_l}{2ir} \left[(-1)^{l+1} e^{-ikr} + e^{2i\delta_l} e^{ikr} \right] P_l\left(\cos\theta\right).$$

Finally, the total scattering cross-section σ can be computed. Taking the orthogonality of the Legendre polynomials into account, the integral appearing in (1.12) can be easily computed, yielding

$$\sigma\left(k\right) = \sum_{l=0}^{+\infty} \sigma_l\left(k\right), \quad \text{with} \quad \sigma_l\left(k\right) = \frac{4\pi}{k^2}\left(2l+1\right) \sin^2\left[\delta_l\left(k\right)\right].$$

Up to now, the bosonic character of the particles has not been yet considered. In order to take that particularity into account, the asymptotic expression for the scattering amplitude has to be modified to be rewritten [11]

$$\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right) \sim \frac{e^{ikz} + e^{-ikz}}{\sqrt{2}} + \frac{f\left(k, \theta\right) + f\left(k, \pi - \theta\right)}{\sqrt{2}} \frac{e^{ikr}}{r}$$

rather than as the expression given in (1.11), and leads to a differential cross-section given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| f\left(k, \theta\right) + f\left(k, \pi - \theta\right) \right|^2 .$$

The only partial waves contributing to the scattering cross-section for polarized bosons correspond to even values of l. The symmetrization principle doubles the contribution of the even partial waves, and cancels that of the odd ones, leading to

$$\sigma\left(k\right) = \frac{8\pi}{k^2} \sum_{l \text{ even}} \left(2l + 1\right) \sin^2\left[\delta_l\left(k\right)\right].$$

The final question that remains to be answered to is the exact expression of $\delta_l\left(k\right)$. It can be difficult to obtain their exact form but fortunately, for a potential scaling as $1/r^n$, an asymptotic expression of these phase shifts is known [21]

$$\delta_l\left(k\right) = \begin{cases} k^{2l+1} & \text{for } 2l + 3 < n \\ k^{n-2} & \text{otherwise.} \end{cases}$$

Since alkali atoms are generally considered in Bose-Einstein condensation experiments, which interact through a Van der Waals force (scaleing as r^{-6} at large distances), the total scattering cross-section at low energy is given by $\lim_{k \to 0} \sigma_{l=0}\left(k\right) = 8\pi a^2$, where the scattering length a is defined by

$$a = -\lim_{k \to 0} \frac{\tan\left[\delta_0\left(k\right)\right]}{k},$$

which shows that the interactions are described by a single parameter.

1.4.3 The pseudo-potential

For the previous computations to hold, it was assumed that the potential had a finite range of action b and decreased towards 0 sufficiently fast enough. However, the real potential between two particles is known to behave as $1/r^6$ at large distances, meaning an infinite range.

Working with such a potential is not easy, however, since

- the exact expression of the scattering potential is difficult to compute,

- a small error in the exact expression of V may result in a drastic difference in the scattering length a.

- A potential behaving as $1/r^6$ at infinity cannot be treated in the Born approximation, and implies that mean field approximations (*i.e.*, approximations that neglect the relations between the particles) cannot be used. Indeed, the Van der Waals interaction is strongly repulsive at short distances, attractive at medium distances, and has many bound molecular states [11].

Therefore, the idea is to replace the exact potential by another one, preserving the scattering properties of the exact potential at low energy and that can be treated in the Born approximation, since the many-body description then depends only on the scattering length, and not on the detailed interatomic potential. The easiest potential satisfying those requirements is the zero-range pseudo-potential, which has the following action on a 2-body wavefunction

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | V | \psi_{1,2} \rangle = g \delta \left(\boldsymbol{r}_1 - \boldsymbol{r}_2 \right) \left\{ \frac{\partial}{\partial r_{12}} \left[r_{12} \psi_{1,2} \left(\boldsymbol{r}_1, \boldsymbol{r}_2 \right) \right] \right\} \Bigg|_{r_{12}=0},$$

with g the coupling constant used to model the exact scattering potential. Introducing that expression for the pseudo-potential into the expression (1.13) yields

$$\psi_{\boldsymbol{k}} \left(\boldsymbol{r} \right) \sim \exp \left(i \boldsymbol{k} \cdot \boldsymbol{r} \right) - g \frac{\mu}{2\pi\hbar^2} \frac{\exp \left(ikr \right)}{r} \frac{\partial}{\partial r} \left[r \psi_{\boldsymbol{k}} \left(\boldsymbol{r} \right) \right] \Bigg|_{r=0}.$$

The second term of the right hand side can be easily computed, and gives

$$\frac{\partial}{\partial r} \left[r \psi_{\boldsymbol{k}} \left(r \right) \right] \Bigg|_{r=0} = \frac{1}{1 + ik \frac{\mu g}{2\pi\hbar^2}}.$$

The scattering state can thus be rewritten under the form

$$\psi_{\boldsymbol{k}} \left(\boldsymbol{r} \right) = \exp \left(i \boldsymbol{k} \cdot \boldsymbol{r} \right) - f \left(k \right) \frac{\exp \left(ikr \right)}{r}, \quad \text{with} \quad f \left(k \right) = g \frac{\mu}{2\pi\hbar^2} \frac{1}{1 + ik \frac{\mu g}{2\pi\hbar^2}}.$$

Considering the very low temperature (which is equivalent to consider the low-energy limit $k \to 0$) of the system, the scattering state can finally be rewritten under the form $\psi_{k \to 0} \left(\boldsymbol{r} \right) = 1 - \frac{a}{r}$, and the constant g given by $g = \frac{2\pi\hbar^2 a}{\mu}$.

1.4.4 Dynamics

It is now time to tackle the problem of the dynamics of the condensate. Taking interactions into account, the Hamiltonian of the system takes the form

$$\hat{H} = \int \hat{\psi}^\dagger \left(\boldsymbol{r} \right) \left[-\frac{\hbar^2}{2m} \nabla_{\boldsymbol{r}}^2 + V_{\text{trap}} \left(\boldsymbol{r} \right) \right] \hat{\psi} \left(\boldsymbol{r} \right) \mathrm{d}\boldsymbol{r} + \frac{1}{2} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}' \hat{\psi}^\dagger \left(\boldsymbol{r} \right) \hat{\psi}^\dagger \left(\boldsymbol{r}' \right) V \left(\boldsymbol{r} - \boldsymbol{r}' \right) \hat{\psi} \left(\boldsymbol{r}' \right) \hat{\psi} \left(\boldsymbol{r} \right).$$

In the Heisenberg representation of quantum mechanics, the evolution of the condensate field operator takes the form [32]

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi} \left(\boldsymbol{r}, t \right) = \left[\hat{\Psi} \left(\boldsymbol{r}, t \right), \hat{H} \right]$$
$$= \left[-\frac{\hbar^2}{2m} \nabla_{\boldsymbol{r}}^2 + V_{\text{trap}} \left(\boldsymbol{r} \right) + \int \mathrm{d}\boldsymbol{r}' \hat{\Psi}^\dagger \left(\boldsymbol{r}', t \right) V \left(\boldsymbol{r} - \boldsymbol{r}' \right) \hat{\Psi} \left(\boldsymbol{r}', t \right) \right] \hat{\Psi} \left(\boldsymbol{r}, t \right). \quad (1.15)$$

To go further, the field operator has to be replaced by the "classical" part Ψ_0. Such a replacement in the integral containing the atom-atom interaction is usually a poor approximations when short distances are $\| \boldsymbol{r} - \boldsymbol{r}' \|$ are involved. However, in a cold dilute gas, only binary interactions at low energy are relevant, and can be characterized by a single parameter (the s-wave scattering length). This allows to replace the real potential $V \left(\boldsymbol{r} - \boldsymbol{r}' \right)$ by the effective potential $g \delta \left(\boldsymbol{r} - \boldsymbol{r}' \right)$, with the coupling constant g related to the scattering length through the relation $g = \frac{4\pi\hbar^2}{m} a$ (the expression is different from what was previously derived because now particles having identical masses are considered).

By using such a pseudo-potential in (1.15) in combination with the replacement of $\hat{\Psi}(\boldsymbol{r}, t)$ by Ψ_0 leads to the well known Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\Psi_0(\boldsymbol{r}, t) = \left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + V_{\text{trap}} + g\left|\Psi_0(\boldsymbol{r}, t)\right|^2\right]\Psi_0(\boldsymbol{r}, t), \qquad (1.16)$$

derived independently by Gross [15, 16] and Pitaevskii [31]. That equation can also be determined by applying a variational procedure, consisting in computing

$$i\hbar\frac{\partial}{\partial t}\Psi_0(\boldsymbol{r}, t) = \frac{\delta E}{\delta\Psi_0^*},$$

with the energy functional $E[\Psi_0]$ given by

$$E[\Psi_0] = \int \mathrm{d}\boldsymbol{r} \left[\frac{\hbar^2}{2m}\left|\nabla\Psi_0(\boldsymbol{r}, t)\right|^2 + V_{\text{trap}}(\boldsymbol{r})\left|\Psi_0(\boldsymbol{r}, t)\right|^2 + \frac{g}{2}\left|\Psi_0(\boldsymbol{r}, t)\right|^4\right].$$

The first term of that equation accounts for the kinetic energy of the gas, while the second and last term are the energy due to the trap and the mean-field interaction energy, respectively. It should be noted that the derivation of the Gross-Pitaevskii equation eq. (1.16) is valid only in the dilute regime, *i.e.* the regime in which the product $\overline{n}a^3 \ll 1$, with $\overline{n}$ the average density of the gas.

Applying eq. (1.16) to an order paramater having the form $\Psi(\boldsymbol{r}, t) = \psi_0(\boldsymbol{r})\exp\left(-i\frac{\mu}{\hbar}t\right)$, with μ the chemical potential and $\psi_0(\boldsymbol{r})$ real and normalized to the number of particles $\int \psi_0^2(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = N$, yields the time-independent Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + V_{\text{trap}}(\boldsymbol{r}) + g\psi_0^2(\boldsymbol{r})\right]\psi_0(\boldsymbol{r}) = \mu\psi_0(\boldsymbol{r}),$$

which has the form of a cubic nonlinear Schrödinger equation, the nonlinearity arising from the mean-field term, proportional to the local density $n(\boldsymbol{r}) = \psi_0^2(\boldsymbol{r})$. By solving that equation, the ground state of the system can be determined. It can be shown by re-expressing that last equation in term of dimensionless variables that the term $\frac{N|a|}{a_{ho}}$, with $a_{ho} = \sqrt{\frac{\hbar}{m\sqrt[3]{\omega_x\omega_y\omega_z}}}$ the characteristic size of the harmonic oscillator, dictates the importance of the interactions [9].

On the other hand, if other states than the ground state are sought, the order parameter can be written under the form, considering the low-temperature limit where the properties of the excitations are not influenced by the temperature, $\Psi_0(\boldsymbol{r}, t) = \left[\psi_0(\boldsymbol{r}) + u(\boldsymbol{r})e^{-i\omega t} + v^*(\boldsymbol{r})e^{i\omega t}\right]e^{-i\mu t/\hbar}$, which correspond to small oscillations of the condensate around the ground state. Injecting that expression for the order parameter into eq. (1.16) yields the system

$$\begin{cases} \hbar\omega u(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + V_{\text{ext}}(\boldsymbol{r}) - \mu + 2g\psi_0^2(\boldsymbol{r})\right]u(\boldsymbol{r}) + g\psi_0^2(\boldsymbol{r})v(\boldsymbol{r}), \\ -\hbar\omega v(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + V_{\text{ext}}(\boldsymbol{r}) - \mu + 2g\psi_0^2(\boldsymbol{r})\right]v(\boldsymbol{r}) + g\psi_0^2(\boldsymbol{r})u(\boldsymbol{r}). \end{cases} \qquad (1.17)$$

That system allows to determine the eigenfrequencies ω, and thus the energy of the excitations. An equivalent way of doing things is to diagonalize the Hamiltonian of the system in Bogoliubov approximation, which consists in rewriting the non-condensed part of the field operator as a linear combination of creation and annihilation operators of quasiparticles, *i.e.* writing

$$\delta\hat{\Psi}(\boldsymbol{r}, t) = \sum_j \left[u_j(\boldsymbol{r})\hat{\alpha}_j(t) + v_j^*(\boldsymbol{r})\hat{\alpha}_j^\dagger(t)\right].$$

By imposing that those operators follow the commutation relations (1.5), the quasiparticles amplitude $u(\mathbf{r})$ and $v(\mathbf{r})$, the normalization condition to which those amplitudes are submitted read

$$\begin{cases} \int \left[u_i^*(\mathbf{r}) u_j(\mathbf{r}) - v_i^*(\mathbf{r}) v_j(\mathbf{r}) \right] \mathrm{d}\mathbf{r} = \pm \delta_{ij}, \\ \int \left[u_i(\mathbf{r}) v_j(\mathbf{r}) - v_i(\mathbf{r}) u_j(\mathbf{r}) \right] = 0 \end{cases} \quad \forall i, j \in \mathbb{N}_0$$

The PDE system (1.17) cannot be easily solved analytically because of the term $\psi_0(\mathbf{r})$, which is not known, excepted for particular cases, like the Thomas-Fermi regime (in which the kinetic energy is negligible with respect to the interaction energy), or the free gas case, for which $\psi_0(\mathbf{r}) = \sqrt{n(\mathbf{r})}$ and $\mu = gn$.

In the case of the free gas, the system (1.17) takes a rather simple form, *i.e.*

$$\begin{cases} \hbar \omega u(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + gn(\mathbf{r}) \right] u(\mathbf{r}) + gn(\mathbf{r}) v(\mathbf{r}), \\ -\hbar \omega v(\mathbf{r}) = \left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + gn(\mathbf{r}) \right] v(\mathbf{r}) + gn(\mathbf{r}) u(\mathbf{r}), \end{cases}$$

which can be easily solved to give the dispersion relation

$$\omega_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\hbar} \sqrt{\frac{\hbar^2 k^2}{2m} \left[\frac{\hbar^2 k^2}{2m} + 2gn(\mathbf{r}) \right]}.$$

This dispersion relation shows that for high momenta $\hbar \|\mathbf{k}\|$, the dispersion relation is identical to that of a quantum particle, *i.e.* $\omega_{\mathbf{k}}(\mathbf{r}) = \omega_{\mathbf{k}} = \frac{\hbar k^2}{2m}$, while for small momenta, the dispersion relation becomes $\omega_{\mathbf{k}}(\mathbf{r}) = c(\mathbf{r}) k$, with c the spped of sound in the condensate, given by the expression

$$c(\mathbf{r}) = \sqrt{\frac{gn(\mathbf{r})}{m}}.$$

1.4.5 Hydrodynamic analogy

In the previous derivations, it was supposed that the system was close to its equilibrium state. It is now time to remove that hypothesis and see how the local density $n(\mathbf{r}, t)$ then evolves. It will be shown that the density evolution can be described by an equation looking like the equation describing the movement of a classical fluid.

By writing the local density as $n(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$, the Gross-Pitaevskii equation eq. (1.16) can be rewritten under the form

$$i\hbar \frac{\partial \psi}{\partial t}(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V_{\text{ext}}(\mathbf{r}, t) + gn(\mathbf{r}, t) \right] \psi(\mathbf{r}, t). \tag{1.18}$$

By noting that $\partial_t n(\mathbf{r}, t) = \psi^*(\mathbf{r}, t) \partial_t \psi(\mathbf{r}, t) + \psi(\mathbf{r}, t) \partial_t \psi^*(\mathbf{r}, t)$, the time variation of the density is obtained by summing the product of eq. (1.18) with $\psi^*(\mathbf{r}, t)$ and the complex conjugate of the same equation, multiplied by $\psi(\mathbf{r}, t)$, which leads to the expression

$$\frac{\partial n}{\partial t}(\mathbf{r}, t) = -\frac{\hbar}{2mi} \left[\psi^*(\mathbf{r}, t) \nabla_{\mathbf{r}}^2 \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \nabla_{\mathbf{r}}^2 \psi^*(\mathbf{r}, t) \right],$$

which can be linked to the density of current vector $\mathbf{J}(\mathbf{r}, t)$, defined as

$$\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{2mi} \left[\psi^*(\mathbf{r}, t) \boldsymbol{\nabla}_{\mathbf{r}} \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \boldsymbol{\nabla}_{\mathbf{r}} \psi^*(\mathbf{r}, t) \right] \tag{1.19}$$

by taking its divergence. The final results is a continuity equation for the density, which reads

$$\frac{\partial n}{\partial t}(\mathbf{r}, t) + \boldsymbol{\nabla} \cdot \mathbf{J}(\mathbf{r}, t) = 0.$$

If the sought wavefunction $\psi(\boldsymbol{r}, t)$ is written under the form $\psi(\boldsymbol{r}, t) = \sqrt{n(\boldsymbol{r}, t)}e^{i\theta(\boldsymbol{r}, t)}$, with $\theta(\boldsymbol{r}, t)$ a local phase, the current density defined in (1.19) takes the form

$$\boldsymbol{J}(\boldsymbol{r}, t) = \frac{\hbar}{m}n(\boldsymbol{r}, t)\nabla_{\boldsymbol{r}}\theta(\boldsymbol{r}, t),$$

which allows to define a local velocity $\boldsymbol{v}(\boldsymbol{r}, t) = \frac{\boldsymbol{J}(\boldsymbol{r}, t)}{n(\boldsymbol{r}, t)} = \frac{\hbar}{m}\nabla_{\boldsymbol{r}}\theta(\boldsymbol{r}, t)$, which means that the velocity of the condensate is curl-free, like the velocity field of a non-viscous classical fluid. From there, the time evolution of that speed can be computed. By taking the time derivative of the new form of $\psi(\boldsymbol{r}, t)$, the left hand side of the Gross-Pitaevskii equation can be computed, and is given by

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r}, t) = \left[i\hbar\frac{\partial}{\partial t}\sqrt{n(\boldsymbol{r}, t)} - \hbar\sqrt{n(\boldsymbol{r}, t)}\frac{\partial}{\partial t}\theta(\boldsymbol{r}, t)\right]e^{i\theta(\boldsymbol{r}, t)}.$$

From there, the time variation of the phase $\theta(\boldsymbol{r}, t)$ can be easily extracted by taking the following combination

$$i\hbar\left[\psi^*(\boldsymbol{r}, t)\frac{\partial}{\partial t}\psi(\boldsymbol{r}, t) - \psi(\boldsymbol{r}, t)\frac{\partial}{\partial t}\psi^*(\boldsymbol{r}, t)\right] = -2\hbar n(\boldsymbol{r}, t)\frac{\partial}{\partial t}\theta(\boldsymbol{r}, t).$$

The left hand side of that equation can be computed thanks to the Gross-Pitaevskii equation. The first term to compute is the Laplacian $\nabla_{\boldsymbol{r}}^2\psi(\boldsymbol{r}, t) = \nabla_{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{r}}\psi(\boldsymbol{r}, t)$, which gives

$$\nabla_{\boldsymbol{r}}^2\psi(\boldsymbol{r}, t) = \left\{\nabla_{\boldsymbol{r}}^2\sqrt{n(\boldsymbol{r}, t)} + 2i\left[\nabla_{\boldsymbol{r}}\sqrt{n(\boldsymbol{r}, t)}\right] \cdot \nabla_{\boldsymbol{r}}\theta(\boldsymbol{r}, t) + i\sqrt{n(\boldsymbol{r}, t)}\nabla_{\boldsymbol{r}}^2\theta(\boldsymbol{r}, t)\right.$$
$$\left. - \sqrt{n(\boldsymbol{r}, t)}\left[\nabla_{\boldsymbol{r}}\theta(\boldsymbol{r}, t)\right]^2\right\}e^{i\theta(\boldsymbol{r}, t)}$$

By further manipulations described in [8], the time evolution of the phase $\theta(\boldsymbol{r}, t)$ or, equivalently, of the speed, reads

$$m\frac{\partial}{\partial t}\boldsymbol{v}(\boldsymbol{r}, t) = -\nabla_{\boldsymbol{r}}\left\{V_{\text{ext}}(\boldsymbol{r}, t) + gn(\boldsymbol{r}, t) + \frac{m\|\boldsymbol{v}(\boldsymbol{r}, t)\|^2}{2} + \frac{\hbar^2}{2m}\frac{1}{\sqrt{n(\boldsymbol{r}, t)}}\nabla_{\boldsymbol{r}}^2\left[\sqrt{n(\boldsymbol{r}, t)}\right]\right\},$$
$$(1.20)$$

which looks like the classical second Newton's law of motion for a system submitted to a potential given by the expression between $\{\}$. The different terms of that expression are

- $V_{\text{ext}}(\boldsymbol{r}, t)$, the external confining potential,

- $gn(\boldsymbol{r}, t)$, the mean interaction potential between the particles of the system,

- $\frac{m\|\boldsymbol{v}(\boldsymbol{r}, t)\|^2}{2}$, the kinetic energy of the system,

- $\frac{\hbar^2}{2m}\frac{1}{\sqrt{n(\boldsymbol{r}, t)}}\nabla_{\boldsymbol{r}}^2\left[\sqrt{n(\boldsymbol{r}, t)}\right]$, a purely quantum term (has the prefactor $\hbar^2$ clearly indicates), called *quantum pressure*.

Chapter 2

Bose-Einstein condensation in reduced dimensionality

Introduction

The phase transition a system can undergo, as well as the types of order existing in physical system is strongly influenced by its dimensionality. For instance, it is known in condensed matter physics that no (anti)ferromagnetism can exist in one or two dimensional systems for arbitrarily small positive temperatures [23].

Even though it was strictly proven that no Bose-Einstein condensate could be formed in a 2D Bose gas, with or without interactions [18], because of the enhanced effect of thermal fluctuations, a phase transition can still occur for small finite temperatures in a 2D interacting system. This phase transition from a normal state to a superfluid one can be studied in the general framework of the Berezinski-Kosterlitz-Thouless phase transition, and take place because the thermal fluctuations are not strong enough to kill the superfluidity of the system.

The first half of this part is dedicated to the Bose gas in 2 dimensions. Going from an ideal uniform infinite gas, the analysis is pushed further to include the effects of interactions between particles. Pushing further the analysis, the case of a gas trapped in an harmonic trap will be discussed. Some particular effects, such as the transition from a normal state to a superfluid state, or the Josephson effect, will be briefly discussed

The second half of this part is dedicated to the 1D Bose gas. In particular, the transition from a traditional Bose gas to a gas of impenetrable bosons, which acts as a fermion gas, will be briefly discussed.

2.1 The 2D Bose gas

Introduction

It was already stated that the 2D Bose gas is an interesting system because of the phase transition that can happen: even though no true condensate can be realized in such a system, it can however exhibit a superfluid behaviour, well-studied in the BKT phase transition regime.

Attention should nevertheless be paid when a 2D Bose gas is evoked: indeed, two situations have to be distinguished

(i) the case in which the gas is geometrically bidimensional, but locally behaves as a tridimensional object, which means that one degree of freedom is frozen out by a thigh confinement but the inter-particle scattering is still tridimensional, and

(ii) the case in which the gas is truly bidimensional, which means that one degree of freedom has been frozen out and that the scattering amplitude depends logarithmically on the energy [17].

2.1.1   The infinite uniform Bose gas at low temperature

If an ideal gas gas is considered, it is known that its energy is purely kinetic. From that fact, using the occupation number of state with energy $\boldsymbol{k}$ given by relation (1.7), the mean number of particles contained in the system is given by

$$\overline{\left\langle \hat{N} \right\rangle} = \sum_{\boldsymbol{k}} \frac{1}{\exp\left[\beta\left(\epsilon_{\boldsymbol{k}} - \mu\right)\right] - 1}, \quad \text{with } \epsilon_{\boldsymbol{k}} = \frac{\hbar^2 \left\|\boldsymbol{k}\right\|^2}{2m}.$$

Once again, using the semiclassical approximation (which allows to rewrite the sum as an integral), identifying the geometrical progression and permuting the summation and the integration, the phase space density can be written

$$n\lambda_T^2 = -\ln\left[1 - \exp\left(\beta\mu\right)\right], \tag{2.1}$$

where the equality $g_1\left(z\right) = -\ln\left(1 - z\right)$ was used. The previous relation can be inverted to give the expression of the chemical potential as a function of the density, i.e.

$$\mu = k_B T \ln\left[1 - \exp\left(-n\lambda_T^2\right)\right].$$

This relation shows that for any non-infinite density, there exist a negative chemical potential μ, which means that no Bose-Einstein condensate can be realized in the case of an infinite 2D Bose gas.

An interesting quantity interesting to consider is the first order correlation function, giving the coherence length of the system, i.e. the length over the gas can be described by a single wavefunction. For a gas contained in a box, this quantity is nothing else than the Fourier transform of the momentum space distribution function since it is defined by $g^{(1)}\left(\boldsymbol{r}, \boldsymbol{r}', t\right) = \left\langle \hat{\psi}^{\dagger}\left(\boldsymbol{r}, t\right) \hat{\psi}\left(\boldsymbol{r}', t\right) \right\rangle$, with the basis functions appearing in the field operator being plane waves, and thus read

$$g^{(1)}\left(\boldsymbol{r}, \boldsymbol{r}'\right) = \frac{1}{\left(2\pi\right)^2} \int \frac{1}{\exp\left[\beta\left(\epsilon_{\boldsymbol{k}} - \mu\right)\right] - 1} \exp\left[-i\boldsymbol{k} \cdot \left(\boldsymbol{r} - \boldsymbol{r}'\right)\right] \mathrm{d}\boldsymbol{k}.$$

To check the behaviour of that quantity, two distinct regimes have to be considered: the non-degenerate gas (in which case the wavefunctions of the different particles do not overlap), and the degenerate gas (in which case the wavefunctions of the different particles do overlap).

The non degenerate gas

In such a case, the density $n\lambda_T^2$ is very low, $n\lambda_T^2 \ll 1$. This allows to rewrite expression (2.1) under the form $\exp\left(\beta\mu\right) \approx n\lambda_T^2$, which is obtained by inverting (2.1) into the form $\exp\left(\beta\mu\right) = 1 - \exp\left(-n\lambda_T^2\right)$, and by using a Taylor expansion of the exponential.

In this regime, the chemical potential is $\left|\mu\right| \gg k_B T$, and thus all momentum states are weakly occupied, which leads to a momentum distribution having a Boltzmann shape, i.e. $n_{\boldsymbol{k}} \approx \exp\left[-\beta\left(\epsilon_{\boldsymbol{k}} - \mu\right)\right]$. Combining that expression with the asymptotic form of $e^{\beta\mu} \approx n\lambda_T^2$, the momentum distribution can be written

$$n_{\boldsymbol{k}} \approx n\lambda_T^2 \exp\left(-\beta\frac{\hbar\left\|\boldsymbol{k}\right\|^2}{2m}\right) = n\lambda_T^2 \exp\left(-\frac{\lambda_T^2\left\|\boldsymbol{k}\right\|^2}{4\pi}\right) \ll 1 \quad \forall\boldsymbol{k}.$$

From that expression, it is clear that the first order correlation function is Gaussian, since it is the Fourier transform of $n_{\boldsymbol{k}}$, which is itself Gaussian. This Gaussian behaviour of $g^{(1)}\left(r\right)$ indicates that correlations are only short range, over a range $\xi = \lambda_T/\sqrt{\pi}$, since $g^{(1)}\left(r\right) \propto n e^{-\pi r^2/\lambda_T^2}$.

The degenerate gas

In such a case, the density $n\lambda_T^2$ is very high, $n\lambda_T^2 \gg 1$. This allows to rewrite expression (2.1) under the form $\exp(\beta\mu) \approx 1$, which means that $\beta\mu \ll 1$. Using that same relation with a Taylor expansion of the exponential leads to $n\lambda_T^2 \approx \ln(k_B T / |\mu|)$.

In that regime, the occupation of the high-energy modes (with $\beta\epsilon_{\boldsymbol{k}} \gg 1$) is still small and given by a Boltzmann expression, while the low-energy modes (with $\beta\epsilon_{\boldsymbol{k}} \ll 1$) become highly populated. This yield

$$\text{(high-energy modes)} \quad n_{\boldsymbol{k}} \approx \exp(-\beta\epsilon_{\boldsymbol{k}}) = \exp\left(-\frac{\lambda_T^2 \|\boldsymbol{k}\|^2}{4\pi}\right) \ll 1, \quad \text{for } \|\boldsymbol{k}\|^2 \gg \frac{4\pi}{\lambda_T^2},$$

$$\text{(low-energy modes)} \quad n_{\boldsymbol{k}} \approx \frac{k_B T}{\epsilon_{\boldsymbol{k}} + |\mu|} = \frac{4\pi}{\lambda_T^2} \frac{1}{\|\boldsymbol{k}\|^2 + k_c^2} \gg 1, \quad \text{for } \|\boldsymbol{k}\|^2 \ll \frac{4\pi}{\lambda_T^2},$$

with $k_c^2 = 2m|\mu|/\hbar^2$, a critical wavenumber giving the separation between the high and low energy modes. Because the behaviour of the momentum distribution changes from Gaussian to Lorentzian, the correlation function is expected to be bimodal. For distances up to λ_T, it is still Gaussian. However, at large distances, the Fourier transform of the Lorentzian gives an approximately exponential decrease of $g^{(1)}(r)$, following the law [17]

$$g^{(1)}(r) \approx \exp\left(-\frac{r}{l}\right), \quad \text{with } l = k_c^{-1} \approx \frac{\lambda_T}{\sqrt{4\pi}} \exp\left(\frac{n\lambda_T^2}{2}\right). \tag{2.2}$$

The corresponding partial densities are then given by

$$\mathcal{D}_G \approx \frac{\lambda_T^2}{(2\pi)^2} \int_{\sqrt{4\pi/\lambda_T^2}}^{+\infty} n_{\boldsymbol{k}} \mathrm{d}\boldsymbol{k} \approx \frac{1}{e} \ll n\lambda_T^2,$$

$$\mathcal{D}_L = \approx \frac{\lambda_T^2}{(2\pi)^2} \int_0^{\sqrt{4\pi/\lambda_T^2}} n_{\boldsymbol{k}} \mathrm{d}\boldsymbol{k} \approx n\lambda_T^2,$$

with $\mathcal{D}_G$ corresponding to the Gaussian part and $\mathcal{D}_L$ to the Lorentzian one. It is thus seen that, even if no phase transition occurs in the system, the correlation function $g^{(1)}(r)$ goes from a Gaussian with short correlation length in the non-degenerated regime, to an exponential in the degenerated one. Moreover, in the case of a high density $n\lambda_T^2 > 1$, the correlation length l, which is proportional to $e^{n\lambda_T^2}$, grows. This shows that the scale over which $g^{(1)}(r)$ decays can become exponentially big for a strongly degenerated system, owing to the equalities appearing in (2.2).

2.1.2 The interacting 2D Bose gas

The idea here is to see how the particles in a gas with a frozen movement along one direction (say, the z-direction) interact. At low temperature, and thus low energy, the asymptotic form of the scattering state of two particles with relative wave vector $\boldsymbol{k}$ is a combination of the incoming wave and the scattered circular wave, given by

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) \approx \left[\exp(i\boldsymbol{k}\cdot\boldsymbol{r}) - \sqrt{\frac{i}{8\pi k}} f(k) \frac{\exp(ikr)}{\sqrt{r}}\right] \varphi_0(z), \quad (\|\boldsymbol{r}\| \to +\infty) \tag{2.3}$$

with $f(k)$ the scattering amplitude, depending on the relative momentum of the scattered particles and not on the angle between the momentum of the particles, since at low temperature the scattering is isotropic and $\varphi_0(z) = (1/2\pi l_0^2)^{1/4} \exp(-z^2/4l_0^2)$ the eigenfunction corresponding

to the ground state of the harmonic oscillator along the z-direction (with $l_0 = \sqrt{\hbar/m\omega_z}$ the characteristic size of the oscillator along that direction).

As in the previous 3D case, the atoms interact through a radial, finite range, potential $U(\boldsymbol{r})$. To get the exact scattering state of the problem, the 2D radial Schrödinger has then to be solved, $i.e.$ the equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) + U(z) - \frac{\hbar\omega_0}{2}\right]\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \epsilon\psi_{\boldsymbol{k}}(\boldsymbol{r}), \tag{2.4}$$

with $\epsilon = \hbar^2 k^2/2m$ the energy [30].

Taking into account the fact that the gas is at a very low temperature, the thermal de Broglie wavelength (which scales as $1/k$) of the particles greatly exceed the range of interaction R_e. In the case where $kR_e \ll 1$, the scattering problem is determined through the sole contribution of the s-wave. It has to be kept in mind that the atoms are tightly confined along z, which means that the the length l_0 plays an analogue role λ_T along that direction, which leads to the the supplementary condition $l_0 \gg R_e$, which ensures that the harmonic confinement does not influence the relative motion of atoms.

Solving eq. (2.4) in the case of a large interparticle separation, $i.e.$ in the case $r \gg R_e$, the interaction potential $U(\boldsymbol{r})$ can safely be set equal to 0. This means that the in-plane motion is free, while the motion along the z-direction is dictated by the harmonic confinement along that direction. The solution to the radial Schrödinger equation then reads [30]

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \varphi_0(z)J_0(kr) - \frac{f(k)}{\theta(0)}G(\boldsymbol{r},0),$$

with θ the scattering angle and $G(\boldsymbol{r},\boldsymbol{r}')$ the Green function corresponding to the Schrödinger equation, $i.e.$ the function verifying [2]

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E\right)G(\boldsymbol{r},\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}')$$

and having solution $G(\boldsymbol{r},\boldsymbol{r}') = -i\frac{m}{2\hbar}H_0^{(1)}(k\|\boldsymbol{r}-\boldsymbol{r}'\|)$, where $H_0^{(1)}$ is a Hankel function.

For an infinite interparticle separation, the asymptotic expression of the scattering state is recovered [30]. In the regime $R_e \ll r \ll l_0$, the scattering state is, up to a constant multiplying constant, equal to the 3D scattering state derived previously, $i.e.$

$$\psi_{\boldsymbol{k}}(r) \approx \eta\varphi(0)\left(1 - \frac{a}{r}\right).$$

Combining that expression with the asymptotic form of the Green function for $r \to 0$ given in [29] allows to find the expression of the scattering amplitude $f(k)$, which then reads [30]

$$f(k) = \frac{2\sqrt{2\pi}}{\frac{l_0}{a} + \frac{1}{\sqrt{2\pi}}\left[i\pi + \ln\left(\frac{2m\omega_z}{\pi\hbar k^2}B\right)\right]}, \quad B \approx 0.915.$$

This last expression shows that, contrary to the 3D case, the 2D scattering problem is characterized by a scattering amplitude which depends on the energy. In the low energy limit, that scattering amplitude is rewritten [5]

$$f(k) = \frac{4\pi}{i\pi - \ln(kd_*)}, \tag{2.5}$$

with d_* linked to the 3D scattering length through the relation

$$d_* = \sqrt{\frac{\pi}{B}}l_0\exp\left(-\sqrt{\frac{\pi}{2}}\frac{l_0}{a}\right).$$

A remarquable feature of the expression of the scattering amplitude is that the corresponding total scattering cross-section becomes infinite in the 0 energy limit, *i.e.*

$$\lim_{k\to 0} \sigma\left(k\right) = \lim_{k\to 0} \frac{\left|f\left(k\right)\right|^2}{4k} \to +\infty.$$

Having found the expression of the scattering amplitude, the scattering potential can be replaced by an approximation which as the same effect as the exact one, in an analogous way to what was done in 3D. This leads to the value

$$g = \frac{4\pi\hbar^2}{m} \frac{1}{\sqrt{2\pi}\frac{l_0}{a} + \ln\left(\frac{2m\omega_z}{\pi\hbar k^2}B\right)},$$

showing that the interaction between the particles is a function of their relative energy, unlike in the 3D case.

As in the previous 3D case, a finite range potential decreasing towards zero sufficiently fast enough is considered. Using again the Rayleigh expansion for the incoming wave

$$\exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right) = \exp\left(ikr\cos\theta\right) = \sum_{m=0}^{+\infty} \epsilon_m i^m \cos\left(m\theta\right) J_m\left(kr\right), \quad \text{with } \epsilon_m = \begin{cases} 1 & \text{for } m=0 \\ 2 & \text{otherwise} \end{cases} \quad (2.6)$$

and the asymptotic expressions of the Bessel and Neumann functions, given by

$$J_m\left(kr\right) \overset{r\to+\infty}{\longrightarrow} \sqrt{\frac{2}{\pi kr}} \cos\left(kr - m\frac{\pi}{2} - \frac{\pi}{4}\right),$$

$$N_m\left(kr\right) \overset{r\to+\infty}{\longrightarrow} \sqrt{\frac{2}{\pi kr}} \sin\left(kr - m\frac{\pi}{2} - \frac{\pi}{4}\right),$$

the scattering state $\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right)$ can be expressed in term of the phase shifts introduced by the scattering potential, as was the case for the three dimensional problem [2]. The asymptotic expression for the scattering state is then given by

$$\psi_{\boldsymbol{k}}\left(\boldsymbol{r}\right) \overset{r\to+\infty}{\longrightarrow} \frac{1}{\sqrt{kr}} \sum_{m=0}^{+\infty} A_m \cos\left(m\theta\right) \cos\left(kr - m\frac{\pi}{2} + \delta_m\right),$$

with δ_m the scattering phase shifts, which of course depend on the energy, *i.e.* $\delta_m = \delta_m\left(k\right)$. Substituting that last expression into relation (2.3), and using the Rayleigh expansion (2.6), combined with the asymptotic expressions for the Bessel and Neumann functions, yields

$$A_m = \sqrt{\frac{2}{\pi}}\epsilon_m i^m \exp\left(i\delta_m\right) \quad \text{and} \quad f\left(k\right) = \sqrt{\frac{2}{\pi}} \sum_{m=0}^{+\infty} \epsilon_m e^{i\delta_m} \sin\left(\delta_m\right).$$

In the low energy limit, the scattering amplitude becomes [5]

$$f\left(k\right) = \frac{4\pi}{2\ln\left(\frac{1}{ka_2}\right) + i\pi}, \tag{2.7}$$

where a_2 is the 2D scattering length. A remarkable feature of that expression is that it vanishes in the 0 energy limit, *i.e.* $\lim_{k\to 0} f\left(k\right) = 0$, while it gave the non-zero result $\lim_{k\to 0} f\left(k\right) = -a$ in 3D. Moreover, the total cross section tends towards infinity in that same limit

$$\lim_{k\to 0} \sigma\left(k\right) = \lim_{k\to 0} \frac{\left|f\left(k\right)\right|^2}{4k} \to +\infty.$$

By equating the relations (2.5) and (2.7), the expression of the bi-dimensional scattering length can be expressed in terms of the 2D scattering length of the confined gas. The relation between the two is given by

$$a_2 = \sqrt{\frac{d_*}{k}},$$

which shows that, even for a free gas, the 2D scattering length is related to the energy.

2.1.3   The trapped Bose gas

Introducing a confining potential with a frequency ω_z along the z-direction such that $\hbar\omega_z \gg k_B T$ allows the formation of a pancake-shaped cloud. Because the trapping frequency along the z-direction is very high compared to the thermal energy, the movement of the particles in the gas along that direction is frozen out, realizing a 2D system.

The mean number of particles contained in the system is then given by

$$\overline{\left\langle \hat{N} \right\rangle} = \sum_{\boldsymbol{k}} \frac{1}{\exp\left[\beta\left(\epsilon_{\boldsymbol{k}} - \mu\right)\right] - 1},$$

where the energy spectrum is given by

$$\epsilon_{\boldsymbol{n}} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y$$

for a harmonic trapping having the form $V_{\text{ext}}\left(\boldsymbol{r}\right) = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2\right)$. Following the developments that were made for the 3D trapped Bose gas, a new chemical potential $\tilde{\mu}$ is defined, which takes the zero-point energy into account, and allow to rewrite the expression of the mean number of particles contained in the system under the form

$$\overline{\left\langle \hat{N} \right\rangle} = \sum_{\boldsymbol{n}} \frac{1}{\exp\left[\beta\hbar\left(n_x\omega_x + n_y\omega_y - \tilde{\mu}\right)\right] - 1}.$$

Separating the lowest energy state from the rest of the series and invoking once again the semiclassical approximation, the series can be replaced by an integral. Following further the line sketched in the 3D case, the integrand is then replaced by the corresponding geometric progression, and the mean number of particles contained in the system is finally given by

$$\overline{\left\langle \hat{N} \right\rangle} = \overline{\left\langle \hat{N}_0 \right\rangle} + \frac{1}{\omega_x\omega_y}\left(\frac{k_B T}{\hbar}\right)^2 \sum_{j=1}^{+\infty} \frac{\exp\left(j\beta\tilde{\mu}\right)}{j^2}.$$

From that expression, the critical temperature can be computed, and is given by

$$T_c = \sqrt{\frac{6N}{\pi^2}\omega_x\omega_y}\,\frac{\hbar}{k_B}.$$

The temperature dependence of the number of particles contained in the system can be written under the form [28]

$$N\left[1 - \left(\frac{T}{T_c}\right)^2\right] = N_0 - \frac{1}{\omega_x\omega_y}\left(\frac{k_B T}{\hbar}\right)^2 \frac{1 + \ln\left(N_0\right)}{N_0}. \tag{2.8}$$

This last expression shows that there exist 2 regimes, namely

- $T < T_c$: the last term of (2.8) can be neglected, and the occupation of the ground state is approximatively given by

$$N_0 \approx N \left[1 - \left(\frac{T}{T_c} \right)^2 \right],$$

which as a similar form to what was found in 3D, except for the value of the exponent.

- $T > T_c$: the first term of (2.8) can be neglected, and the occupation of the ground state is approximatively given by the expression

$$N \left[1 - \left(\frac{T}{T_c} \right)^2 \right] \approx -\frac{1}{\omega_x \omega_y} \left(\frac{k_B T}{\hbar} \right)^2 \frac{1 + \ln (N_0)}{N_0}.$$

It should be noted that for $T = T_c$, the thermal de Broglie wavelength becomes comparable to the mean distance between the particles, which scales as $\sqrt{\frac{T_c}{N m \omega_x \omega_y}}$, and is the condition for entering in the quantum regime.

A graphical representation of the ground state population as a function of temperature for different values of N is given in fig. 2.1. As can be seen from this figure, the effect of a finite
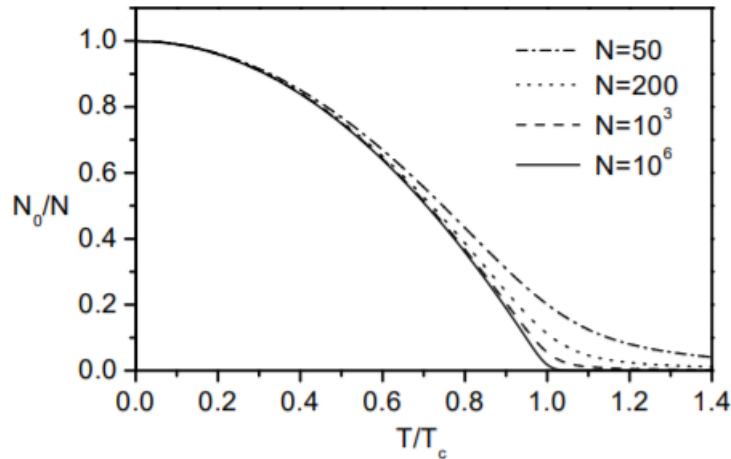

Figure 2.1 – Ground state population of the trapped 2D Bose gas as a function of temperature for different values of the total number of particles N. Figure from [28].

number of particles in the system has the same effect than in 3D, namely is changes the value of the critical temperature and leads to a smoother transition.

The previous calculations were performed in a basis in which the Hamiltonian was diagonal, but they can also be performed in real space. In that case, phase-space density relation linking the density to the chemical potential reads

$$n (\boldsymbol{r}) \lambda_T^2 = -\ln \left\{ 1 - e^{\beta [\tilde{\mu} - V_{\text{ext}} (\boldsymbol{r})]} \right\},$$

which shows that, in the centre of the trap at $\boldsymbol{r} = \boldsymbol{0}$, no condensation is possible as the density on that point tends towards infinity. However, condensation away from the centre of the trap cannot be excluded.

2.1.4 Some applications

Superfluidity

As already stated, one of the most striking feature of the 2D Bose gas is the absence of true long range order for a temperature different from the absolute 0. Nevertheless, a quasi-long

range order exists for temperatures small enough, which manifests itself by an algebraic decays of the one-body correlation function.

At strictly 0 K, a weakly interacting 2D Bose gas is condensed and can be described by a macroscopic wavefunction $\psi(\boldsymbol{r}, t) = n(\boldsymbol{r}, t) e^{i\theta(\boldsymbol{r}, t)}$, where $n(\boldsymbol{r}, t)$ and $\theta(\boldsymbol{r}, t)$ are real classical fields. If the temperature is raised from 0 K to a higher value, both the amplitude and the phase of $\psi(\boldsymbol{r}, t)$ will show some fluctuations around an equilibrium value.

Even though the amplitude, and thus the density, oscillates when the temperature is reached, those oscillations are suppressed for low enough temperature, leaving only a fluctuating phase. If only contact interactions are considered between free particles, the Hamiltonian of the system is given by

$$\hat{H} = \frac{\hbar^2}{2m} \int [\nabla_{\boldsymbol{r}} \psi^*(\boldsymbol{r})] [\nabla_{\boldsymbol{r}} \psi(\boldsymbol{r})] \, \mathrm{d}\boldsymbol{r} + \frac{g}{2} \int [\psi^*(\boldsymbol{r})]^2 [\psi(\boldsymbol{r})]^2 \, \mathrm{d}\boldsymbol{r}. \tag{2.9}$$

The dynamics of the wavefunction describing the system is dictated by the the Gross-Pitaevskii equation, which was derived previously and is given by eq. (1.16).

In order to find the local phase $\theta(\boldsymbol{r}, t)$, the sought wavefunction is written under the form $\psi(\boldsymbol{r}, t) = |\psi(\boldsymbol{r}, t)| e^{i\theta(\boldsymbol{r}, t)}$, with the amplitude linked to the local density through the relation $|\psi(\boldsymbol{r}, t)|^2 = n[1 + 2\eta(\boldsymbol{r}, t)]$, with the small perturbation $\eta(\boldsymbol{r}, t)$ verifying $\eta \ll 1$ and $\int \eta(\boldsymbol{r}, t) \, \mathrm{d}\boldsymbol{r} = 0$. Injecting those expression in expression (2.9) lead to the following form for the Hamiltonian

$$\hat{H} = \frac{n\hbar^2}{2m} \int \left\{ [1 + 2\eta(\boldsymbol{r}, t)] [\nabla_{\boldsymbol{r}} \theta(\boldsymbol{r}, t)]^2 + \frac{[\nabla_{\boldsymbol{r}} \eta(\boldsymbol{r}, t)]^2}{1 + 2\eta(\boldsymbol{r}, t)} \right\} \mathrm{d}\boldsymbol{r} + \frac{gn^2}{2} \int \left[1 + 4\eta(\boldsymbol{r}, t) + 4\eta^2(\boldsymbol{r}, t) \right] \mathrm{d}\boldsymbol{r}.$$

Neglecting the constant term $gn^2 L^2/2$ and using the assumption $\eta \ll 1$, the final expression of the Hamiltonian is

$$\hat{H} = \frac{n\hbar^2}{2m} \int \left\{ [\nabla_{\boldsymbol{r}} \theta(\boldsymbol{r}, t)]^2 + [\nabla_{\boldsymbol{r}} \eta(\boldsymbol{r}, t)]^2 \right\} \mathrm{d}\boldsymbol{r} + 2gn^2 \int \eta^2(\boldsymbol{r}, t) \, \mathrm{d}\boldsymbol{r}.$$

Moreover, the time evolution of $\theta(\boldsymbol{r}, t)$ and $\eta(\boldsymbol{r}, t)$ is given by the solution to the coupled system

$$\frac{\partial \theta}{\partial t}(\boldsymbol{r}, t) = \frac{\hbar^2}{2m} \nabla^2 \eta(\boldsymbol{r}, t) - \frac{gn}{\hbar} [1 + 2\eta(\boldsymbol{r}, t)],$$
$$\frac{\partial \eta}{\partial t}(\boldsymbol{r}, t) = -\frac{\hbar}{2m} \nabla^2 \theta(\boldsymbol{r}, t).$$

In order to solve that system, the unknowns can be expanded in Fourier series as

$$\theta(\boldsymbol{r}, t) = \sum_{\boldsymbol{k}} c_{\boldsymbol{k}}(t) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \quad \text{and} \quad \eta(\boldsymbol{r}, t) = \sum_{\boldsymbol{k}} d_{\boldsymbol{k}}(t) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}.$$

It should be noted that, by hypothesis, $\theta(\boldsymbol{r}, t)$ and $\eta(\boldsymbol{r}, t)$ are real, and so the coefficients appearing in the Fourier expansions verify the relations $c_{\boldsymbol{k}}^*(t) = c_{-\boldsymbol{k}}(t)$ and $d_{\boldsymbol{k}}^*(t) = d_{-\boldsymbol{k}}(t)$. Moreover, by using the conservation of particles $\int \eta(\boldsymbol{r}, t) \, \mathrm{d}\boldsymbol{r} = 0$, the first term in the series expansion of $\eta(\boldsymbol{r}, t)$ must be null, *i.e.* $d_0(t) = 0$.

Using the Fourier expansion of the density and the phase in the Hamiltonian and the coupled system, the Hamiltonian in Fourier space reads [17]

$$\hat{H} = nL^2 \sum_{\boldsymbol{k}} \left[\frac{\hbar^2 k^2}{2m} |c_{\boldsymbol{k}}(t)|^2 + \left(\frac{\hbar^2 k^2}{2m} + 2gn \right) |d_{\boldsymbol{k}}(t)|^2 \right], \tag{2.10}$$

while the system giving the time evolution of the density and the phase becomes $\dot{c}_0 = -\frac{gn}{\hbar}$ for $\boldsymbol{k} = \boldsymbol{0}$ and

$$\dot{c}_{\boldsymbol{k}} = -\left(\frac{\hbar k^2}{2m} + \frac{2gn}{\hbar}\right) d_{\boldsymbol{k}},$$

$$\dot{d}_{\boldsymbol{k}} = \frac{\hbar k^2}{2m} c_{\boldsymbol{k}}$$

for $\boldsymbol{k} \neq \boldsymbol{0}$. From there, the dispersion relation is found and is given by

$$\omega_{\boldsymbol{k}} = \sqrt{\frac{\hbar k^2}{2m}\left(\frac{\hbar k^2}{2m} + \frac{2gn}{\hbar}\right)},$$

which is nothing else than the Bogoliubov dispersion relation, which was already found in the part concerned with the dynamics of a 3D Bose gas.

The Hamiltonian given in (2.10) gives insight on the importance of the density and phase fluctuations. Indeed, by checking the coefficients in front of $\langle|d_{\boldsymbol{k}}(t)|^2\rangle$ and $\langle|c_{\boldsymbol{k}}(t)|^2\rangle$, which gives

$$\frac{\langle|d_{\boldsymbol{k}}(t)|^2\rangle}{\langle|c_{\boldsymbol{k}}(t)|^2\rangle} = \frac{\hbar^2 k^2/2m}{\hbar^2 k^2/2m + 2gn},$$

it is clear that long wavelengths ($\equiv k \to 0$) involve only phase fluctuations, and short wavelengths ($\equiv k \to +\infty$) involve phase and density variations in equal parts. Moreover, the Hamiltonian shows that the phase fluctuations do not cost energy in the $k \to 0$ limit, whereas the energetic cost of density fluctuations do not vanish in the same limit because of the interactions.

Since the gas is very cold, the most important part in the Hamiltonian (2.10) is the part containing the phase fluctuations, but it has to be kept in mind that if only that part is kept, short distance effects cannot be represented and a cutoff momentum $k_{\max} = 1/\xi$, with $\xi = 1/\sqrt{gn}$, is introduced. To incorporate the short-distance physics, the total density can be replaced by the superfluid density, leading to an Hamiltonian having the form

$$\hat{H} \approx n_s L^2 \sum_{\substack{\boldsymbol{k} \\ \|\boldsymbol{k}\|<\xi^{-1}}} \frac{\hbar^2 k^2}{2m}|c_{\boldsymbol{k}}|^2 = n_s \frac{\hbar^2}{2m}\int[\nabla_{\boldsymbol{r}}\theta(\boldsymbol{r},t)]^2\,\mathrm{d}\boldsymbol{r}.$$

It was shown that at low temperature, only phase fluctuations are important. However, the mechanism leading to the phase transition from the superfluid state to the normal state have not been yet explained. It should be noted that even though the density fluctuations are small compared to the phase fluctuations, those alone cannot explain the transition since at a given critical point, the phonons, which are responsible for those fluctuations, destroy the long-range order in a very smooth and "slow" way, since the first-order correlation function reads [17]

$$g^{(1)}(r) = n_s\left(\frac{\xi}{r}\right)^{1/\left(n_s\lambda_T^2\right)}.$$

Phase fluctuations are due to two different sources. The first one, already identified previously, are the long wavelengths phonons. The other source of phase fluctuation, which is a key ingredient in the BKT theory of superfluidity, is the apparition of vortices. Such vortices are points where the superfluid density vanishes and around which the phase varies by a multiple of 2π.

For those vortices, two distinct regimes exist. The first one is the regime in which the temperature is lower than some critical value, the BKT temperature T_{BKT}. In such a case, the vortices form pairs of opposite circulations, which means that the pair does not carry a net

charge and that there is no phase fluctuation along a path greater than the size of the pair. Such pairs do not influence the behaviour of $\rho(r)$ at large distance and fall in the "short-range" physics, together with the density fluctuations. The other regime is reached when $T > T_{BKT}$, in which case the pairs break and individual free vortices proliferate in the gas, creating a disordered gas of phase defect, which means that a well-defined phase θ can no longer be assigned to the gas.

Josephson effect

Another application of the bidimensional Bose gas is the realization of a Josephson effect, consisting in the exchange of atoms between 2 BECs. The principle is illustrated in fig. 2.2.
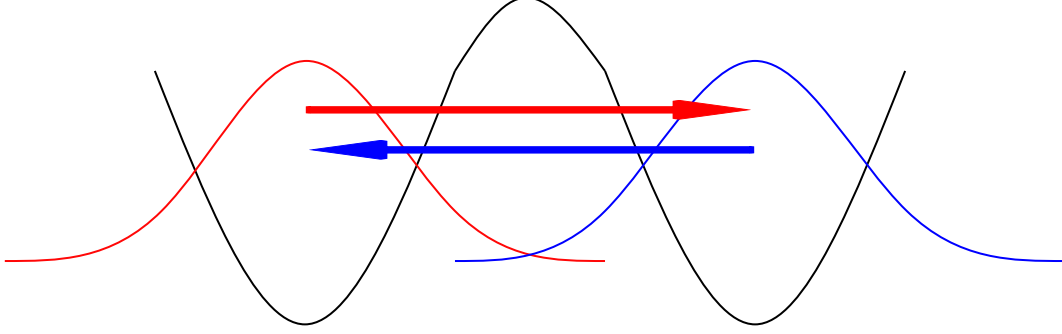

Figure 2.2 – Schematic illustration of the principle of the Josephson effect between 2 BECs.

If the potential separating the two condensates is symmetric, an approximate solution to the Gross-Pitaevskii equation can be constructed[1]. By solving the GPE for N_a and N_b atoms for the different wells, the wavefunction of the system can be written

$$\psi(\boldsymbol{r}, t) = \psi_a(\boldsymbol{r}, N_a(t)) e^{i\theta_a(\boldsymbol{r}, t)} + \psi_b(\boldsymbol{r}, N_b(t)) e^{i\theta_b(\boldsymbol{r}, t)}.$$

The total number of atoms in the system $N = N_a(t) + N_b(t)$ stays, of course, constant. Using that wavefunction, an atomic current $I = \frac{\partial}{\partial t} N_a = -\frac{\partial}{\partial t} N_b$ between the wells exists, given that the phase difference between the two condensates $\Phi(\boldsymbol{r}, t) = \theta_b(\boldsymbol{r}, t) - \theta_a(\boldsymbol{r}, t)$ is nonzero. If the double well potential is considered to be symmetric around the $z = 0$ position, the current is given by [32]

$$I(\boldsymbol{r}, t) = -I_J \sin\left[\Phi(\boldsymbol{r}, t)\right], \tag{2.11}$$

with the amplitude I_J given by

$$I_J = \frac{\hbar}{m} \int dx\, dy\, \left[\psi_a(\boldsymbol{r}, t) \frac{\partial \psi_b}{\partial z}(\boldsymbol{r}, t) - \psi_b(\boldsymbol{r}, t) \frac{\partial \psi_a}{\partial z}(\boldsymbol{r}, t)\right]\Bigg|_{z=0}.$$

To get the exact expression of the tunnelling current, an equation for the phase $\Phi(\boldsymbol{r}, t)$ is needed. Fortunately, it is known that the time dependence of the phase of the wavefunction describing a BEC is in general defined by [32]

$$\hbar \frac{\partial \theta}{\partial t}(\boldsymbol{r}, t) = -\left(\frac{m}{2} v_s^2 + \mu\right),$$

with $v_s = \frac{\hbar}{m} \nabla_{\boldsymbol{r}} \theta(\boldsymbol{r}, t)$ the superfluid velocity. Considering the system of the two condensates and neglecting the (small) superfluid velocity created by the Josephson current, the equation for the phase of the total system reads

$$\frac{\partial \Phi}{\partial t}(\boldsymbol{r}, t) = -\frac{1}{\hbar}(\mu_b - \mu_a), \tag{2.12}$$

---

[1]This holds if the overlap of the wavefunctions associated to each condensate is small, which is indeed the case if the barrier separating those BECs is "thick" enough.

with $\mu_{a,b}$ the chemical potential of the condensate in well a, b. It should be noted that this last equation is only valid in the case of two well-separated condensates.

If the variations of $N_a(t)$ and $N_b(t)$ around their equilibrium value $N/2$ is small, a small parameter k, defined as

$$k(t) = \frac{N_a(t) - N_b(t)}{N}, \quad \text{with } |k(t)| \ll 1,$$

allows to rewrite eqs. (2.11) and (2.12) under the form

$$\frac{\partial k}{\partial t}(\boldsymbol{r}, t) = -I_J \sin[\Phi(\boldsymbol{r}, t)] \quad \text{and} \quad \frac{\partial \Phi}{\partial t}(\boldsymbol{r}, t) = \frac{E_c}{\hbar} k(\boldsymbol{r}, t), \tag{2.13}$$

with $E_c = 2\frac{\mathrm{d}\mu_a}{\mathrm{d}N_a}$. To get those new forms, the current $I(\boldsymbol{r}, t)$ appearing in eq. (2.11) is re-expressed under the form $I(\boldsymbol{r}, t) = \frac{\partial N_a}{\partial t} = \frac{\partial N_a}{\partial k}\frac{\partial k}{\partial t}$, while the new expression for the phase $\Phi(\boldsymbol{r}, t)$ is obtained by combining the Taylor expansion of the chemical potentials around their equilibrium value with the fact that $\frac{\mathrm{d}\mu_a}{\mathrm{d}N_a} = -\frac{\mathrm{d}\mu_b}{\mathrm{d}N_b}$, *i.e.*

$$\mu_{a,b} = \mu_{a,b}^{\mathrm{eq}} + k\frac{\mathrm{d}\mu_{a,b}}{\mathrm{d}N_{a,b}} \quad \text{and} \quad \frac{\mathrm{d}\mu_a}{\mathrm{d}N_a} = -\frac{\mathrm{d}\mu_b}{\mathrm{d}N_b}.$$

The set of equations (2.13) have the same form as the equations of motion of a classical pendulum, and the solution depends on the initial conditions.

First, if the phase and k are small, the equations appearing in (2.13) can be linearised, leading to an oscillatory solution with frequency

$$\omega_{pl} = \sqrt{\frac{I_J E_c}{\hbar}},$$

which is the classical oscillation frequency between the wells. If $|k| > \sqrt{2\hbar I_J/E_c}$, the solutions to the equations correspond to a full rotation of the phase. Finally, if $|k| \gg \sqrt{2\hbar I_J/E_c}$, the phase evolves linearly in time according to the relation $\Phi = tE_c k_0/\hbar$, with k_0 an equilibrium value around which k oscillates according to the law

$$k = k_0\left[1 + \frac{\hbar I_J}{E_c k_0^2}\cos\left(\frac{E_c k_0}{\hbar}t\right)\right],$$

which is possible only if $\sqrt{\frac{N^2 E_c}{\hbar I_J}} \gg 1$, given the condition $|k| \ll N$. It was already stressed that the above results are valid for a weak overlap of the condensates. In fact, in order to decouple the Josephson motion from the oscillations of each of the condensates, k and Φ should vary on timescales bigger than $1/\omega_{ho}$, the trap frequency, which leads to the condition $\sqrt{\hbar I_J E_c} \ll \hbar\omega_{ho}$.

All this discussion was to highlight the fact that a tunnelling current exists between two spatially separated BECs, in an analogous way to the tunnelling current that exists between two superconductors separated by a thin enough insulator. However, if the wells are separated by a big barrier, then the tunnelling of atoms can be considered as negligible, and the system acts as if it where an insulator.

2.2   The 1D Bose gas

Introduction

After having discussed the 3D and 2D Bose gas, a natural extension is to discuss the 1D case. In such a configuration, the behaviour of the gas can be dramatically different from the previous

discussed cases as it can behave as a Fermi gas. Other strange effect, such as solitonic ones, can manifest themselves.

If the confining potential is given by $V_{\text{ext}}(\boldsymbol{r}) = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$, the condition to freeze out the oscillations along the x- and y- directions is $\hbar\omega_x, \hbar\omega_y \gg k_B T$ and $\omega_x, \omega_y \gg \omega_z$, while the oscillation energy along the remaining direction is of the order of the thermal energy, i.e. $\hbar\omega_z \approx k_B T$.

2.2.1 The ideal gas

If the particles constituting the gas do not interact and are totally free to move along one dimension, there is only kinetic energy in the system, which reads $\epsilon_k = \frac{\hbar^2 k^2}{2m} + \frac{\hbar}{2}\left(\omega_x + \omega_y\right)$. In this case, the mean number of particles contained in the system is given by

$$\left\langle \hat{N} \right\rangle = \sum_k \frac{1}{\exp\left[\beta\left(\epsilon_k - \mu\right)\right] - 1}.$$

Following the by now standard procedure, the sum can be replaced by an integral, yielding

$$\left\langle \hat{N} \right\rangle = \frac{L}{\lambda_T} g_{1/2}\left(e^{\beta\tilde{\mu}}\right),$$

with $\tilde{\mu} = \mu - \frac{\hbar}{2}\left(\omega_x + \omega_y\right)$, which leads to the density $n\lambda_T = g_{1/2}\left(e^{\beta\tilde{\mu}}\right)$. If a condensate were realized, that equality would become $n\lambda_T = \zeta\left(1/2\right)$, which means that an infinite density would be needed to reach condensation, since $\zeta\left(x\right)$ diverges for $x \le 1$. This shows that no condensate can be realized in a perfect uniform infinite 1D Bose gas, in good agreement with the Hohenberg theorem.

Even though no real condensate can be formed in low dimensional systems, it was shown previously that a 2D Bose gas could nevertheless exhibit a superfluid behaviour under a given temperature and that a harmonic confinement could change the behaviour of the gas. It is thus instructing to check whether a 1D Bose gas can undergo a phase transition to a superfluid state and if a harmonic confinement can change the conclusions with respect to what was concluded for the ideal free case.

2.2.2 The trapped Bose gas

The case of a gas confined by a harmonic potential along the previously free space direction is now considered. The energy spectrum of the Hamiltonian is thus $\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_z + \frac{\hbar}{2}\left(\omega_x + \omega_y\right)$. In the case of a one-dimensional system, the density of states reads $\rho\left(\epsilon\right) = 1/\hbar\omega_z$ and the total number of particles contained in the system is given by

$$N = N_0 + \int \frac{\rho\left(\epsilon\right)}{\exp\left[\beta\left(\epsilon - \tilde{\mu}\right)\right] - 1}\mathrm{d}\epsilon,$$

with $\tilde{\mu} = \mu - \frac{\hbar}{2}\left(\omega_x + \omega_y + \omega_z\right)$. The problem with such an expression is that the integrand diverges for $\tilde{\mu} \to 0$. This divergence comes from the fact that the discrete nature of the energy spectrum was not correctly taken into account. To correct this, low energy modes have to be separated from high energy modes, yielding

$$N = N_0 + k_B T \sum_{n=1}^{M} \frac{1}{n\hbar\omega_z - \tilde{\mu}} + \sum_{n=M+1}^{+\infty} \frac{1}{\exp\left[\beta\left(n\hbar\omega_z - \tilde{\mu}\right)\right] - 1}, \tag{2.14}$$

with the number M satisfying $1 \ll M \ll k_B T / \hbar \omega_z$. The last term of the right hand-side can be transformed to an integral to give

$$\sum_{n=M+1}^{+\infty} \frac{1}{\exp\left[\beta\left(n\hbar\omega_z - \tilde{\mu}\right)\right] - 1} \approx \int_M^{+\infty} \frac{\mathrm{d}n}{\exp\left[\beta\left(n\hbar\omega_z - \tilde{\mu}\right)\right] - 1}.$$

Using the by now well-known trick to replace the integrand by the corresponding geometric progression and then permuting the summation with the integration leads to

$$\frac{k_B T}{\hbar \omega_z} \sum_{j=1}^{+\infty} \frac{\exp\left[-j\beta\left(M\hbar\omega_z - \tilde{\mu}\right)\right]}{j} = -\frac{k_B T}{\hbar \omega_z} \ln\left[1 - e^{-\beta(M\hbar\omega_z - \tilde{\mu})}\right].$$

To compute the first sum appearing in eq. (2.14), the digamma function $\psi(z)$ has to be used, which leads to [30]

$$\sum_{n=1}^{M} \frac{1}{n - \tilde{\mu}/\hbar\omega_z} = \psi\left(M + 1 - \frac{\tilde{\mu}}{\hbar\omega_z}\right) - \psi\left(1 - \frac{\tilde{\mu}}{\hbar\omega_z}\right).$$

Injecting all those results in eq. (2.14), the total number of particles contained can be computed and is given by

$$N = N_0 + \psi\left(M + 1 - \frac{\tilde{\mu}}{\hbar\omega_z}\right) - \psi\left(1 - \frac{\tilde{\mu}}{\hbar\omega_z}\right) - \frac{k_B T}{\hbar \omega_z} \ln\left[1 - e^{-\beta(M\hbar\omega_z - \tilde{\mu})}\right].$$

By further taking into account that when the system is in the lowest state, $\tilde{\mu} \to 0$, which means that the chemical potential is linked to the lowest energy population by the relation $\tilde{\mu} = -\frac{k_B T}{N_0}$ (obtained by Taylor expanding the repartition function), the expression for the number of particles in the system can be approximated by the expression

$$N \approx N_0 + \frac{k_B T}{\hbar \omega_z} \ln(N_0) + \frac{k_B T}{\hbar \omega_z} \ln\left(\frac{k_B T}{N_0 \hbar \omega_z}\right) - \psi\left(1 + \frac{k_B T}{N_0 \hbar \omega_z}\right)$$

$$= N_0 + \frac{k_B T}{\hbar \omega_z} \ln\left(\frac{k_B T}{\hbar \omega_z}\right) - \psi\left(1 + \frac{k_B T}{N_0 \hbar \omega_z}\right).$$

As was previously the case in 2D, there are two distinct regimes, separated by a temperature given by [30]

$$T_{1D} \approx \frac{N}{\ln(N)} \hbar \omega_z.$$

2.2.3 The interacting 1D Bose gas

It is now time to include interactions between the particles of the gas. As in all previous cases, the only interactions that will be considered are pairwise, since the gas is supposed to be dilute. The case of the 1D interacting gas is quite different from its 2D and 3D counterparts, since there are not an infinity of directions in which the scattered particles can go.

As was the case for higher dimensions, the scattering state of the system has to solve the radial Schrödinger equation, which in this case reads

$$\left[-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right] \psi_k(x) = E\psi_k(x),$$

with $V(x)$ a symmetric finite range potential, and $E = \frac{\hbar^2 k^2}{2m}$ the energy. Moreover, the asymptotic behaviour of the scattering state is the superposition of the incoming plane wave and the scattered one, which reads

$$\psi_k(x) \approx \exp(ikx) + \frac{i}{k} f_k(\epsilon) \exp(ikx_0), \quad (x \to +\infty),$$

with $\epsilon = x/x_0$ and x_0 the range of the potential [4]. In order to define the partial wave decomposition, which will allow to find the partial wave projections of $\psi_k(x)$ and the phase shifts $\delta(k)$ introduced by the potential, the asymptotic form for the scattering state is parametrized as

$$\psi_k(x) \approx \sum_{j=0}^{L} \epsilon^j A_j \cos\left[kx_0 + j\frac{\pi}{2} + \delta_j\left(k^2\right)\right], \quad (x \to +\infty),$$

where the A_j's are unknown coefficients, and where the sum contains only 2 terms because there are only two possible scattering directions. Comparing the asymptotic form of $\psi_k(x)$ with its partial wave decomposition and using the decomposition $\exp(ikx) = \cos(kx_0) + i\epsilon \sin(kx_0)$ allows to identify [4]

$$A_j = (-i)^j \exp(i\delta_j) \quad \text{and} \quad f_k(\epsilon) = k \sum_{j=0}^{1} \epsilon^j \exp(i\delta_j) \sin(\delta_j).$$

The total scattering cross section can then be computed, and read $\sigma(k) = 2\sum_{j=0}^{1} \sin^2(\delta_j)$, where the expression of the partial scattering amplitude $f_j = k \exp(i\delta_j) \sin(\delta_j)$ was used.

Another way of doing things is to consider that, like in the 3D case, the pairwise interactions between atoms are modelled by the pseudopotential

$$U(r) = g\delta(\boldsymbol{r}) \frac{\partial}{\partial r}(r\cdot),$$

with $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ the vector going from one particle to the other, $g = \frac{2\pi\hbar^2 a}{\mu}$ the strength of the pseudopotential, a the s-wave scattering length of the true interaction and μ the reduced mass. Since the confining potential is harmonic, the center-of-mass motion can be decoupled from the relative motion, which obeys the Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + g\delta(\boldsymbol{r})\frac{\partial}{\partial r}(r\cdot) + \frac{\mu}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2\right)\right]\psi = E\psi.$$

To proceed further, the sought wavefunction is assumed to have the following asymptotic behaviour

$$\psi(z, \rho) \approx \left\{e^{ikz} + [f_{\text{even}} + \text{sign}(z)] e^{ik|z|}\right\} \phi_{0,0}(\rho), \quad (z \to +\infty),$$

with $\rho = \sqrt{x^2 + y^2}$, $f_{\text{even/odd}}$ the scattering amplitudes for the even/odd partial waves and $\phi_{0,0}(\rho)$ the lowest energy eigenmode of the transverse harmonic oscillator. Following the developments of [24], it can be shown that

$$f_{\text{even}} \approx -\frac{1}{1 + ika_{\text{1D}}} \quad \text{and} \quad f_{\text{odd}} = 0,$$

with a_{1D} the one-dimensional scattering length, given by the relation

$$a_{\text{1D}} = -\frac{a_\perp^2}{2a}\left(1 - C\frac{a}{a_\perp}\right), \quad \text{with } a_\perp^2 = \frac{\hbar}{m\sqrt{\omega_x\omega_y}}, C \approx 1.4603.$$

2.2.4 Dynamics

Rather than describe an application of the 1D interacting Bose gas (as was previously done for a bidimensional gas), the one-dimensional Gross-Pitaevskii equation will be derived. It will be shown that the expression obtained for the time evolution of the wavefunction along the z-direction is the same as in 3D, the only difference being the value of the constant g.

The full three-dimensional Gross-Pitaevskii equation takes the form given in eq. (1.16). Since the motion is frozen out along the x- and y-directions, the wavefunction of the system can be written under the form

$$\psi(\boldsymbol{r}, t) = \phi_{0,0}(x, y)\psi(z, t)$$
$$= \phi_0(x)\phi_0(y)\psi(z, t), \tag{2.15}$$

where $\phi_0(x)$ and $\phi_0(y)$ are the lowest-energy wavefunction of the harmonic oscillator along x and y, respectively given by

$$\phi_0(x) = \sqrt{\frac{1}{a_x\sqrt{\pi}}}\exp\left(-\frac{x^2}{2a_x^2}\right) \quad \text{and} \quad \phi_0(y) = \sqrt{\frac{1}{a_y\sqrt{\pi}}}\exp\left(-\frac{y^2}{2a_y^2}\right),$$

with a_x and a_y the characteristic size along the x- and y-directions, respectively. Injecting the ansatz (2.15) into the full Gross-Pitaevskii equation leads to

$$i\hbar\phi_0(x)\phi_0(y)\frac{\partial}{\partial t}\psi(z, t) =$$
$$-\frac{\hbar^2}{2m}\left\{\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_0(x)\right]\phi_0(y)\psi(z, t) + \left[\frac{\mathrm{d}^2}{\mathrm{d}y^2}\phi_0(y)\right]\phi_0(x)\psi(z, t) + \left[\frac{\partial^2}{\partial z^2}\psi(z, t)\right]\phi_0(x)\phi_0(y)\right\}$$
$$+\frac{m}{2}\left\{\left[\omega_x^2 x^2\phi_0(x)\right]\phi_0(y)\psi(z, t) + \left[\omega_y^2 y^2\phi_0(y)\right]\phi_0(x)\psi(z, t) + \left[\omega_z^2 z^2\psi(z, t)\right]\phi_0(x)\phi(y)\right\}$$
$$+ g\left|\psi(z, t)\right|^2\psi(z, t)\phi_0^3(x)\phi_0^3(y).$$

To keep only the equation for the wavefunction along the z-direction, only the terms having coefficients $\phi_0^n(x)\phi_0^n(x)$ are kept (with n being equal to 1 or 3 here). The corresponding equation is then averaged by multiplying both sides by $\phi_0(x)\phi_0(y)$ and integrating over the whole space. The final expression, which corresponds to an effective 1D Gross-Pitaevskii equation then takes the form

$$i\hbar\frac{\partial}{\partial t}\psi(z, t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{1}{2}m\omega_z^2 z^2 + \tilde{g}\left|\psi(z, t)\right|^2\right]\psi(z, t), \tag{2.16}$$

which has exactly the same form as the full 3D GPE eq. (1.16), except for the parameter $\tilde{g}$, which takes the form $\tilde{g} = 2a\hbar\sqrt{\omega_x\omega_y}$. This equation can be made adimensional. By calling $a_\perp = \sqrt{\frac{\hbar}{m\sqrt{\omega_x\omega_y}}}$ the radial extension of the condensate and by introducing the adimensional variables

$$\tilde{t} = \omega_z t, \quad \tilde{z} = \frac{z}{a_\perp}, \quad \text{and} \quad \tilde{\psi}(\tilde{z}, \tilde{t}) = \sqrt{a_\perp}\psi(z, t),$$

the expression of the adimensional 1D Gross-Pitaevskii equation takes the form

$$i\epsilon\frac{\partial}{\partial\tilde{t}}\tilde{\psi}(\tilde{z}, \tilde{t}) = \left[-\frac{\epsilon^2}{2}\frac{\partial^2}{\partial\tilde{z}^2} + \frac{1}{2}\tilde{z}^2 + \delta\right]\tilde{\psi}(\tilde{z}, \tilde{t}),$$

where ϵ and δ are adimensional quantities given by

$$\epsilon = \frac{\hbar}{m\omega_z a_\perp^2} \quad \text{and} \quad \delta = \frac{\tilde{g}}{m\omega_z^2 a_\perp^2}.$$

3

Chapter

Solitons

3.1 Generalities

In the literature, the distinction between solitary wave and soliton is blurred, and that those terms are used interchangeably. It is thus convenient to start the discussion by defining[1] precisely what a solitary wave and a soliton are.

Definition 1 (Solitary wave) *A solitary wave is a localized non-singular solution to any non-linear field equation (or system of coupled equations if several fields are involved) with a localized energy density behaving as*

$$\epsilon\left(\boldsymbol{x},t\right) = \epsilon\left(\boldsymbol{x} - \boldsymbol{v}t\right),$$

with $\boldsymbol{v}$ a velocity vector.

This definition of the solitary wave shows that the energy density moves undisturbed with a constant speed in space, and shows that any time-independent localized solution is a solitary wave with velocity $\boldsymbol{v} = \boldsymbol{0}$.

Definition 2 (Soliton) *Consider some (possibly coupled) non-linear equation(s). Let them have a solitary wave solution whose energy density is some localized function $\epsilon_0\left(\boldsymbol{x} - \boldsymbol{v}t\right)$. Consider any other solution of this system which in the far past consists of N such solitary waves, with arbitrary initial velocities and positions. Then the energy density $\epsilon\left(\boldsymbol{x},t\right)$ of this solution will have the form*

$$\epsilon\left(\boldsymbol{x},t\right) \to \sum_{i=1}^{N} \epsilon_0\left(\boldsymbol{x} - \boldsymbol{x}_i - \boldsymbol{v}_i t\right), \quad \left(t \to -\infty\right).$$

Given this configuration at $t = -\infty$, it will then evolve in time as governed by the non-linear equations. Suppose this evolution is such that

$$\epsilon\left(\boldsymbol{x},t\right) \to \sum_{i=1}^{N} \epsilon_0\left(\boldsymbol{x} - \boldsymbol{x}_i - \boldsymbol{v}_i t + \boldsymbol{\delta}_i\right), \quad \left(t \to +\infty\right),$$

where $\boldsymbol{\delta}_i$ are some constant vectors. Then such a solitary wave is called a soliton.

The definition of a soliton is thus a solitary wave whose energy density profile is asymptotically restored to its initial profile, with the possibility of a spatial shift. That definition of a soliton can be understood in a less formal way: if N infinitely hard particles are considered and collide,

---

[1]Those definition are from [33].

they will continue to move with the same speed, only their trajectories are possibly modified. Such particles can be seen as solitons. An interesting point, particularly true for solitons in Bose-Einstein condensates, is that, even if the governing equation(s) is/are wave equations, the behaviour of the solution is particle-like.

With those definitions, it is now clear what is a soliton. A last general remark that can be made is that, depending on the sign of the nonlinearity in the one-dimensional Gross-Pitaevskii equation ($g < 0$ for attractive interactions and $g > 0$ for repulsive ones), different behaviours are observed. In particular, for repulsive interactions, *dark* solitons can be generated, while, for attractive interactions, *bright* solitons can be generated.

The free 1D Nonlinear Schrödinger equation is a field equation that is exactly integrable in the sense that its solutions possess an infinite number of conserved quantities (such as energy, momentum, number of particles, *etc.*). Bree 1D Gross-Pitaevskii equation is exactly integrable, a complete spectrum of solution exist, hence solitonic solutions are plausible existing solution (that arise due to the nonlinearity). Those solitonic solution can be obtained in the general framework of the *Inverse Scattering Transform*. That technique, introduced by Zakharov and Shabat, consists in drawing an analogy between the studied equation and a system of the form

$$i\zeta \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix} = \begin{bmatrix} -\frac{\partial}{\partial x} & \psi(x,t) \\ -\psi^*(x,t) & \frac{\partial}{\partial x} \end{bmatrix} \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}.$$

with $\psi(x,t)$ is the solution to the 1D Gross-Pitaevskii equation. The solution to such a problem consists in three mains steps:

- first, the eigenvalues of the above matrix have to be found at an initial time t_i, with $\psi(x,t_i)$ as initial condition. The spectrum of the problem consists in a set of discrete eigenvalues, and a continuous component, corresponding to the solitons and the radiations, respectively.

- Then, the quantities $u(x,t)$ and $u(x,t)$ can be chosen such that the compatibility condition $\frac{\partial}{\partial xt}\left[u(x,t),v(x,t)\right]^{\mathrm{T}} = \frac{\partial}{\partial tx}\left[u(x,t),v(x,t)\right]^{\mathrm{T}}$ ensures that $\psi(x,t)$ solves the equation.

- Finally, the time evolution of $\psi(x,t)$ can be found by inverting the scattering problem given initially.

3.2 Dark soliton

3.2.1 Generalities

In the previous section, it was explained that a dark soliton is realized in a BEC if the interaction between particles is negative, *i.e.* $g < 0$. What was not said is that, even for such attractive interactions, two distinct solutions exist: dark solitons, and grey solitons. The first ones can be associated to a hole in the gas, in the sense that it correspond to a locally null density. The other one can be associated to a "quasi-hole" in the sense that, locally, the density is lowered with respect to its equilibrium value, but does not go to 0.

In the following, rather than considering the form of the previously derived 1D GPE eq. (2.16), a slight modification of the equation will be considered, in order to stick to the literature and to the code that has been written to deal with bright solitons (see later). The new form is expressed in natural units, *i.e.* units in which $\hbar = 1$ and $m = 1$. The equation then reads

$$i\frac{\partial}{\partial t}\psi(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V(z) + |\psi(z,t)|^2\right]\psi(z,t). \tag{3.1}$$

In the case in which there is no trapping potential, the simpler non-trivial solution to the former equation takes the form of a plane wave,

$$\psi(z,t) = \sqrt{n_0} \exp\left[i\left(kz - \omega t + \theta_0\right)\right],$$

where n_0 is the equilibrium density and θ_0 an arbitrary phase. Injecting that solution into the last equation leads to the dispersion relation $\omega = \frac{1}{2}k^2 - n_0$. As explained in [13], the dark soliton solutions can be seen as strong nonlinear excitations of the plane wave solution given previously. In the most general case in which the density moves, a single dark soliton solution may be expressed as

$$\psi(z,t) = \sqrt{n_0}\left[B\tanh\left(\zeta\right) + iA\right]\exp\left[i\left(kz - \omega t + \theta_0\right)\right],$$

where $\zeta = \sqrt{n_0}B\left[z - z_0(t)\right]$, with $z_0(t) = z_0 + vt$ the position of the centre of the soliton (with v the relative speed of the soliton and the moving density, given by $v = A\sqrt{n_0} + k$).

In the simpler case where the background density is at rest $(k = 0)$, the square of the modulus of the wavefunction is given by

$$|\psi(z,t)|^2 = n_0\left[1 - B^2\operatorname{sech}^2(\zeta)\right]$$
$$= n_0\left[1 - \cos^2(\phi)\operatorname{sech}^2(\zeta)\right]$$

where the fundamental relation $\cosh^2(z) + \sinh(z)$ was used and where, sticking to [13], the angle ϕ is introduced so as to verify $A = \sin(\phi)$ and $B = \cos(\phi)$.

3.2.2 Link with the Korteweg - de Vries equation

In the case of a small amplitude black soliton, which travels with a speed close to the speed of sound [13], the black soliton can be described by an effective KdV equation, which reads, for a field $u(z,t)$,

$$\frac{\partial}{\partial t}u(z,t) + 6u(z,t)\frac{\partial}{\partial z}u(z,t) + \frac{\partial^3}{\partial z^3}u(z,t) = 0$$

and has a single-soliton solution of the form

$$u(z,t) = 2\kappa^2\operatorname{sech}^2\left[\kappa\left(z - 4\kappa^2 t\right)\right],$$

with κ, an arbitrary constant.

In order to see the similarities, the adimensional generalized free 1D GPE

$$i\frac{\partial}{\partial t}\psi(z,t) = -\frac{1}{2}\frac{\partial^2}{\partial 2^2}\psi(z,t) + f(n)\psi(n),$$

is used, with $f(n)$ a nonlinear function that take into account the fact that the transverse density can depend upon the longitudinal coordinate z, is used. Injecting the Madelung transformation $\psi(z,t) = \sqrt{n(z,t)}\exp\left[i\theta(z,t)\right]$ into that equation leads to the following nonlinear coupled system of equations

$$\begin{cases} \dfrac{\partial}{\partial t}n(z,t) = -\dfrac{\partial}{\partial z}\left[n(z,t)\dfrac{\partial}{\partial z}\theta(z,t)\right], \\ \dfrac{\partial}{\partial t}\theta(z,t) = \dfrac{1}{2}\dfrac{1}{\sqrt{n(z,t)}}\dfrac{\partial^2}{\partial z^2}\sqrt{n(z,t)} - \dfrac{1}{2}\left[\dfrac{\partial}{\partial z}\theta(z,t)\right]^2 - f(n). \end{cases} \tag{3.2}$$

The simplest solution of that system is a constant density $n(z,t) = |\psi(z,t)|^2 = n_0$ and a phase evolving linearly with time, i.e. $\theta(z,t) = f(n_0)t$. To get a more general solution to that system

of equations, a perturbation method approach can be undertaken. By using a Taylor expansion around their equilibrium values, the functions $n(z,t)$, $\theta(z,t)$ and $f(n)$ take the form

$$
\begin{cases}
n(Z,T) = n_0 + \epsilon n_1(Z,T) + \epsilon^2 n_2(Z,T) + \dots, \\
\theta(Z,T) = -f(n_0)t + \epsilon^{1/2}\theta_1(Z,T) + \epsilon^{3/2}\theta_2(Z,T) + \dots, \\
f(n) = f(n_0) + \epsilon n_1(Z,T) \left.\frac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0} + \epsilon^2 \left[\frac{n_1^2(Z,T)}{2}\left.\frac{\mathrm{d}^2 f}{\mathrm{d}n^2}\right|_{n=n_0} + n_2(Z,T)\left.\frac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0}\right] + \mathcal{O}(\epsilon^3),
\end{cases}
$$

where ϵ is a small parameter and the spatial and temporal variations of the functions are assumed to be smooth, allowing to rescale space and time to the new variables

$$
Z = \epsilon^{1/2}(z - ct) \quad \text{and} \quad T = \epsilon^{3/2}t.
$$

Thanks to those rescaled quantities, and by using the chain rule for the derivatives, the derivatives can be re-expressed under the form

$$
\frac{\partial}{\partial z} = \frac{\partial}{\partial Z}\frac{\partial Z}{\partial z} \qquad\qquad \frac{\partial}{\partial t} = \frac{\partial}{\partial Z}\frac{\partial Z}{\partial T}\frac{\partial T}{\partial t} + \frac{\partial}{\partial T}\frac{\partial T}{\partial t}
$$
$$
= \epsilon^{1/2}\frac{\partial}{\partial Z} \qquad\qquad\qquad = -\epsilon^{1/2}c\frac{\partial}{\partial Z} + \epsilon^{3/2}\frac{\partial}{\partial T}
$$

Combining those new expressions with the Taylor development of $\sqrt{n(z,t)}$ and $\frac{1}{\sqrt{n(z,t)}}$, the equations appearing in (3.2) can be re-expressed. Keeping the $\mathcal{O}(\epsilon^{3/2})$ term in the first equation and the $\mathcal{O}(\epsilon)$ term in the second equation leads to the system

$$
\begin{cases}
c\dfrac{\partial}{\partial Z}n_1(Z,T) = n_0\dfrac{\partial^2}{\partial Z^2}\theta_1(Z,T), \\
\dfrac{\partial}{\partial Z}\theta_1(Z,T) = n_1(Z,T)\left.\dfrac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0},
\end{cases}
$$

while, if the terms of order $\mathcal{O}(\epsilon^{5/2})$ and $\mathcal{O}(\epsilon^2)$ are kept, the system becomes

$$
\begin{cases}
\dfrac{\partial}{\partial T}n_1(Z,T) - c\dfrac{\partial}{\partial Z}n_2(Z,T) = -n_0\dfrac{\partial^2}{\partial Z^2}\theta_2(Z,T) - \dfrac{\partial}{\partial Z}\left[n_1(Z,T)\dfrac{\partial}{\partial Z}\theta_1(Z,T)\right], \\
\dfrac{\partial}{\partial T}\theta_1(Z,T) - c\dfrac{\partial}{\partial Z}\theta_2(Z,T) = \\
\qquad \dfrac{1}{4n_0}\dfrac{\partial^2}{\partial Z^2}n_1(Z,T) - \dfrac{1}{2}\left[\dfrac{\partial}{\partial Z}\theta_1(Z,T)\right]^2 - \left[\dfrac{n_1^2(Z,T)}{2}\left.\dfrac{\mathrm{d}^2 f}{\mathrm{d}n^2}\right|_{n=n_0} + n_2(Z,T)\left.\dfrac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0}\right].
\end{cases}
$$

The compatibility condition linked to that system reads $c^2 = n_0 \left.\frac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0}$, along with a KdV equation for the unknown density $n_1(Z,T)$ [13]

$$
2c\frac{\partial}{\partial T}n_1(Z,T) + \left[3\left.\frac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0} + n_0\left.\frac{\mathrm{d}^2 f}{\mathrm{d}n^2}\right|_{n=n_0}\right]n_1(Z,T)\frac{\partial}{\partial Z}n_1(Z,T) - \frac{1}{4}\frac{\partial^3}{\partial Z^3}n_1(Z,T) = 0.
$$

The density of a shallow dark soliton can thus be expressed as a KdV soliton. Returning to the original coordinates, n_1 takes the form

$$
n_1(z,t) = -\frac{3\kappa^2}{2\left[3\left.\frac{\mathrm{d}f}{\mathrm{d}n}\right|_{n=n_0} + n_0\left.\frac{\mathrm{d}^2 f}{\mathrm{d}n^2}\right|_{n=n_0}\right]}\operatorname{sech}^2\left[\epsilon^{1/2}\kappa(z - vt)\right],
$$

where κ is an arbitrary constant, and v is the soliton's speed given by the relation $v = c - \epsilon \frac{\kappa^2}{2c}$, which shows that the soliton moves slower than the speed of sound. Because of the minus sign appearing in the expression of the density $n_1(z, t)$, the dark soliton corresponds in a dip in density. The phase can also be found and is given by [13]

$$\theta_1(z, t) = -\frac{3\kappa c}{2n_0 \left[3 \left. \frac{df}{dn} \right|_{n=n_0} + n_0 \left. \frac{d^2 f}{dn^2} \right|_{n=n_0} \right]} \tanh \left[\epsilon^{1/2} \kappa (z - vt) \right]$$

Those relations shows that, as was stated in the beginning, a dark soliton is characterized by a dip in its density. It is also seen, from the last relation, that a sharp phase difference exists at the point of minimum density. Only in the case of a static soliton is the phase shift between the two sides of the density minimum equal to $\Delta\theta = \pi$ [7].

3.2.3 Effect of the potential

In the previous discussion, the effect of the trapping potential was neglected. It is now time to include its effect and see how it affects the conclusions of the previous discussion. First, by considering the ansatz

$$\psi(z, t) = \phi(z) \exp(-i\mu t + i\theta_0)$$

and injecting it in the adimensional 1D GPE eq. (3.1), the following expression arises

$$\mu\phi(z) + \frac{1}{2} \frac{d^2}{dz^2} \phi(z) - \phi^3(z) = V(z)\phi(z). \tag{3.3}$$

The next step is to seek a solution of eq. (3.1) on top of the inhomogeneous background that satisfy eq. (3.3). Such a solution is sought through the ansatz $\psi(z, t) = \phi(z) \exp(-i\mu t + i\theta_0) \psi_s(z, t)$, where $\psi_s(z, t)$ is an unknown wavefunction representing a dark soliton. Injecting that ansatz in eq. (3.1), in combination with (3.3) leads to the new expression

$$i\frac{\partial}{\partial t} \psi_s(z, t) + \frac{1}{2} \frac{\partial^2}{\partial z^2} \psi_s(z, t) - \phi^2(z) \left[|\psi_s(z, t)|^2 - 1 \right] \psi_s(z, t) = -\frac{d}{dz} \ln[\phi(z)] \frac{\partial}{\partial z} \psi_s(z, t).$$

Since the relation (3.3) was used, it is clear that if the potential $V(z)$ varies slowly on the length scale of the soliton, the right hand side of that equation, as well as a part of the nonlinear term can be treated as a perturbation. Following the suggestion of [13], the perturbation is rewritten under an explicit form thanks to the Thomas-Fermi approximation (which consists in writing the background density under the form $\phi(z) = \sqrt{1 - V(z)}$). The logarithm is then approximated by the expression

$$-\frac{d}{dz} \ln[\phi(z)] \approx \frac{1}{2} \left[1 + V(z) + V^2(z) \right] \frac{d}{dz} V(z),$$

and the perturbed equation can then be rewritten under the form

$$i\frac{\partial}{\partial t} \psi_s(z, t) + \frac{1}{2} \frac{\partial^2}{\partial z^2} \psi_s(z, t) - \left[|\psi_s(z, t)|^2 - 1 \right] \psi_s(z, t) = Q[\psi_s(z, t)],$$

where the perturbation is given by

$$Q[\psi_s(z, t)] = -\left[|\psi_s(z, t)|^2 - 1 \right] V(z) \psi_s(z, t) + \frac{1}{2} \frac{\partial}{\partial z} \psi_s(z, t) \left[1 + V(z) + V^2(z) \right] \frac{d}{dz} V(z).$$

In the case where there is no potential, it is known that the solution to the unperturbed equation takes the form of a dark soliton

$$\psi_s(z, t) = \cos(\theta) \tanh(\zeta) + i \sin(\theta),$$

with $\zeta = \cos(\theta)[x - \sin(\theta)t]$ [13]. From there, a soliton moving adiabatically is expected to have parameters that move slowly with time t. This means that the soliton's phase becomes $\theta(t)$ and that the soliton's coordinate becomes $\zeta(t) = \cos[\theta(t)][z - z_0(t)]$, with $z_0(t)$ the centre of the soliton connected to the phase by the relation

$$\frac{\mathrm{d}}{\mathrm{d}t} z_0(t) = \sin[\theta(t)]. \tag{3.4}$$

This last relation shows that in order to find the time evolution of the soliton's position, the time evolution of the phase has to be known. To get that equation, the normalized soliton energy can be used, whose time evolution can be found thanks to the perturbation $Q[\psi_s(z,t)]$ and is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} E(t) = -\int_{\mathbb{R}} \left\{ Q[\psi_s(z,t)] \frac{\partial}{\partial t}\psi_s^*(z,t) + Q^*[\psi_s(z,t)] \frac{\partial}{\partial t}\psi_s(z,t) \right\} \mathrm{d}z.$$

From there, the time evolution of the phase is given by [20]

$$\frac{\mathrm{d}}{\mathrm{d}t} \theta(t) = \frac{1}{2\cos^2[\theta(t)]\sin[\theta(t)]} \mathrm{Re}\left\{ \int_{\mathbb{R}} Q[\psi_s(z,t)] \frac{\partial}{\partial t}\psi_s^*(z,t)\,\mathrm{d}z \right\}.$$

Going further in the developments and considering that the soliton moves near the trap centre, a Taylor expansion of the potential around z_0 allows to neglect the terms in $V(z)$ and $V^2(z)$ in the perturbation $Q[\psi_s(z,t)]$, which allows to write

$$\frac{\mathrm{d}}{\mathrm{d}t} \theta(t) = -\frac{1}{2}\cos[\theta(t)]\frac{\partial V}{\partial z_0}.$$

Considering a small phase, the approximation $\cos[\theta(t)] \approx \theta(t)$ can be used. Combining that approximation with eq. (3.4), the last equality can be rewritten under the form

$$\frac{\partial^2}{\partial t^2} z_0(t) = -\frac{1}{2}\frac{\partial V}{\partial z_0},$$

which indicates that the centre of the soliton moves like a classical particle in the potential V: indeed, the equation has the form of the Newton equation of motion for a particle of mass $m = 2$ in the external potential V. Furthermore, if the trapping potential is harmonic, the equation becomes the classical equation of motion of a linear oscillator

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} z_0(t) = -\frac{1}{2}\omega_z^2 z_0^2(t),$$

which shows that the centre of the dark soliton oscillates with a frequency given by $\omega_{\mathrm{osc}} = \omega_z/\sqrt{2}$, *i.e.* it oscillates with a smaller frequency than the trapping potential.

3.2.4 Experimental realization techniques

Phase imprinting

The first technique that can be mentioned to create a dark soliton in the phase imprinting method. It consists in manipulating the phase of the condensate without touching its density. To achieve that result, a part of the condensate is illuminated by a short off-resonance laser beam pulse. The procedure can be described in the framework of the 1D Gross-Pitaevskii equation, with a potential that is the sum of the confining potential and a potential of the

form $V(z,t) \propto \theta(z) f(t)$, where $f(t)$ is the function describing the evolution of the laser pulse envelope and $\theta(z)$ is the imprinted phase, given by [7]

$$\theta(z) = \frac{\Delta\theta}{2} \left[1 + \tanh\left(\frac{z - z_*}{bW} \right) \right],$$

where $\Delta\theta$ is the phase gradient, W is the width of the pulse that sets the phase gradient at location z_*, and b is an experimental factor.

Density engineering

If a black soliton can be created by simply modifying the phase of the BEC, it should be possible to create such a soliton by just changing the condensate's density. This is the philosophy of density engineering method. A classical analogy is the creation of dark optical solitons by modulating the intensity of a light field that propagated in a nonlinear medium.

Engineering the density of a BEC is not difficult experimentally: it can be achieved by modifying the trapping potential, for example.

Quantum state engineering method

The quantum state engineering method is a combination of both the phase and density engineering, *i.e.* a method in which both the condensate's phase and density are modified. The techniques requires two steps: first, a density minimum is created by adiabatically illuminating a uniform BEC with a focused laser beam. That laser beam is then abruptly switched off and a second far-detuned laser beam, with uniform intensity, is shone on half of the BEC, which is responsible for imprinting a certain phase on that part of the gas. The density minimum then acquires the desired phase distribution.

3.3 Bright soliton

3.3.1 Generalities

As can be read in a previous section, so-called *bright* soliton can be formed in the case of a Gross-Pitaevskii equation with attractive interactions. Before analysing the behaviour of such solitons, it can be instructive to check whether those structures are stable or not. To see this, as scaling analysis can be conducted. The starting point of such an analysis is the D-dimensional Gross-Pitaevskii equation, given by the expression

$$i\hbar \frac{\partial}{\partial \boldsymbol{r}, t} = \left[-\frac{\hbar^2}{2m} \nabla_{\boldsymbol{r}}^2 + V_{\text{ext}}(\boldsymbol{r}) - g_{DD} |\psi(\boldsymbol{r}, t)|^2 \right] \psi(\boldsymbol{r}, t)$$

where $\boldsymbol{r}$ is now a D-dimensional vector. The corresponding energy functional is given by

$$E[\psi(\boldsymbol{r}, t)] = \int \left[\frac{\hbar^2}{2m} |\nabla_{\boldsymbol{r}} \psi(\boldsymbol{r}, t)|^2 + V_{\text{ext}}(\boldsymbol{r}) |\psi(\boldsymbol{r}, t)|^2 - \frac{g_{DD}}{2} |\psi(\boldsymbol{r}, t)|^4 \right] \mathrm{d}\boldsymbol{r}.$$

Considering that energy functional, along with the normalization condition $\int |\psi(\boldsymbol{r}, t)|^2 \mathrm{d}\boldsymbol{r} = N$, the different terms scale as, for a system with typical size L

- for the wavefunction itself: $\psi(\boldsymbol{r}, t) \sim 1/L^{D/2}$,

- for the kinetic energy: $E_{\text{kin}} \sim 1/L^2$,

- for the potential energy (for $V(\boldsymbol{r}) \sim r^n$): $E_{\mathrm{pot}} \sim L^D$,

- and for the interaction energy: $E_{\mathrm{int}} \sim 1/L^D$.

Considering those scaling laws and a harmonic-like confining potential, it is directly seen that, in 1D, the energy scales as

$$E \sim \frac{c_{\mathrm{kin}}}{L^2} + c_{\mathrm{pot}}L^2 - \frac{c_{\mathrm{int}}}{L},$$

while it scale as

$$E \sim \frac{c_{\mathrm{kin}}}{L^2} + c_{\mathrm{pot}}L^3 - \frac{c_{\mathrm{int}}}{L^3} \qquad \text{and} \qquad E \sim \frac{c_{\mathrm{kin}} - c_{\mathrm{int}}}{L^2} + c_{\mathrm{pot}}L^2$$

for $D = 3$ and $D = 2$, respectively. Those scaling laws show that there exist a L for which the energy is minimum in 1D, while there exist a critical number of atoms in the condensate above which a collapse occur [1].

3.4 Numerics

3.4.1 Linear stability analysis

In this section, a linear stability analysis is performed around a steady-state solution to the Gross-Pitaevskii equation. If $\psi_0(x)$ is a steady-state solution, its linear stability is studied by checking its behaviour if it is slightly perturbed. That perturbed function can be written

$$\psi(z,t) = \left\{ \psi_0(z) + \epsilon \left[u(z) e^{-i\omega t} + v^*(z) e^{i\omega^* t} \right] \right\} \exp\left(-i\frac{\mu}{\hbar}t\right),$$

where μ is the chemical potential an ϵ is a small perturbation. The perturbation is thus time dependent with frequency ω and complex amplitudes $u(x)$, $v(x)$. It should be noted than in order for the solution to not blow up exponentially with time, the frequency should verify $\mathrm{Im}\{\omega\} < 0$.

Injecting the ansatz into the 1D Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi(z,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_{\mathrm{ext}}(z) + g\left|\psi(z,t)\right|^2 \right]\psi(z,t)$$

and keeping only the first order in ϵ leads to the following system

$$\begin{bmatrix} \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_{\mathrm{ext}}(z) + 2g\left|\psi_0(z)\right|^2 - \mu\right] & \psi_0^2(z) \\ -\psi_0^2(z) & -\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_{\mathrm{ext}}(z) + 2g\left|\psi_0(z)\right|^2 - \mu\right] \end{bmatrix} \begin{bmatrix} u(z) \\ v(z) \end{bmatrix} = \hbar\omega \begin{bmatrix} u(z) \\ v(z) \end{bmatrix}.$$

The Laplace operator appearing in the matrix of the left hand side has to be discretized, using a finite-difference approximation method, for example. This procedure will allow to compute the eigenvalues of the system. It can however already be seen that the matrix representing the system will be extremely sparse and have a diagonal-like shape.

3.4.2 Discretization

Generalities

Formally, the GPE can be written under the form

$$i\hbar\frac{\partial}{\partial t}\psi(z,t) = \left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)\psi(z,t),$$

where $\hat{\mathcal{T}}$ and $\hat{\mathcal{V}}$ are the kinetic energy operator and the potential energy operators, respectively. The solution to that equation is simply

$$\psi(z,t) = \exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right]\psi(z,0) \tag{3.5}$$

$$= \exp\left\{-\frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_{\text{ext}}(z) + g\left|\psi(z,t)\right|^2\right]t\right\}\psi(z,0).$$

Written like that, the solution to the equation does not seem easy to handle. However, if the solution is written under the form

$$\psi(z,t) = \exp\left(-\frac{i}{\hbar}\hat{\mathcal{T}}t\right)\exp\left(-\frac{i}{\hbar}\hat{\mathcal{V}}t\right)\psi(z,0), \tag{3.6}$$

the solution becomes much more easy to handle since, owing to the spectral theorem, it is known that applying a function to an operator is equivalent to applying the same function to the eigenvalues of that operator if it is expressed in a basis in which its expression is diagonal. The next question is then to know if such bases exist for $\hat{\mathcal{T}}$ and $\hat{\mathcal{V}}$. Fortunately, the potential energy operator is diagonal in space representation, while the kinetic energy operator is diagonal in the reciprocal space. There is, however, one point that has not been discussed: the transition from the expression appearing in (3.5) to that appearing in (3.6) is allowed only if the operators $\hat{\mathcal{T}}$ and $\hat{\mathcal{V}}$ commute, which is not the case here. In order to be able to perform computations, something has to be done to approximate in the right way the expression of the solution (3.5).

The BCH approximation

The Baker-Campbell-Hausdorff (BCH) approximation is very handy in the present case since it allows to write [35]

$$\exp\left(\hat{\mathcal{T}}\right)\exp\left(\hat{\mathcal{V}}\right) = \exp\left\{\hat{\mathcal{T}} + \hat{\mathcal{V}} + \frac{1}{2}\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right] + \frac{1}{12}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right] + \left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right) + \ldots\right\}.$$

Thanks to that relation, the expression appearing in (3.6) can be re-expressed into another form. Applying the above BCH approximation, the following expressions arise

$$e^{-\frac{i}{\hbar}\hat{\mathcal{T}}t}e^{-\frac{i}{\hbar}\hat{\mathcal{V}}t} = \exp\left\{-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t - \frac{t^2}{\hbar^2}\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right] + i\frac{t^3}{12\hbar^3}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right] + \left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right) + \cdots\right\}$$

$$\approx \exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right]\exp\left(-\frac{t^2}{2\hbar^2}\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right)\exp\left\{i\frac{t^3}{12\hbar^3}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right] + \left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right)\right\}.$$

By further using the equalities

$$\exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right] \approx$$

$$\exp\left\{-\frac{i}{\hbar}\hat{\mathcal{T}}t\right\}\exp\left\{-\frac{i}{\hbar}\hat{\mathcal{V}}t\right\}\exp\left\{\frac{t^2}{2\hbar^2}\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right\}\exp\left\{-i\frac{t^3}{12\hbar^3}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right] + \left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right)\right\}$$

$$\exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right] \approx$$

$$\exp\left\{-\frac{i}{\hbar}\hat{\mathcal{V}}t\right\}\exp\left\{-\frac{i}{\hbar}\hat{\mathcal{T}}t\right\}\exp\left\{\frac{t^2}{2\hbar^2}\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right\}\exp\left\{-i\frac{t^3}{12\hbar^3}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right] + \left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right)\right\}$$

and the fact that $\exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right]$ can be rewritten under the form

$$\exp\left[-\frac{i}{\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right] = \exp\left[-\frac{i}{2\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right]\exp\left[-\frac{i}{2\hbar}\left(\hat{\mathcal{T}} + \hat{\mathcal{V}}\right)t\right],$$

The expression appearing in (3.5) can be rewritten under the form

$$\psi(z,t) \approx$$
$$\exp\left(-\frac{i}{2\hbar}\hat{\mathcal{V}}t\right)\exp\left(-\frac{i}{\hbar}\hat{\mathcal{T}}t\right)\exp\left(-\frac{i}{2\hbar}\hat{\mathcal{V}}t\right)\exp\left\{-i\frac{t^3}{48\hbar^3}\left(\left[\hat{\mathcal{T}},\left[\hat{\mathcal{T}},\hat{\mathcal{V}}\right]\right]+\left[\hat{\mathcal{V}},\left[\hat{\mathcal{V}},\hat{\mathcal{T}}\right]\right]\right)\right\}\psi(z,0),$$
$$(3.7)$$

which, once the last term Taylor-expanded, shows that the discretization is $\mathcal{O}(t^3)$. Those developments allowed to re-express the exact solution into a suitable approximation. The action of the operators appearing inside the different exponentials have still to be determined. Those actions will be determined in the following.

Action of the operators

The spectral theorem has already been evoked, and it is now time to use it. The discretization of the Laplacian by a centred difference method was evoked, and will thus be used. Considering a one-dimensional straight line composed of elements of length Δz, the position of the ith point x_i is then

$$z_i = z_0 + i\Delta z,$$

with z_0 the origin of the grid. Time can be approximated in the same way: $t_n = t_0 + n\Delta t$, with t_0 the origin of time and Δt the time interval between iterations. With those notations, the exact value of the wavefunction at point x_i and time t_n is given by $\psi(x_i, t_n)$, while its approximate value is noted, at the same point and time, ψ_i^n. With those notations, the discrete equivalent of (3.7) is

$$\psi(z_i, t_{n+1}) \approx \exp\left(-\frac{i}{2\hbar}\hat{\mathcal{V}}\Delta t\right)\exp\left(-\frac{i}{\hbar}\hat{\mathcal{T}}\Delta t\right)\exp\left(-\frac{i}{2\hbar}\hat{\mathcal{V}}\Delta t\right)\psi(z_i, t_n). \qquad (3.8)$$

To now get the action of the operators on the wavefunction, the periodicity of the domain has to be taken into account. Decomposing the unknown wavefunction in a discrete Fourier series according to the definition given in [14] (with N the number of nodes contained in the domain) leads to

$$\tilde{\psi}(k_i, t_n) = \frac{1}{\sqrt{N}}\sum_{l=0}^{N-1}\psi(z_l, t_n)\exp\left(-2i\pi\frac{k_i}{N}l\right).$$

From there, the action of the kinetic energy operator $\hat{\mathcal{T}}$ can be computed. It reads

$$\left(\hat{\mathcal{T}}\psi\right)_j = -\mathcal{J}\left(\psi_{j+1} - 2\psi_j + \psi_{j-1}\right), \quad \text{with } \mathcal{J} = \frac{\hbar^2}{2m\left(\Delta z\right)^2}.$$

Applying the operator on the Fourier transform of ψ gives

$$\left(\hat{\mathcal{T}}\tilde{\psi}\right)_j = \frac{1}{\sqrt{N}}\sum_{l=0}^{N-1}\left(\hat{\mathcal{T}}\psi\right)_j\exp\left(-2i\pi\frac{k_i}{N}l\right)$$
$$= -\frac{\mathcal{J}}{\sqrt{N}}\sum_{l=0}^{N-1}\left(\psi_{j+1} - 2\psi_j + \psi_{j-1}\right)\exp\left(-2i\pi\frac{k_i}{N}l\right).$$

By further taking the periodic boundary conditions into account, that last expression can be

re-expressed nuder the form

$$\left(\hat{\mathcal{T}}\tilde{\psi}\right)_j = -\frac{\mathcal{J}}{\sqrt{N}} \sum_{l=0}^{N-1} \psi_l \left[\exp\left(-2i\pi k_i \frac{l+1}{N}\right) - 2\exp\left(-2i\pi k_i \frac{l}{N}\right) + \exp\left(-2i\pi k_i \frac{l-1}{N}\right)\right]$$

$$= -\frac{\mathcal{J}}{\sqrt{N}} \sum_{l=0}^{N-1} 2\psi_l \exp\left(-2i\pi k_i \frac{l}{N}\right) \left[\cos\left(2\pi \frac{k_i}{N}\right) - 1\right]$$

$$= -2\frac{\mathcal{J}}{\sqrt{N}} \left[\cos\left(2\pi \frac{k_i}{N}\right) - 1\right] \tilde{\psi}_j.$$

Those computations show that the eigenvalue of the kinetic energy operator is given by $-2\frac{\mathcal{J}}{\sqrt{N}}\left[\cos\left(2\pi\frac{k_i}{N}\right) - 1\right]$, and is thus the value that has to be placed inside the exponential containing that operator.

Concerning the potential energy operator $\hat{\mathcal{V}}$, the computation of the eigenvalues is straight forward since its eigenbasis is the physical space. It is thus direct to write

$$\left(\hat{\mathcal{V}}\psi\right)_j = \left(V_j + g\left|\psi_j\right|^2\right)\psi_j,$$

with V_j the value of the external potential at node x_j.

Resume of the code

Now that the eigenvalues of the different operators are known, the expression appearing in (3.8) can be rewritten as

$$\psi\left(z_j, t_n\right) \approx \exp\left[-\frac{i}{2\hbar}\left(V_j + g\left|\psi_j\right|^2\right)\right] \mathcal{F}^{-1}\left\{\exp\left[\frac{2i}{\hbar}\frac{\mathcal{J}}{\sqrt{N}}\left(\cos\left(2\pi\frac{k}{N}\right) - 1\right)\Delta t\right]\right.$$
$$\left.\mathcal{F}\left(\exp\left[-\frac{i}{2\hbar}\left(V_j + g\left|\psi_j\right|^2\right)\Delta t\right]\psi_j\right)\right\}$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ represent a Fourier and inverse Fourier transform, respectively.

Results

In order to compute the time evolution of the sought wavefunction, a C-code was written. As is discussed here above, Fourier transforms have to be used. Those were realized thanks to the FFTW[2] library. All the computations were performed on the NIC4 supercomputer, one of the several supercomputers of the CECI[3]. A pseudo-code is given in Algorithm 1. The idea is to vary the number of particles contained in the system and to see how the error between a known analytical expression (see Chapter A) and the numerical approximation obtained thanks to the code described in Algorithm 1 evolves. Those computations can be done for different values of the grid spacing Δx.

However, the implemented space discretization (based on finite differences) does not seem to converge to the exact solution, even for very small time and space steps, which is in good agreement with the results in [27]. To see this, different timesteps (i.e. $\Delta t = 3\cdot10^{-2}$, $\Delta t = 3\cdot10^{-3}$, $\Delta t = 3\cdot10^{-4}$ and $\Delta t = 10^{-4}$) were used and, for each of those timesteps, different spatial steps (i.e. $\Delta x = 6\cdot10^{-2}$, $\Delta x = 6\cdot10^{-3}$, $\Delta x = 3\cdot10^{-3}$ and $\Delta x = 6\cdot10^{-4}$) were tried. Figure 3.1 shows the comparison between the analytic and numerical results for $\Delta t = 10^{-4}$ and $\Delta x = 3\cdot10^{-3}$. On that figure, it is clear that the numerical solution travels with a speed that is different from

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[2]http://www.fftw.org/
[3]http://www.ceci-hpc.be/

Algorithm 1 Compute the time evolution $\psi(z,t)$.

Ensure: Time evolution $\psi(z,t)$

    Initiate L, nbNodes, nbTimesteps, t_{end} and position vector z

    $\Delta x = \frac{L}{\text{nbNodes}}$ and $\Delta t = \frac{t_{\text{end}}}{\text{nbTimesteps}}$

    $\psi(z,t) \leftarrow \psi(z,0)$

    Initiate confining potential $V_{\text{ext}}(z)$

    saveResult = true/false and frequency

    $n = 0$

    while $n < $ nbTimesteps **do**

        $\psi(z,n\Delta t) \leftarrow \text{computeEffectV}\left[V(z), \psi(z,n\Delta t), \Delta t\right]$

        $\tilde{\psi} = \mathcal{F}\left[\psi(z,n\Delta t)\right]$

        $\tilde{\psi} \leftarrow \text{computeEffectT}\left[\tilde{\psi}, \Delta t, \Delta x\right]$

        $\psi(z,n\Delta t) = \mathcal{F}^{-1}\left[\tilde{\psi}\right]$

        $\psi(z,n\Delta t) \leftarrow \text{computeEffectV}\left[V(z), \psi(z,n\Delta t), \Delta t\right]$

        if saveResult && !(n%frequency) **then**

            Save Re$\{\psi(z,t)\}$, Im$\{\psi(z,t)\}$ and $|\psi(z,t)|^2$ at desired iteration

        end if

    end while

    Free all dynamically allocated quantities

---

the analytic solution. Even more, the speed seems to decrease. Those results can come from the fact that the timestep chosen is not small enough to linearise the last exponential appearing in relation (3.7), and consequently numerical errors build up.

The influence of the timestep is illustrated in fig. 3.2, where it is clearly visible that a smaller timestep allows to come closer to the analytic solution. This comes from the fact that the linearisation of the last exponential appearing in relation (3.7) becomes more accurate.
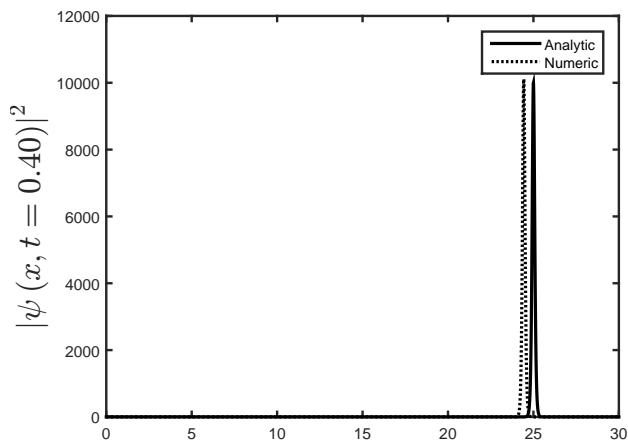
On the contrary, for a free Schrödinger's equation, whose solution is analytically known (see (B)), the numerical results are in very good agreement with the analytic ones, which shows that the nonlinearity appearing in the 1D Gross-Pitaevskii equation needs to be treated more carefully. To see the matching between analytic and numeric results, fig. 3.3 can be checked.
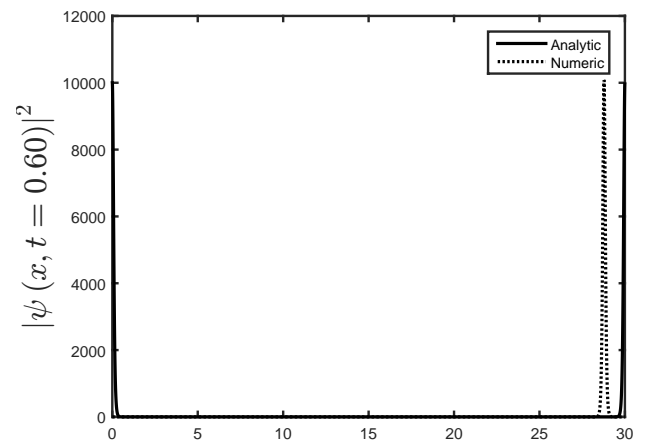
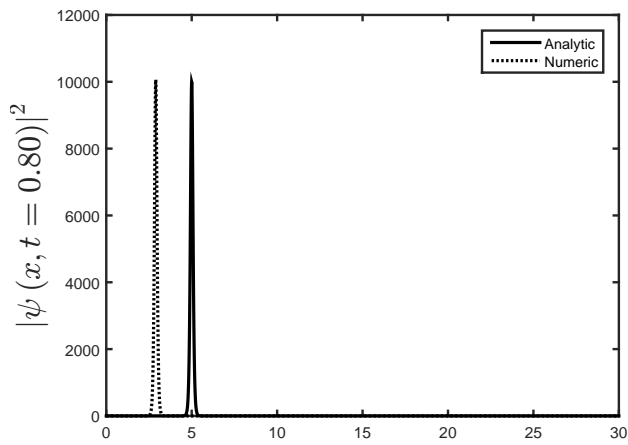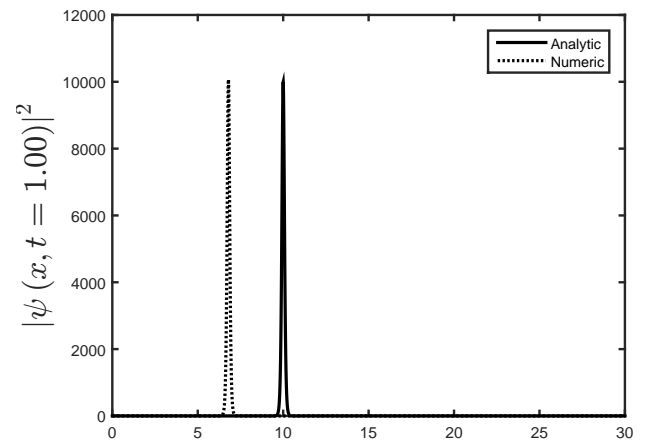**Figure 3.1** – Comparison between analytic and numeric solutions to the 1D GPE for a condensate of 2000 particles and discretization parameters $\Delta t = 10^{-4}$ and $\Delta x = 6 \cdot 10^{-3}$, showing that the numerical solution propagates at a (wrong) decreasing speed.
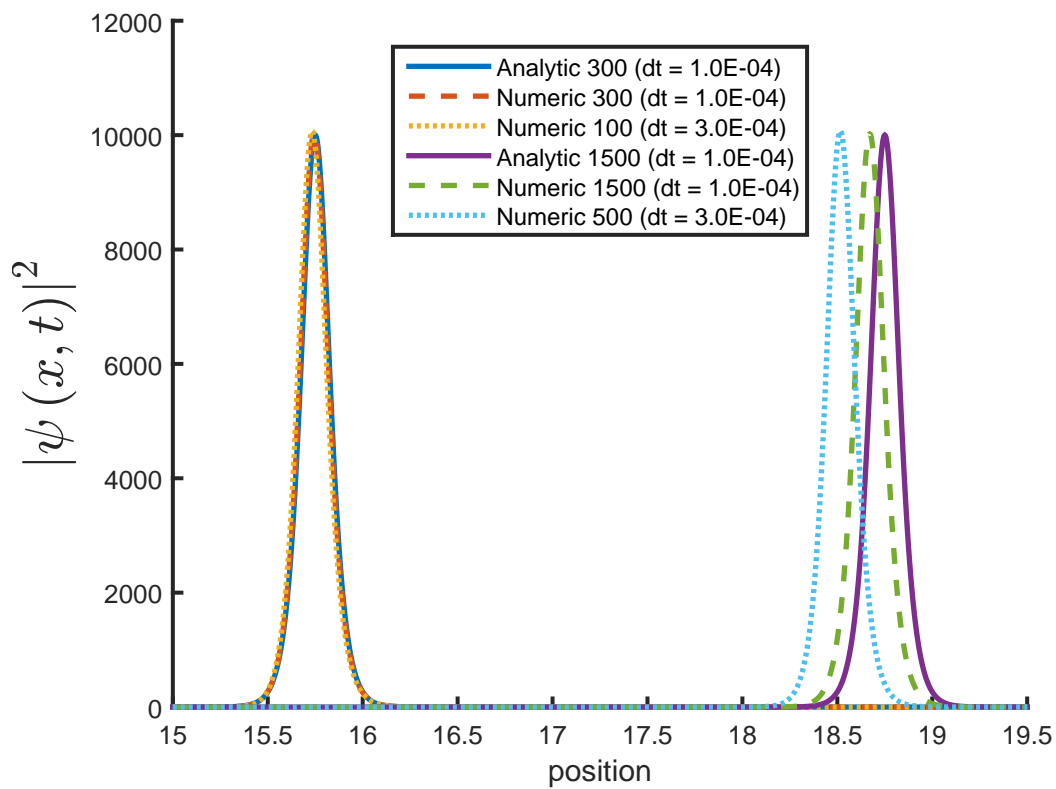
Figure 3.2 – Comparison between the analytic and numerical results for different timesteps and $\Delta x = 3 \cdot 10^{-3}$. The influence of the timestep is clearly visible: a smaller timestep allows to come closer to the analytic solution.
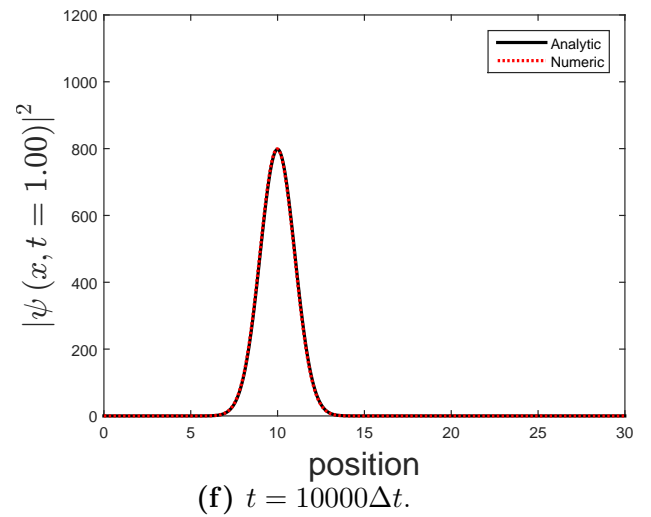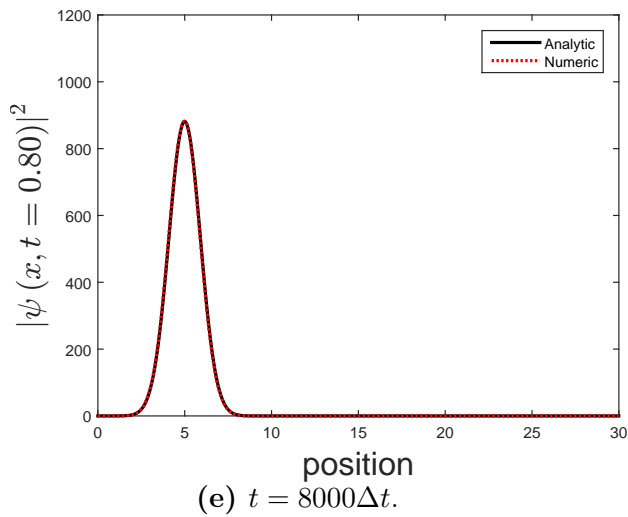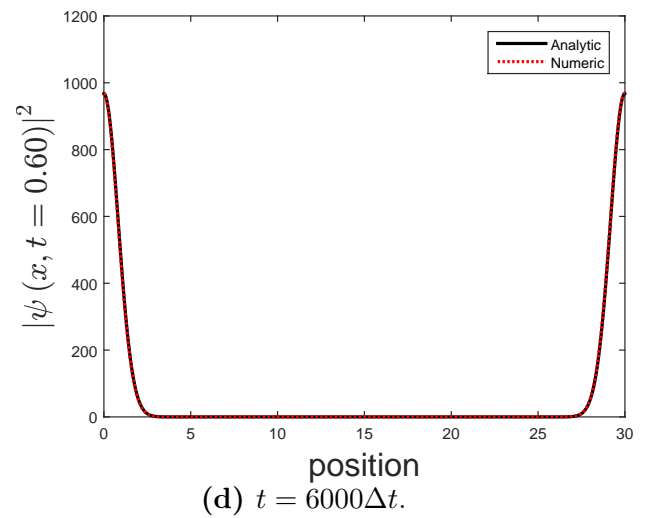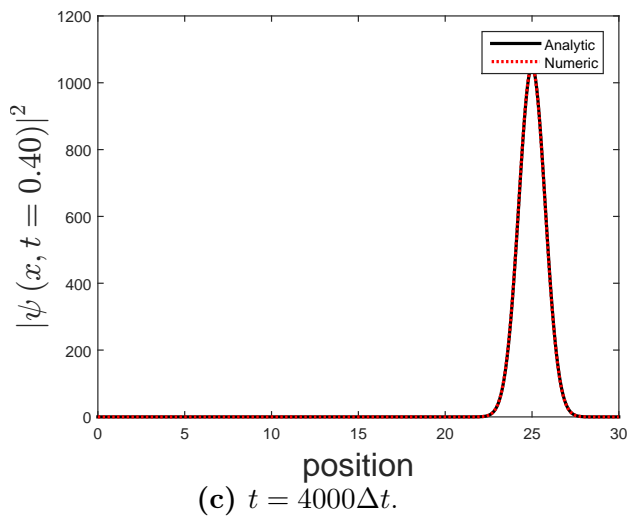
(a) $t = 0$.

(b) $t = 2000\Delta t$.

(c) $t = 4000\Delta t$.

(d) $t = 6000\Delta t$.

(e) $t = 8000\Delta t$.
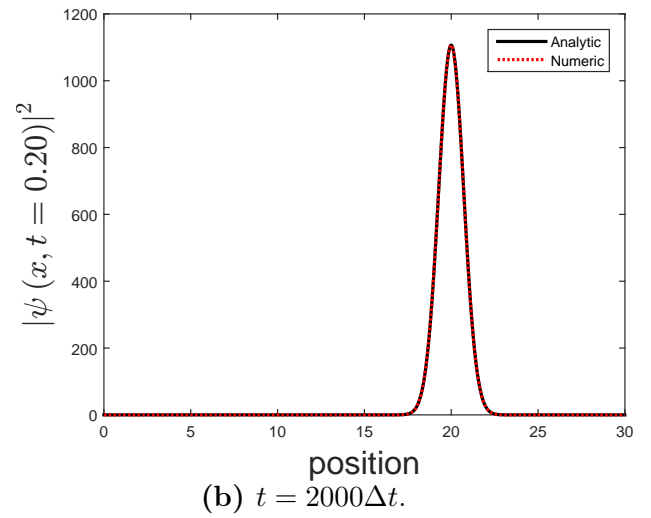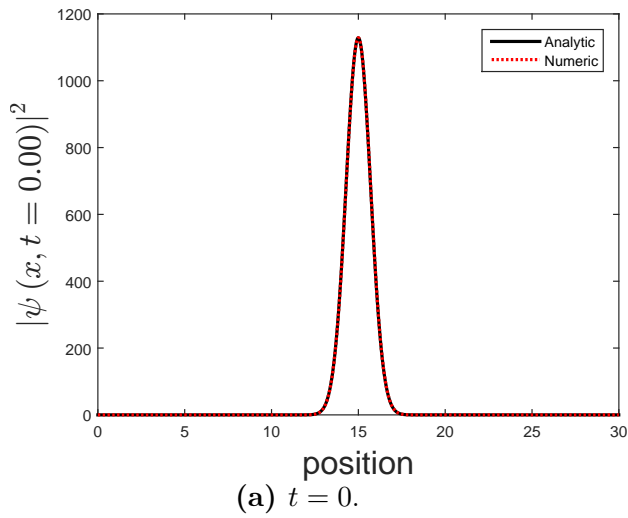
(f) $t = 10000\Delta t$.

Figure 3.3 – Comparison between analytic and numeric solutions to the 1D free Schrödinger equation for a condensate of 2000 particles and discretization parameters $\Delta t = 10^{-4}$ and $\Delta x = 3 \cdot 10^{-3}$, showing the agreement between numerical and analytical results.

Chapter 4

Conclusion

Ultracold atoms is a vast field of physics that spans over many other "subfield". Ranging from theoretical fundamental physics to more "down-to-the-Earth" applications, the possibilities offered by those ultracold systems seems to be extraordinary vast. On of the sub-fields related to Bose-Einstein condensates is that of fundamental nonlinear excitations known as solitons.

Such solitons are excitations well known in nonlinear optics, where they appear in nonlinear dispersive media, such as optical fibres. However, their experimental observation in Bose-Einstein condensates is much more recent than their optical colleges, mainly because the first experimental realization of BEC dates back from the mid-90s. Since then, solitons have effectively been observed in condensates. This masters thesis tries to fit in that field of research by providing a quite general picture of solitons in BECs described by a mean-field theory.

In order to sketch that general picture, different steps had to be undertaken, and can be resumed as follow:

- In the first chapter, the necessary tools to understand the basics about the Bose-Einstein condensation phenomenon were introduced. From there, general relations were derived, such as the mean number of particles contained in the system, the mean energy contained in that system, or even its specific heat, both in the cases of free and trapped three dimensional ideal Bose gas. The next step is to take interactions between particles into account to see how they modify the previously derived results. Even if a proper treatment of those interactions imply to solve the full many-body Schrödinger equation, it was shown that, given the low temperature of the system, the interactions can be described by a single parameter. From there, considering that the system can be described by a unique wavefunction, the well-known Gross-Pitaevskii equation, which gives access to the time evolution of that wave function, was derived. Further considering that at low temperature the wavefunction oscillates around its ground state, the Bogoliubov-de Gennes system was obtained, which gives a picture of the collective mode of the condensate and the dispersion relation. That dispersion relation allows to notice that two different regimes exist: for high momenta, the dispersion relation is the same as a quantum particle, whereas at low momenta, it becomes linear, the proportionality constant being the speed of sound in the condensate. The last part was concerned with an extension of the theory to case out of thermal equilibrium. In particular, by using the Madelung transformation, it can be seen that the dynamics of the condensates is dictated by a Newtonian like law (see eq. (1.20)), with a purely quantum contribution coming from the kinetic part of the Hamiltonian.

- The next step before being able to talk about solitons in BEC is to consider such gases in lower dimensions, for reasons that will be explained later on. Beginning with Bose gases in two-dimensional configurations, the cases of infinite ideal and interacting systems is considered. In particular, it is shown that an ideal gas cannot undergo a phase transition

to the condensate state, but that the first order correlation function is bimodal in the degenerated gas, which means that long range effects can still exist. From there, interactions are added to this picture, in two types of configurations: configurations in which the system is geometrically 2D but locally behaves as a 3D object, and configurations that are truly two-dimensional. In particular, the relation between the 2 scattering length is derived, which allows to express the "true" bidimensional system in function of the scattering length of the "false" one, and vis-versa. The computations are then repeated for a trapped bidimensional gas. Finally, two applications those 2D systems are discussed (superfluidity and the Josephson efect). For the first one, it is shown that it is the fluctuations of the phase that destroy the long range order characteristic of a condensate. The second effect is just a short presentation of the phenomenon. The last part is concerned with 1D systems. In particular, the corresponding Gross-Pitaevskii is derived, and is shown to have the same aspect as the full three dimensional one, the difference between the two being the expression of the interaction parameter g.

- Those considerations lead to the study of the solitons themselves. First, some definitions are given in order to make a clear distinction between solitary waves and solitons. From there, the case of dark and bright solitons are treated separately. For the first ones, the derivations are purely analytical, while for the second ones, only numerical tests and results are provided. For the bright solitons, the discussion starts with generalities showing that bright solitons cannot exist in a 3D system, while it could exist in lower dimensional systems under certain conditions. The discussion then continues with numerical considerations. In particular, the discussion starts with the scheme used to discretize time, the so-called spectral method. From there, the action of the different operators appearing in the Gross-Pitaevskii are derived. It is then shown that the choice of discretization technique does not lead to convergence when interactions between particles are taken into account, meaning that a more involved numerical method is needed.

As a final remark, it has to be said that all the developments and results of this work were derived in the framework of a mean field theory. Such a theory is, however, not strictly speaking, applicable to solitons since they generally contain a limited number of particles. A more realistic model should be used and full quantum computations should be performed numerically to get trustable results.

Appendices

A

Soliton: analytical derivation

In this appendix, the solution to the 1D Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi\left(x,t\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\left(x,t\right) + V_{\text{trap}}\left(x\right)\psi\left(x,t\right) + g\left|\psi\left(x,t\right)\right|^2\psi\left(x,t\right), \qquad (A.1)$$

will be derived thanks to the ansatz

$$\psi\left(x,t\right) = A\left(x-vt\right)\exp\left\{i\left[B\left(x-vt\right)+Ct\right]\right\}, \qquad (A.2)$$

with B and C, two independent real constants. Injecting the ansatz into Equation (A.1) and renaming $x - vt = X$ yields different parts:

- the kinetic energy

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\left(x,t\right) = -\frac{\hbar^2}{2m}\left\{\frac{\mathrm{d}^2 A\left(X\right)}{\mathrm{d}X^2} + 2iB\frac{\mathrm{d}A\left(X\right)}{\mathrm{d}X} + B^2 A\left(X\right)\right\}\exp\left[i\left(BX+Ct\right)\right]$$

- the trapping energy

$$V_{\text{trap}}\left(x\right)\psi\left(x,t\right) = A\left(X\right)\exp\left[i\left(BX+Ct\right)\right]V_{\text{trap}}\left(x\right)$$

- the interaction energy

$$g\left|\psi\left(x,t\right)\right|^2\psi\left(x,t\right) = g\left|A\left(X\right)\right|^2 A\left(X\right)\exp\left[i\left(BX+Ct\right)\right]$$

Putting all those different parts together yields a new equation for the amplitude $A\left(X\right)$ reading

$$i\hbar\left[-v\frac{\mathrm{d}A\left(X\right)}{\mathrm{d}X} + i\left(C-vB\right)A\left(X\right)\right] = -\frac{\hbar^2}{2m}\left[\frac{\mathrm{d}^2 A\left(X\right)}{\mathrm{d}X^2} + 2iB\frac{\mathrm{d}A\left(X\right)}{\mathrm{d}X} - B^2 A\left(X\right)\right]$$
$$+ V_{\text{trap}}\left(X+vt\right)A\left(X\right) + g\left|A\left(X\right)\right|^2 A\left(X\right).$$

By regrouping the different derivative orders together, and by replacing $\frac{\mathrm{d}}{\mathrm{d}X}$ by $'$, the last expression takes the form

$$-\frac{\hbar^2}{2m}A'' + i\hbar\left(v-\frac{\hbar}{m}B\right)A' + g\left|A\right|^2 A + \hbar\left(C-vB+\frac{\hbar}{2m}B^2+V_{\text{trap}}\right) = 0.$$

The constants B and C being arbitrary, the above expression can be somewhat simplified by choosing $B = \frac{m}{\hbar}v$, yielding

$$-\frac{\hbar^2}{2m}A'' + g\left|A\right|^2 A + \hbar\left(C-\frac{1}{2}\frac{mv^2}{\hbar}+V_{\text{trap}}\right)A = 0.$$

By further considering that the function $A(X)$ is real, *i.e.* $A(X) \in \mathbb{R}$, the modulus can be removed in the last expression, yielding

$$-\frac{\hbar^2}{2m}A'' + gA^3 + \hbar\left(C - \frac{1}{2}\frac{mv^2}{\hbar} + V_{\text{trap}}\right)A = 0. \tag{A.3}$$

This last equation is absolutely not trivial to solve, since the potential energy term V_{trap} is a function of X rather than a constant. In what follows, it will thus be considered that there is no trapping potential. In such a case, eq. (A.3) can be solved by multiplying both sides by A' and integrating with respect to X, which gives

$$-\frac{1}{2}\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}A(X)}{\mathrm{d}X}\right)^2 + \frac{g}{4}A^4(X) + \frac{1}{2}\hbar\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)A^2 = E = 0,$$

where E is the integration constant representing the total energy of the system. Such an equation can be rewritten under the form

$$\frac{\mathrm{d}A}{\mathrm{d}X} = \pm\sqrt{\frac{mg}{\hbar^2}A^4 + \frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)A^2},$$

which is separable, and can be directly integrated to give

$$\int \frac{\mathrm{d}A}{\sqrt{\frac{mg}{\hbar^2}A^4 + \frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)A^2}} = \pm(x - vt) + C_1.$$

That expression can be further simplified by writing

$$\int \frac{\mathrm{d}A}{A\sqrt{A^2 + \frac{2m}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}} = \pm\sqrt{\frac{mg}{\hbar^2}}(x - vt) + C_2 \tag{A.4}$$

To proceed further, two cases have to be considered, namely (i) the repulsive interaction ($g > 0$), and (ii) the attractive interaction ($g < 0$). Those cases will be treated separately.

Repulsive interactions

In this case, eq. (A.4) can be easily computed. By first performing the change of variable $u \mapsto \frac{1}{A}$, eq. (A.4) becomes

$$-\int \frac{\mathrm{d}u}{\sqrt{1 + \frac{2m}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)u^2}} = \pm\sqrt{\frac{mg}{\hbar^2}}(x - vt) + C_2.$$

By performing the new change of variable $u \mapsto \frac{\sinh(y)}{\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}}$, the integral becomes

$$-\int \frac{1}{\sqrt{1 + \sinh^2(y)}}\frac{\cosh(y)}{\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}}\mathrm{d}y = \pm\sqrt{\frac{mg}{\hbar^2}}(x - vt) + C_2,$$

which finally leads to

$$y = \mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}(x - vt) + C_4,$$

or, by keeping in mind all the previous changes of variable,

$$A = \sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)} \frac{1}{\sinh\left[\mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,(x - vt) + C_4\right]}, \qquad (A.5)$$

which, once injected in the ansatz (A.2), leads to the expression

$$\psi(x,t) = \sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)} \frac{1}{\sinh\left[\mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,(x - vt) + C_4\right]} \exp\left\{i\left[\frac{m}{\hbar}v\,(x - vt) + Ct\right]\right\}.$$

The final step is to determine the expression of the constant C, which is done through the normalization condition $\int |\psi(x,t)|^2\,\mathrm{d}x = \int |\psi(x,0)|^2\,\mathrm{d}x = N$, which leads to

$$\frac{Ng}{2\hbar}\frac{1}{C - \frac{1}{2}\frac{mv^2}{\hbar}} = \int \frac{1}{\sinh^2\left[\mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,x + C_4\right]}\,\mathrm{d}x$$

$$= \frac{1}{\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}} \int \frac{\mathrm{d}}{\mathrm{d}x}\cotanh\left[\pm\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,x + C_4\right]\mathrm{d}x$$

Attractive interactions

In this case, g should be replaced by $-g$ in eq. (A.4), leading to the equation

$$\int \frac{\mathrm{d}A}{A\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right) - A^2}} = \pm\sqrt{\frac{mg}{\hbar^2}}\,(x - vt) + C_5.$$

By performing the change of variable $u \mapsto \frac{1}{A}$, this last expression becomes

$$-\int \frac{\mathrm{d}u}{\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)u^2 - 1}} = \pm\sqrt{\frac{mg}{\hbar^2}}\,(x - vt) + C_5.$$

By performing the new change of variable $u \mapsto \dfrac{\cosh(y)}{\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}}$, the last expression becomes

$$-\int \frac{1}{\sqrt{\cosh^2(y) - 1}}\frac{\sinh(y)}{\sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}}\,\mathrm{d}y = \pm\sqrt{\frac{mg}{\hbar^2}}\,(x - vt) + C_5,$$

and finally leads to the expression

$$y = \mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,(x - vt) + C_6.$$

Keeping in mind all the previous changes of variable, that last expression can be rewritten under the form

$$A = \sqrt{\frac{2\hbar}{g}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,\mathrm{sech}\left[\mp\sqrt{\frac{2m}{\hbar}\left(C - \frac{1}{2}\frac{mv^2}{\hbar}\right)}\,(x - vt) + C_6\right],$$

which, once injected in the ansatz (A.2), leads to

$$\psi\left(x,t\right)=\sqrt{\frac{2\hbar}{g}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}\ \text{sech}\left[\mp\sqrt{\frac{2m}{\hbar}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}\left(x-vt\right)+C_6\right]\exp\left\{i\left[\frac{m}{\hbar}v\left(x-vt\right)+Ct\right]\right\}.$$

The last step is to determine the constant C through the normalization condition $\int\left|\psi\left(x,t\right)\right|^2\mathrm{d}x=\int\left|\psi\left(x,0\right)\right|^2\mathrm{d}x=N$, which yields

$$\frac{Ng}{2\hbar}\frac{1}{C-\frac{1}{2}\frac{mv^2}{\hbar}}=\int\text{sech}^2\left[\mp\sqrt{\frac{2m}{\hbar}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}x+C_6\right]\mathrm{d}x$$

$$=\frac{1}{\sqrt{\frac{2m}{\hbar}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}}\int\frac{\mathrm{d}}{\mathrm{d}x}\tanh\left[\mp\sqrt{\frac{2m}{\hbar}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}x+C_6\right]\mathrm{d}x$$

$$=\frac{2}{\sqrt{\frac{2m}{\hbar}\left(C-\frac{1}{2}\frac{mv^2}{\hbar}\right)}}.$$

From this expression, the value of C can be found and reads

$$\boxed{C=\frac{1}{2}\frac{m}{\hbar}\left(v^2+\frac{N^2g^2}{4\hbar^2}\right).}$$

B

Schrödinger's equation: analytical solution

Let the problem to consider be

$$
\begin{cases}
i\hbar \frac{\partial}{\partial t}\psi\left(x,t\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\left(x,t\right) & \text{on } \mathbb{R}\times\left]0,+\infty\right[, \\
\psi\left(x,0\right) = \sqrt{\frac{N}{\sigma_0\sqrt{\pi}}}\exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right]e^{ik_0 x} & \text{on } \mathbb{R}\times\left\{t=0\right\}.
\end{cases}
\tag{B.1}
$$

It is known that such a problem can be solved thanks to Fourier transforms. In Fourier space, the solution to that equation reads

$$
\tilde{\psi}\left(k,t\right) = \tilde{\psi}\left(k,0\right)\exp\left(-i\frac{\hbar k^2}{2m}t\right),
$$

where $\tilde{\psi}\left(k,0\right)$ is the Fourier transform of the initial condition of the problem. It is given by

$$
\tilde{\psi}\left(k,0\right) = \sqrt{\frac{N}{\sigma_0\sqrt{\pi}}}\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right]e^{ik_0 x}\exp\left(-ikx\right),\mathrm{d}x,
$$

$$
\overset{X=x-x_0}{=\!=\!=}\sqrt{\frac{N}{2\sigma_0\pi^{3/2}}}\exp\left[-i\left(k-k_0\right)x_0\right]\int_{\mathbb{R}}\exp\left(-\frac{X^2}{2\sigma_0^2}\right)\exp\left[-i\left(k-k_0\right)X\right]\mathrm{d}X.
$$

By putting the exponentials together, the expression can be identified to a second order expression. This allows to rewrite

$$
\tilde{\psi}\left(k,0\right) = \sqrt{\frac{N}{2\sigma_0\pi^{3/2}}}e^{-i(k-k_0)x_0}e^{-\frac{\sigma_0^2}{2}(k-k_0)^2}\int_{\mathbb{R}}\exp\left\{-\left[\frac{X}{\sqrt{2}\sigma_0}+i\frac{\sigma_0}{\sqrt{2}}\left(k-k_0\right)\right]^2\right\}\mathrm{d}X.
$$

By making the change of variable $Y\mapsto\frac{X}{\sqrt{2}\sigma_0}+i\frac{\sigma_0}{\sqrt{2}}\left(k-k_0\right)$ and using the result of the Poisson integral, the Fourier transform of the initial condition reads

$$
\tilde{\psi}\left(k,0\right) = \sqrt{\frac{\sigma_0 N}{\sqrt{\pi}}}\exp\left[-i\left(k-k_0\right)\right]\exp\left[-\frac{\sigma_0^2}{2}\left(k-k_0\right)^2\right],
$$

which leads to the final result in Fourier space

$$
\tilde{\psi}\left(k,t\right) = \sqrt{\frac{\sigma_0 N}{\sqrt{\pi}}}\exp\left[-i\left(k-k_0\right)\right]\exp\left[-\frac{\sigma_0^2}{2}\left(k-k_0\right)^2\right]\exp\left(-i\frac{\hbar k^2}{2m}t\right).
$$

To get the final solution to the problem (B.1), that last expression has to be re-expressed in the physical space, which is done by performing an inverse Fourier transform. The result is given by

$$\psi\left(x,t\right)=\sqrt{\frac{\sigma_0 N}{2\pi^{3/2}}}\int_{\mathbb{R}}\exp\left[-i\left(k-k_0\right)x_0\right]\exp\left[-\frac{\sigma_0^2}{2}\left(k-k_0\right)^2\right]\exp\left(-i\frac{\hbar k^2}{2m}t\right)\exp\left(ikx\right)\mathrm{d}k,$$

$$\stackrel{K=k-k_0}{=}\sqrt{\frac{\sigma_0 N}{2\pi^{3/2}}}\int_{\mathbb{R}}\exp\left(-iKx_0\right)\exp\left(-\frac{\sigma_0^2}{2}K^2\right)\exp\left[-i\frac{\hbar t}{2m}\left(K+k_0\right)^2\right]\exp\left[i\left(K+k_0\right)x\right]\mathrm{d}K,$$

$$=\sqrt{\frac{\sigma_0 N}{2\pi^{3/2}}}\exp\left(-i\frac{\hbar k_0^2}{2m}t\right)\exp\left(ik_0 x\right)\int_{\mathbb{R}}\exp\left[-\left(\frac{\sigma_0^2}{2}+i\frac{\hbar t}{2m}\right)K^2+i\left(x-x_0-\frac{\hbar k_0}{m}t\right)K\right]\mathrm{d}K.$$

Once again, the expression of the argument of the exponential can be associated to a second order expression. By performing the same kind of computations as was done to find the expression of $\tilde{\psi}\left(k,t\right)$, the final result to the problem (B.1) reads

$$\boxed{\psi\left(x,t\right)=\sqrt{\frac{\sigma_0 N}{2\sqrt{\pi}}}\frac{\exp\left(ik_0 x\right)}{\sqrt{\frac{\sigma_0^2}{2}+i\frac{\hbar t}{2m}}}\exp\left(-i\frac{\hbar k_0^2}{2m}t\right)\exp\left[-\frac{\left(x-x_0-\frac{\hbar k_0}{m}t\right)^2}{4\left(\frac{\sigma_0^2}{2}+i\frac{\hbar t}{2m}\right)}\right].}$$

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