Bose-Einstein condensates in atomic gases: simple theoretical results

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Contents

1   Introduction

1.1   1925: Einstein's prediction for the ideal Bose gas

Einstein considered N non-interacting bosonic and non-relativistic particles in a cubic box of volume L^3 with periodic boundary conditions. In the *thermodynamic limit*, defined as

$$N, L \to \infty \quad \text{with} \quad \frac{N}{L^3} = \rho = \text{constant}, \tag{1}$$

a phase transition occurs at a temperature T_c defined by:

$$\rho \lambda_{dB}^3(T_c) = \zeta(3/2) = 2.612... \tag{2}$$

where we have defined the thermal de Broglie wavelength of the gas as function of the temperature T:

$$\lambda_{dB}(T) = \left(\frac{2\pi\hbar^2}{mk_BT} \right)^{1/2} \tag{3}$$

and where $\zeta(\alpha) = \sum_{k=1}^{\infty} 1/k^\alpha$ is the Riemann Zeta function.

The order parameter of this phase transition is the fraction N_0/N of particles in the ground state of the box, that is in the plane wave with momentum $\vec{p} = \vec{0}$. For temperatures lower than T_c this fraction N_0/N remains finite at the thermodynamic limit, whereas it tends to zero when $T > T_c$:

$$T > T_c \qquad\qquad \frac{N_0}{N} \to 0 \tag{4}$$

$$T < T_c \qquad\qquad \frac{N_0}{N} \to 1 - \left(\frac{T}{T_c} \right)^{3/2}. \tag{5}$$

For $T < T_c$ the system has formed a Bose-Einstein condensate in $\vec{p} = \vec{0}$. The number N_0 of particles in the condensate is on the order of N, that is macroscopic. As we will

see, the *macroscopic population of a single quantum state* is the key feature of a Bose-Einstein condensate, and gives rise to interesting properties, e.g. coherence (as for the laser).

1.2   Experimental proof?

The major problem encountered experimentally to verify Einstein's predictions is that at densities and temperatures required by Eq.(2) at thermodynamic equilibrium almost all materials are in the solid state.

An exception is He ^{4} which is a fluid at $T = 0$. However He ^{4} is a strongly interacting system. In He ^{4} in sharp contrast with the prediction for the ideal gas Eq.(5), $N_0/N < 10\%$ even at zero temperature [1]. [1]

The solution which victoriously led to Bose-Einstein condensation in atomic gases is to bring the system to extremely low densities (much lower than in a normal gas) and to cool it rapidly enough so that it has no time to recombine and solidify. The price to pay for an ultralow density is the necessity to cool at extremely low temperatures. Typically one has in the experiments with condensates:

$$\rho \quad < \quad 10^{15}\text{atoms/cm}^3 \tag{6}$$

$$T \quad < \quad 1\mu K. \tag{7}$$

The critical temperatures range from 20 nK to the μ K range.

Bose-Einstein condensation was achieved for the first time in atomic gases in 1995. The group of Eric Cornell and Carl Wieman at JILA was first, with ^{87} Rb atoms [2]. They were closely followed by the group of Wolfgang Ketterle at MIT with ^{23} Na atoms [3] and the group of Randy Hulet at Rice University with ^{7} Li atoms [4]. Nowadays there are many condensates mainly with rubidium or sodium atoms. No other alkali atoms than the ones of year 1995 has been condensed. Atomic hydrogen has been condensed in 1998 at MIT in the group of Dan Kleppner [5]; the experiments on hydrogen were actually the first ones to start and played a fundamental pioneering role in developing many of

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[1] Amusingly the ideal gas prediction Eq.(2) does not give a too wrong result for the transition temperature in helium. Note that the condensate fraction N_0/N should not be confused with the superfluid fraction: at $T = 0$ the superfluid fraction is equal to unity.

the experimental techniques having led the alkalis atoms to success, such as magnetic trapping and evaporative cooling of atoms.

In our lectures we do not consider the experimental techniques used to obtained and to study Bose-Einstein condensates as they are treated in the lectures of Wolgang Ketterle and of Eric Cornell at this school.

1.3 Why interesting?

1.3.1 Simple systems for the theory

An important theoretical frame for Bose-Einstein condensation in interacting systems was developed in the 50's by Beliaev, Bogoliubov, Gross, Pitaevskii in the context of superfluid helium. This theory however is supposed to work better if applied to Bose condensed gases where the interactions are much weaker.

The interactions in ultracold atomic gases can be described by a single parameter a, the so-called *scattering length*, as interactions take place between atoms with very low relative kinetic energy. The gaseous condensates are *dilute* systems as the mean interparticle separation is much larger than the scattering length a:

$$\rho |a|^3 \ll 1. \tag{8}$$

This provides a small parameter to the theory and, as we shall see, simple mean field approaches can be used with success to describe most of the properties of the atomic condensates.

1.3.2 New features

Atomic gases offer some new interesting features with respect to superfluid helium 4:

- *Spatial inhomogeneity*: This feature can be used as a tool to detect the presence of a Bose-Einstein condensate inside the trap: in an inhomogeneous gas Bose-Einstein condensation occurs not only in momentum space but also in position space!

- *Finite size effects*: The number of atoms in condensates of alkali gases is usually $N_0 < 10^7$. The hydrogen condensate obtained at MIT by Kleppner is larger $N_0 \simeq 10^9$. Interesting finite size effects, that is effects which disappear at the

thermodynamic limit, such as Bose-Einstein condensates with effective attractive interactions ($a < 0$), can be studied in relatively small condensates.

It is also interesting to consider small condensates where some interesting quantum aspects concerning coherence properties of the condensates, such as collapses and revivals of the relative phase between two condensates [6], could perhaps be measured [7].

- *Tunability*: Condensates in atomic gases can be manipulated and studied using the powerful techniques of atomic physics (see the lectures of Wolfgang Ketterle and Eric Cornell). Almost all the parameters can be controlled at will, including the interaction strength a between the particles. The atoms can be imaged not only in position space, but also in momentum space, allowing one to see the momentum distribution of atoms in the condensate! One can also tailor the shape and intensity of the trapping potential containing the condensate.

2 The ideal Bose gas in a trap

Let us consider a gas of non-interacting bosonic particles trapped in a potential $U(\vec{r})$ at thermal equilibrium. As the particles do not interact thermal equilibrium has to be provided by coupling to an external reservoir. In the grand-canonical ensemble the state of the gas is described by the equilibrium N-body density matrix

$$\hat{\rho} = \frac{1}{\Xi} \exp[-\beta \left(\hat{H} - \mu \hat{N} \right)] \tag{9}$$

where Ξ is a normalization factor, $\hat{H}$ is the Hamiltonian containing the kinetic energy and trapping potential energy of all the particles, $\hat{N}$ is the operator giving the total number of particles, $\beta = 1/k_B T$ where T is the temperature, and μ is the chemical potential. One more conveniently introduces the fugacity:

$$z = \exp[\beta\mu]. \tag{10}$$

2.1 Bose-Einstein condensation in a harmonic trap

Let us consider the case of a harmonic trapping potential $U(\vec{r})$:

$$U(\vec{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \tag{11}$$

We wish to determine the properties of the trapped gas at thermal equilibrium; the calculations can be done in the basis of harmonic levels or in position space.

2.1.1 In the basis of harmonic levels

Let us consider the single particle eigenstates of the harmonic potential with eigenvalues $\epsilon_{\vec{l}}$ labeled by the vector:

$$\vec{l} = (l_x, l_y, l_z) \qquad l_\alpha = 0, 1, 2, 3... \; (\alpha = x, y, z). \tag{12}$$

One has:

$$\epsilon_{\vec{l}} = l_x \hbar \omega_x + l_y \hbar \omega_y + l_z \hbar \omega_z \tag{13}$$

where the zero-point energy $(\hbar/2)(\omega_x + \omega_y + \omega_z)$ has been absorbed for convenience in the definition of the chemical potential. Let us consider the case of an isotropic potential for which all the ω_α 's are equal to ω , so that $\epsilon_{\vec{l}} = l\hbar\omega$ with $l \equiv l_x + l_y + l_z$.

The mean occupation number of each single particle eigenstate in the trap is given by the Bose distribution:

$$n_{\vec{l}} = \frac{1}{\exp[\beta(\epsilon_{\vec{l}} - \mu)] - 1} = \left[\frac{1}{z} \exp(\beta l \hbar \omega) - 1 \right]^{-1} . \tag{14}$$

Since $n_{\vec{l}}$ has to remain positive (for $l = 0, 1, 2 ...$), the range of variation of the fugacity z is given by

$$0 < z < 1. \tag{15}$$

The average total number of particles N is obtained by summing over all the occupation numbers: $N = \sum_{\vec{l}} n_{\vec{l}}$, a relation that can be used in principle to eliminate z in terms of N . It is useful to keep in mind that for a fixed temperature T , N is an increasing function of z .

In the limit $z \to 0$ one recovers Boltzmann statistics: $n_{\vec{l}} \propto \exp(-\beta \epsilon_{\vec{l}})$. We are interested here in the opposite, quantum degenerate limit where the occupation number of the ground state $l = 0$ of the trap, given by

$$N_0 = n_{\vec{0}} = \frac{z}{1 - z}, \tag{16}$$

diverges when $z \to 1$, which indicates the presence of a Bose-Einstein condensate in the ground state of the trap.

We wish to watch the formation of the condensate when z is getting closer to one, that is when one gradually increases the total number of particles N. The essence of Bose-Einstein condensation is actually the phenomenon of *saturation* of the population of the excited levels in the trap, a direct consequence of the Bose distribution function. Consider indeed the sum of the occupation numbers of the single particle excited states in the trap:

$$N' = \sum_{\vec{l} \neq \vec{0}} n_{\vec{l}} \, . \tag{17}$$

The key point is that for a given temperature T, N' is bounded from above:

$$N' = \sum_{\vec{l} \neq \vec{0}} \left[\frac{1}{z} \exp(\beta l \hbar \omega) - 1 \right]^{-1} < \sum_{\vec{l} \neq \vec{0}} [\exp(\beta l \hbar \omega) - 1]^{-1} \equiv N'_{\max} \, . \tag{18}$$

Note that we can safely set z = 1 since the above sum excludes the term $l = 0$.

If the temperature T is fixed and we start adding particles to the system, particles will be forced to pile up in the ground state of the trap when $N > N'_{\max}$, where they will form a condensate. Let us now estimate the "critical" value of particle number $N'_{\max}$.

We will restrict to the interesting regime $k_B T \gg \hbar \omega$: in this regime Bose statistics allows one to accumulate most of the particles in a single quantum state of the trap while having the system in contact with a thermostat at a temperature much higher than the quantum of oscillation $\hbar \omega$, a very counter-intuitive result for someone used to Boltzmann statistics! On the contrary the regime $k_B T \ll \hbar \omega$ would lead to a large occupation number of the ground state of the trap even for Boltzmann statistics.

A first way to calculate $N'_{\max}$ is to realize that the generic term of the sum varies slowly with l as $k_B T \gg \hbar \omega$ so that one can replace the discrete sum $\sum_{\vec{l} \neq \vec{0}}$ by an integral $\int_{l_\alpha \geq 0} d^3 \vec{l}$. As we are in the case of a three-dimensional harmonic trap there is no divergence of the integral around $\vec{l} = \vec{0}$.

We will rather use a second method, which allows one to calculate also the first correction to the leading term in $k_B T / \hbar \omega$. We use the series expansion

$$\frac{1}{e^x - 1} = \frac{e^{-x}}{1 - e^{-x}} = \sum_{k=1}^{\infty} e^{-kx} \tag{19}$$

which leads to the following expression for $N'_{\max}$, if one exchanges the summations over

$\vec{l}$ and k :

$$N'_{\text{max}} = \sum_{k=1}^{\infty} \sum_{\vec{l} \neq \vec{0}} \exp[-k\beta\hbar\omega \sum_{\alpha} l_{\alpha}] = \sum_{k=1}^{\infty} \left[\left(\frac{1}{1 - \exp[-\beta\hbar\omega k]} \right)^3 - 1 \right].$$ (20)

We now expand the expression inside the brackets for small x :

$$\left[\left(\frac{1}{1 - \exp[-x]} \right)^3 - 1 \right] = \frac{1}{x^3} + \frac{3}{2x^2} + \dots$$ (21)

and we sum term by term to obtain

$$N'_{\text{max}} = \left(\frac{k_B T}{\hbar\omega} \right)^3 \zeta(3) + \frac{3}{2} \left(\frac{k_B T}{\hbar\omega} \right)^2 \zeta(2) + \dots$$ (22)

Note that the exchange of summation over k and summation over the order of expansion in Eq.(21) is no longer allowed for the next term $1/x$, which would lead to a logarithmic divergence (that one can cut "by hand" at $k \simeq k_B T/\hbar\omega$).

One then finds to leading order for the fraction of population in the single particle ground state:

$$\frac{N_0}{N} \simeq \frac{N - N'_{\text{max}}}{N} \simeq 1 - \zeta(3) \left(\frac{k_B T}{\hbar\omega} \right)^3 \frac{1}{N} = 1 - \left(\frac{T}{T_c^0} \right)^3$$ (23)

where the critical temperature T_c^0 is defined by:

$$\zeta(3) \left(\frac{k_B T_c^0}{\hbar\omega} \right)^3 = N$$ (24)

and $\zeta(3) = 1.202...$. Note that the universal law (23) differs from the one obtained in the homogeneous case (5) usually considered in the literature.

The present calculation is easily extended to the case of an anisotropic harmonic trap. To leading order one finds

$$N'_{\text{max}} \simeq \left(\frac{k_B T}{\hbar\bar{\omega}} \right)^3 \zeta(3)$$ (25)

where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trap frequencies. One can also calculate N'_{max} in two-dimensional and one-dimensional models. One also finds in these cases a finite value for N'_{max} : the saturation of population in the single particle excited states applies as well and one can form a condensate, a situation very different from the thermodynamical limit in the homogeneous 1D and 2D cases.

2.1.2 Comparison with the exact calculation

One can see in figure 1 that the first two terms in the expansion Eq.(22), combined with the approximation $N_0/N \simeq 1 - N'_{max}/N$, give a very good approximation to the exact condensate fraction for $N = 1000$ particles only.
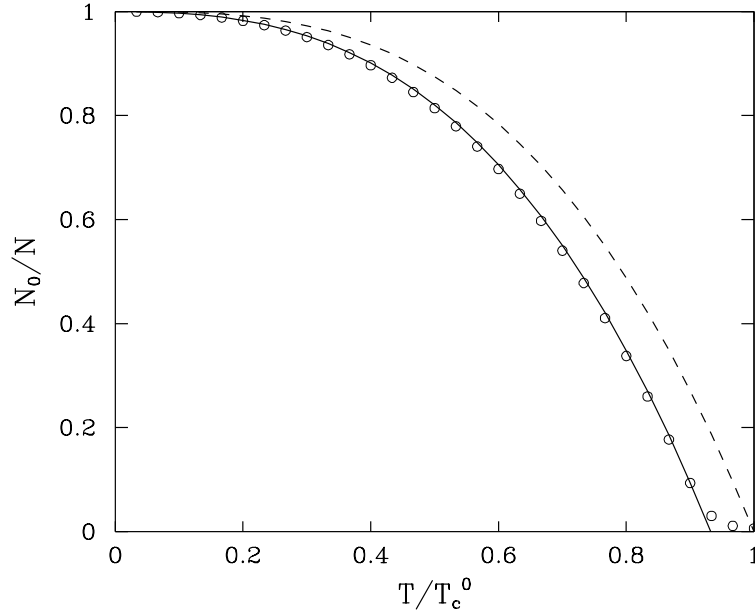
Figure 1: Condensate fraction versus temperature for an ideal Bose gas in a spherically symmetric trap with $N = 1000$ particles. The circles correspond to the exact quantum calculation. The solid line corresponds to the prediction $N_0/N \simeq 1-N'_{max}/N$ with N'_{max} given by the two terms in the expansion Eq.(22). The dashed line corresponds to the prediction $N_0/N \simeq 1 - N'_{max}/N$ with N'_{max} given by the leading term in Eq.(22). This figure was taken from [8].

2.1.3 In position space

A very important object in the description of the state of the gas is the so-called one-body density matrix. We can define it as follows.

Consider a one-body observable

$$\mathcal{X} = \sum_{i=1}^{\hat{N}} X(i) \tag{26}$$

where $X(i)$ is the observable for particle number i and where $\hat{N}$ is the operator giving the total number of particles. The one-body density matrix $\hat{\rho}_1$ is defined by the requirement that for any X:

$$\langle \mathcal{X} \rangle \equiv \mathrm{Tr}[\hat{\rho}_1 X(1)]. \tag{27}$$

For the particular case of X equal to the identity it follows $\mathcal{X} = \hat{N}$ and $\langle \mathcal{X} \rangle = \mathrm{Tr}[\hat{\rho}_1] = \langle \hat{N} \rangle$ so that our one-body density matrix is normalized to the mean number of particles in the system.

An equivalent definition of $\hat{\rho}_1$ in the second quantized formalism is simply

$$\langle \vec{r}' | \hat{\rho}_1 | \vec{r} \rangle = \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}') \rangle \tag{28}$$

where $\hat{\psi}(\vec{r})$ is the atomic field operator, annihilating an atom in $\vec{r}$.

At thermal equilibrium in the grand-canonical ensemble, the one-body density matrix of the ideal Bose gas is given by

$$\hat{\rho}_1 = \frac{1}{z^{-1} \exp(\beta \hat{h}_1) - 1} \tag{29}$$

where the single-particle Hamiltonian in the case of a spherically symmetric harmonic trap is

$$\hat{h}_1 = \frac{\vec{p}^2}{2m} + \frac{1}{2} m \omega^2 \vec{r}^2 - \frac{3}{2} \hbar \omega. \tag{30}$$

Here again we have subtracted the zero-point energy for convenience. The Bose formula Eq.(14) corresponds to the diagonal element of $\hat{\rho}_1$ in the eigenbasis of the harmonic oscillator (the off-diagonal elements of course vanish). In position space the diagonal term

$$\langle \vec{r} | \hat{\rho}_1 | \vec{r} \rangle = \rho(\vec{r}) \tag{31}$$

gives the mean spatial density of the gas.

In order to calculate the density we use the series expansion Eq.(19) to rewrite $\hat{\rho}_1$ as follows:

$$\hat{\rho}_1 = \sum_{k=1}^{\infty} z^k e^{-\beta k \hat{h}_1}. \tag{32}$$

This writing takes advantage of the fact that the matrix elements

$$\langle \vec{r} | e^{-\beta k \hat{h}_1} | \vec{r}' \rangle \tag{33}$$

are known for an harmonic oscillator potential [9]. One then obtains explicitly:

$$\rho(\vec{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \sum_{k=1}^{\infty} z^k \left(1 - \exp(-2\beta k\hbar\omega)\right)^{-3/2} \exp\left[-\frac{m\omega r^2}{\hbar}\tanh\left(\frac{\beta k\hbar\omega}{2}\right)\right] \qquad (34)$$

One can identify the contribution of the condensate to this sum when $z \to 1^-$. When the summation index k is large, what determines the convergence of the series is indeed the factor z^k. Replacing the other factors in the summand by their asymptotic value for $k \to +\infty$ we identify the diverging part when $z = 1$:

$$\left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \sum_{k=1}^{\infty} z^k \exp\left[-\frac{m\omega r^2}{\hbar}\right] = \frac{z}{1-z}|\phi_{0,0,0}(\vec{r})|^2 = N_0|\phi_{0,0,0}(\vec{r})|^2 \qquad (35)$$

where $\phi_{0,0,0}(\vec{r})$ is the ground state wave function of the harmonic oscillator.

Numerically we have calculated the total density $\rho(\vec{r})$ for a fixed temperature $k_B T = 20\hbar\omega$ and for increasing number of particles (see figure 2). Here the maximal number of particles one can put in the excited states of the trap is $N'_{\max} \simeq \zeta(3)(k_B T/\hbar\omega)^3 \simeq 10^4$. When $N \ll N'_{\max}$ the effect of an increase of N is mainly to multiply the density by some global factor (the curves in logarithmic scale in figure 2 are parallel one to the other). When N is becoming larger than $N'_{\max}$ a peak in density grows around $r = 0$, indicating the formation of the condensate, whereas the far wings of the density distribution saturate, which reflects the saturation of the population of the excited levels of the trap.

2.1.4 Relation to Einstein's condition $\rho\lambda_{dB}^3 = \zeta(3/2)$

In the limit $k_B T \gg \hbar\omega$ we can actually calculate the value $\rho'_{\max}(\vec{r})$ to which the density $\rho'(\vec{r})$ of particles in the excited states of the trap saturates when $z \to 1$. We simply use the expansion Eq.(34), subtracting from the total density $\rho(\vec{r})$ the contribution of the condensate $N_0|\phi_{0,0,0}(\vec{r})|^2$. The resulting series is converging even for $z = 1$ so that we can take safely the semiclassical limit $k_B T \gg \hbar\omega$ term by term in the sum:

$$\rho'(\vec{r}) \simeq \frac{1}{\lambda_{dB}^3} \sum_{k=1}^{\infty} \frac{z^k}{k^{3/2}} \exp\left(-\frac{1}{2}k\beta m\omega^2 r^2\right) = \frac{1}{\lambda_{dB}^3} g_{3/2}\left[z\exp\left(-\beta\frac{1}{2}m\omega^2 r^2\right)\right] \qquad (36)$$

where

$$g_\alpha(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^\alpha}. \qquad (37)$$
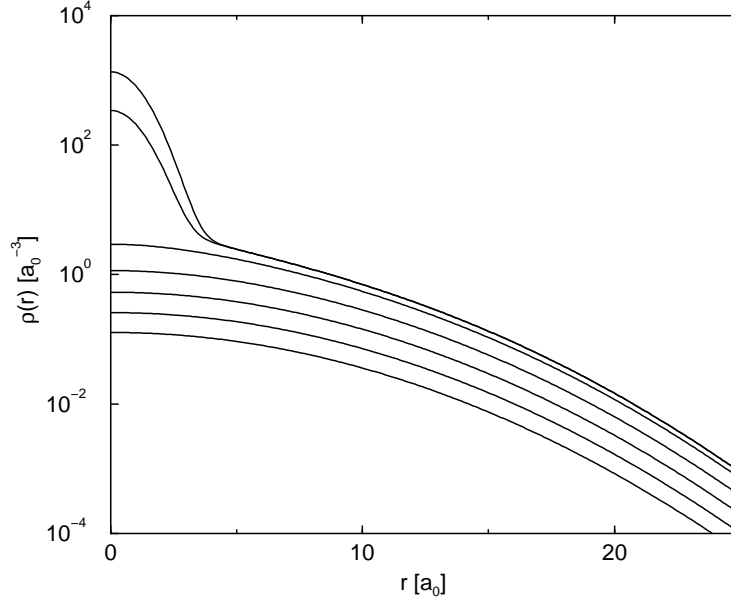
Figure 2: Spatial density for an ideal Bose gas at thermal equilibrium in a harmonic trap of frequency ω. The temperature is fixed to $k_B T = 20\hbar\omega$ and the number of particles ranges from $N = 500$ to $N = 32000$ between the lowest curve and the upper curve, with a geometrical reason equal to 2. The unit of length for the figure is $a_0 = (\hbar/2m\omega)^{1/2}$, that is the spatial radius of the ground state of the trap.

We term this approximation semiclassical as (i) one can imagine that the classical limit $\hbar \to 0$ is taken in each term k of the sum, giving the usual Gaussian distribution for the density of a classical harmonic oscillator at temperature $k_B T/k$, but (ii) the distribution still reflects the quantum Bose statistics.

If now we set $z = 1$ in (36) to express the fact that a condensate is formed we obtain

$$\rho'_{\max}(\vec{r} = \vec{0}) \simeq \frac{1}{\lambda_{dB}^3} g_{3/2}(1) = \frac{\zeta(3/2)}{\lambda_{dB}^3}. \tag{38}$$

We therefore recover Einstein's condition provided one replaces the density ρ of the homogeneous case by the density at the center of the trap.

2.2   Bose-Einstein condensation in a more general trap

We now extend the idea of the previous semiclassical limit to more general non-harmonic potentials. This allows to find the condition for Bose-Einstein condensation in presence

of a non-harmonic potential. This will prove useful in presence of interactions between the particles where the non-harmonicity is provided by the mean field potential.

2.2.1 The Wigner distribution

The idea is to find a representation of the one-body density matrix having a simple (non pathological) behavior when $\hbar \to 0$. Let us take as an example a single harmonic oscillator. The density matrix is then of the form:

$$\hat{\sigma} = \frac{1}{Z} e^{-\beta \hat{H}_{\text{ho}}} \tag{39}$$

where $\hat{H}_{\text{ho}}$ is the harmonic oscillator Hamiltonian. As shown in [9] all the matrix elements of $\hat{\sigma}$ can be calculated exactly:

$$\langle \vec{r} | \hat{\sigma} | \vec{r}' \rangle = \frac{1}{(2\pi)^{3/2}(\Delta r)^3} \exp\left[-\frac{[(\vec{r} + \vec{r}')/2]^2}{2(\Delta r)^2} \right] \exp\left[-\frac{(\vec{r} - \vec{r}')^2}{2\xi^2} \right] \tag{40}$$

The relevant length scales are the spatial width of the cloud Δr:

$$(\Delta r)^2 = \frac{\hbar}{2m\omega} \coth\left(\frac{\hbar\omega}{2k_B T} \right) \tag{41}$$

and the coherence length ξ:

$$\xi^2 = \frac{2\hbar}{m\omega} \tanh\left(\frac{\hbar\omega}{2k_B T} \right). \tag{42}$$

If we now take the classical limit $\hbar \to 0$ (in more physical terms the limit $\hbar\omega \ll k_B T$) then:

$$(\Delta r)^2 \quad \to \quad \frac{k_B T}{m\omega^2} \tag{43}$$

$$\xi^2 \quad \sim \quad \frac{\hbar^2}{m k_B T} = \frac{\lambda_{dB}^2}{2\pi}. \tag{44}$$

In the limit $\hbar \to 0$ the $\hbar$ dependence of ξ causes $\langle \vec{r} | \hat{\sigma} | \vec{r}' \rangle \to 0$ for fixed values of $\vec{r}, \vec{r}'$ unless $\vec{r} = \vec{r}'$: the limit is singular.

To avoid this problem one can use the Wigner representation of the density matrix, introduced also in the lectures of Zurek and Paz:

$$W[\hat{\sigma}](\vec{r}, \vec{p}) = \int \frac{d^3\vec{u}}{h^3} \langle \vec{r} - \frac{\vec{u}}{2} | \hat{\sigma} | \vec{r} + \frac{\vec{u}}{2} \rangle e^{i\vec{p}\cdot\vec{u}/\hbar}. \tag{45}$$

The Wigner distribution is the quantum analog of the classical phase space distribution. In particular one can check that the Wigner distribution is normalized to unity and that

$$\int d^3\vec{r}\, W(\vec{r},\vec{p}) = \langle \vec{p}|\hat{\sigma}|\vec{p}\rangle \tag{46}$$

$$\int d^3\vec{p}\, W(\vec{r},\vec{p}) = \langle \vec{r}|\hat{\sigma}|\vec{r}\rangle. \tag{47}$$

An important caveat is that W is not necessarily positive.

For the harmonic oscillator at thermal equilibrium the integral over $\vec{u}$ in Eq.(45) is Gaussian and can be performed exactly:

$$W(\vec{r},\vec{p}) = \frac{1}{(2\pi\Delta r \Delta p)^3} \exp(-\frac{r^2}{2(\Delta r)^2}) \exp(-\frac{p^2}{2(\Delta p)^2}) \tag{48}$$

where $\Delta p \equiv \hbar/\xi$. If we take now the limit $\hbar \to 0$:

$$(\Delta r)^2 \rightarrow \frac{k_B T}{m\omega^2} \tag{49}$$

$$(\Delta p)^2 \rightarrow mk_B T \tag{50}$$

so that $W(\vec{r},\vec{p})$ tends to the classical phase space density.

2.2.2 Critical temperature in the semiclassical limit

Let us turn back to our problem of trapped atoms in a non-harmonic trap where the single particle Hamiltonian is given by

$$\hat{h}_1 = \frac{\vec{p}^2}{2m} + U(\vec{r}) \tag{51}$$

and the one-body density matrix is given by Eq.(32). For $\hbar \to 0$ we have:

$$W[e^{-\beta k \hat{h}_1}](\vec{r},\vec{p}) \simeq \frac{1}{h^3} \exp\left[-k\beta\left(\frac{p^2}{2m} + U(\vec{r})\right)\right]. \tag{52}$$

As we did before we put apart the contribution of the condensate. One then gets for the one-body density matrix of the non-condensed fraction of the gas in the semiclassical limit:

$$W[\hat{\rho}_1']_{sc} = \frac{1}{h^3} \sum_{k=1}^{+\infty} z^k \exp\left[-k\beta\left(\frac{p^2}{2m} + U(\vec{r})\right)\right] \tag{53}$$

$$= \frac{1}{h^3} \left\{\frac{1}{z} \exp\left[\beta\left(\frac{p^2}{2m} + U(\vec{r})\right)\right] - 1\right\}^{-1}. \tag{54}$$

We are now interested in the spatial density of the non-condensed particles in the semiclassical limit. By integrating Eq.(53) over p we obtain:

$$\rho'_{sc}(\vec{r}) = \frac{1}{\lambda_{dB}^3} g_{3/2}(\mathrm{z}e^{-\beta U(\vec{r})}) \tag{55}$$

where g_α is defined in Eq.(37). The condition for Bose-Einstein condensation is $\mathrm{z} \to e^{\beta U_{\min}}$ where $U_{\min} = \min_{\vec{r}} U(\vec{r})$ is the minimal value of the trapping potential, achieved in the point $\vec{r}_{\min}$. For $\mathrm{z} = e^{\beta U_{\min}}$ the semiclassical approximation for the non-condensed density gives in this point:

$$\rho'_{sc}(\vec{r}_{\min}) = \frac{1}{\lambda_{dB}^3} g_{3/2}(1) \tag{56}$$

or

$$\rho \lambda_{dB}^3 = 2.612... \tag{57}$$

Again Einstein's formula is recovered with ρ being the maximal density of the non-condensed cloud, that is the non-condensed density at the center of the trap.

The semiclassical calculation that we have just presented was initially put forward in [10]. We do not discuss in details the validity of this semi-classical approximation. Intuitively a necessary condition is $k_B T \gg \Delta E$ where ΔE is the maximal level spacing of the single particle Hamiltonian among the states thermally populated. Some situations, where the trapping potential is not just a single well, may actually require more care. The case of Bose-Einstein condensation in a periodic potential is an interesting example that we leave as an exercise to the reader.

2.3   Is the ideal Bose gas model sufficient: experimental verdict

2.3.1   Condensed fraction as a function of temperature

The groups at MIT and JILA have measured the condensate fraction N_0/N as function of temperature for a typical number of particles $N = 10^5$ or larger. We reproduce here the results of JILA [11] (see figure 3). This figure shows that the leading order prediction of the ideal Bose gas Eq.(23) is quite good, even if there is a clear indication from the experimental data that the actual transition temperature is lower than T_c^0. This deviation may be due to finite size effects and interaction effects but the large experimental error has not allowed yet a fully quantitative comparison to theory.
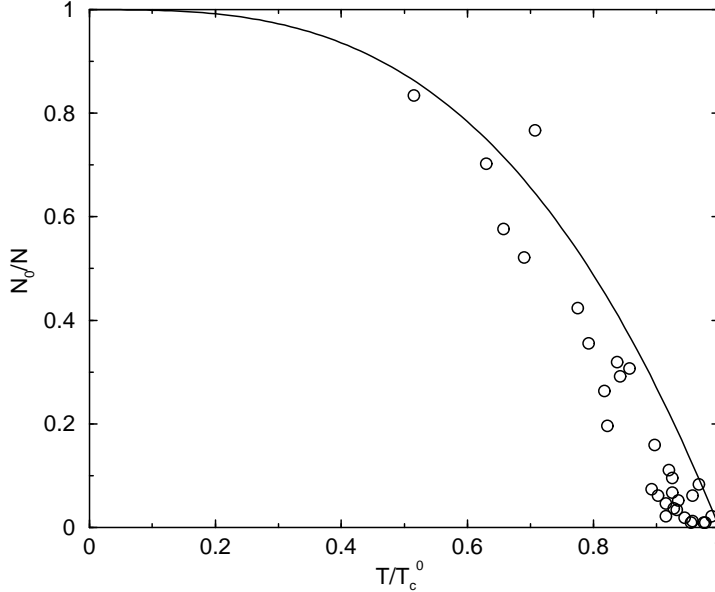
Figure 3: Condensate fraction N_0/N as function of T/T_c^0 where T_c^0 is the leading order ideal Bose gas prediction Eq.(24). Circles are the experimental results of [11] while the dashed line is Eq.(23).

2.3.2 Energy of the gas as function of temperature and number of particles

In the experiments one produces first a Bose condensed gas at thermal equilibrium. Then one switches off suddenly the trapping potential. The cloud then expands ballistically, and after a time long enough that the expansion velocity has reached a steady state value one measures the kinetic energy of the expanding cloud.

Suppose that the trap is switched off at $t = 0$. For $t = 0^-$ the total energy of the gas can be written as

$$E_{\text{tot}}(0^-) = E_{\text{kin}} + E_{\text{trap}} + E_{\text{int}}, \tag{58}$$

that is as the sum of kinetic energy, trapping potential energy and interaction energy. At time $t = 0^+$ there is no trapping potential anymore so that the total energy of the gas reduces to

$$E_{\text{tot}}(0^+) = E_{\text{kin}} + E_{\text{int}}. \tag{59}$$

In the limit $t \to +\infty$ the gas expands, the density and therefore the interaction energy drop, and all the energy $E_{\text{tot}}(0^+)$ is converted into kinetic energy, which is measured.

In figure 4 we show the results of JILA for $E_{\text{tot}}(0^+)$ for temperatures around T_c^0 [11] together with the ideal Bose gas prediction. The main feature of the ideal Bose gas prediction is a change in the slope of the energy as function of temperature when T crosses T_c. One observes indeed a change of slope in the experimental results (see the magnified inset)!

For $T > T_c$ the ideal Bose gas model is in good agreement with the experiment. For $T < T_c$ we observe however that the experiment significantly deviates from the ideal Bose gas.
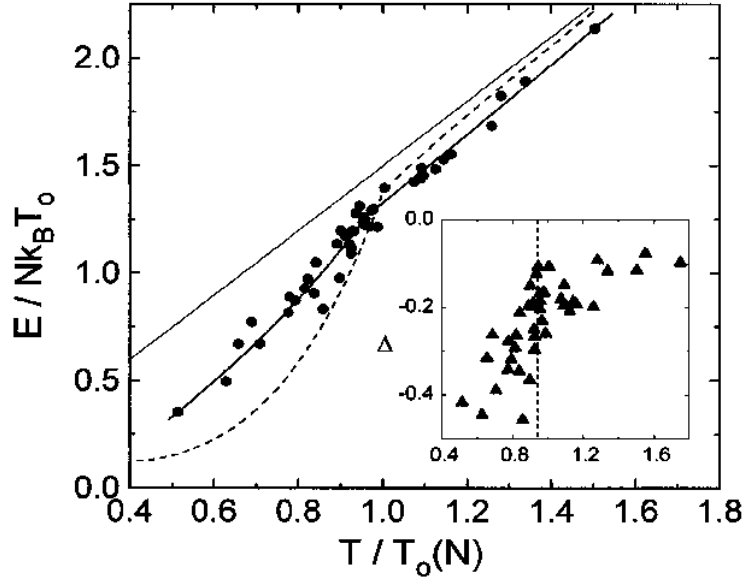
Figure 4: Expansion energy of the gas $E_{\text{tot}}(0^+)$ per particle and in units of $k_B T_c^0$ as function of the temperature in units of T_c^0. The disks correspond to the experimental results of [11]. The straight solid line is the prediction of Boltzmann statistics. The dashed curve exhibiting a change of slope is the ideal Bose gas prediction. The curved solid line is a piecewise polynomial fit to the data. The inset is a magnification showing the change of slope of the energy as function of T close to $T = T_c^0$. The figure is taken from [11].

What happens at even lower values of T/T_c^0? We show in figure 5 the expansion energy of the condensate per particle in the regime of an almost pure condensate [12]. This energy then depends almost only on the number of condensate particles N_0, in a non-linear fashion. This is in complete violation with the ideal Bose gas model, which

predicts an energy per particle in the condensate independent of N_0. More precisely the ideal Bose gas prediction would be $\hbar(\omega_x + \omega_y + \omega_z)/4$ where the ω_α's are the trap frequencies. In units of k_B this would be in the 10 nK range, an order of magnitude smaller than the measured values.
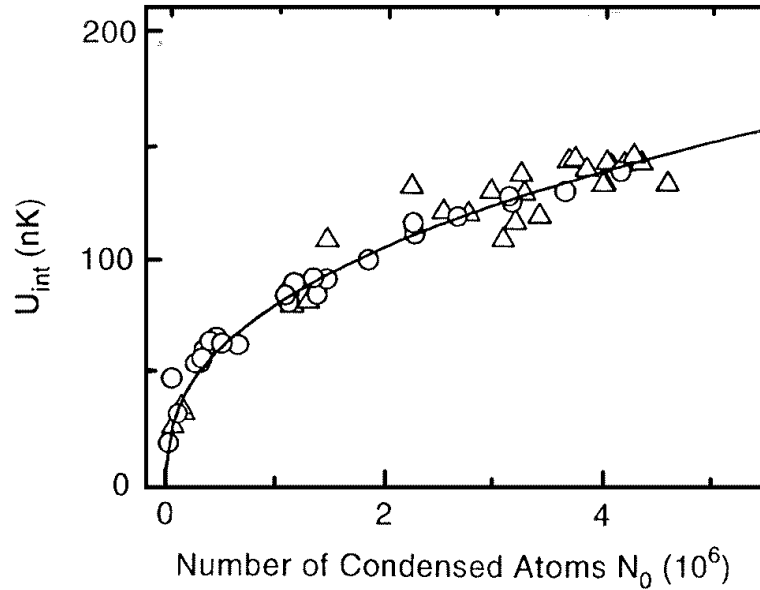
Figure 5: Expansion energy of the condensate per particle in the condensate, divided by k_B, as a function of the number of particles in the condensate. The experiment is performed at temperatures $T \ll T_c$. The triangles correspond to cases where the non-condensed cloud was not visible experimentally. The disks correspond to case where the non-condensed cloud could be seen. The figure is taken from [12]. The solid line is a fit of the interacting Bose gas prediction of §5.

2.3.3 Density profile of the condensate

The group of Lene Hau at Rowland Institute has measured the density profile of the condensate in a cigar-shaped trap, along the weakly confining axis z of the trap. As imaging with a light beam is used the actual density obtained in the experiment is the density integrated along the direction y of propagation of the laser beam, plotted in figure 6 for $x = 0$ as function of z [13]. The measured profile is very different from and

much broader than the Gaussian density profile of the ground state wavefunction of the harmonic oscillator.
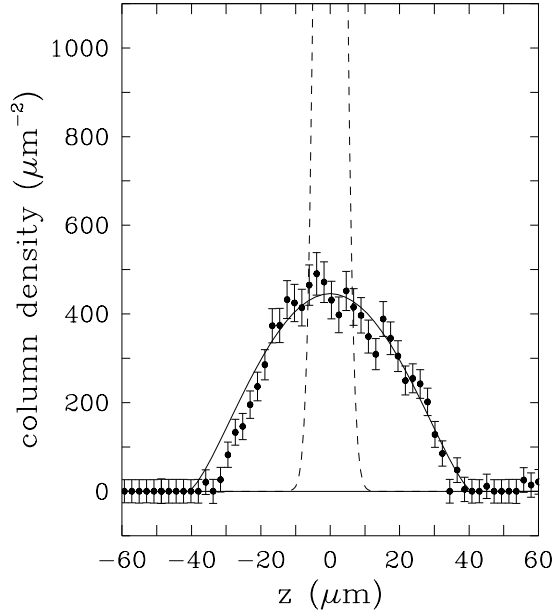
Figure 6: Column density profile (see text) of a condensate along the weak axis z of a cigar-shaped trap. The experimental results of [13] (dots) are very different from the ideal Bose gas prediction (dashed line). The solid line corresponds to the theoretical prediction of §5.

2.3.4 Response frequencies of the condensate

By modulating the harmonic frequencies of the trapping potential one can excite breathing modes of the condensate. For example the group at MIT modulated the trap frequency along the slow axis z of a cigar-shaped trap and observed at $T \ll T_c$ subsequent breathing of the condensate at a frequency $1.569(4)\omega_z$. This frequency is not an integer multiple of ω_z and can therefore not be obtained in the ideal Bose gas model.

In conclusion the ideal Bose gas model may be acceptable as long as no significant condensate has been formed. If a condensate is formed interaction effects become important, and dominant at $T \ll T_c$. This serves as a motivation to the next sections of this lecture, which will deal with the interacting Bose gas problem.

3 A model for the atomic interactions

The previous section 2 has shown that the ideal Bose gas model is insufficient to explain the experimental results when a condensate is formed. In this section we choose the model potential to be used in this lecture to take into account the atomic interactions. The reader interested in a more careful discussion of real interaction potentials is referred to [14].

3.1 Reminder of scattering theory

We consider two particles of mass m interacting in free space via the potential $V(\vec{r_1}-\vec{r_2})$ depending on the positions $\vec{r_1},\vec{r_2}$ only through the relative vector $\vec{r_1}-\vec{r_2}$. The center of mass of the two particles is then decoupled from their relative motion, and the evolution of the relative motion is governed by the Hamiltonian:

$$H_{\text{rel}} = \frac{\vec{p}^2}{2\mu} + V(\vec{r}) \tag{60}$$

where $\vec{r} = \vec{r_1} - \vec{r_2}$ is the vector of coordinates of the relative motion, $\vec{p} = (\vec{p_1} - \vec{p_2})/2$ is the relative momentum and $\mu = m/2$ is the reduced mass. We assume in what follows that the potential $V(\vec{r})$ is vanishing in the limit $r \to \infty$.

3.1.1 General results of scattering theory

The scattering states $\psi(\vec{r})$ of the relative motion of the two particles are the eigenstates of H_{rel} with positive energy E. Writing $E = \hbar^2 k^2/2\mu$ and multiplying the eigenvalue equation by $2\mu/\hbar^2$ we obtain

$$(\Delta + k^2)\psi(\vec{r}) = \frac{2\mu}{\hbar^2}V(\vec{r})\psi(\vec{r}). \tag{61}$$

One has also to specify boundary conditions on ψ to get the full description of a scattering state. This is achieved by means of an integral formulation of the eigenvalue equation.

- *Integral equation*

To obtain the integral formulation of the scattering problem we write the right hand side of the eigenvalue equation Eq.(61) as a continuous sum of Dirac distributions:

$$(\Delta + k^2)\psi(\vec{r}) = \int d^3\vec{r}'\frac{2\mu}{\hbar^2}V(\vec{r}')\psi(\vec{r}')\delta(\vec{r} - \vec{r}'). \tag{62}$$

We then find a solution of this equation with a single Dirac distribution on the right hand side:

$$(\Delta_{\vec{r}} + k^2)\psi_G(\vec{r}) = \delta(\vec{r} - \vec{r}')$$

(63)

having the form of an outgoing spherical wave for $r \to \infty$:

$$\psi_G(\vec{r}) = -\frac{1}{4\pi}\frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}.$$

(64)

This is actually a Green's function of the operator $\Delta + k^2$. The scattering state of the full problem can then be written as

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{2\mu}{4\pi\hbar^2}\int d^3\vec{r}'\frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}V(\vec{r}')\psi(\vec{r}')\,.$$

(65)

The first term ψ_0 is the incoming free wave of the collision, solving $(\Delta + k^2)\psi_0 = 0$; we simply assume here that the incoming wave is a plane wave of wavevector $\vec{k}$:

$$\psi_0(\vec{r}) = \exp[i\vec{k} \cdot \vec{r}].$$

(66)

The remaining part of ψ is then simply the scattered wave.

- *Born expansion*

When the interaction potential is weak one sometimes expands the scattering state ψ in powers of V. In the integral formulation Eq.(65) of the eigenvalue equation this corresponds to successive iterations of the integral, the approximation for ψ at order $n + 1$ in V being obtained by replacing ψ by its approximation at order n in the right-hand side of the integral equation. E.g. to zeroth order in V, $\psi = \psi_0$, and to first order in V we get the so-called Born approximation:

$$\psi_{\text{Born}}(\vec{r}) = \psi_0(\vec{r}) - \frac{2\mu}{4\pi\hbar^2}\int d^3\vec{r}'\,\frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|}V(\vec{r}')\psi_0(\vec{r}').$$

(67)

3.1.2 Low energy limit for scattering by a finite range potential

Some results can be obtained in a simple way when the potential V has a finite range b, that is when it vanishes when $r > b$.

- *asymptotic behavior for large* r

As the integration over the variable $\vec{r}'$ is limited to a range of radius b one can expand the distance from $\vec{r}$ to $\vec{r}'$ in powers of r when $r \gg b$:

$$|\vec{r} - \vec{r}'| = r - \vec{r}' \cdot \vec{n} + O\left(\frac{1}{r}\right) \tag{68}$$

where $\vec{n} = \vec{r}/r$ is the direction of scattering. The neglected term, scaling as b^2/r, has a negligible contribution to the phase $\exp[ik|\vec{r} - \vec{r}'|]$ when $r \gg kb^2$. One then enters the asymptotic regime for ψ:

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \frac{e^{ikr}}{r} f_{\vec{k}}(\vec{n}) + O\left(\frac{1}{r^2}\right) \tag{69}$$

where the factor $f_{\vec{k}}$, the so-called scattering amplitude, does not depend on the distance r:

$$f_{\vec{k}}(\vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3\vec{r}' \; e^{-ik\vec{n}\cdot\vec{r}'} V(\vec{r}')\psi(\vec{r}'). \tag{70}$$

If the mean distance between the particles in the gas, on the order of $\rho^{-1/3}$, where ρ is the density, lies in the asymptotic regime for ψ (that is $\rho^{-1/3} \gg b, kb^2$) the effect of binary interactions on the macroscopic properties of the gas will be sensitive to the scattering amplitude $f_{\vec{k}}$, and no longer to the details of the scattering potential. This is the key property that we shall use later in this low density regime to replace the exact interaction potential by a model potential having approximately the same scattering amplitude.

- *limit of low energy collisions*

Another simplification comes from the fact that collisions take place at low energy in the Bose condensed gases: as $\hbar^2 k^2/2\mu$ is on the order of $k_B T$ in the thermal gas, k becomes small at low temperature.

If $kb \ll 1$ the phase factor $\exp[-ik\vec{n}\cdot\vec{r}']$ becomes close to one in the integral Eq.(70) giving the scattering amplitude. The scattering amplitude $f_{\vec{k}}$ then no longer depends on the scattering direction $\vec{n}$, the asymptotic part of the scattered wave becomes spherically symmetric (even if the scattering potential is not!): one then says that scattering takes place in the s-wave only.

Going to the mathematical limit $k \to 0$ we get for the scattering amplitude:

$$f_{\vec{k}}(\vec{n}) \to -a. \tag{71}$$

The quantity a is the so-called scattering amplitude; it will be the only parameter of our theory describing the interactions between the particles, and our model potential will be adjusted to have the same scattering length as the exact potential. When k is going to zero, the scattering state converges to the zero energy scattering state, behaving for large r as

$$\psi_{E=0}(\vec{r}) = 1 - \frac{a}{r} + O\left(\frac{1}{r^2}\right). \tag{72}$$

A numerical calculation of this zero energy scattering state is an efficient way of calculating a for a given potential V. Note that there is of course no connection between a and b, except for particular potentials like the hard sphere potential.

3.1.3 Power law potentials

In real life the interaction potential between atoms is not of finite range, as it contains the Van der Waals tail scaling as $1/r^6$ for large r [2]. It is fortunately possible to show for the class of power-law potentials, scaling as $1/r^n$, that several of our conclusions, obtained in the finite range case, hold provided that $n > 3$. E.g. in the limit of small k's only the s-wave scattering survives, and $f_{\vec{k}}$ has a well defined limit for $k \to 0$, allowing one to define the scattering length.

3.2 The model potential used in this lecture

3.2.1 Why not keep the exact interaction potential ?

For alkali atoms the exact interaction potential has a repulsive hard core, is very deep (as deep as 10^3 Kelvins times k_B for ^{133} Cs), has a minimum at a distance r_{12} on the order of 6 Å(for cesium), and contains many bound states corresponding to molecular states of two alkali atoms (see figure 7).

There are several disadvantages to use the exact interaction potential in a theoretical treatment of Bose-Einstein condensation:

1. V is difficult to calculate precisely, and a small error on V may result in a large error on the scattering length a. In practice a is measured experimentally, and this is the most relevant information on V in the low density, low temperature limit.

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[2]or even as $1/r^7$ if r is larger than the optical wavelength.
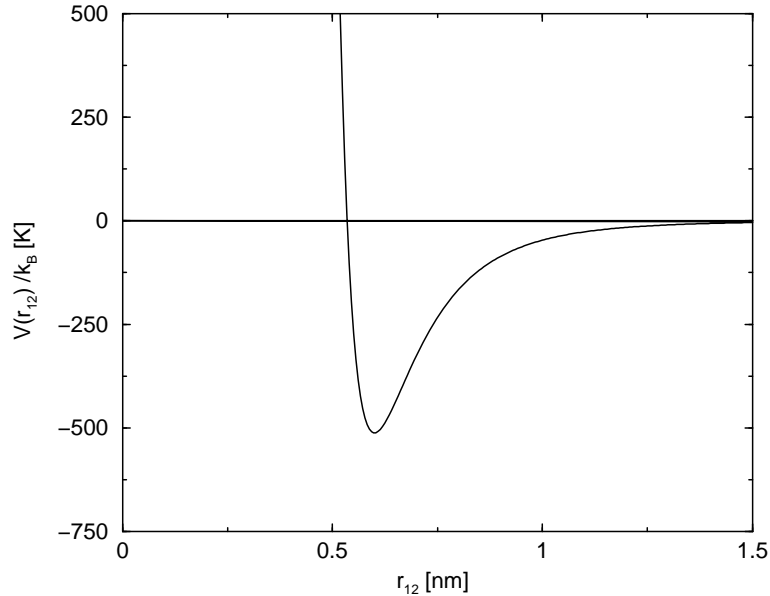
Figure 7: Typical shape of the interaction potential between two atoms, as function of the interatomic distance r_{12}. The numbers are indicative and correspond to cesium.

2. the presence of bound states of V with a binding energy much smaller than the temperature of the gas (there are 9 orders of magnitude between the potential depth 10^3 K and the gas temperature $\simeq 1\mu$ K) clearly indicates that the Bose condensed gases are in a metastable state; at the experimental temperatures and densities the complete thermal equilibrium of the system would be a solid. Direct thermal equilibrium theory, such as the thermal N-body density matrix $\exp[-\beta H]$, cannot therefore be used with V. This is why even in the exact Quantum Monte Carlo calculations performed for alkali gases [15] V is replaced by a hard sphere potential. Such a complication was absent for liquid helium, where the well-known exact V can be used [16].

3. V can not be treated in the Born approximation, because it is very strongly repulsive at short distances and has many bound states: even if the scattering length was zero, one would have to resum the whole Born series to obtain the correct result [We recall that for a potential as gentle as a square well of radius b, the Born approximation applies when the zero-point energy for confinement within a domain of

radius b, $\hbar^2/2\mu b^2$, is much larger than the potential depth, which implies that no bound state is present in the well.] As a consequence naive mean field approximations, which neglect the correlations between particles due to interactions, implicitly relying on the Born approximation, cannot be used with the exact V.

The key idea is therefore to replace the exact interaction potential by a model potential (i) having the same scattering properties at low energy, that is the same scattering length, and (ii) which should be treatable in the Born approximation, so that naive mean field approaches apply.

The model potential satisfying these requirements with the minimal number of parameters (one!) is the zero-range pseudo-potential initially introduced by Enrico Fermi [17, 18] and having the following action on any two-body wavefunction:

$$\langle \vec{r_1}, \vec{r_2} | V | \psi_{1,2} \rangle \equiv g\delta(\vec{r_1} - \vec{r_2}) \left[\frac{\partial}{\partial r_{12}} \left(r_{12} \psi_{1,2}(\vec{r_1}, \vec{r_2}) \right) \right]_{r_{12}=0}. \tag{73}$$

The factor g is the so-called coupling constant

$$g = \frac{4\pi\hbar^2}{m} a \tag{74}$$

where a is the scattering length of the exact potential. The pseudo-potential involves a Dirac distribution and a regularizing operator.

- *Effect of regularization*

When the wavefunction $\psi_{1,2}$ is regular close to $\vec{r_1} = \vec{r_2}$, one can check that the regularizing operator has no effect, so that the pseudo-potential can be viewed as a mere contact potential $g\delta(\vec{r_1} - \vec{r_2})$.

When the wavefunction $\psi_{1,2}$ has a $1/r_{12}$ divergence:

$$\psi_{1,2}(\vec{r_1}, \vec{r_2}) = \frac{A(\vec{r_1} + \vec{r_2})}{r_{12}} + \text{regular} \tag{75}$$

where A is the function of the center of mass coordinates only the regularizing operator removes the diverging part:

$$\frac{\partial}{\partial r_{12}} \left(r_{12} \frac{A(\vec{r_1} + \vec{r_2})}{r_{12}} \right) = 0. \tag{76}$$

In this way we have extended the Hilbert space of the state vectors of the particles with wave functions diverging as $1/r_{12}$; note that these wavefunctions remain square integrable, as the element of volume scales as r_{12}^2 in 3D. As we shall see this $1/r_{12}$ divergence is a consequence of the zero-range of the pseudo-potential.

3.2.2 Scattering states of the pseudo-potential

Turning back to the relative motion of two particles we now derive the scattering states of the pseudo-potential from the integral equation Eq.(65). As the pseudo-potential involves a Dirac $\delta(\vec{r}')$ the integral over $\vec{r}'$ can be performed explicitly:

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - a\frac{e^{ikr}}{r}\left[\frac{\partial}{\partial\vec{r}'}\left(r'\psi(\vec{r}')\right)\right]_{r'=0}. \tag{77}$$

As the factor

$$C = \left[\frac{\partial}{\partial\vec{r}'}\left(r'\psi(\vec{r}')\right)\right]_{r'=0} \tag{78}$$

does not depend on $\vec{r}$ we find that ψ has the standard asymptotic behavior of a scattering state in r but *everywhere* in space, not only for large r. This is due to the zero-range of the pseudo-potential. To calculate C, we multiply Eq.(77) by r, we take the derivative with respect to r and set r to zero. On the left hand side we recover the constant C by definition. We finally obtain:

$$C = 1 - aCik \tag{79}$$

so that $C = 1/(1 + ika)$ and the scattering states of the pseudo-potential are exactly given by

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{a}{1 + ika}\frac{e^{ikr}}{r}. \tag{80}$$

The corresponding scattering amplitude,

$$f_k = -\frac{a}{1 + ika} \tag{81}$$

does not depend on the direction of scattering, so that the pseudo-potential scatters only in the s -wave, whatever the modulus k is. The scattering length of the pseudo-potential, $-f_{k=0} = a$, coincides with the one of the exact potential.

Finally we note that the total cross-section for scattering of identical bosons by the pseudo-potential is given by a Lorentzian in k,

$$\sigma = 8\pi |f_{\vec{k}}(\vec{n})|^2 = \frac{8\pi a^2}{1 + k^2 a^2},\tag{82}$$

and that the pseudo-potential obeys the optical theorem.

3.2.3 Bound states of the pseudo-potential

As a mathematical curiosity we now point out that not only the scattering states but also the bound states of the pseudo-potential can be calculated. A first way of obtaining the bound states is a direct solution of Schrödinger's equation. A more amusing way is to use the following closure relation:

$$\int \frac{d^3\vec{k}}{(2\pi)^3} |\psi_{\vec{k}}\rangle\langle|\psi_{\vec{k}}| = 1 - P_{\text{bound}}\tag{83}$$

where $|\psi_{\vec{k}}\rangle$ is the scattering state given in Eq.(80) and P_{bound} is the projector on the bound states of the pseudo-potential.

In calculating the matrix elements of this closure relation between perfectly localized state vectors $|\vec{r}\rangle$ and $|\vec{r}'\rangle$ and using spherical coordinates for the integration over $\vec{k}$ one ultimately faces the following type of integrals:

$$I = \int_{-\infty}^{+\infty} dk\, \frac{e^{ik(r+r')}}{1 + ika}.\tag{84}$$

We calculate I using the residues formula, by extending the integration variable k to the complex plane and closing the contour of integration by a circle of infinite radius, which has to be in the upper half of the complex plane as $r + r' > 0$. As the integrand in I has a pole in $k = i/a$, we find that I vanishes for $a < 0$, as the pole is then in the lower half of the complex plane. For $a > 0$ the pole gives a non-zero contribution to the integral:

$$I = \frac{2\pi}{a} e^{-(r+r')/a}.\tag{85}$$

Finally we find that $P_{\text{bound}} = 0$ for $a < 0$, corresponding to the absence of bound states, and $P_{\text{bound}} = |\psi_{\text{bound}}\rangle\langle\psi_{\text{bound}}|$ for $a > 0$, corresponding to the existence of a single bound state:

$$\psi_{\text{bound}}(\vec{r}) = \frac{1}{\sqrt{2\pi a}} \frac{e^{-r/a}}{r}.\tag{86}$$

From Schrödinger's equation, we find for the energy of the bound state:

$$E_{\text{bound}} = -\frac{\hbar^2}{ma^2}. \tag{87}$$

The existence of a bound state for $a > 0$ and its absence for $a < 0$ is a paradoxical situation. As we shall see in the mean field approximation, the case $a > 0$ corresponds to effective repulsive interactions between the atoms, whereas the case $a < 0$ corresponds to effective attractive interactions. In the purely 1D case, the situation is more intuitive, the potential $g_{1D}\delta(x)$ having a bound state only in the effective attractive case $g_{1D} < 0$. This paradox in 3D comes from the non-intuitive effect of the regularizing operator (an operation not required in 1D), which makes the pseudo-potential different from a delta potential; actually one can shown in 3D that a delta potential viewed as a limit of square well potentials with decreasing width b and constant area does not scattered in the limit $b \to 0$.

3.3 Perturbative vs non-perturbative regimes for the pseudo-potential

3.3.1 Regime of the Born approximation

As we will use mean field approximations requiring that the scattering potential is treatable in the Born approximation, we identify the regime of validity of the Born approximation for the pseudo-potential.

As we have seen in the previous subsection the integral equation for the scattering states of the pseudo-potential can be reduced to the equation for C:

$$C = 1 - ikaC, \tag{88}$$

the scattering state being given by

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - aC\frac{e^{ikr}}{r}. \tag{89}$$

The Born expansion will then reduces to iterations of Eq.(88). To zeroth order in the interaction potential, we obtain $C_0 = 0$ so that $\psi_{\vec{k}}$ reduces to the incoming wave. To first order, we get the Born approximation

$$C_1 = 1 - ikaC_0 = 1. \tag{90}$$

To second order and third order we obtain

$$C_2 = 1 - ikaC_1 = 1 - ika \tag{91}$$

$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2 \tag{92}$$

so that the Born expansion is a geometrical series expansion of the exact result $C = 1/(1 + ika)$ in powers of ika.

The validity condition of the Born approximation is that the first order result is a small correction to the zeroth order result. For the scattering amplitude this requires

$$k|a| \ll 1. \tag{93}$$

For the scattering state this requires

$$r \gg a. \tag{94}$$

If one takes for r the typical distance $\rho^{-1/3}$ between the particles in the gas, where ρ is the density, this leads to

$$\rho^{1/3}|a| \ll 1. \tag{95}$$

- *Are the conditions for the Born approximation satisfied in the experiments ?*

To estimate the order of magnitude of k we average k^2 over a Maxwell-Boltzmann distribution of atoms with a temperature $T = 1\mu$ K, typically larger than the critical temperature for alkali gases; the average gives a root mean square for k equal to

$$\Delta k = \left(\frac{3mk_B T}{2\hbar^2} \right)^{1/2}. \tag{96}$$

For ^{23} Na atoms used at MIT, with a scattering length of $50\, a_{\text{Bohr}}$, where the Bohr radius is $a_{\text{Bohr}} = 0.53$ Å, we obtain $\Delta k\, a = 2 \times 10^{-2}$. For rubidium ^{87} Rb atoms used at JILA, with a scattering length of $110\, a_{\text{Bohr}}$, we obtain $\Delta k\, a = 0.1$.

In the case of an almost pure condensate in a trap, the typical k is given by the inverse of the size R of the condensate, as the condensate wavefunction is not very far from a minimum uncertainty state. Generally this results in a much smaller Δk than Eq.(96), as R is much larger than the thermal de Broglie wavelength. One could however

imagine a condensate in a very strongly confining trap, such that R would become close to a; in this case, not yet realized, the mean field theory has to be revisited.

We turn to the second condition Eq.(95). The typical densities of condensates are on the order of 2×10^{14} atoms per cm^3. For the scattering length of sodium this leads to $\rho^{1/3}a \simeq 0.015 \ll 1$. For the scattering length of rubidium this leads to $\rho^{1/3}a \simeq 0.034 \ll 1$. Both conditions for the Born approximation applied to the pseudo-potential are therefore satisfied.

3.3.2 Relevance of the pseudo-potential beyond the Born approximation

Let us try to determine necessary validity conditions for the substitution of the exact interaction potential by the pseudo-potential.

First one should be in a regime dominated by s-wave scattering, as the pseudo-potential neglects scattering in the other wave. This condition is easily satisfied in the μK temperature range for Rb, Na.

Second the scattering amplitude of the exact potential in s-wave should be well approximated by the pseudo-potential. For isotropic potentials vanishing for large r as $1/r^n$, with $n > 5$, the s-wave scattering amplitude has the following low k expansion:

$$f_k^{s=0} = -\frac{1}{a^{-1} + ik - \frac{1}{2}k^2 r_e + \dots} \tag{97}$$

where r_e is the so-called effective range of the potential. To this order in k the result of the pseudo-potential corresponds to the approximation $r_e = 0$. When r_e is on the order of a (which is the case for a hard sphere potential, but not necessarily true for a more general potential) the term in r_e can be neglected if $k^2 r_e \ll 1/a$, that is $(ka)^2 \ll 1$; there is therefore no meaning to use the pseudo-potential beyond the Born regime.

Consider now the case $r_e \ll |a|$. The term $r_e k^2$ remains small as compared to $1/a$ for $k|a| < 1$. For $k|a| \gg 1$ the term ik dominates over $1/a$; $k^2 r_e$ remains small as compared to ik as long as $kr_e \ll 1$. The use of the pseudo-potential may then extend beyond the Born approximation.

An example of a situation with $r_e \ll |a|$ is the so-called zero energy resonance, where a is diverging. When a bound state of the interaction potential is arbitrarily close to the dissociation limit, the scattering length diverges $a \to +\infty$, the bound state has a large

tail in r scaling as $e^{-r/a}/r$ and the bound state energy scales as $-\hbar^2/ma^2$ [19, 20]. These scaling laws hold for the pseudo-potential, as we have seen.

4 Interacting Bose gas in the Hartree-Fock approximation

Now that we have identified a simple model interaction potential treatable in the Born approximation we use it in the simplest possible mean field approximation, the so-called Hartree-Fock approximation. This approximation was applied to trapped gases for the first time in 1981 (see [21])!

4.1 BBGKY hierarchy

The Hartree-Fock mean field approximation can be implemented in a variety of ways. We have chosen here the approach in terms of the BBGKY hierarchy, truncated to first order.

4.1.1 Few body-density matrices

We have already introduced in §2 the concept of the one-body density matrix. We revisit here this notion and extend it to two-body density matrices.

- *For a fixed total number of particles*

Let us first consider a system with a fixed total number of particles N and let $\sigma_{1,2...N}$ be the N-body density matrix. Starting from $\sigma_{1,2...N}$ we introduce simpler objects as the one-body and two-body density matrices $\hat{\rho}_1$ and $\hat{\rho}_{12}$, by taking the trace over the states of all the particles but one or two:

$$\hat{\rho}_1^{(N)} = N \operatorname{Tr}_{2,3...N}(\sigma_{1,2,...N}) \tag{98}$$

$$\hat{\rho}_{12}^{(N)} = N(N-1) \operatorname{Tr}_{3,4...N}(\sigma_{1,2,...N}). \tag{99}$$

In practice the knowledge of $\hat{\rho}_1$ and $\hat{\rho}_{12}$ is sufficient to describe most of the experimental results. As you know, $\langle \vec{r}|\hat{\rho}_1|\vec{r}\rangle$ is the density of particles and $\langle \vec{r_1}, \vec{r_2}|\hat{\rho}_1|\vec{r_1}, \vec{r_2}\rangle$ is the pair distribution function.

- *For a fluctuating total number of particles*

If N fluctuates according to the probability distribution P_N , we define few-body density matrices by the following averages over N :

$$\hat{\rho}_1 = \sum_N P_N \hat{\rho}_1^{(N)} \tag{100}$$

$$\hat{\rho}_{12} = \sum_N P_N \hat{\rho}_{12}^{(N)} \tag{101}$$

Alternatively on can define directly the one-body and two-body density matrices in second quantization:

$$\langle \vec{r_1} | \hat{\rho}_1 | \vec{r_2} \rangle = \langle \hat{\psi}^\dagger(\vec{r_2}) \hat{\psi}(\vec{r_1}) \rangle \tag{102}$$

$$\langle \vec{r_1}, \vec{r_2} | \hat{\rho}_{12} | \vec{r_3}, \vec{r_4} \rangle = \langle \hat{\psi}^\dagger(\vec{r_3}) \hat{\psi}^\dagger(\vec{r_4}) \hat{\psi}(\vec{r_2}) \hat{\psi}(\vec{r_1}) \rangle. \tag{103}$$

Note that the few-body density matrices are normalized as

$$\mathrm{Tr}[\hat{\rho}_1] = \langle N \rangle \tag{104}$$

$$\mathrm{Tr}[\hat{\rho}_{12}] = \langle N(N-1) \rangle \tag{105}$$

so that one can obtain the variance of the fluctuations in the number of atoms from the one-body and two-body density matrices.

4.1.2 Equations of the hierarchy

The idea of our derivation of the mean field approximation is to get an approximate closed equation for $\hat{\rho}_1$ by closing the hierarchy with some "cooking recipe" giving $\hat{\rho}_{12}$ in terms of $\hat{\rho}_1$.

To derive the first equation of the hierarchy we start from the exact master equation:

$$i\hbar \frac{d}{dt} \sigma_{1,2..N} = [H, \sigma_{1,2..N}] \tag{106}$$

where the Hamiltonian is the sum of one-body and two-body terms:

$$H = \sum_{i=1}^{N} h_i + \frac{1}{2} \sum_{i \neq j; i,j=1}^{N} V_{ij}. \tag{107}$$

The single particle Hamiltonian h_i contains the kinetic and trapping potential energy of the atom i and V_{ij} in the interaction potential between the atoms i and j. Now we take the trace of the master equation over the particles 2,3 ... N and multiply it by N, obtaining

$$i\hbar \frac{d}{dt}\hat{\rho}_1 = [h_1, \hat{\rho}_1] + N\mathrm{Tr}_{2,...N}\left\{\sum_{j=2}^{N}[V_{1j}, \sigma_{1,2....N}]\right\}. \tag{108}$$

We have kept here only the terms involving the atom 1, as the other terms are commutators of vanishing trace. The sum over j amounts to $N-1$ times the same contribution, e.g. the $j = 2$ contribution, as the atoms are indiscernible. We finally obtain the first equation of the hierarchy:

$$i\hbar\frac{d}{dt}\hat{\rho}_1 = [h_1, \hat{\rho}_1] + \mathrm{Tr}_2\{[V_{12}, \hat{\rho}_{12}]\}. \tag{109}$$

The equation Eq.(109) is not closed for $\hat{\rho}_1$, as it involves $\hat{\rho}_{12}$. The next equation of the hierarchy, the equation for $\hat{\rho}_{12}$, involves $\hat{\rho}_{123}$, etc, up to the N-body density matrix, where the hierarchy terminates. The mean field approximation consists in replacing $\hat{\rho}_{12}$ by an ad hoc function of $\hat{\rho}_1$.

4.2 Hartree-Fock approximation for $T > T_c$

4.2.1 Mean field potential for the non-condensed particles

We use the following simple approximation to break the hierarchy:

$$\hat{\rho}_{12} \simeq \hat{\rho}_{12}^{HF} = \left(\frac{1 + P_{12}}{\sqrt{2}}\right)\hat{\rho}_1 \otimes \hat{\rho}_1 \left(\frac{1 + P_{12}}{\sqrt{2}}\right) = (1 + P_{12})\hat{\rho}_1 \otimes \hat{\rho}_1 \tag{110}$$

where P_{12} is the permutation operator exchanging the states of the particles 1 and 2. The last identity in (110) is obtained by using the commutation of P_{12} and $\hat{\rho}_1 \otimes \hat{\rho}_1$, and the fact that $P_{12}^2 = 1$.

The factorized prescription $\hat{\rho}_{12} = \hat{\rho}_1 \otimes \hat{\rho}_1$ is the Hartree approximation. It assumes weak correlations between the particles. Indeed at short distances r_{12}, the real $\hat{\rho}_{12}$ is expected to be a statistical mixture of scattering states of the interaction potential. Neglecting the correlations in $\hat{\rho}_{12}$ between particles 1 and 2 amounts to considering only separable, plane wave scattering states, which corresponds to the zeroth order in the Born expansion of the scattering theory. Actually $\hat{\rho}_{12}$ appears in Eq.(109) inside a commutator with V_{12}, so that taking the zeroth order approximation for the scattering

states in $\hat{\rho}_{12}$ corresponds to the first order of the Born approximation in the equation for $\hat{\rho}_1$.

As we are dealing with bosons we have supplemented the Hartree approximation by a bosonic symmetrization procedure, involving the permutation operator P_{12}. Note that the symmetrization as it was written works only for particles 1 and 2 in orthogonal states:

$$\frac{1 + P_{12}}{\sqrt{2}} |\alpha\rangle |\beta\rangle = \frac{|\alpha\rangle |\beta\rangle + |\beta\rangle |\alpha\rangle}{\sqrt{2}} \tag{111}$$

as the factor $\sqrt{2}$ is the correct normalization factor only in this case. This is almost true for a non-degenerate Bose gas. This restriction forces us to treat separately the case in which a condensate is present ($T < T_c$).

We now insert the Hartree-Fock ansatz for $\hat{\rho}_{12}$ in the hierarchy [3]

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = [h_1, \hat{\rho}_1] + \text{Tr}_2\{[V_{12}, \hat{\rho}_{12}^{HF}]\}. \tag{112}$$

In the commutator with V_{12} we will encounter

$$\delta(\vec{r_1} - \vec{r_2})(1 + P_{12}) = (1 + P_{12})\delta(\vec{r_1} - \vec{r_2}) = 2\delta(\vec{r_1} - \vec{r_2}). \tag{113}$$

The fact that P_{12} commutes with V_{12} is due to the parity of the delta distribution, and P_{12} acting on a state with two particles at the same position can be replaced by the identity. As a consequence, with our zero-range interaction potential, the Fock term simply doubles the Hartree term. We finally obtain

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + \mathcal{V}(\vec{r}), \hat{\rho}_1 \right] \tag{114}$$

where $\mathcal{V}(\vec{r})$ is the mean field potential

$$\mathcal{V}(\vec{r}) = 2g\langle \vec{r} | \hat{\rho}_1 | \vec{r} \rangle = 2g\rho(\vec{r}). \tag{115}$$

The Hartree-Fock Hamiltonian is then

$$h^{HF}(1) = \frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}). \tag{116}$$

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[3]Note that for the present calculation the regularization of the pseudo-potential is not necessary. Indeed by considering plane waves as scattering states in $\hat{\rho}_{12}$ we suppress any problem of divergences in the commutator with V_{12}, and we can then take V_{12} as a simple delta distribution.

The problem is then formally reduced to the one of an ideal Bose gas moving in a self-consistent potential. For $g > 0$ the mean field corresponds to repulsive interactions, as $2g\rho(\vec{r})$ expels the atoms from the region of high density, while for $g < 0$ the mean field corresponds to attractive interactions.

4.2.2 Effect of interactions on T_c

Let us now consider the Hartree-Fock one-body density matrix at thermal equilibrium; we use the same formula as the ideal Bose gas Eq.(29), replacing h_1 by the Hartree-Fock Hamiltonian:

$$\hat{\rho}_1 = \{\exp\left[\beta\left(h^{HF}(1) - \mu\right)\right] - 1\}^{-1}. \tag{117}$$

For $k_B T \gg \Delta E$ where where ΔE is the level spacing of h^{HF} we can perform the semiclassical approximation. We obtain for the spatial density as in Eq.(55):

$$\rho_{sc}(\vec{r}) = \frac{1}{\lambda_{dB}^3} g_{3/2}(\text{z}\exp[-\beta(U(\vec{r}) + 2g\rho_{sc}(\vec{r}))]) \tag{118}$$

At $T = T_c$ the argument of $g_{3/2}$ goes to 1 in the point $\vec{r}_{\min}$ where the potential is minimal, so that Einstein's condition still holds in the Hartree-Fock approximation:

$$\rho_{sc}(\vec{r}_{\min})\lambda_{dB}^3 = \zeta(3/2). \tag{119}$$

For the harmonic trap $U(\vec{r}) = m\omega^2 r^2/2$ the minimum occurs at the center of the trap, $\vec{r}_{\min} = \vec{0}$ so that the chemical potential at the phase transition is given by

$$\mu = 2g\rho_{sc}(\vec{0}). \tag{120}$$

It is shifted by the mean field effect with respect to the ideal Bose gas. Using as a small parameter $\rho_{sc}(\vec{0})g/k_B T_c^0$, one can derive at constant N [22] the first order change in the critical temperature with respect to T_c^0, the transition temperature of the ideal Bose gas:

$$\frac{\delta T_c}{T_c^0} = -2.5\rho_{sc}^{1/3}(\vec{0})a = -1.33\frac{a}{(\hbar/m\omega)^{1/2}}N^{1/6}. \tag{121}$$

For $N = 10^7$ atoms of ^{23}Na in a trap of harmonic frequency $\omega = 2\pi \times 100$ Hz, with a scattering length $a = 50\,a_{\text{Bohr}}$ we find $T_c^0 \simeq 1\mu$ K, and $\delta T_c/T_c^0 \simeq -2.5 \times 10^{-2}$, an effect for the moment smaller than the experimental accuracy. The fact that δT_c is negative

for effective repulsive interactions ($a > 0$) is intuitive: for fixed values of N and T the interacting gas has a lower density at the center of the trap than the ideal Bose gas, so that one needs to further cool the gas to get Bose-Einstein condensation.

- *A calculation of δT_c beyond mean field*

The purest situation to study the effect of the interactions on the critical temperature T_c is the case of atoms trapped in a flat bottom potential; in this case the density is uniform, the previously mentioned intuitive mean field effect is suppressed, and our Hartree-Fock theory predicts the same critical temperature as the ideal Bose gas. This prediction is actually not correct, and rigorous results for the first order correction of T_c in $a\rho^{1/3}$ have been obtained recently, by a combination of perturbative theory and Quantum Monte Carlo calculations [23]:

$$\frac{\delta T_c^{\text{box}}}{T_c^0} = (2.2 \pm 0.25)a\rho^{1/3} + o(a\rho^{1/3}). \tag{122}$$

Recent calculations in the many body Green's function formalism confirm this result [24]. This effect, if heuristically extended to the trap, is of opposite sign and of the same order of magnitude as the mean-field prediction.

4.3 Hartree-Fock approximation in presence of a condensate

4.3.1 Improved Hartree-Fock Ansatz

As already emphasized in the previous subsection the symmetrization procedure of the Hartree-Fock prescription Eq.(110) has to be modified in presence of a condensate. To this end we split the one-body density matrix as

$$\hat{\rho}_1 = \langle N_0 \rangle |\phi\rangle\langle\phi| + \hat{\rho}_1' \tag{123}$$

where ϕ is the condensate wavefunction, $\langle N_0 \rangle$ is the mean number of particles in the condensate and $\hat{\rho}_1'$ is the one-body density matrix of the non-condensed fraction. The Hartree approximation for the two-body density matrix now reads:

$$\hat{\rho}_1 \otimes \hat{\rho}_1 = \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi| + \text{remaining Hartree part.} \tag{124}$$

The first term in the right hand size is already symmetrized; the second term can be symmetrized as in Eq.(110) as it does not involve coexistence of two atoms in the (only) macroscopically populated state ϕ. We therefore put forward the following Hartree-Fock ansatz:

$$\hat{\rho}_{12}^{HF} = \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi| + \left(\frac{1 + P_{12}}{\sqrt{2}}\right) \text{remaining Hartree part} \left(\frac{1 + P_{12}}{\sqrt{2}}\right). \quad (125)$$

Eliminating the remaining Hartree part with the help of Eq.(124), we finally obtain

$$\hat{\rho}_{12}^{HF} = \left(\frac{1 + P_{12}}{\sqrt{2}}\right) \hat{\rho}_1 \otimes \hat{\rho}_1 \left(\frac{1 + P_{12}}{\sqrt{2}}\right) - \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi|. \quad (126)$$

In this way we have avoided the double counting of the condensate contribution that would have resulted from the prescription Eq.(110).

4.3.2   Mean field seen by the condensate

We replace $\hat{\rho}_{12}$ in the first equation of the hierarchy by the improved Hartree-Fock ansatz. The first bit of the ansatz gives the same result as in the case $T > T_c$, the second bit involves the term:

$$\text{Tr}_2 \left([\delta(\vec{r_1} - \vec{r_2}), |\phi, \phi\rangle\langle\phi, \phi|]\right) = [|\phi(\vec{r_1})|^2, |\phi\rangle\langle\phi|]. \quad (127)$$

Splitting $\hat{\rho}_1$ as condensate and non-condensed contribution we arrive at

$$i\hbar\frac{d}{dt}\hat{\rho}_1 = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}) - \langle N_0 \rangle g|\phi(\vec{r})|^2, \langle N_0 \rangle|\phi\rangle\langle\phi|\right] \quad (128)$$

$$+ \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}), \hat{\rho}_1'\right]. \quad (129)$$

The non-condensed particles still move in the mean field potential $2g\rho(\vec{r})$. On the contrary the atoms in the condensate see a different mean field potential:

$$2g\rho(\vec{r}) - g\langle N_0 \rangle|\phi(\vec{r})|^2 = 2g\rho'(\vec{r}) + g\langle N_0 \rangle|\phi(\vec{r})|^2 \quad (130)$$

where ρ' is the non-condensed density and $\langle N_0 \rangle|\phi|^2$ is the condensate density. [4] This result can be interpreted as follows: An atom in the condensate interacts with non-

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[4]A careful reader may argue that we forget here the condition of orthogonality of the eigenstates of $\hat{\rho}_1'$ to ϕ. Inclusion of this condition is beyond accuracy of the Hartree-Fock approximation. It will be carefully included in the more precise number conserving Bogoliubov approach of §7.

condensed particles with the effective coupling constant $2g$, and it interacts with another particle of the condensate with the effective coupling constant g.

For repulsive effective interactions ($g > 0$) this is at the basis of Nozières'argument against fragmentation of the condensate in several orthogonal states: in a box of size L in the thermodynamical limit, transferring a finite fraction of condensate particles from the plane wave $\vec{p} = \vec{0}$ to an excited plane wave $p = O(\hbar/L)$ costs a negligible amount of kinetic energy per particle but a finite amount of interaction energy. The transferred fraction would indeed be repelled with a stronger amplitude ($2g$ rather than g) by the atoms remaining in the condensate.

4.3.3 At thermal equilibrium

At thermal equilibrium the one-body density matrix of non-condensed atoms is given by the usual Bose distribution for the ideal Bose gas, with the trapping potential being supplemented by the mean-field potential:

$$\hat{\rho}_1' = \frac{1}{\exp\left\{\beta\left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}) - \mu\right]\right\} - 1} \tag{131}$$

The condensate wave function has to be a steady state of the total, mean field plus trapping potential seen by an atom in the condensate:

$$\lambda\phi(\vec{r}) = -\frac{\hbar^2}{2m}\Delta\phi + [U(\vec{r}) + g\langle N_0\rangle|\phi(\vec{r})|^2 + 2g\rho'(\vec{r})]\phi(\vec{r}). \tag{132}$$

The Hartree-Fock single particle energy λ should not be confused with the energy per particle in the condensate, as it will become clear in the next section. The occupation number of the condensate is related to λ by the Bose formula:

$$\langle N_0\rangle = \frac{1}{e^{\beta(\lambda-\mu)} - 1}. \tag{133}$$

We now have to solve in a self consistent way the three equations Eq.(131,132, 133). In practice, when $\langle N_0\rangle$ is already large, one can assume $\lambda = \mu$, which eliminates one unknown λ and one equation Eq.(133).

4.4   Comparison of Hartree-Fock to exact results

4.4.1   Quantum Monte Carlo calculations

The Quantum Monte Carlo method developed by David Ceperley and others allows to sample in an exact way the N-body distribution function of a gas of N interacting bosons at thermal equilibrium. I.e. the algorithm generates random positions $\vec{r_1}, ..., \vec{r_N}$ for the N particles with a probability distribution given by the exact N-body distribution function of the atoms.

On the figure 8 the Hartree-Fock prediction for the radial density of particles in a spherical harmonic trap, $r^2\rho(r)$, is compared to the Quantum Monte Carlo result for several temperatures below T_c. The Hartree-Fock prediction is in good agreement with the exact result, except close to T_c where it tends to underestimate the number of particles in the condensate [25].
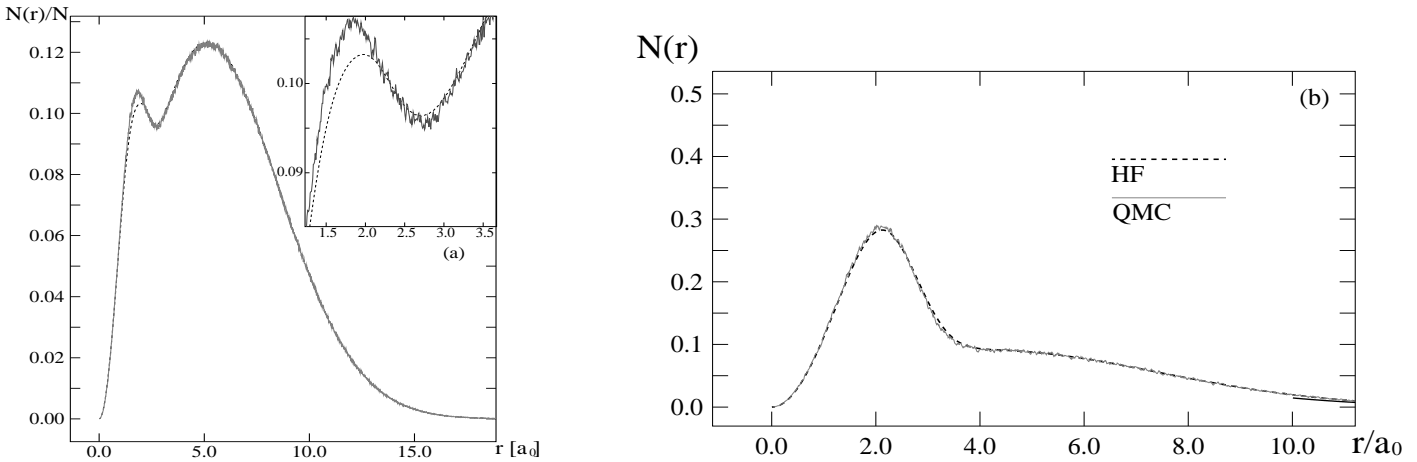
Figure 8: Radial density of particles, $r^2\rho(r)$, for an interacting Bose gas at thermal equilibrium in an isotropic harmonic trap. Noisy lines: results of a Quantum Monte Carlo simulation. Smooth solid lines: Hartree-Fock prediction. The curves corresponds to the temperatures $T/T_c^0 = 0.88$ (a), $T/T_c^0 = 0.7$ (b). The number of particles is $N = 10^4$ and the parameters are the ones of ^{87}Rb. These figures are taken from [25].

4.4.2 Experimental results for the energy of the gas

At JILA the sum of kinetic and interaction energy of the atoms was measured as function of temperature, as we have already explained in §2.3. Whereas the ideal Bose gas model was clearly getting wrong for $T < T_c$, the Hartree-Fock prediction [26] is consistent with the experimental results over the whole considered temperature range (see figure 9).
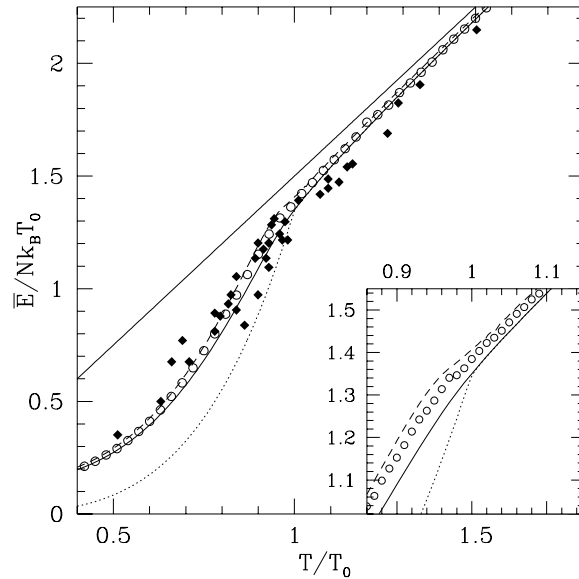
Figure 9: Expansion energy of the gas per particle and in units of $k_B T_c^0$ as function of the temperature in units of T_c^0 . The filled rhombi correspond to the experimental results of [11]. The straight solid line is the prediction of Boltzmann statistics. The dotted curve is the ideal Bose gas prediction. The circles are the numerical solution to the Hartree-Fock approach. The curved solid line and the dashed line are approximate solutions to the Hartree-Fock equations. The inset is a magnification showing the change of slope of the energy as function of T close to $T = T_c^0$. The figure is taken from [26].

At very low temperatures ($T < T_c/2$), measurements at MIT have shown that the same energy becomes mainly a function of the number of particles N_0 in the condensate. By setting $\rho' = 0$ in the Hartree-Fock approximation, and using approximations presented in the coming section §5.3, an analytical expression can be obtained for the energy, in excellent agreement with the experimental results (see figure 5): the energy per particle has a power law dependence with N_0 , with an exponent $2/5$, to be contrasted with the

constant ideal Bose gas result, and has typical values an order of magnitude larger than the zero-point energy of the harmonic oscillator.

5 Properties of the condensate wavefunction

In this section we consider the regime of an almost pure condensate, where the non-condensed cloud has a negligible effect on the condensate. At thermal equilibrium with temperature T this regime corresponds to the limit $T \ll T_c$. As we shall see most of the experimental results obtained with almost pure condensates can be well reproduced by a single equation for the condensate wavefunction, the so-called Gross-Pitaevskii equation, derived independently by Gross [27] and Pitaevskii [28].

5.1 The Gross-Pitaevskii equation

5.1.1 From Hartree-Fock

Let us assume that the density of non-condensed particles is much smaller than the density of condensate particles over the spatial width of the condensate:

$$\rho'(\vec{r}) \ll N_0 |\phi(\vec{r})|^2 \tag{134}$$

where N_0 is the mean number of particles in the condensate, ϕ is the condensate wavefunction normalized to unity:

$$\int d^3 \vec{r} \, \phi(\vec{r}, t) \phi^*(\vec{r}, t) = 1. \tag{135}$$

In the Hartree-Fock expression of the mean field potential seen by the condensate, derived in the previous section §4, we can drop the contribution of the non-condensed particles, to get for the evolution of the condensate contribution to the 1-body density matrix:

$$i\hbar \frac{d}{dt}(N_0 |\phi\rangle\langle\phi|) = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}, t) + g N_0 |\phi(\vec{r}, t)|^2, N_0 |\phi\rangle\langle\phi| \right]. \tag{136}$$

This equation leads to $N_0 = $ constant and to the evolution equation for the condensate wavefunction:

$$i\hbar \partial_t \phi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m}\Delta + U(\vec{r}, t) + N_0 g |\phi(\vec{r}, t)|^2 - \xi(t) \right] \phi(\vec{r}, t). \tag{137}$$

This non-linear Schrödinger equation is the so-called time dependent Gross-Pitaevskii equation. This equation is determined from our Hartree-Fock approach up to an arbitrary real function of time, $\xi(t)$, as Eq.(136) involves a commutator to which $\xi(t)$ does not contribute. In general the precise value of $\xi(t)$ is considered as a matter of convenience, as it can be absorbed in a redefinition of the global phase of ϕ. The knowledge of the value of $\xi(t)$ can become important when one is interested in the evolution of the relative phase of *two* Bose-Einstein condensates. The value of $\xi(t)$ has been derived in [29] assuming a well defined number of particles in the condensate. If the condensate is assumed to be in a Glauber coherent state that is a quasi-classical state of the atomic field with a well defined relative phase (see §8) one obtains $\xi(t) = 0$ as we will see in §5.1.3.

When the gas is at thermal equilibrium, the only time dependence left for ϕ is a global phase dependence. The most convenient choice is to assume $\partial_t \phi = 0$ so that $\xi(t)$ is a constant. As shown in §4.3.3 this constant is very close to the chemical potential of the gas as N_0 is large so that we get the so-called time independent Gross-Pitaevskii equation:

$$\mu\phi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\Delta + U(\vec{r}) + N_0 g|\phi(\vec{r})|^2 \right] \phi(\vec{r}). \tag{138}$$

Both the time independent and the time dependent Gross-Pitaevskii equations can be solved numerically. But, as explained in the next part of this section, the fact that the trap is harmonic allows one to find very good approximate analytical solutions.

5.1.2   Variational formulation

Variational calculus turns out to be a very fruitful approximate technique in the solution of the Gross-Pitaevskii equation. We therefore derive here a variational formulation of the Gross-Pitaevskii equation.

- *Time independent case*

The time independent Gross-Pitaevskii equation can be obtained from extremalization over ϕ of the so-called Gross-Pitaevskii energy functional:

$$E[\phi, \phi^*] = N_0 \int d^3\vec{r} \left[\frac{\hbar^2}{2m}|\vec{\text{grad}}\,\phi|^2 + U(\vec{r})|\phi(\vec{r})|^2 + \frac{1}{2}N_0 g|\phi(\vec{r})|^4 \right] \tag{139}$$

with the constraint that ϕ is normalized to unity.

Proof: We take into account the normalization constraint with the method of Lagrange multiplier, so that we simply have to express the fact that ϕ extremalizes without constraint the functional:

$$X[\phi, \phi^*] = E[\phi, \phi^*] - \lambda N_0 \int d^3\vec{r}\, \phi(\vec{r})\phi^*(\vec{r}). \tag{140}$$

The parameter λ is the Lagrange multiplier. We calculate the first order variation of X due to an infinitesimal arbitrary variation of the condensate wavefunction:

$$\phi(\vec{r}) \to \phi(\vec{r}) + \delta\phi(\vec{r}). \tag{141}$$

We obtain:

$$\delta X = N_0 \int d^3\vec{r}\, \left[\frac{\hbar^2}{2m}\vec{\mathrm{grad}}\,\delta\phi^* \cdot \vec{\mathrm{grad}}\,\phi + U(\vec{r})\delta\phi^*\phi + N_0 g\delta\phi^*\phi^*\phi^2 - \lambda\delta\phi^*\phi \right] + \text{c.c.} \tag{142}$$

We modify the variation of the kinetic energy term by integrating by part, assuming that ϕ vanishes at infinity:

$$\int d^3\vec{r}\, (\vec{\mathrm{grad}}\,\delta\phi^* \cdot \vec{\mathrm{grad}}\,\phi + \text{c.c.}) = -\int d^3\vec{r}\, (\delta\phi^*\Delta\phi + \text{c.c.}). \tag{143}$$

The variation δX has to vanish for any $\delta\phi$. We can take as independent variables the real part and the imaginary part of $\delta\phi$, or equivalently $\delta\phi$ and $\delta\phi^*$ as it amounts to considering independent linear superpositions of the real and imaginary part. We therefore obtain:

$$N_0 \left[-\frac{\hbar^2}{2m}\Delta + U(\vec{r}) + N_0 g|\phi(\vec{r})|^2 - \lambda \right] \phi(\vec{r}) = 0. \tag{144}$$

We recover the time independent Gross-Pitaevskii equation, with $\lambda = \mu$, which gives a physical interpretation to the Lagrange multiplier λ.

- *Time dependent case*

The time dependent Gross-Pitaevskii equation with the choice $\xi(t) \equiv 0$ is obtained over a time interval $[t_1, t_2]$ from extremalization of the action:

$$A = \int_{t_1}^{t_2} dt\, \left[\frac{i\hbar}{2}\left(\langle\phi|\frac{d}{dt}|\phi\rangle - \text{c.c.} \right) N_0 - E[\phi(t), \phi^*(t)] \right] \tag{145}$$

with fixed values of $|\phi(t = t_1)\rangle$ and $|\phi(t = t_2)\rangle$.

- *Physical interpretation of the Gross-Pitaevskii energy functional*

We now show that $E[\phi, \phi^*]$ is simply the mean energy of the gas in the Hartree-Fock approximation in the limit of a pure condensate. As the N-body Hamiltonian is a sum of one-body and two-body (binary interaction) terms,

$$H = \sum_{i=1}^{N} h_i + \frac{1}{2} \sum_{i \neq j} V_{ij} \tag{146}$$

the mean energy of the gas involves the one-body and two-body density matrices:

$$\langle H \rangle = \text{Tr}[h_1 \hat{\rho}_1] + \frac{1}{2} \text{Tr}[V_{12} \hat{\rho}_{12}]. \tag{147}$$

In the limit of a pure condensate we keep only the condensate contribution to $\hat{\rho}_1$:

$$\hat{\rho}_1 \simeq N_0 |\phi\rangle\langle\phi| \tag{148}$$

and we approximate $\hat{\rho}_{12}$ by the Hartree ansatz

$$\hat{\rho}_{12} \simeq \hat{\rho}_1 \otimes \hat{\rho}_1. \tag{149}$$

We then obtain $E[\phi, \phi^*] = \langle H \rangle$. It was actually clear from the start that $E[\phi, \phi^*]$ was the sum of kinetic energy, trapping potential energy and mean field interaction energy of the condensate.

A different and interesting point of view at zero temperature is to use directly a Hartree-Fock ansatz for the ground state wavefunction $|\Psi\rangle$ of the gas, assuming that all the particles are in the condensate:

$$|\Psi\rangle = |N : \phi\rangle = |\phi\rangle \otimes \ldots \otimes |\phi\rangle. \tag{150}$$

The mean energy of $|\Psi\rangle$ for the interaction potential $g\delta(\vec{r}_1 - \vec{r}_2)$ is then

$$E[\phi, \phi^*] = N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\text{grad}}\, \phi|^2 + U(\vec{r})|\phi(\vec{r})|^2 + \frac{1}{2}(N-1)g|\phi(\vec{r})|^4 \right], \tag{151}$$

which differs from Eq.(139) in the limit $N_0 = N$ only by the occurrence of a factor $(N-1)$ rather than N in front of the coupling constant g, ensuring that the interaction term disappears for $N = 1$!

• *What is the chemical potential ?*

At zero temperature, assuming a pure condensate $N_0 \simeq N$, the usual thermodynamical definition of the chemical potential μ reduces to:

$$\mu = \frac{d\langle H \rangle}{dN} \simeq \frac{d}{dN_0} E[\phi, \phi^*, N_0] \tag{152}$$

where we have made appear the explicit dependence of E on N_0. When one takes the total derivative of E with respect to N_0, one gets in principle a contribution from the implicit dependence of E on N_0 through the N_0 dependence of ϕ, ϕ^*; actually this contribution vanishes as the variation of E due to a change in ϕ, ϕ^* vanishes to first order in this change. We therefore get

$$
\begin{aligned}
\frac{d}{dN_0} E[\phi, \phi^*, N_0] &= \frac{\partial}{\partial N_0} E[\phi, \phi^*, N_0] \\
&= \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\mathrm{grad}}\, \phi|^2 + U(\vec{r})|\phi(\vec{r})|^2 + N_0 g |\phi(\vec{r})|^4 \right].
\end{aligned}
\tag{153}
$$

This quantity coincides with the chemical potential indeed, as can be checked by multiplying the time independent Gross-Pitaevskii equation by ϕ^* and integrating over the whole space. As g does not have the factor $1/2$ in Eq.(153), whereas it is multiplied by $1/2$ in the expression for $E[\phi, \phi^*]$, we see that in the interacting case $g \neq 0$:

$$\mu \neq \frac{E}{N_0} \tag{154}$$

that is the chemical potential μ differs from the mean energy per particle.

5.1.3   The fastest trick to recover the Gross-Pitaevskii equation

Starting from the second quantized form of the Hamiltonian,

$$H = \int d1\, \hat{\psi}^\dagger(1) h_1 \hat{\psi}(1) + \frac{1}{2} \int d1 \int d2\, \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2) V_{12} \hat{\psi}(2)\hat{\psi}(1) \tag{155}$$

where 1 and 2 stand for three-dimensional coordinates in real space, one first derives the Heisenberg equation of motion for the field operator:

$$
\begin{aligned}
i\hbar \frac{d}{dt}\hat{\psi}(1) &= [\hat{\psi}(1), H] = \partial_{\hat{\psi}^\dagger(1)} H \tag{156} \\
&= h_1 \hat{\psi}(1) + \int d2\, \hat{\psi}^\dagger(2) V_{12}\hat{\psi}(2)\hat{\psi}(1) \tag{157}
\end{aligned}
$$

and then replaces the quantum field operator by a classical field:

$$\hat{\psi} \rightarrow \psi = \sqrt{N_0}\phi. \tag{158}$$

As V_{12} is the pseudo-potential, the equation that we get for ϕ is the time dependent Gross-Pitaevskii equation with $\xi(t) \equiv 0$.

This sheds a new light on the Gross-Pitaevskii equation: the Gross-Pitaevskii equation is the equation of motion of the atomic field in the classical approximation, neglecting quantum fluctuations of the field. A Bose-Einstein condensate is a classical state of the atomic field, in a way similar to the laser being a classical state of the electromagnetic field.

5.2 Gaussian Ansatz

In this subsection we look for a variational solution to the Gross-Pitaevskii equation in a harmonic trap, using a Gaussian ansatz for ϕ [30]. The choice of a Gaussian is natural in the non-interacting limit $g \rightarrow 0$, where it becomes exact. It turns out to give also interesting results in presence of strong interactions.

5.2.1 Time independent case

Consider for simplicity an isotropic harmonic trap, where the atoms have the oscillation frequency ω. We assume the following Gaussian for the condensate wavefunction:

$$\phi(\vec{r}) = \frac{1}{\pi^{3/4}\sigma^{3/2}}e^{-r^2/2\sigma^2} \tag{159}$$

the spatial width σ being the only variational parameter. The mean energy per particle can be calculated exactly for this ansatz:

$$\varepsilon \equiv \frac{E[\phi, \phi^*]}{N_0} = \frac{3\hbar^2}{4m\sigma^2} + \frac{3}{4}m\omega^2\sigma^2 + \frac{\hbar^2}{m}\frac{N_0 a}{\sigma^3}\frac{1}{\sqrt{2\pi}}. \tag{160}$$

The form of the result is intuitive: the kinetic energy term scales as Δp_x^2, where $\Delta p_x = \hbar/(2\Delta x) = \hbar/(\sqrt{2}\sigma)$; the trapping potential energy scales as σ^2 and the interaction energy per particle is proportional to the coupling constant $g = 4\pi\hbar^2 a/m$ and to the typical density of atoms in the gas, N_0/σ^3. Taking the harmonic oscillator length $(\hbar/m\omega)^{1/2}$

as a unit of length and the harmonic quantum of vibration $\hbar\omega$ as a unit of energy we get the simple form:

$$\varepsilon = \frac{3}{4}\left[\frac{1}{\sigma^2} + \sigma^2\right] + \frac{\chi}{2\sigma^3} \tag{161}$$

where the only physical parameter left is

$$\chi = \sqrt{\frac{2}{\pi}}\frac{N_0 a}{\sqrt{\hbar/m\omega}}. \tag{162}$$

This parameter χ measures the effect of the interactions on the condensate density: The case $\chi \ll 1$ corresponds to the weakly interacting regime, close to the ideal Bose gas limit $\chi = 0$; the case $\chi \gg 1$ corresponds to the strongly interacting regime.

- case $a > 0$

In the case of effective repulsive interactions between the particles, the dependence of ε with σ is plotted in figure 10. In the limit $\sigma \to 0$, the energy ϵ is dominated by the positively diverging repulsive interaction ($\sim 1/\sigma^3$). For large σ the trapping potential term $\sim \sigma^2$ dominates. The function ε has a single minimum, in $\sigma = \sigma_0$, solving

$$\frac{d\varepsilon}{d\sigma}(\sigma_0) = 0 \to \sigma_0^5 = \sigma_0 + \chi. \tag{163}$$

For $\chi \ll 1$ one recovers the ground state of the harmonic trap, with $\sigma_0 = 1$. For $\chi \gg 1$ the condensate cloud becomes much broader than the ground state of the harmonic trap,

$$\sigma_0 \simeq \chi^{1/5} \propto N_0^{1/5}. \tag{164}$$

In this regime one can check that the kinetic energy term becomes negligible as compared to the trapping energy:

$$\frac{E_{\text{kin}}}{E_{\text{trap}}} = \frac{1}{\sigma^4} \simeq \frac{1}{\chi^{4/5}} \tag{165}$$

so that the steady state of the condensate is an equilibrium between the trapping potential and the repulsive interactions between particles. This regime will be studied in detail in the next subsection.

- case $a < 0$
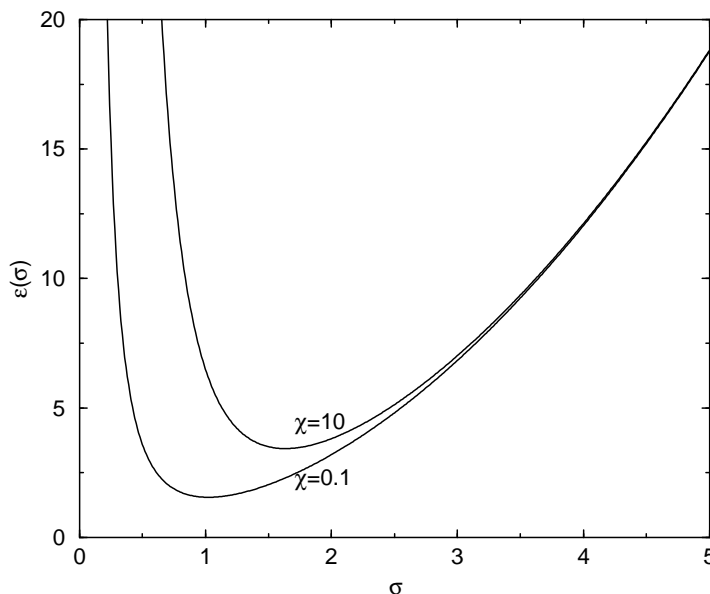
Figure 10: Energy per particle in the condensate in units of $\hbar\omega$ as function of the variational width σ in units of $(\hbar/m\omega)^{1/2}$. Case of effective repulsive interactions $a > 0$.

For effective attractive interactions between the particles the shape of ε as function of σ depends on the balance between kinetic and interaction energy (see figure 11). The interaction energy is negatively diverging as $\sigma \to 0$ always faster than the positively diverging kinetic energy so that $\sigma = 0$ is always a minimum of ε, with $\varepsilon = -\infty$: the condensate is in a spatially collapsed state ! Of course the Gross-Pitaevskii equation not longer applies for a too small σ, as the validity of the Born approximation requires $k|a| \simeq |a|/\sigma \ll 1$. For $|\chi|$ larger than some critical value $|\chi_c|$, this collapsed minimum is the only one of $\varepsilon(\sigma)$ so that we do not find any stable solution for the condensate wavefunction. When $|\chi|$ is smaller than $|\chi_c|$ the kinetic energy term, which is opposed to spatial compression of the gas, is able to beat the attractive energy over some range of σ, so that a local minimum of $\varepsilon(\sigma)$ appears, in $\sigma = \sigma_0$, separated from the collapsed minimum by a barrier.

To calculate $|\chi_c|$ we express the fact that the stationary point of ε in $\sigma = \sigma_0$ has now a vanishing curvature (inflexion point of ε):

$$\left(\frac{d\varepsilon}{d\sigma}\right)^{\chi=\chi_c}_{\sigma=\sigma_0} = 0 \tag{166}$$
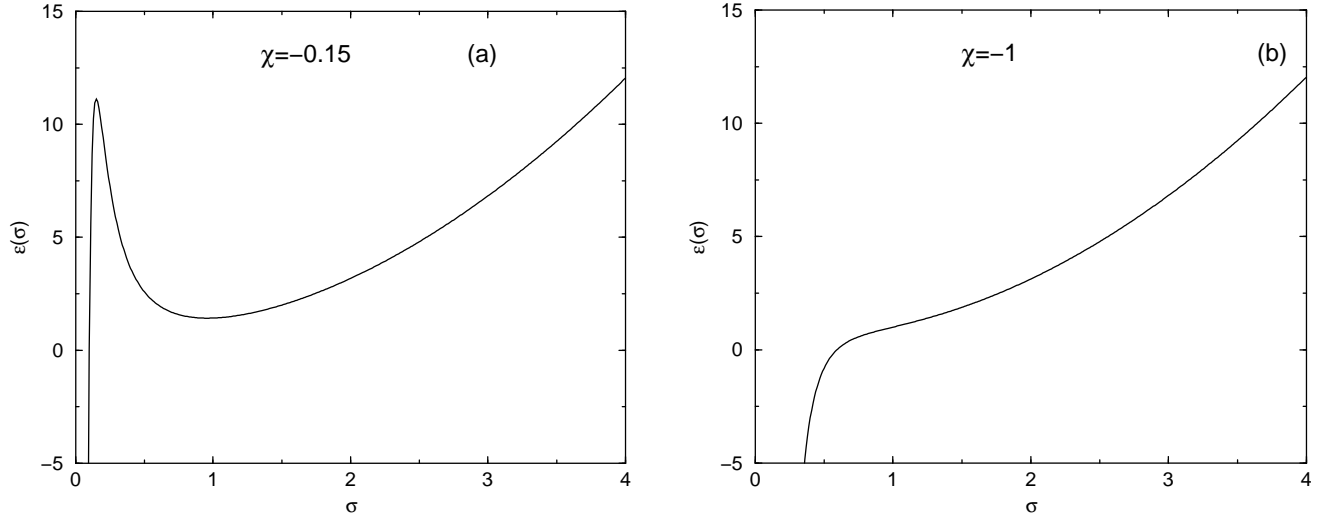
Figure 11: For an effective attractive interaction $a < 0$ between the particles energy per particle in the condensate in units of $\hbar\omega$ as function of the variational width σ in units of $(\hbar/m\omega)^{1/2}$. The curve has two possible shapes, (a) with two minima when $|\chi|$ is smaller than a critical value $|\chi_c|$, and (b) with a single minimum for $|\chi| > |\chi_c|$.

$$\left(\frac{d^2\varepsilon}{d\sigma^2}\right)^{\chi=\chi_c}_{\sigma=\sigma_0} = 0 \tag{167}$$

By eliminating σ_0 between these two equations we obtain

$$\chi_c = -\frac{4}{5^{5/4}} = -0.5350... \tag{168}$$

This result can be rephrased in terms of a maximal number of atoms N_0^c that can be put in the condensate without inducing a collapse, according to a Gaussian ansatz:

$$\frac{N_0^c |a|}{\sqrt{\hbar/m\omega}} = \left(\frac{\pi}{2}\right)^{1/2} |\chi_c| \simeq -0.67. \tag{169}$$

A more precise result has been obtained by a numerical solution of Gross-Pitaevskii equation, not restricting to the subspace of Gaussian wavefunctions [31]: no solution of the time independent Gross-Pitaevskii equation is obtained for $N_0 > N_0^c$, where

$$\frac{N_0^c |a|}{\sqrt{\hbar/m\omega}} \simeq -0.57. \tag{170}$$

By a generalization of the Gaussian ansatz to the case of a non-isotropic harmonic trap one can also get a prediction of N_0^c for the parameters of the lithium experiment of Hulet's group [32]. In the experiment the traps frequencies are $\omega_z = 2\pi \times 117$ Hz and $\omega_{x,y} = 2\pi \times 163$ Hz, and the scattering length is $a = -27$ Bohr radii. The Gaussian prediction is then $N_0^c \simeq 1500$, consistent with the experimental results.

- *Physical origin of the stabilization for $a < 0$*

In a harmonic trap, the energy of the ground state level is separated from the energy of excited states by $\hbar\omega$. At low values of χ the mean interaction energy per particle, $\sim \rho|g|$, where ρ is the density, is much smaller than $\hbar\omega$ so that it cannot efficiently induce a transition from the ground harmonic level to excited harmonic levels. Initiation of collapse on the contrary requires that the wavefunction ϕ expands on many excited levels in the trap, so that the density $|\phi|^2$ can exhibit a high density peak narrower than $\sqrt{\hbar/m\omega}$. We therefore intuitively reformulate the non-collapse condition as

$$\rho|g| < \hbar\omega. \tag{171}$$

Estimating ρ as $N_0/(\hbar/m\omega)^{3/2}$ we recover a N_0^c scaling as $\sqrt{\hbar/m\omega}/|a|$. This reasoning also applies to the gas confined in a cubic box with periodic boundary conditions, as we shall see in section §6 of the lecture.

5.2.2 Time dependent case

As done in [33, 34] the Gaussian ansatz can be generalized to the time dependent case. We assume here for simplicity that the condensate, initially in steady state, is excited only by a temporal variation of the trap frequencies $\omega_\alpha(t)$; then no oscillation of the center of mass motion of the condensate takes place, ϕ remaining of vanishing mean position and momentum. The Gaussian ansatz then contains only exponential of terms quadratic with position, its does not involve exponential of terms linear with position:

$$\phi(\vec{r}, t) = \frac{e^{i\delta(t)}}{\pi^{3/4} \left[\prod_\alpha \sigma_\alpha(t)\right]^{1/2}} \exp\left[-\sum_\alpha \frac{r_\alpha^2}{2\sigma_\alpha^2(t)} + i\sum_\alpha r_\alpha^2 \gamma_\alpha(t) \right]. \tag{172}$$

We do not assume that the trap is isotropic, so we have as variational parameters 3 spatial widths σ_α ($\alpha = x, y, z$), 3 factors γ_α governing the spatially quadratic phase and a global phase δ.

One gets time evolution equations for the variational parameters by inserting the ansatz for ϕ in the action A of Eq.(145) and by writing the Lagrange equations expressing the stationarity condition. It turns out that γ_α can be expressed in terms of the widths and their time derivatives:

$$\gamma_\alpha = -\frac{m\dot{\sigma}_\alpha}{2\hbar\sigma_\alpha} \tag{173}$$

so that one is left with equations for the σ_α's. Taking ω^{-1} as a unit of time, $\sqrt{\hbar/m\omega}$ as a unit of length, where ω is an arbitrary reference frequency, we get:

$$\ddot{\sigma}_\alpha + \nu_\alpha^2\sigma_\alpha = \frac{1}{\sigma_\alpha^3} + \frac{\chi}{\sigma_\alpha\sigma_x\sigma_y\sigma_z} \tag{174}$$

where the trap frequencies are $\omega_\alpha = \nu_a\omega$ and χ is defined in Eq.(162). In the absence of interaction ($\chi = 0$) these evolution equations become exact, and give a remarkable (and known !) result for the time dependent harmonic oscillator. In the interacting case ($\chi \neq 0$) these equations can be cast in Hamiltonian form as the "force" seen by the variable σ_α derives from a potential. The corresponding dynamics is non linear and non trivial; chaotic behavior has been obtained in [35] in the limiting regime of $\chi \gg 1$ where the $1/\sigma_\alpha^3$ can be neglected.

One can use Eq.(174) to study the response of the condensate to a weak excitation, the trap frequency ω_α in the experiments being typically slightly perturbed from its steady state value $\omega_\alpha(0)$ for a finite excitation time. Linearizing the evolution equations in terms of the deviations of the σ's from their steady state value:

$$\sigma_\alpha(t) = \sigma_\alpha^{\text{st}} + \delta\sigma_\alpha(t) \tag{175}$$

one gets a three by three system of second order differential equations for the $\delta\sigma$'s. Looking for eigenmodes of this system, one finds three eigenfrequencies [34]. Their values have been compared to experimental results at JILA [36], see Fig.12: the agreement is very good, not only in the weakly interacting regime $\chi \ll 1$ but also in the regime $\chi \gg 1$, where the Gaussian ansatz for the condensate wavefunction has no reason to be a good one! The explanation of this mystery is given in §5.4.1.

5.3   Strongly interacting regime: Thomas-Fermi approximation

In this subsection we focus on the strongly interacting regime: the scattering length is positive, with the dimensionless parameter χ of Eq.(162) much larger than one. This
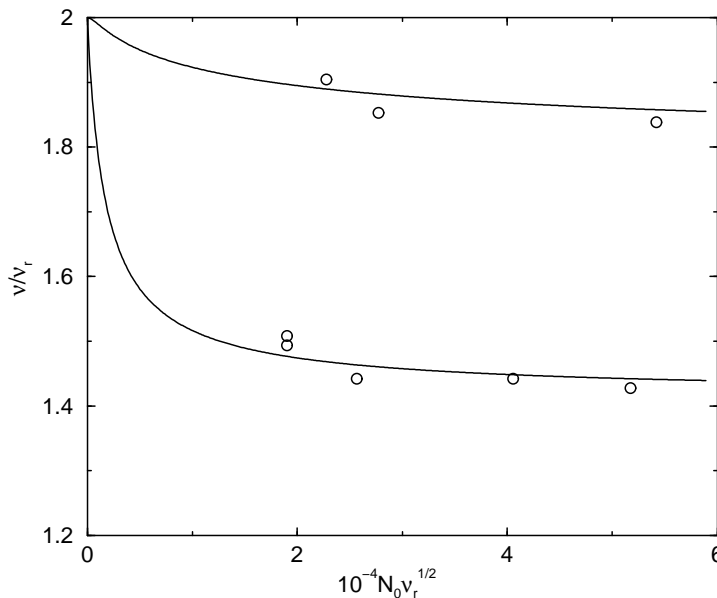
Figure 12: Frequencies of two eigenmodes of a condensate in a cylindrically symmetric harmonic trap, in units of the radial trap frequency ν_r, as a function of a parameter proportional to χ measuring the strength of the interactions. Plotting symbols: measurements at JILA [36]. Solid lines : predictions of the Gaussian Ansatz [34].

regime is the so-called Thomas-Fermi regime. As we now see analytical results can be obtained in this limit.

5.3.1   Time independent case

If we put a large enough number of particles into the condensate the atoms will experience repulsive interactions that will increase the spatial radius of the condensate to a value R much larger than the one of the ground state of the harmonic trap:

$$R \gg \left(\frac{\hbar}{m\omega} \right)^{1/2} . \tag{176}$$

For increasing value of N_0, R increases so that the momentum width of the condensate, scaling as $\hbar/R$ as ϕ_0 is a non-oscillating function of the position, is getting smaller and smaller. More precisely we find that the typical kinetic energy of the condensate becomes

much smaller than the typical harmonic potential energy of the condensate:

$$\frac{E_{\text{kin}}}{E_{\text{harm}}} \simeq \frac{\frac{\hbar^2}{mR^2}}{m\omega^2 R^2} \simeq \left(\frac{\hbar}{m\omega R^2}\right)^2 \ll 1. \tag{177}$$

The mechanical equilibrium of the condensate in the trap then comes mainly from the balance between the expelling effect of the repulsive interactions and the confining effect of the trap.

In this large R regime we neglect the kinetic energy term in the Gross-Pitaevskii energy functional, which leads to a functional of the condensate density only (similarly to the Thomas-Fermi approximation for electrons). This approximation amounts to neglecting the $\Delta\phi$ term in the Gross-Pitaevskii equation:

$$\mu\phi(\vec{r}) \simeq U(\vec{r})\phi(\vec{r}) + N_0 g|\phi(\vec{r})|^2\phi(\vec{r}). \tag{178}$$

Taking ϕ to be real we find that

$$\phi(\vec{r}) = \left(\frac{\mu - U(\vec{r})}{N_0 g}\right)^{1/2} \tag{179}$$

in the points of space where $\mu > U(\vec{r})$, otherwise we have $\phi(\vec{r}) = 0$.

This very important, Thomas-Fermi result Eq.(179) can also be obtained in a local density approximation point of view. A spatially uniform condensate with a chemical potential μ and in presence of a uniform external potential U has a density $N_0|\phi|^2 = (\mu - U)/g$. Applying this formula with a $\vec{r}$ dependent potential U gives again Eq.(179). A local density approximation can be used only if the density of the condensate varies slowly at the scale of the so-called "healing length" ξ, introduced in §5.3.4; one can check that the condition $\xi \ll R$ is indeed satisfied in the Thomas-Fermi regime.

We specialize Eq.(179) to the case of a harmonic but not necessarily isotropic trap:

$$U(\vec{r}) = \frac{1}{2}m\sum_\alpha \omega_\alpha^2 r_\alpha^2 \tag{180}$$

where $\alpha = x, y, z$ label the eigenaxis of the trap. The boundary of the condensate $\mu = U(\vec{r})$ is then an ellipsoid with a radius R_α along axis α given by:

$$\mu = \frac{1}{2}m\omega_\alpha^2 R_\alpha^2. \tag{181}$$

The condensate wavefunction can be rewritten in terms of these radii:

$$\phi(\vec{r}) = \left(\frac{\mu}{N_0 g}\right)^{1/2} \left(1 - \sum_\alpha \frac{r_\alpha^2}{R_\alpha^2}\right)^{1/2}. \tag{182}$$

Using the normalization condition of ϕ to unity we can also express the "normalization" factor $\sqrt{\mu/N_0 g}$ in terms of the radii. The integral of $|\phi|^2$ can be calculated in spherical coordinates after having made the change of variable $u_\alpha = r_\alpha/R_\alpha$. This leads to

$$\left(\frac{\mu}{N_0 g}\right)^{1/2} = \left(\frac{15}{8\pi \prod_\alpha R_\alpha}\right)^{1/2}. \tag{183}$$

Eliminating R_α in terms of μ thanks to Eq.(181) we can calculate the chemical potential:

$$\mu = \frac{1}{2}\hbar\bar{\omega} \left[15 \frac{N_0 a}{(\hbar/m\bar{\omega})^{1/2}}\right]^{2/5} \tag{184}$$

where $\bar{\omega}$ is the geometrical mean of the trap frequencies:

$$\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}. \tag{185}$$

We can now see that in the limit $\chi \gg 1$ the chemical potential μ satisfies

$$\mu \gg \hbar\bar{\omega}, \tag{186}$$

which is a convenient way of defining the Thomas-Fermi regime.

We can now compare these Thomas-Fermi predictions to the MIT experimental results on the energy of the condensate [12]. In the experiment the trapping potential is switched off abruptly, so that the energy of the gas abruptly reduces to $E_{\text{red}} = E_{\text{kin}} + E_{\text{int}} \simeq E_{\text{int}}$; afterwards the cloud ballistically expands, E_{int} is converted in kinetic expansion energy that can be measured. In the Thomas-Fermi approximation the integral of $N_0^2 g |\phi|^4/2$ can be done, which leads to

$$E_{\text{int}} \simeq \frac{2}{7} N_0 \mu \propto N_0^{7/5}. \tag{187}$$

The resulting dependence in N_0 is in good agreement with the MIT results, see Fig.5.

From the expression of the chemical potential we can also calculate the total energy of the condensate in the trap , as $\mu = \partial_{N_0} E$: integrating over N_0 gives

$$E \simeq \frac{5}{7}\mu N_0. \tag{188}$$

One can then check explicitly that $\mu \neq E/N_0$!

5.3.2 How to extend the Thomas-Fermi approximation to the time dependent case ?

We would like to analyze time dependent situations encountered in the experiments, *e.g.*

- ballistic expansion of the gas: this is a crucial example, as it is a standard experimental imaging technique of the condensate

- collective excitations: response of the condensate to a modulation of the trap frequencies

in the strongly interacting regime. An immediate generalization of the Thomas-Fermi approximation consisting in neglecting the kinetic energy of the condensate is now too naive! In the case of ballistic expansion for example the interaction energy is gradually transformed into kinetic energy when the cloud expands so kinetic energy becomes important!

The trick is actually to split the kinetic energy in two contributions, one of them remaining small and negligible in the time dependent case. This is performed using the so-called hydrodynamic representation of the condensate classical field, split in a modulus and a phase:

$$N_0^{1/2}\phi(\vec{r}) = \rho^{1/2}(\vec{r})e^{iS(\vec{r})/\hbar} \tag{189}$$

where S has the dimension of an action and ρ is simply the condensate density. The mean kinetic energy of the condensate then writes

$$
\begin{aligned}
E_{\text{kin}}[\phi, \phi^*] &= \int d^3\vec{r}\, \frac{\hbar^2}{2m}|\vec{\text{grad}}\,\phi|^2 \\
&= \int d^3\vec{r}\left[\frac{\hbar^2}{2m}\left(\vec{\text{grad}}\sqrt{\rho}\right)^2 + \rho\frac{\left(\vec{\text{grad}}\,S\right)^2}{2m}\right].
\end{aligned}
\tag{190}
$$

As we shall see during ballistic expansion of the condensate the density ρ remains a smooth, slowly varying function of the position so that it has a very small contribution to the kinetic energy; most of the kinetic energy induced from interaction energy is stored in the spatial variation of the phase of the condensate wavefunction.

5.3.3 Hydrodynamic equations

In this subsection we rewrite the time dependent Gross-Pitaevskii equation in terms of the density ρ and the phase S. This can be done of course by a direct insertion of Eq.(189) in the Gross-Pitaevskii equation.

A more elegant way is to use the covariant nature of the Lagrangian formulation of the Gross-Pitaevskii equation, Eq.(145). We rewrite the density of Lagrangian in terms of ρ and S:

$$\mathcal{L} = -\left[\rho\partial_t S + \frac{\hbar^2}{2m}\left(\vec{\mathrm{grad}}\sqrt{\rho}\right)^2 + \rho\frac{\left(\vec{\mathrm{grad}}\,S\right)^2}{2m} + U(\vec{r},t)\rho + \frac{g}{2}\rho^2\right]. \tag{191}$$

An evolution equation for an arbitrary coordinate $Q(\vec{r},t)$ of the field is obtained from the Lagrange equation:

$$\partial_t\left(\frac{\partial\mathcal{L}}{\partial(\partial_t Q)}\right) + \sum_\alpha \partial_{r_\alpha}\left(\frac{\partial\mathcal{L}}{\partial(\partial_{r_\alpha} Q)}\right) = \frac{\partial\mathcal{L}}{\partial Q}. \tag{192}$$

We first specialize the Lagrange equations to the choice $Q = \sqrt{\rho}$; dividing the resulting equation by $2\sqrt{\rho}$ we obtain

$$\partial_t S + \frac{1}{2m}\left(\vec{\mathrm{grad}}\,S\right)^2 + U + \rho g = \frac{\hbar^2}{2m}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}. \tag{193}$$

Then we set $Q = S$ in the Lagrange equations which leads to

$$\partial_t\rho + \mathrm{div}\left[\frac{\rho}{m}\vec{\mathrm{grad}}\,S\right] = 0. \tag{194}$$

This last equation looks like a continuity equation. This is confirmed by the following physical interpretation of $\vec{\mathrm{grad}}\,S$. It is known in basic quantum mechanics that the probability current density associated to a single particle wavefunction ϕ is

$$\vec{j}_{\mathrm{proba}} = \frac{\hbar}{2im}\left[\phi^*\vec{\mathrm{grad}}\,\phi - \mathrm{c.c.}\right]. \tag{195}$$

Multiplying this expression by N_0, as there are N_0 particles in the condensate, and introducing the (ρ, S) representation of ϕ we get the following expression for the current density of condensate particles:

$$\vec{j} = \rho\frac{\vec{\mathrm{grad}}\,S}{m} \equiv \rho\,\vec{v} \tag{196}$$

where $\vec{v}$ is the so-called local velocity field in the gas.

Equation (194) is therefore the usual continuity equation:

$$\partial_t \rho + \operatorname{div}\left[\rho \vec{v}\right] = 0. \tag{197}$$

The other equation (193) can be turned into an evolution equation for the velocity field by taking its spatial gradient:

$$m\partial_t \vec{v} + \vec{\operatorname{grad}}\left[\frac{1}{2}mv^2 + U(\vec{r}) + g\rho(\vec{r}) - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right] = 0. \tag{198}$$

This looks like the Navier-Stockes equation used in classical hydrodynamics, in the limiting case of a fluid with no viscosity. The term $\vec{\operatorname{grad}}(\frac{1}{2}mv^2)$ looks unusual but using the fact that $\vec{v}$ is the gradient of a function S/m one can put it in the usual form of a convective term:

$$\vec{\operatorname{grad}}\left(\frac{1}{2}mv^2\right) = m(\vec{v}\cdot\vec{\operatorname{grad}})\vec{v}. \tag{199}$$

A difference with classical hydrodynamics is the so-called quantum pressure term, involving

$$-\frac{\hbar^2}{2m}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}, \tag{200}$$

the only term in the equations (197,198) where $\hbar$ appears.

5.3.4 Classical hydrodynamic approximation

The classical hydrodynamic approximation consists precisely in neglecting the quantum pressure term Eq.(200) in the equation (198) for the velocity field of the condensate.

We can estimate simply the validity condition of this approximation. Denoting d a typical length scale for the variation of the condensate density $\rho(\vec{r})$ we obtain the estimate

$$\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \sim \frac{1}{d^2}. \tag{201}$$

Comparing the quantum pressure term Eq.(200) to the classical mean field term ρg yields the condition

$$\frac{\hbar^2}{md^2} \ll g\rho(\vec{r}) \sim \rho_{\max}g \tag{202}$$

where ρ_{max} is the maximal density (usually at the center of the trap). This validity condition can be reformulated in terms of the healing length,

$$d \gg \xi \equiv \left(\frac{\hbar^2}{2m\rho_{\mathrm{max}}g} \right)^{1/2}. \tag{203}$$

Note that ξ is sometimes also called coherence length, which can be confusing.

Why this name of healing length for ξ? Imagine that you cut with an infinite wall a condensate in an otherwise uniform potential. Right at the wall the condensate density vanishes; far away from the wall the density of the condensate is uniform. The condensate density adapts from zero to its constant bulk value over a length typically on the order of ξ. This can be checked by an explicit solution of the Gross-Pitaevskii equation:

$$N_0^{1/2}\phi(x,y,z) = \rho_{\mathrm{max}}^{1/2} \tanh\left(\frac{z}{\sqrt{2}\xi} \right) \tag{204}$$

where $z = 0$ is the plane of the infinite wall. This explicit solution shows that at a distance $z \gg \xi$ from the infinite wall there is no more any effect of the boundary condition $\phi(x,y,z=0) = 0$. This is to be contrasted with the case of the ideal Bose gas: the ground state between infinite walls separated by the length L then scales as $\sin(\pi z/L)$ and depends dramatically on L.

For a moderate excitation of the condensate by a modulation of the trap frequencies, or in the course of ballistic expansion of the condensate, we shall see that the only typical length scale for the variation of the condensate density is the radius R of the condensate itself. One can then check that in the Thomas-Fermi regime the classical hydrodynamic approximation indeed applies:

$$\frac{R}{\xi} \simeq \left(\frac{2\mu}{m\omega^2} \right)^{1/2} \times \left(\frac{2m\mu}{\hbar^2} \right)^{1/2} = \frac{2\mu}{\hbar\omega} \gg 1. \tag{205}$$

In the Thomas-Fermi regime we therefore neglect the quantum pressure term to obtain

$$m\left[\partial_t + \left(\vec{v} \cdot \vec{\mathrm{grad}} \right) \right] \vec{v}(\vec{r},t) = -\vec{\mathrm{grad}}\left(U(\vec{r},t) + g\rho(\vec{r},t) \right) \equiv \vec{F}(\vec{r},t). \tag{206}$$

This equation is then a purely classical equation, Newton's equation in presence of the force field $\vec{F}$ written in Euler's point of view. The operator between square brackets is simply the so-called convective derivative.

It is instructive to rewrite Eq.(206) in Lagrange's point of view. One then follows a small piece of the fluid in course of its motion. Denoting $\vec{r}(t)$ the trajectory of the small piece of fluid we directly write Newton's equation:

$$m\frac{d^2}{dt^2}\vec{r}(t) = \vec{F}(\vec{r}(t), t) = -\left[\vec{\mathrm{grad}}\,(U + g\rho)\right](\vec{r}(t), t). \tag{207}$$

This equation automatically implies the continuity equation (197) and the Euler equation (206). The unusual feature is that the force field depends itself on the density of the gas, so that we are facing here a self-consistent classical problem, corresponding formally to the mean field approximation for a collisionless classical gas! A surprising conclusion, knowing that we are actually studying the motion of a Bose-Einstein condensate!

5.4 Recovering time dependent experimental results

5.4.1 The scaling solution

It turns out that the self-consistent classical problem Eq.(207) can be solved exactly for the particular conditions of a gas initially at rest and in a harmonic trap.

At time $t = 0$ we assume a steady state Bose-Einstein condensate in the trap, of course in the Thomas-Fermi regime so that the classical hydrodynamic approximation is reasonable. The steady state of Eq.(207) corresponds to a force field $\vec{F}$ vanishing everywhere, so that

$$U(\vec{r}) + g\rho(\vec{r}) = \mathrm{constant}. \tag{208}$$

One recovers the stationary Thomas-Fermi density profile, the constant being determined from the normalization condition of ρ and therefore coinciding with the Thomas-Fermi approximation for μ.

At time $t > 0$ the trapping potential remains harmonic with the same eigenaxis [37] but the eigenfrequencies of the trap can have any time dependence:

$$U(\vec{r}, t) = \frac{1}{2}\sum_{\alpha=x,y,z} m\omega_\alpha^2(t)r_\alpha^2. \tag{209}$$

Then any small piece of the fluid with initial positions $r_\alpha(0)$ along axis α will move according to the trajectory

$$r_\alpha(t) = \lambda_\alpha(t)r_\alpha(0) \tag{210}$$

where the scaling factors $\lambda_\alpha(t)$ depend only on time, not on the initial position of the small piece of fluid. In other words the density of the gas will experience a mere (possibly anisotropic) dilatation

$$\rho(\vec{r}, t) = \frac{1}{\lambda_x(t)\lambda_y(t)\lambda_z(t)} \rho\left(\{\frac{r_\alpha}{\lambda_\alpha(t)}\}, t = 0\right). \tag{211}$$

We can see simply why the ansatz Eq.(210) solves indeed Eq.(207) for a harmonic trap. As the initial density in the trap has a quadratic dependence on position, so will have the density at time t. The gradient $-\vec{\mathrm{grad}}(\rho g)$ appearing in the expression of the force field will then be a linear function of the coordinates; so is the harmonic force $-\vec{\mathrm{grad}}\, U(\vec{r}, t)$. Newton's equation is therefore linear in the coordinates; dividing it by $r_\alpha(0)$ one then gets equations for $\lambda_\alpha(t)$ irrespective of the initial coordinates $r_\alpha(0)$!

More details are given in [38, 39], we give here the equations for the scaling parameters:

$$\frac{d^2}{dt^2}\lambda_\alpha(t) = \frac{\omega_\alpha^2(0)}{\lambda_\alpha \lambda_x \lambda_y \lambda_z} - \omega_\alpha^2(t)\lambda_\alpha(t), \quad \alpha = x, y, z \tag{212}$$

with the initial conditions

$$\lambda_\alpha(0) \;=\; 0 \tag{213}$$

$$\frac{d}{dt}\lambda_\alpha(0) \;=\; 0 \tag{214}$$

since the condensate is initially at rest.

Finally we make the connection between these scaling solutions and the equations for the spatial widths σ_α obtained in Eq.(174) from a time dependent variational Gaussian ansatz for the condensate wavefunction. We are here in the Thomas-Fermi regime $\chi \gg 1$ so that the $1/\sigma_\alpha^3$ terms can be neglected in Eq.(174). The steady state solutions for the σ_α's are then $\sigma_\alpha(0) \simeq \chi^{1/5}\bar{\nu}^{3/5}/\nu_\alpha(0)$ where $\bar{\nu}$ is the geometrical mean of the initial frequencies $\nu_\alpha(0)$, and the quantities $\sigma_\alpha(t)/\sigma_\alpha(0)$ then obey the same equations as the λ_α's! The Gaussian ansatz, which has the wrong shape in the Thomas-Fermi regime, is however able to capture the right scaling nature of the solution! This explains why the collective mode frequencies obtained from Eq.(174) are a good approximation, not only when $\chi \ll 1$, where the Gaussian ansatz was expected to hold, but also in the strongly interacting regime $\chi \gg 1$.

5.4.2 Ballistic expansion of the condensate

At time $t = 0^+$ the trapping potential is turned off suddenly. The scaling parameters then satisfy the simpler equations

$$\frac{d^2}{dt^2}\lambda_\alpha(t) = \frac{\omega_\alpha^2(0)}{\lambda_\alpha\lambda_x\lambda_y\lambda_z}. \tag{215}$$

These equations are still difficult to solve analytically. In the experimentally relevant regime of cigar-shaped traps, with $\omega_z(0) \ll \omega_x(0) = \omega_y(0)$, one can find an approximate solution [38].

Experimentally the scaling predictions have been tested carefully. First one can see if the ballistically expanded condensate density has indeed the shape of an inverted parabola [38]. Second one can measure the radii of the condensate as function of time to see if they fit the scaling predictions [40]. Both tests confirm the scaling predictions in the Thomas-Fermi regime.

5.4.3 Breathing frequencies of the condensate

A typical excitation sequence of breathing modes of the condensate proceeds as follows. One starts with a steady state condensate in the trapping potential. Then one modulates one of the trap frequencies for some finite time t_{exc}, at a frequency close to an expected resonance of the condensate. Then one lets the excited condensate evolve in the unperturbed trap for some adjustable time t_{osc}. Finally one can perform imaging of the cloud, *e.g.* by performing a ballistic expansion of the condensate and measuring the aspect ratio of the expanded cloud. By repeating the whole sequence for different values of t_{osc} one can reconstruct the aspect ratio as function of t_{osc}.

Such a procedure has been used at JILA and at MIT. In figure 13 are shown results obtained at MIT in a cigar-shaped trap, for a modulation of the trap frequency along the slow (that is weakly confining) axis z. The solid line corresponds to the prediction of scaling theory, the input parameters being (i) the oscillation frequencies ω_α of the atoms in the trap, (ii) the precise way the excitation is performed, and (iii) the duration of ballistic expansion; the agreement between theory and experiment is good, considering the fact that there is no fitting parameter [38].

If one is interested only in the frequencies of the breathing eigenmodes of the condensate it is sufficient to linearize the equations of the scaling parameters around their steady

state value:

$$\frac{d^2}{dt^2}\delta\lambda_\alpha = -2\omega_\alpha^2(0)\delta\lambda_\alpha - \omega_\alpha^2(0)\sum_\beta \delta\lambda_\beta \tag{216}$$

and find the eigenvalues of the corresponding three by three linear system (see also §6.3.3). For a trap with cylindrical symmetry one gets the eigenfrequencies $\Omega = \sqrt{2}\omega_\perp(0)$ and

$$\Omega^2 = \frac{1}{2}\left[3\omega_z^2(0) + 4\omega_\perp^2(0) \pm \left(9\omega_z^4(0) + 16\omega_\perp^4(0) - 16\omega_z^2(0)\omega_\perp^2(0)\right)^{1/2}\right]. \tag{217}$$

The mode observed at MIT corresponds to the $-$ sign in the above expression; as the trap was cigar-shaped in the experiment, $\omega_\perp(0) \gg \omega_z(0)$ so that one has the approximate formula

$$\Omega \simeq \left(\frac{5}{2}\right)^{1/2} \omega_z(0). \tag{218}$$
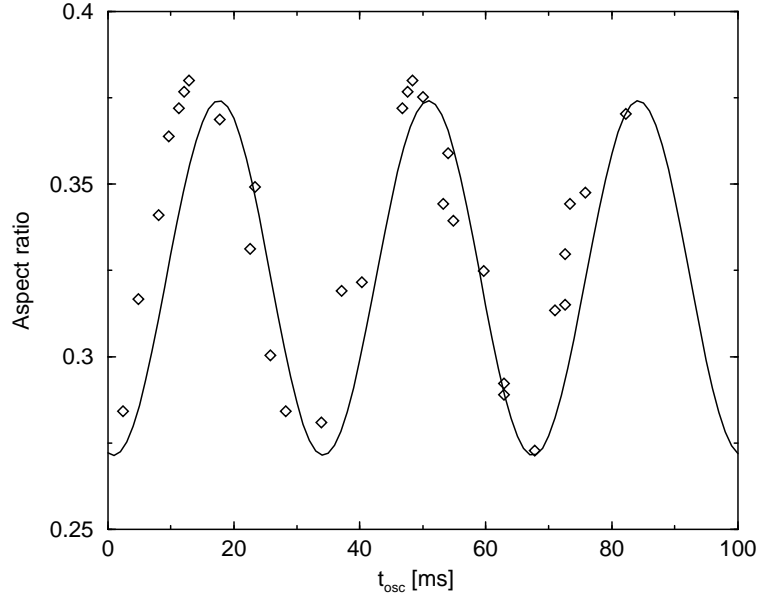
Figure 13: Aspect ratio of the excited and ballistically expanded condensate as a function of free oscillation time t_{osc}. The expansion time is 40 ms, the unperturbed trap frequencies are $\omega_\perp(0) = 2\pi \times 250$ Hz, $\omega_z(0) = 2\pi \times 19$ Hz. Solid line: theory. Diamonds: experimental data obtained at MIT.

6 What we learn from a linearization of the Gross-Pitaevskii equation

There are several important motivations to perform a linearization of the Gross-Pitaevskii equation around a steady state solution ϕ_0 :

- as the Gross-Pitaevskii equation is a non-linear equation it is crucial to check the so-called "dynamical" stability of the steady state solution. More precisely one has to check with a linear stability analysis that any small deviation $\delta\phi$ of the condensate wavefunction from ϕ_0 does not diverge exponentially with time. Otherwise ϕ_0 may not be physically considered as a steady state as even very small perturbations will eventually induce an evolution of the condensate wavefunction far from ϕ_0 .

- as a byproduct of linear stability analysis we obtain a linear response theory for the condensate very useful to interpret experiments which apply a weak perturbation to the condensate.

- another important byproduct is the Bogoliubov approach which gives a description of the state of the non-condensed particles that is still approximate but more accurate at low temperature (typically $k_B T < \mu$) that the Hartree-Fock approach. This allows to check the so-called "thermodynamical stability" of the condensate and will be the subject of §7.

6.1 Linear response theory for the condensate wavefunction

6.1.1 Linearize the Gross-Pitaevskii solution around a steady state solution

Let $\phi_0(\vec{r})$ be a steady state solution of the Gross-Pitaevskii solution in the time independent trapping potential $U_0(\vec{r})$:

$$0 = \left[-\frac{\hbar^2}{2m}\Delta + U_0 + gN_0|\phi_0|^2 - \mu \right] \phi_0. \tag{219}$$

The trapping potential is then slightly modified by a time dependent perturbation $\delta U(\vec{r}, t)$, resulting in a total trapping potential

$$U(\vec{r}, t) = U_0(\vec{r}) + \delta U(\vec{r}, t). \tag{220}$$

The condensate wavefunction, initially equal to ϕ_0, evolve according to

$$i\hbar\partial_t\phi = \left[-\frac{\hbar^2}{2m}\Delta + U + gN_0|\phi|^2 - \mu\right]\phi. \tag{221}$$

As δU is so small we assume that ϕ experiences only a small deviation from ϕ_0:

$$\phi(\vec{r},t) = \phi_0(\vec{r}) + \delta\phi(\vec{r},t) \tag{222}$$

so that we can linearize Eq.(221) in terms of $\delta\phi$. Neglecting the second order product of $\delta\phi$ and δU we obtain:

$$i\hbar\partial_t\delta\phi = \left[-\frac{\hbar^2}{2m}\Delta + U_0 - \mu\right]\delta\phi + 2gN_0\phi_0^*\phi_0\delta\phi + gN_0\phi_0^2\delta\phi^* + \delta U\phi_0. \tag{223}$$

Note the presence of the factor 2 in front of the term proportional to $g\delta\phi$; it turns out (and this should become clear in the Bogoliubov approach) that this factor 2 has the same origin as the one in the Hartree-Fock potential Eq.(115) for the non-condensed particles. As ϕ remains normalized to unity, as ϕ_0 was, we note that to first order in $\delta\phi$,

$$\int d^3\vec{r}\ [\delta\phi(\vec{r},t)\phi_0^*(\vec{r}) + \phi_0(\vec{r})\delta\phi^*(\vec{r},t)] = 0. \tag{224}$$

A peculiar feature of Eq.(223) is that, though it is obtained from a linearization procedure, it is not a linear equation for $\delta\phi$ in the strict mathematical sense: if $\delta\phi$ is a particular solution of the homogeneous part of this equation (set $\delta U = 0$), the function $\alpha\delta\phi$ (where α is a constant complex number) is generally not a solution of the homogeneous part anymore because of the coupling of $\delta\phi$ to $\delta\phi^*$. There are several possibilities to restore this linearity. A first one is to consider as unknown functions the real part and the imaginary part of $\delta\phi$. A second, more elegant method, more common in the literature, is to introduce formally as unknown the two-component column vector:

$$\left(\begin{array}{c} \delta\phi(\vec{r},t) \\ \delta\phi^*(\vec{r},t) \end{array}\right) \tag{225}$$

the functions $\delta\phi$ and $\delta\phi^*$ being now considered as independent. We then rewrite Eq.(223) as the linear system:

$$i\hbar\partial_t\left(\begin{array}{c} \delta\phi(\vec{r},t) \\ \delta\phi^*(\vec{r},t) \end{array}\right) = \mathcal{L}_{GP}\left(\begin{array}{c} \delta\phi(\vec{r},t) \\ \delta\phi^*(\vec{r},t) \end{array}\right) + \left(\begin{array}{c} S(\vec{r},t) \\ -S^*(\vec{r},t) \end{array}\right) \tag{226}$$

with a source term $S(\vec{r}, t) = \delta U(\vec{r}, t)\phi_0(\vec{r})$ and a linear operator

$$\mathcal{L}_{GP} = \begin{pmatrix} H_{GP} + gN_0|\phi_0|^2 & gN_0\phi_0^2 \\ -gN_0\phi_0^{*2} & -\left[H_{GP} + gN_0|\phi_0|^2\right]^* \end{pmatrix} \tag{227}$$

where we have introduced the Gross-Pitaevskii Hamiltonian:

$$H_{GP} \equiv -\frac{\hbar^2}{2m}\Delta + U_0 + gN_0|\phi_0|^2 - \mu. \tag{228}$$

Note the presence of complex conjugation in the second line of $\mathcal{L}_{GP}$; it also applies to the potential U_0 , without effect here as U_0 , hermitian function of $\vec{r}$, is real; it should not be forgotten if situations where the potential contains a complex term such as $-\Omega L_z$ where L_z is the angular momentum operator (inertial term in a frame rotating at angular velocity Ω).

As the operator $\mathcal{L}_{GP}$ is time independent the general method to determine the time evolution of $\delta\phi$ is to diagonalize $\mathcal{L}_{GP}$ and expand $\delta\phi$ on the corresponding eigenmodes. At this stage one faces a slight difficulty: it turns out that $\mathcal{L}_{GP}$ is not diagonalizable, that is the set of all eigenvectors of $\mathcal{L}_{GP}$ does not form a basis (in general one vector is missing to span the whole functional space). Mathematically this can be solved by putting $\mathcal{L}_{GP}$ into the so-called Jordan normal form. Here we use the more physical following procedure.

6.1.2 Extracting the "relevant part" from $\delta\phi$

We split $\delta\phi$ on a component along ϕ_0 and a part orthogonal to ϕ_0 :

$$\delta\phi(\vec{r}, t) = \eta(t)\phi_0(\vec{r}) + \delta\phi_\perp(\vec{r}, t). \tag{229}$$

From Eq.(224) valid to first order in $\delta\phi$ we realize that $\eta = \langle\phi_0|\delta\phi\rangle$ is such that $\eta(t) + \eta^*(t) = 0$, so that $\eta(t)$ is purely imaginary and can be reinterpreted as a change of phase of ϕ_0 :

$$\phi(\vec{r}, t) \simeq e^{\eta(t)}\phi_0(\vec{r}) + \delta\phi_\perp(\vec{r}, t). \tag{230}$$

One then sees that this change of phase has no consequence on the one-body density matrix of the condensate, up to first order in $\delta\phi$:

$$|\phi\rangle\langle\phi| \simeq |\phi_0\rangle\langle\phi_0| + |\phi_0\rangle\langle\delta\phi_\perp| + |\delta\phi_\perp\rangle\langle\phi_0|. \tag{231}$$

After a little algebra we turn Eq.(226) into a closed equation for $\delta\phi_\perp$:

$$i\hbar\partial_t \left(\begin{array}{c} \delta\phi_\perp(\vec{r},t) \\ \delta\phi_\perp^*(\vec{r},t) \end{array} \right) = \mathcal{L} \left(\begin{array}{c} \delta\phi_\perp(\vec{r},t) \\ \delta\phi_\perp^*(\vec{r},t) \end{array} \right) + \left(\begin{array}{c} S_\perp(\vec{r},t) \\ -S_\perp^*(\vec{r},t) \end{array} \right). \tag{232}$$

Introducing the projection operators orthogonally to ϕ_0 and ϕ_0^* :

$$Q = 1 - |\phi_0\rangle\langle\phi_0| \tag{233}$$

$$Q^* = 1 - |\phi_0^*\rangle\langle\phi_0^*| \tag{234}$$

we have $S_\perp = QS$ and

$$\mathcal{L} = \left(\begin{array}{cc} H_{GP} + gN_0 Q|\phi_0|^2 Q & gN_0 Q\phi_0^2 Q^* \\ -gN_0 Q^*\phi_0^{*2} Q & -\left[H_{GP} + gN_0 Q|\phi_0|^2 Q \right]^* \end{array} \right) \tag{235}$$

where the Gross-Pitaevskii Hamiltonian H_{GP} is defined in Eq.(228). In general the operator $\mathcal{L}$ is diagonalizable.

6.1.3 Spectral properties of $\mathcal{L}$ and dynamical stability

Consider an eigenvector of $\mathcal{L}$ with eigenvalue ϵ_k :

$$\mathcal{L} \left(\begin{array}{c} u_k \\ v_k \end{array} \right) = \epsilon_k \left(\begin{array}{c} u_k \\ v_k \end{array} \right) \tag{236}$$

The free evolution of this mode, that is for $\delta U = 0$, is given by the phase factor $\exp(-i\epsilon_k t/\hbar)$. This factor remains bounded in time provided that the imaginary part of ϵ_k is negative, which leads to the dynamical stability condition

$$\mathrm{Im}(\epsilon_k) \leq 0 \quad \text{for all} \quad k. \tag{237}$$

One has the following three interesting spectral properties.

1. ϵ_k^* is also an eigenvalue of $\mathcal{L}$.

2. $\left(\begin{array}{c} v_k^* \\ u_k^* \end{array} \right)$ is also an eigenvector of $\mathcal{L}$, with eigenvalue $-\epsilon_k^*$.

3. $\left(\begin{array}{c} u_k \\ -v_k \end{array} \right)$ is an eigenvector of $\mathcal{L}^\dagger$ with eigenvalue ϵ_k .

The last two of these three properties can be checked by direct substitution. They can be viewed more elegantly as a consequence of the symmetry properties:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{L} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1} = -\mathcal{L}^* \tag{238}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{L} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{-1} = \mathcal{L}^\dagger. \tag{239}$$

As we shall see this last property involving $\mathcal{L}^\dagger$ is useful to write $\mathcal{L}$ in diagonal form.

The first of these properties is easy to prove when ϕ_0 is real. In this case the operator $\mathcal{L}$ is a real operator (as Q, U_0, ϕ_0^2, Δ are real) so that complex eigenvalues come by pairs of complex conjugates. When ϕ_0 is complex one can use the following mathematical fact: if ϵ_k is an eigenvalue of an arbitrary operator $\mathcal{L}$, ϵ_k^* is an eigenvalue of the operator $\mathcal{L}^\dagger$. Here $\mathcal{L}^\dagger$ differs from $\mathcal{L}$ by a unitary transform (239) so that it has the same spectrum as $\mathcal{L}$. This property of the spectrum is actually known in classical mechanics for a linearized Hamiltonian system, and the Gross-Pitaevskii equation can be viewed as a classical Hamiltonian equation for a continuous set of conjugate coordinates $q = \mathrm{Re}(\phi), p = \mathrm{Im}(\phi)$.

As a consequence of this first spectral property of $\mathcal{L}$ the dynamical stability condition Eq.(237) can be reformulated as

$$\mathrm{Im}(\epsilon_k) = 0 \ \ \text{for all} \ \ k \tag{240}$$

that is all the eigenvalues of $\mathcal{L}$ have to be real to have a dynamically stable condensate wavefunction. We assume that this property is satisfied in the remaining part of this subsection 6.1.

6.1.4   Diagonalization of $\mathcal{L}$

As $\mathcal{L}$ is not a Hermitian operator the eigenbasis of $\mathcal{L}$ is not orthogonal (see the minus sign in the second line of $\mathcal{L}$, due to Bose statistics; one does not have this sign in the BCS theory for interacting fermions).

To write $\mathcal{L}$ in diagonal form the knowledge of the eigenvectors is then *a priori* not sufficient. One generally proceeds as follows:

Reminder: *Let M be a diagonalizable but not necessarily Hermitian operator. Then the diagonal form of M can be written as*

$$M = \sum_k m_k |\psi_k^R\rangle\langle\psi_k^L| \tag{241}$$

where $|\psi_k^R\rangle$ is a right eigenvector of M with eigenvalue m_k :

$$M|\psi_k^R\rangle = m_k|\psi_k^R\rangle \tag{242}$$

and $\langle\psi_k^L|$ is a left eigenvector of M with eigenvalue m_k :

$$\langle\psi_k^L|M = m_k\langle\psi_k^L| \tag{243}$$

or equivalently

$$M^\dagger|\psi_k^L\rangle = m_k^*|\psi_k^L\rangle. \tag{244}$$

The normalization of the left and right eigenvectors is such that

$$\langle\psi_k^L|\psi_{k'}^R\rangle = \delta_{k,k'}. \tag{245}$$

$|\psi_k^L\rangle$ *is then called the adjoint vector of* $|\psi_k^R\rangle$.

We apply this reminder to $\mathcal{L}$. We have already defined the right eigenvector:

$$|\psi_k^R\rangle = \begin{pmatrix} |u_k\rangle \\ |v_k\rangle \end{pmatrix}, \quad \text{eigenvalue of } \mathcal{L} \; : \; \epsilon_k. \tag{246}$$

From the third of the above spectral properties of $\mathcal{L}$ we can easily obtain the corresponding left eigenvector up to a normalization factor:

$$|\psi_k^L\rangle = \mathcal{N}_k \begin{pmatrix} |u_k\rangle \\ -|v_k\rangle \end{pmatrix}, \quad \text{eigenvalue of } \mathcal{L}^\dagger \; : \; \epsilon_k^* = \epsilon_k. \tag{247}$$

The normalization condition Eq.(245) imposes

$$\langle\psi_k^L|\psi_k^R\rangle = 1 = \mathcal{N}_k^*[\langle u_k|u_k\rangle - \langle v_k|v_k\rangle]. \tag{248}$$

It is then natural to normalize the right eigenvectors in such a way that the quantity between square brackets is ± 1 , leading to $\mathcal{N}_k = \pm 1$.

We therefore group the eigenvectors of $\mathcal{L}$ in three families:

- the $+$ family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = +1$

- the $-$ family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = -1$

- the 0 family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = 0$.

From the spectral property number 2 we see that there is a duality between the $+$ family and the $-$ family. Conventionally we will refer to eigenvectors of the $+$ family as (u_k, v_k) (eigenvalue ϵ_k) and the eigenvectors of the $-$ family will be expressed as (v_k^*, u_k^*) (eigenvalue $-\epsilon_k$).

Generally there are only the following two members in the 0 family:

$$\begin{pmatrix} \phi_0 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ \phi_0^* \end{pmatrix}. \tag{249}$$

One can check that these two vectors are eigenvectors of $\mathcal{L}$ with the eigenvalue zero. [In the case of $\mathcal{L}_{GP}$ one finds in general only one zero-energy eigenmode, the missing one leads to the non-diagonalizability]. In general these two vectors span the whole 0 family. As they are also eigenmodes of the operator $\mathcal{L}^\dagger$ with the eigenvalue zero they are actually their own conjugate vectors! From Eq.(245) we then get the important property:

$$\langle \phi_0 | u_k \rangle = \langle \phi_0^* | v_k \rangle = 0 \quad \text{for all } k \text{ in } + \text{ family.} \tag{250}$$

It is important to note that the $+$ in the denomination "$+$ family" refers *a priori* to the sign of $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle$ and **not** to the sign of ϵ_k !

6.1.5 General solution of the linearized problem

We expand the unknown column vector of Eq.(232) onto eigenmodes of $\mathcal{L}$. We assume that the only modes of the 0 family are the ones of Eq.(249); these modes do not contribute to the expansion as $\langle \phi_0 | \delta \phi_\perp \rangle = \langle \phi_0^* | \delta \phi_\perp^* \rangle = 0$. We then get the expansion

$$\begin{pmatrix} \delta \phi_\perp(\vec{r}, t) \\ \delta \phi_\perp^*(\vec{r}, t) \end{pmatrix} = \sum_{k \in +\text{family}} b_k(t) \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + b_k^*(t) \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix} \tag{251}$$

with the coefficients

$$b_k(t) = (\langle u_k |, -\langle v_k |) \begin{pmatrix} |\delta \phi_\perp(t)\rangle \\ |\delta \phi_\perp^*(t)\rangle \end{pmatrix} = \int d^3\vec{r} \, [u_k^*(\vec{r}) \delta \phi_\perp(\vec{r}, t) - v_k^*(\vec{r}) \delta \phi_\perp^*(\vec{r}, t)]. \tag{252}$$

As the second component of the expanded column vector is the complex conjugate of the first component the amplitudes on the $-$ family modes are the complex conjugates of the amplitudes b_k on the $+$ family modes, that is b_k^* .

Similarly one expands the source term of Eq.(232) on the eigenmodes of $\mathcal{L}$. The components on the $+$ family modes are given by

$$s_k(t) = \int d^3\vec{r} \; [u_k^*(\vec{r})S_\perp(\vec{r},t) + v_k^*(\vec{r})S_\perp^*(\vec{r},t)] . \tag{253}$$

Note the absence of $-$ sign here, due to the fact that the second component of the source column vector is the opposite of the complex conjugate of the first component. Finally the projection of Eq.(232) on the eigenmodes of the $+$ family gives the set of equations:

$$i\hbar\frac{d}{dt}b_k(t) = \epsilon_k b_k(t) + s_k(t) \tag{254}$$

which can be integrated including the initial condition $\delta\phi_\perp(t_0) = 0$:

$$b_k(t) = \int_0^{t-t_0} \frac{d\tau}{i\hbar} s_k(t-\tau)e^{-i\epsilon_k\tau/\hbar}. \tag{255}$$

6.1.6 Link between eigenmodes of $\mathcal{L}_{GP}$ and eigenmodes of $\mathcal{L}$

The linear operators $\mathcal{L}$ and $\mathcal{L}_{GP}$ describe the same physical problem, so that one expects in particular that their spectra, which correspond to the linear response frequencies of the condensate, are the same.

This expectation is confirmed by the simple result, that one can check by direct substitution: if $(|u_k^{GP}\rangle, |v_k^{GP}\rangle)$ is an eigenvector of $\mathcal{L}_{GP}$ with the eigenvalue ϵ_k then $(Q|u_k^{GP}\rangle, Q^*|v_k^{GP}\rangle)$ is an eigenvector of $\mathcal{L}$ with the *same* eigenvalue ϵ_k .

6.2 Examples of dynamical instabilities

We consider simple stationary solutions of the Gross-Pitaevskii equations that are dynamically unstable, that is with non-real eigenfrequencies $\epsilon_k/\hbar$. The situations considered correspond to a gas trapped in a cubic box with periodic boundary conditions; analytical calculations can then be performed. The conclusions remain qualitatively correct for harmonic traps.

6.2.1 Condensate in a box

The atoms are trapped in a cubic box of size L, and we assume periodic boundary conditions. An obvious solution of the time independent Gross-Pitaevskii equation is then the plane wave with vanishing momentum,

$$\phi_0(\vec{r}) = \frac{1}{L^{3/2}}. \tag{256}$$

It has a chemical potential

$$\mu = gN_0|\phi_0|^2 = \rho_0 g \tag{257}$$

where $\rho_0 = N_0/L^3$ is the density of condensate atoms.

To obtain the linear response frequencies of the condensates we calculate the spectrum of $\mathcal{L}_{GP}$, this operator takes here the very simple form:

$$\mathcal{L}_{GP} = \begin{pmatrix} -\dfrac{\hbar^2}{2m}\Delta + \rho_0 g & \rho_0 g \\[2ex] -\rho_0 g & -\left[-\dfrac{\hbar^2}{2m}\Delta + \rho_0 g\right] \end{pmatrix}. \tag{258}$$

Using the translational invariance of this operator we seek its eigenvectors in the form of plane waves:

$$\begin{pmatrix} u_{\vec{k}}^{GP}(\vec{r}) \\[2ex] v_{\vec{k}}^{GP}(\vec{r}) \end{pmatrix} = \frac{e^{i\vec{k}\cdot\vec{r}}}{L^{3/2}} \begin{pmatrix} U_{\vec{k}} \\[2ex] V_{\vec{k}} \end{pmatrix}. \tag{259}$$

Within the subspace of plane waves with wave vector $\vec{k}$, $\mathcal{L}_{GP}$ is represented by the 2×2 non-Hermitian matrix:

$$\mathcal{L}_{GP}[\vec{k}] = \begin{pmatrix} \dfrac{\hbar^2 k^2}{2m} + \rho_0 g & \rho_0 g \\[2ex] -\rho_0 g & -\left[\dfrac{\hbar^2 k^2}{2m} + \rho_0 g\right] \end{pmatrix}. \tag{260}$$

For $\vec{k} \neq \vec{0}$ this matrix can be diagonalized, giving one eigenvector of $+$ family, with the eigenvalue

$$\epsilon_{\vec{k}} = \left[\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2\rho_0 g\right)\right]^{1/2} \tag{261}$$

and one eigenvector of $-$ family with the eigenvalue $-\epsilon_{\vec{k}}$. The eigenvector of the $+$ family can be chosen as

$$
\begin{aligned}
U_{\vec{k}} + V_{\vec{k}} &= \left(\frac{\dfrac{\hbar^2 k^2}{2m}}{\dfrac{\hbar^2 k^2}{2m} + 2\rho_0 g} \right)^{1/4} \\[2em]
U_{\vec{k}} - V_{\vec{k}} &= \left(\frac{\dfrac{\hbar^2 k^2}{2m}}{\dfrac{\hbar^2 k^2}{2m} + 2\rho_0 g} \right)^{-1/4}
\end{aligned}
\tag{262}
$$

with the correct normalization $U_{\vec{k}}^2 - V_{\vec{k}}^2 = 1$.

The spectrum Eq.(261) is the so-called Bogoliubov spectrum, as it was first derived by Bogoliubov. Physically it is a very important result. In the limiting case of the ideal Bose gas ($g = 0$) the spectrum is the usual parabola; for $g \neq 0$ the spectrum is very different, and this deserves a more detailed discussion

- *Bogoliubov spectrum for $g > 0$*

In the case of effective repulsive interactions the Bogoliubov spectrum strongly differs from the one of a free particle in the low momenta domain $\hbar^2 k^2/2m \ll 2\rho_0 g$ as it scales linearly with k:

$$
\epsilon_{\vec{k}} \simeq \hbar k \sqrt{\frac{\rho_0 g}{m}}.
\tag{263}
$$

This linear dispersion relation leads to a propagation of low energy excitations in the condensate in the form of sound waves with a sound velocity c_s given by

$$
c_s = \frac{d\omega_{\vec{k}}}{dk} = \frac{1}{\hbar}\frac{d\epsilon_{\vec{k}}}{dk} = \sqrt{\frac{\rho_0 g}{m}}
\tag{264}
$$

or equivalently by the relativistic type formula

$$
mc_s^2 = \rho_0 g.
\tag{265}
$$

Superfluidity is an important consequence of this linear behavior of the spectrum at low k, as shown by an argument due to Landau and that we explain briefly. Consider a particle (of mass M) sent in the atomic gas with an initial velocity $\vec{u}$. The motion of this

particle can be damped by interaction with the condensate only if the particle can create some excitation of the condensate. Imagine that such an excitation is produced, with momentum $\vec{k}$; the particle experiences a momentum recoil of $-\hbar\vec{k}$ and conservation of energy imposes

$$\epsilon_{\vec{k}} = \frac{1}{2}M\vec{u}^{\,2} - \frac{1}{2M}\left[M\vec{u} - \hbar\vec{k}\right]^2 = \hbar\vec{k}\cdot\vec{u} - \frac{\hbar^2 k^2}{2M}. \tag{266}$$

The velocity u has then to satisfy the inequality:

$$u \geq \left|\frac{\vec{k}\cdot\vec{u}}{k}\right| \geq \frac{\epsilon_{\vec{k}}}{k} \geq c_s. \tag{267}$$

So a particle with an incoming velocity smaller than the sound velocity can move through the condensate without damping, only scattering on thermal excitations of the gas can damp its motion. This prediction has received an experimental confirmation at MIT [41].

At high momenta ($\hbar^2 k^2/2m \gg \rho_0 g$) corresponding to a velocity $\hbar k/m$ much larger than the sound velocity the Bogoliubov spectrum reduces to a shifted parabola

$$\epsilon_{\vec{k}} \simeq \frac{\hbar^2 k^2}{2m} + \rho_0 g = \frac{\hbar^2 k^2}{2m} + 2\rho_0 g - \mu. \tag{268}$$

This approximate form can be obtained by a series expansion of the general formula Eq.(261). It can also be derived more instructively from the observation that the off-diagonal coupling $\rho_0 g$ between the $U_{\vec{k}}$ component and the $V_{\vec{k}}$ component in the 2×2 matrix Eq.(260) becomes very non-resonant at high k (because the diagonal terms for $U_{\vec{k}}$ and $V_{\vec{k}}$ have opposite signs); neglecting this coupling one recovers Eq.(268) with $U_{\vec{k}} \simeq 1$, $V_{\vec{k}} \simeq 0$.

This last high energy property applies also in a non-uniform trapping potential: neglecting the off-diagonal coupling between u_k and v_k one approximates the high energy part of the Bogoliubov spectrum by the eigenvalues of

$$-\frac{\hbar^2}{2m}\Delta + U_0 + 2gN_0|\phi_0|^2 - \mu \tag{269}$$

which (up to the shift $-\mu$) is the Hartree-Fock Hamiltonian for non-condensed particles Eq.(116) in a regime of an almost pure condensate where the density of non-condensed particles is negligible as compared to the condensate density $N_0|\phi_0|^2$.

From this we expect that the Hartree Fock approach is invalid for the low energy fraction of the non-condensed gas (energy typically less than μ); this may become a

problem at temperatures $k_B T < \mu$, where one has to use the more precise Bogoliubov approach of §7.

- *Case of a negative g*

In the case of effective attractive interactions between particles the dynamical stability condition $\text{Im}(\epsilon_{\vec{k}}) = 0$ is satisfied if and only if

$$\frac{\hbar^2 k^2}{2m} + 2g\rho_0 \geq 0 \ \text{ for all } \ k > 0. \tag{270}$$

If one considers the thermodynamical limit of an infinite number of condensate atoms with a fixed mean density $\rho_0 = N_0/L^3$ the stability condition cannot be satisfied as k can be arbitrarily close to 0 in an infinite box. One may then be tempted to conclude that condensates with effective attractive interactions cannot be obtained experimentally, attractive interactions leading to a spatial collapse of the gas.

Experiments with atomic gases can deal however with small number of atoms and the simplifying assumption of a thermodynamical limit is not necessarily a good approximation. In the cubix box of size L with periodic boundary conditions the components of the wavevector $\vec{k}$ of an atom are integer multiples of $2\pi/L$. The smallest but non zero modulus of wavevector that can be achieved is therefore $2\pi/L$ (by taking e.g. $k_x = 2\pi/L, k_y = k_z = 0$). Dynamical stability condition Eq.(270) can then be rewritten as

$$\frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 \geq 2|g|\frac{N_0}{L^3} \tag{271}$$

or equivalently in terms of the scattering length as

$$\frac{N_0|a|}{L} \leq \frac{\pi}{4}. \tag{272}$$

Condensates for $a < 0$ can contain a limited number of atoms proportional to the size of the condensate.

Condition Eq.(271) has a clear physical interpretation: the energy gap in the spectrum of a particle in the box between the ground state and the first excited states should be larger than the mean field energy per particle: stabilization against collapse is thus provided by the discrete spectrum of the atoms in the trapping potential. This condition can thus be qualitatively extended to the case of an isotropic harmonic trap, $\hbar\omega >$

$|g|N_0/a_{\text{ho}}^3$ where ω is the oscillation frequency of the atoms in the trap and $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$ is the typical spatial extension of the ground state of the trap. One then recovers up to a numerical factor the results of §5.2.1.

6.2.2 Demixing instability

We consider here atoms with two internal states a, b; this model is relevant for experiments performed at JILA on binary mixtures of ^{87}Rb condensates, and also (if one includes a third atomic internal level) experiments at MIT in Ketterle's group on spinor ^{23}Na condensates.

To describe the elastic interactions between the atoms with two internal states one needs three coupling constants, all positive in the case of ^{87}Rb: g_{aa} and g_{bb} for interactions between atoms in the same internal state, g_{ab} for interactions between atoms in different internal states:

$$
\begin{aligned}
g_{aa} &: \quad a + a \rightarrow a + a \\
g_{bb} &: \quad b + b \rightarrow b + b \\
g_{ab} &: \quad a + b \rightarrow a + b.
\end{aligned}
\tag{273}
$$

In the JILA experiment internal states a and b correspond to different hyperfine levels of the atoms so that inelastic collisions such as $a+a \rightarrow a+b$ are either strongly endothermic (and do not take place) or strongly exothermic (and result in losses of atoms from the trap); we neglect these inelastic processes.

Omitting for simplicity the regularizing operator in the pseudo-potential we write the interaction Hamiltonian between the atoms in second quantized form as

$$
\begin{aligned}
H_{\text{int}} = \int d^3\vec{r} \quad & \left[\frac{g_{aa}}{2} \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a(\vec{r}) \hat{\psi}_a(\vec{r}) + \frac{g_{bb}}{2} \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_b(\vec{r}) \hat{\psi}_b(\vec{r}) \right. \\
& \left. + \quad g_{ab} \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a(\vec{r}) \hat{\psi}_b(\vec{r}) \right]
\end{aligned}
\tag{274}
$$

where $\hat{\psi}_a$ and $\hat{\psi}_b$ are the atomic field operators for atoms in state a and b respectively. Note the absence of factor $1/2$ in the $a - b$ interaction term, which is best understood in first quantization point of view: all the pairs of atoms of the form $a : i, b : j$, where i running from 1 to N_a labels the atoms in a and j running from 1 to N_b labels the atoms in b, are different so that there is no double counting of these interaction terms and no factor $1/2$ is required.

Using the trick of §5.1.3 we can rapidly derive the Gross-Pitaevskii equations for the condensate wavefunctions ϕ_a in state a and ϕ_b in state b, both wavefunctions being normalized to unity. One simply has to write the Heisenberg equations of motion for the field operators and perform the substitution

$$
\begin{align}
\hat{\psi}_a &\rightarrow N_a^{1/2}\phi_a \tag{275} \\
\hat{\psi}_b &\rightarrow N_b^{1/2}\phi_b \tag{276}
\end{align}
$$

where $N_{a,b}$ are the number of particles in condensates a, b. As in §6.2.1 we restrict to the case of atoms trapped in a cubix box of size L with periodic boundary conditions. We obtain the coupled time dependent Gross-Pitaevskii equations

$$
\begin{align}
i\hbar\partial_t\phi_a &= \left[-\frac{\hbar^2}{2m}\Delta + N_a g_{aa}|\phi_a|^2 + N_b g_{ab}|\phi_b|^2\right]\phi_a \\
i\hbar\partial_t\phi_b &= \left[-\frac{\hbar^2}{2m}\Delta + N_b g_{bb}|\phi_b|^2 + N_a g_{ab}|\phi_a|^2\right]\phi_b. \tag{277}
\end{align}
$$

Consider now a steady state solution of these coupled Gross-Pitaevskii equations. As we have not introduced any coherent coupling between the internal states a and b (no $\hat{\psi}_b^\dagger\hat{\psi}_a$ term in the Hamiltonian) ϕ_a and ϕ_b can have in steady state time dependent phase factors evolving with *different* frequencies:

$$
\begin{align}
\phi_a(\vec{r}, t) &= \phi_{a,0}(\vec{r})e^{-i\mu_a t/\hbar} \tag{278} \\
\phi_b(\vec{r}, t) &= \phi_{b,0}(\vec{r})e^{-i\mu_b t/\hbar} \tag{279}
\end{align}
$$

From a more thermodynamical perspective we can also observe that the number of particles N_a and N_b are separately conserved by the three elastic interactions of Eq.(273) so that *two* distinct chemical potentials μ_a and μ_b are required to describe the equilibrium state.

The time independent Gross-Pitaevskii equations for $\phi_{a,0}$ and $\phi_{b,0}$ in the box have the natural solutions

$$
\phi_{a,0}(\vec{r}) = \phi_{b,0}(\vec{r}) = \frac{1}{L^{3/2}} \tag{280}
$$

leading to the following expressions for the chemical potentials:

$$
\begin{align}
\mu_a &= \rho_{a,0}g_{aa} + \rho_{b,0}g_{bb} \tag{281} \\
\mu_b &= \rho_{b,0}g_{bb} + \rho_{a,0}g_{ab} \tag{282}
\end{align}
$$

where $\rho_{a,b}$ are the condensate densities in a, b. Although we assume here that all the coupling constants are positive it is physically intuitive that these spatially uniform solutions should become instable when the interactions between a and b are very repulsive; one then feels that the two condensates a and b have a tendency to spatially separate.

To test this expectation we linearize the time dependent coupled Gross-Pitaevskii equations around the steady state, setting

$$\phi_a(\vec{r}, t) = e^{-i\mu_a t/\hbar} \left[\phi_{a,0}(\vec{r}) + \delta\phi_a(\vec{r}, t) \right] \tag{283}$$

$$\phi_b(\vec{r}, t) = e^{-i\mu_b t/\hbar} \left[\phi_{b,0}(\vec{r}) + \delta\phi_b(\vec{r}, t) \right]. \tag{284}$$

We obtain

$$i\hbar\partial_t\delta\phi_a = -\frac{\hbar^2}{2m}\Delta\delta\phi_a + \rho_{a,0}g_{aa}[\delta\phi_a + \delta\phi_a^*] + \rho_{b,0}g_{ab}[\delta\phi_b + \delta\phi_b^*] \tag{285}$$

and a similar equation for $\delta\phi_b$ exchanging the role of a and b indices. We look for eigenmodes of these linear equations, with eigenfrequency $\epsilon/\hbar$ and a well defined wavevector $\vec{k}$. This amounts to performing the substitutions

$$\delta\phi_a(\vec{r}, t) \rightarrow u_a e^{i(\vec{k}\cdot\vec{r} - \epsilon t/\hbar)}$$

$$\delta\phi_a^*(\vec{r}, t) \rightarrow v_a e^{i(\vec{k}\cdot\vec{r} - \epsilon t/\hbar)}$$

and equivalent changes for the b components. This leads to the eigensystem

$$\left[\epsilon - \frac{\hbar^2 k^2}{2m}\right]u_a = \left[-\epsilon - \frac{\hbar^2 k^2}{2m}\right]v_a = \rho_{a,0}g_{aa}\left[u_a + v_a\right] + \rho_{b,0}g_{ab}\left[u_b + v_b\right] \tag{286}$$

and similar equations obtained by exchanging the indices a and b. Taking as new variables the sums and the differences between u and v and using the first identity in Eq.(286) we eliminate the differences as functions of the sums:

$$u_a - v_a = \frac{2m\epsilon}{\hbar^2 k^2}\left[u_a + v_a\right]. \tag{287}$$

We get from the second equality in Eq.(286) (and $a \leftrightarrow b$) a two by two system for the sums $u_a + v_a$, $u_b + v_b$:

$$\left\{\frac{\hbar^2 k^2}{2m}\left[1 - \left(\frac{2m\epsilon}{\hbar^2 k^2}\right)^2\right] \text{Id} + M\right\}\begin{pmatrix} u_a + v_a \\ u_b + v_b \end{pmatrix} = 0 \tag{288}$$

where we have introduced the two by two matrix

$$M = \begin{pmatrix} \rho_{a,0} g_{aa} & \rho_{b,0} g_{ab} \\ \rho_{a,0} g_{ab} & \rho_{b,0} g_{bb} \end{pmatrix}. \tag{289}$$

This leads to the following condition for the spectrum:

$$\epsilon^2 = \left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\eta_{1,2} \right) \right] \tag{290}$$

where $\eta_{1,2}$ are the eigenvalues of M.

In the thermodynamical limit the mixture of condensates with uniform densities is dynamically stable provided that both eigenvalues $\eta_{1,2}$ are positive. This is equivalent to the requirement that the symmetric matrix M is positive. As $g_{aa} > 0$ here this is ensured provided that the determinant of M is positive:

$$\det M = \rho_{a,0} \rho_{b,0} \left[g_{aa} g_{bb} - g_{ab}^2 \right] \geq 0. \tag{291}$$

The mixture of spatially uniform condensates is therefore stable if

$$g_{ab} \leq (g_{aa} g_{bb})^{1/2}. \tag{292}$$

In this case one can check that the spectrum of the $+$ family is given by the positive solutions ϵ to Eq.(290). The spectrum of the binary mixtures of condensates is then made of two branches, which are both linear at low momenta with sound velocities $(\eta_{1,2}/m)^{1/2}$.

What happens when this stability condition is not satisfied ? The condensates a and b have a tendency to separate spatially. This happens in the JILA experiment [42]. Actually our model in a box is too crude to be applied to the experimental case of particles in a harmonic trap, the stability condition Eq.(292) being marginally satisfied for ^{87} Rb; a numerical solution of the time dependent Gross-Pitaevskii equations is required in this case [43].

The occurrence of demixing when Eq.(292) is violated can be connected with the following simple energy argument. Consider a demixed configuration with all the N_a atoms in the left part of the box in a volume νL^3 and all the N_b atoms in the right part of the box in the complementary volume $(1-\nu)L^3$. The condensate densities vanish on a scale on the order of the healing length ξ of the gas, this leads to "surface" kinetic and

interaction energies negligible in the thermodynamical limit as compared to the volume interaction energy

$$\frac{N_a^2 g_{aa}}{2\nu L^3} + \frac{N_b^2 g_{bb}}{2(1-\nu)L^3}. \tag{293}$$

We minimize this energy over ν to obtain

$$E_{\text{demix}} = \frac{1}{2L^3} \left[N_a^2 g_{aa} + N_b^2 g_{bb} + 2N_a N_b (g_{aa}g_{bb})^{1/2} \right]. \tag{294}$$

We find that the demixed configuration has an energy lower than the one of the spatially uniform configuration

$$E_{\text{unif}} = \frac{1}{2L^3} \left[N_a^2 g_{aa} + N_b^2 g_{bb} + 2N_a N_b g_{ab} \right] \tag{295}$$

precisely when the stability condition Eq.(292) of the uniform configuration is violated.

6.3 Linear response in the classical hydrodynamic approximation

We consider in this subsection the case of a condensate in a harmonic trap. The eigenmodes of the linearized Gross-Pitaevskii equation can then in general be determined only numerically. In the Thomas-Fermi regime however approximate results can be obtained for the low energy eigenmodes of the system from the classical hydrodynamic approach, as we shall see now.

6.3.1 Linearized classical hydrodynamic equations

The classical hydrodynamic equations for the position dependent condensate density $\rho(\vec{r})$ and velocity field $\vec{v}(\vec{r})$ have been derived in §5.3.4:

$$\partial_t \rho + \text{div}\left[\rho\, \vec{v}\right] = 0 \tag{296}$$

$$m\left(\partial_t + \vec{v}\cdot\vec{\text{grad}}\right)\vec{v} = -\vec{\text{grad}}[U + \rho g]. \tag{297}$$

We linearize these equations around their steady state solution with density ρ_0 and vanishing velocity field $\vec{v}_0 = \vec{0}$ in the unperturbed trapping potential U_0. Writing the trap potential as a perturbation of U_0:

$$U(\vec{r},t) = U_0(\vec{r}) + \delta U(\vec{r},t) \tag{298}$$

and splitting ρ and $\vec{v}$ as

$$\rho(\vec{r}, t) = \rho_0(\vec{r}) + \delta\rho(\vec{r}, t) \tag{299}$$

$$\vec{v}(\vec{r}, t) = \vec{0} + \delta\vec{v}(\vec{r}, t) \tag{300}$$

we obtain the linearized equations:

$$\partial_t \delta\rho + \text{div}\left[\rho_0 \delta\vec{v}\right] = 0$$

$$m\partial_t \delta\vec{v} + \vec{\text{grad}}[\delta\rho g] = -\vec{\text{grad}}\,\delta U. \tag{301}$$

Taking the time derivative of the first equation we obtain a term $\partial_t \delta\vec{v}$ that we can eliminate with the second equation. This results in a closed equation for the perturbation of density:

$$\partial_t^2 \delta\rho - \text{div}\left[\frac{\rho_0 g}{m}\vec{\text{grad}}\,\delta\rho\right] = \text{div}\left[\frac{\rho_0}{m}\vec{\text{grad}}\,\delta U\right]. \tag{302}$$

The homogeneous part of this equation can be rewritten in a more suggestive way by introducing the position dependent velocity c_s given by

$$mc_s^2(\vec{r}) = \rho_0(\vec{r})g. \tag{303}$$

The homogeneous part of Eq.(302) then reads

$$\partial_t^2 \delta\rho - \text{div}\left[c_s^2(\vec{r})\vec{\text{grad}}\,\delta\rho\right] \tag{304}$$

which corresponds to the propagation of sound waves with a position dependent sound velocity $c_s(\vec{r})$. Note that the expression (303) could be expected from the result Eq.(265) obtained in the spatially homogeneous case.

The propagation of sound waves in a cigar shaped trapped condensate has been observed in Ketterle's group at MIT; the condensate was excited mechanically by the dipole force induced by a far detuned laser beam focused at the center of the trap. It is instructive to note that to predict theoretically the velocity of sound obtained in the experiment one has to carefully solve Eq.(302), rather than to take naively the sound velocity on the axis of the trap; the naive expectation would be wrong by a factor of $\sqrt{2}$ [44, 45].

6.3.2 Validity condition of the linearized classical hydrodynamic equations

The classical hydrodynamic equations have been obtained from the time dependent Gross-Pitaevskii equation in hydrodynamic point of view by neglecting the quantum pressure

term (see §5.3.4). If we keep this term and linearize the resulting equation we get extra terms with respect to Eq.(301). One of the extra terms is

$$\frac{\hbar^2}{m\rho_0}\Delta\delta\rho \tag{305}$$

which should be small as compared to the "classical" pressure term $g\delta\rho$:

$$\frac{\hbar^2}{m\rho_0}|\Delta\delta\rho| \ll g|\delta\rho|. \tag{306}$$

If we denote by k a typical wavevector for the spatial variation of $\delta\rho$, $\Delta\delta\rho \sim -k^2\delta\rho$ and the condition for neglecting the quantum pressure term reads

$$\frac{\hbar^2 k^2}{m} \ll g\rho_0. \tag{307}$$

This condition can be rewritten in a variety of ways. It claims that the wavevector k should satisfy

$$k\xi \ll 1 \tag{308}$$

where $\xi = \hbar/(2m\rho_0 g)^{1/2}$ is the healing length of the condensate. Eq.(302) cannot be used to describe perturbations of the condensate at a length scale on the order of ξ or smaller.

The validity condition can also be written as

$$\hbar k \ll mc_s \quad \text{or} \quad \hbar k c_s \ll mc_s^2 = \rho_0 g \sim \mu \tag{309}$$

In terms of the Bogoliubov spectrum for the homogeneous condensate this means that the wavevector k has to be in the *linear* part of the excitation spectrum. The energy of the corresponding eigenmode $\sim \hbar k c_s$ has to be much smaller than μ. Therefore only the eigenmodes of Eq.(302) with eigenenergy much less than μ are relevant:

$$\epsilon \ll \mu \tag{310}$$

the higher energy modes are not an acceptable approximation of the exact eigenmodes of the condensate. Note that as shown in [46, 47], Eq.(310) is a necessary but not sufficient condition in a trap.

6.3.3 Approximate spectrum in a harmonic trap

We look for eigenmodes of the homogeneous part of Eq.(302) with eigenenergy ϵ. They solve the eigenvalue equation

$$-\epsilon^2 \delta\rho = \operatorname{div}\left[c_s^2(\vec{r})\vec{\operatorname{grad}}\,\delta\rho\right]. \tag{311}$$

In the present Thomas-Fermi regime c_s^2 is a quadratic function of the coordinates as it is proportional to the condensate density ρ_0. We can therefore solve the eigenvalue equation using an ansatz for $\delta\rho$ polynomial in the spatial coordinates x, y, z. If $\delta\rho$ is a polynomial of total degree n, $\vec{\operatorname{grad}}\,\delta\rho$ is a polynomial of total degree $n-1$; after multiplication by c_s^2 and action of the div operator we get a polynomial of total degree $(n-1)+2-1 = n$. The subspace of polynomials of degree $\leq n$ is therefore stable.

For low values of the total degree n an analytical calculation is possible. For example in a general harmonic trap with atomic oscillation frequencies $\omega_x, \omega_y, \omega_z$ one can check that the polynomials $\delta\rho = x, y, z$ (respectively) are eigenvectors with eigenvalues $\epsilon = \hbar\omega_x, \hbar\omega_y, \hbar\omega_z$ (respectively). These three modes correspond to the oscillation of the center of mass of the gas, which is exactly decoupled from all the relative coordinates of the particles in a harmonic trap; for this specific example the frequencies (but not the modes!) predicted by classical hydrodynamics are exact. These "sloshing" modes are used experimentally to determine accurately the trap frequencies $\omega_{x,y,z}$.

Another important example is the case of a total degree $n=2$. One can check that the subclass of polynomials involving the monomials x^2, y^2, z^2 and 1 is stable, which corresponds to the ansatz

$$\delta\rho(\vec{r}) = B + \sum_{\alpha=x,y,z} A_\alpha r_\alpha^2. \tag{312}$$

By inserting this ansatz into Eq.(311) we arrive at the eigenvalue system

$$(\epsilon/\hbar)^2 A_\alpha = 2\omega_\alpha^2 A_\alpha + \omega_\alpha^2 \sum_\beta A_\beta. \tag{313}$$

This eigenvalue system can be obtained more directly as in Eq.(216) by a linearization of the equations Eq.(212) for the scaling parameters λ_α around their steady state value $\lambda_\alpha = 1$. Physically the modes identified by the ansatz (312) are therefore breathing modes of the condensate. The frequency of one of these modes (the one of §5.4.3) has been measured with high precision at MIT in a cigar-shaped trap, it differs from the Thomas-Fermi prediction $\simeq (5/2)^{1/2}\omega_z$ (see Eq.(218)) by less than one percent [48].

In the case of an isotropic harmonic trap all the eigenenergies ϵ can be calculated analytically (keeping in mind that modes with $\epsilon > \mu$ are not properly described by classical hydrodynamics !). As shown in [49] one uses the rotational symmetry of the problem, as in the case of Schrödinger's equation for the hydrogen atom, with the ansatz

$$\delta\rho(\vec{r}) = Y_l^m(\theta, \phi) r^l P_{l,n}(r) \tag{314}$$

where θ, ϕ are the polar and azimuthal angles of spherical coordinates, Y_l^m is the spherical harmonic of angular momentum l. The last factor $P_{l,n}(r)$ is a polynomial of degree n in r. As $P_{l,n}$ is a polynomial the recurrence relation obtained from Eq.(311) for the coefficients of the monomials r^j should terminate at $j = n$. This leads to the eigenfrequencies $\Omega = \epsilon/\hbar$ such that

$$\Omega^2 = (2n^2 + 2nl + 3n + l)\omega^2 \text{ for any } n, l \geq 0 \tag{315}$$

where ω is the oscillation frequency of the atoms in the trap. For $l = 1, n = 0$ we recover the sloshing modes with frequency $\Omega = \omega$.

7 Bogoliubov approach and thermodynamical stability

Imagine that we have already checked the dynamical stability of a steady state solution ϕ_0 of the Gross-Pitaevskii equation for the condensate wavefunction. We cannot relax yet and be sure that the condensate will remain in state ϕ_0 in the long run.

What is missing is a check that interaction of the condensate with the non-condensed cloud does not induce an evolution of the condensate far from the predicted ϕ_0. We have to check what is called thermodynamical stability of the condensate as it involves the "thermal", non-condensed component of the gas.

This check will be performed in the low temperature domain ($T \ll T_c$) using the Bogoliubov approach. We will then present examples of thermodynamical instabilities.

We give here a summarized account of the $U(1)$-symmetry preserving Bogoliubov approach developed in [50, 51]. In contrast to the almost general attitude in the literature this approach does not assume a symmetry breaking state with $\langle \hat{\psi} \rangle \neq 0$ but considers instead a state with a fixed total number of particles. A different $U(1)$-symmetry preserving Bogoliubov approach was developed long ago in [52].

This allows to eliminate a technical problem of the symmetry breaking approach: if $\langle\hat{\psi}\rangle(t=0)\neq 0$ the state of the system necessarily involves a coherent superposition of states with different total number of particles; such a state *cannot be stationary* (as states with different number of particles have also different energies) and it experiences a phase collapse $\langle\hat{\psi}\rangle(t)\to 0$ making the description of the evolution of the system more involved.

7.1   Small parameter of the theory

We restrict in this section to a steady state regime where most of the atoms of the gas are in the condensate. We split the atomic field operator as

$$\hat{\psi}(\vec{r}) = \phi_0(\vec{r})\hat{a}_{\phi_0} + \delta\hat{\psi}(\vec{r}) \tag{316}$$

where ϕ_0 is the condensate wavefunction and $\hat{a}_{\phi_0}$ annihilates a particle in the mode ϕ_0. The idea is to treat $\delta\hat{\psi}$ as a perturbation with respect to $\phi_0\hat{a}_{\phi_0}$: Let us compare indeed the typical matrix elements of these two operators:

$$\delta\hat{\psi} \sim \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle^{1/2} \sim (\rho')^{1/2} \tag{317}$$

where ρ' is the density of non-condensed particles whereas

$$\phi_0\hat{a}_{\phi_0} \sim N_0^{1/2}\phi_0 \sim \rho_0^{1/2} \tag{318}$$

where ρ_0 is the condensate density. We will therefore assume

$$\rho' \ll \rho_0 \tag{319}$$

and even more

$$N' = \int d^3\vec{r}\,\rho'(\vec{r}) \ll N_0 \simeq N \tag{320}$$

where N is the total number of particles in the gas. Using these two assumptions a systematic expansion of the field equations in powers of the small parameter

$$\varepsilon = (N'/N_0)^{1/2} \ll 1 \tag{321}$$

can be performed. We give here a somewhat simplified presentation.

The following identities are important properties of $\delta\hat{\psi}$. First, $\delta\hat{\psi}$ is the part of the atomic field operator transverse to the condensate wavefunction:

$$\int d^3\vec{r}\,\phi_0{}^*(\vec{r})\delta\hat{\psi}(\vec{r}) = 0. \tag{322}$$

As a consequence the bosonic commutation relation obeyed by $\delta\hat{\psi}$ involves matrix elements of the projector Q orthogonal to ϕ_0 rather than the identity operator:

$$[\delta\hat{\psi}(\vec{r_1}), \delta\hat{\psi}^\dagger(\vec{r_2})] = \langle\vec{r_1}|Q|\vec{r_2}\rangle = \delta(\vec{r_1} - \vec{r_2}) - \phi_0(\vec{r_1})\phi_0^*(\vec{r_2}). \tag{323}$$

Second, there should be no coherence in the one-body density matrix between the condensate and the non-condensed modes, or equivalently ϕ_0 should be an eigenstate of the one-body density matrix (with eigenvalue N_0):

$$\langle\hat{a}_{\phi_0}^\dagger\delta\hat{\psi}\rangle = 0. \tag{324}$$

This last identity is used to calculate the condensate wavefunction order by order in the small parameter [50, 51].

7.2 Zeroth order in ε: Gross-Pitaevskii equation

To zeroth order in ε all the particles are supposed to be in the condensate. In steady state one then recovers the time independent Gross-Pitaevskii equation with the further approximation $N_0 \simeq N$:

$$\mu\phi_0 = \left[-\frac{\hbar^2}{2m}\Delta + U + gN|\phi_0|^2\right]\phi_0. \tag{325}$$

7.3 Next order in ε: linear dynamics of non-condensed particles

Calculation to first order in ε corresponds to a linearization of the Heisenberg field equations around $\phi_0\hat{a}_{\phi_0}$ keeping terms up to first order in $\delta\hat{\psi}$. Equivalently it corresponds to a quadratization of the Hamiltonian around $\phi_0\hat{a}_{\phi_0}$ keeping terms up to second order in $\delta\hat{\psi}$.

We use this quadratization approach here. At this order of the calculation the regularizing operator of the pseudo-potential can be neglected, divergences due the use of

the non-regularized $g\delta$ potential coming at the next order ε^2. We therefore take the Hamiltonian

$$\hat{H} = \int d^3\vec{r} \left[\hat{\psi}^\dagger h_1 \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right]. \tag{326}$$

The one-body Hamiltonian h_1 contains the kinetic energy and the trapping potential energy:

$$h_1 = -\frac{\hbar^2}{2m} \Delta + U. \tag{327}$$

It does not contain any $-\mu$ term as we use here in the canonical rather than grand canonical point of view, the total number of particles being fixed to N.

We substitute expansion (316) for Eq.(326) and we keep terms up to quadratic in $\delta\hat{\psi}$.

• The contribution of h_1 is quadratic in $\hat{\psi}$ so that all the terms should be kept. One of the contributions is

$$(\int d^3\vec{r} \, \phi_0^* h_1 \phi_0) \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}. \tag{328}$$

One can use the following trick to express this quantity in terms of $\delta\hat{\psi}$: from Eq.(322) one sees that the total number of particles operator can be written as

$$\hat{N} \equiv \int d^3\vec{r} \, \hat{\psi}^\dagger \hat{\psi} = \hat{n}_{\phi_0} + \delta\hat{N} \tag{329}$$

that is the sum of the number operator of condensate particles:

$$\hat{n}_{\phi_0} = \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \tag{330}$$

and the number operator of non-condensed particles:

$$\delta\hat{N} = \int d^3\vec{r} \, \delta\hat{\psi}^\dagger \delta\hat{\psi}. \tag{331}$$

We therefore obtain

$$\hat{n}_{\phi_0} = \hat{N} - \delta\hat{N}. \tag{332}$$

• The expansion of the interaction term gives the following up to quadratic contributions:

$$\begin{aligned}
\frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \rightarrow \quad & \frac{g}{2} |\phi_0|^4 \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \hat{a}_{\phi_0} \\
+ \quad & g[\phi_0^* \phi_0^* \phi_0 \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \delta\hat{\psi} + \text{h.c.}] \\
+ \quad & \frac{g}{2} [\phi_0^* \phi_0^* \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \delta\hat{\psi} \delta\hat{\psi} + \text{h.c.}] \\
+ \quad & 2g \phi_0^* \phi_0 \hat{a}_{\phi_0}^\dagger \delta\hat{\psi}^\dagger \delta\hat{\psi} \hat{a}_{\phi_0}.
\end{aligned} \tag{333}$$

The first line of this expression is transformed using Eq.(332):

$$\hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \hat{a}_{\phi_0} = \hat{n}_{\phi_0}(\hat{n}_{\phi_0} - 1) = \hat{N}(\hat{N} - 1) - 2\hat{N}\delta\hat{N} + \dots \tag{334}$$

with $N \simeq N - 1$. When we group the above term in $\delta\hat{N}$ with the one coming from h_1 and we replace $\hat{N}$ by N we obtain

$$-\delta\hat{N} \left[\int d^3\vec{r}\, \phi_0{}^* h_1 \phi_0 + N g |\phi_0|^4 \right] = -\mu\delta\hat{N} \tag{335}$$

as ϕ_0 solves the Gross-Pitaevskii equation (325). This is amusing: we obtain formally a grand canonical Hamiltonian for the non-condensed particles, the reservoir being formed by the condensate particles! In the second line of Eq.(333) we replace $\hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}$ by N as the corrective term $\delta\hat{N}$ would lead to a cubic contribution in $\delta\hat{\psi}$.

Another important transformation is performed by collecting the terms linear in $\delta\hat{\psi}$ from Eq.(333) and from the contribution of h_1, leading to

$$\int d^3\vec{r}\, \phi_0{}^* \hat{a}_{\phi_0}^\dagger [h_1 + g|\phi_0|^2 N]\delta\hat{\psi} + \text{h.c.} \tag{336}$$

As ϕ_0 solves the Gross-Pitaevskii equation, the operator between brackets, when acting on the left on $\phi_0{}^*$, gives a contribution $\mu\phi_0{}^*$ orthogonal to $\delta\hat{\psi}$ (see Eq.(322)). The sum of all the terms linear in $\delta\hat{\psi}$ therefore vanishes! We shall see later that this could be expected from Eq.(324).

7.4 Bogoliubov Hamiltonian

We now collect all the terms of $\hat{H}$ up to quadratic in $\delta\hat{\psi}$ and express them in terms of the field operator

$$\hat{\Lambda}(\vec{r}) = \frac{1}{\hat{N}^{1/2}} \hat{a}_{\phi_0}^\dagger \delta\hat{\psi}(\vec{r}). \tag{337}$$

This operator commutes with the operator $\hat{N}$ giving the total number of particles: it transfers one non-condensed particle into the condensate. As the operator $\delta\hat{\psi}$, it is transverse to ϕ_0 (see Eq.(322)). By definition of the condensate wavefunction $\hat{\Lambda}$ has a zero mean (see Eq.(324)).

In general it is difficult to exactly eliminate $\delta\hat{\psi}$ in terms of $\hat{\Lambda}$. Fortunately at the present order of the calculation we can use the assumption of a very small non-condensed fraction so that one has for example

$$\delta\hat{\psi}^\dagger \delta\hat{\psi} \simeq \delta\hat{\psi}^\dagger \hat{a}_{\phi_0} \hat{N}^{-1} \hat{a}_{\phi_0}^\dagger \delta\hat{\psi} = \hat{\Lambda}^\dagger \hat{\Lambda}. \tag{338}$$

To the same order of approximation $\hat{\Lambda}$ obeys the same commutation relation Eq.(323) as $\delta\hat{\psi}$.

The final result can be written in term of the operator $\mathcal{L}$ introduced in §6, with the approximation $N_0 \simeq N$:

$$\hat{H}_{\text{quad}} = f(\hat{N}) + \frac{1}{2} \int d^3\vec{r}(\hat{\Lambda}^\dagger, -\hat{\Lambda})\mathcal{L}\left(\begin{array}{c} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{array}\right) \tag{339}$$

where the function f is specified in [51].

From this quadratic Hamiltonian the Heisenberg equations of motion for the field $\hat{\Lambda}$ have the suggestive form

$$i\hbar\frac{d}{dt}\left(\begin{array}{c} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{array}\right) = \mathcal{L}\left(\begin{array}{c} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{array}\right). \tag{340}$$

We note that an hypothetic term of $\hat{H}_{\text{quad}}$ linear in $\hat{\Lambda}$ would give rise to a source term in Eq.(340) preventing one from satisfying Eq.(324) at all times!

The result Eq.(340) is really a crucial one. It shows that the linearized evolution of the non-condensed part $\delta\hat{\psi}$ of the atomic field is formally equivalent to the linearized response of the condensate to a classical perturbation (e.g. of the trapping potential) derived from the Gross-Pitaevskii equation; both treatments indeed exhibit the same operator $\mathcal{L}$ (see Eq.(232)).

All the machinery of §6 can therefore be used. We expand the field operator $\hat{\Lambda}$ on the eigenmodes of $\mathcal{L}$. We assume here dynamical stability and that the only eigenmodes in the 0 family are the zero-energy modes $(\phi_0, 0)$ and $(0, \phi_0{}^*)$ to which the field $\hat{\Lambda}$ is orthogonal according to Eq.(322). We therefore get an expansion similar to Eq.(251):

$$\left(\begin{array}{c} \hat{\Lambda}(\vec{r}) \\ \hat{\Lambda}^\dagger(\vec{r}) \end{array}\right) = \sum_{k\in+\text{family}} \hat{b}_k\left(\begin{array}{c} u_k(\vec{r}) \\ v_k(\vec{r}) \end{array}\right) + \hat{b}_k^\dagger\left(\begin{array}{c} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{array}\right) \tag{341}$$

with the important difference that the coefficients in the expansion are now operators:

$$\hat{b}_k = \int d^3\vec{r}\left[u_k^*(\vec{r})\hat{\Lambda}(\vec{r}) - v_k^*(\vec{r})\hat{\Lambda}^\dagger(\vec{r})\right]. \tag{342}$$

From the normalization condition between the eigenvectors of $\mathcal{L}$ and their adjoint vectors (see §6) one shows that the $\hat{b}_k$ obey bosonic commutation relations:

$$[\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{k,k'} \quad \text{and} \quad [\hat{b}_k, \hat{b}_{k'}] = 0. \tag{343}$$

$\hat{b}_k$ corresponds formally to an annihilation operator; as $|v_k\rangle \neq 0$ in general $\hat{b}_k$ does not simply annihilate a particle as it is a coherent superposition of $\hat{\Lambda}$ (which transfers one non-condensed particle to the condensate) and of $\hat{\Lambda}^\dagger$ (which transfers one condensate particle to the non-condensed fraction). One then says that $\hat{b}_k$ annihilates a *quasi-particle* in mode k.

Finally we rewrite the Hamiltonian Eq.(339) in terms of the $\hat{b}_k$'s:

$$\hat{H}_{\text{quad}} = E_0(\hat{N}) + \sum_{k \in +\text{family}} \epsilon_k \hat{b}_k^\dagger \hat{b}_k. \tag{344}$$

We recall that ϵ_k is the eigenenergy of the mode (u_k, v_k) of the $+$ family. Our quadratic Hamiltonian describes a gas of non-interacting quasi-particles: this is the so-called Bogoliubov Hamiltonian.

The ground state of $\hat{H}_{\text{quad}}$ is obtained when no quasi-particle is present, it corresponds to all the modes k being in vacuum state:

$$\hat{H}_{\text{quad}}|0\rangle = E_0(N)|0\rangle \tag{345}$$

where

$$\hat{b}_k|0\rangle = 0 \quad \forall k. \tag{346}$$

E_0 is therefore the Bogoliubov approximation for the ground state energy of the gas. To get a finite expression for E_0 one has to include the regularizing operator in the pseudo-potential.

The excited states of the system are obtained in the Bogoliubov approximation by successive actions of the $\hat{b}_k^\dagger$'s. For this reason $\hat{b}_k^\dagger$ is said to create an *elementary* excitation k in the system, to distinguish with *collective* excitations involving all the particles of the condensate (induced e.g. by a perturbation δU of the trapping potential). We emphasize again that the elementary excitations of the gas have the same frequency $\epsilon_k/\hbar$ as the collective excitations in the linear response domain (δU small enough). This intriguing property is valid only at the presently considered regime of an almost pure condensate ($T \ll T_c$).

7.5   Order ε^2: corrections to the Gross-Pitaevskii equation

Expanding the Heisenberg field equations for $\hat{\psi}$ keeping terms up to $N^{1/2}\varepsilon^2$ one can calculate the first correction to the prediction Eq.(325) for the condensate wavefunction.

This correction includes (i) the fact that the number of condensate particles N_0 rather than the total number of particles N should appear in the Gross-Pitaevskii equation, and (ii) the mechanical back-action of the non-condensed particles on the condensate in the form of mean field potentials.

The calculations are a bit involved [51] and require the use of the regularizing operator in the pseudo-potential (a fact realized in [53] but not yet in [51]). We give here only the result. The condensate wavefunction is given by an expansion

$$\phi_0 = \phi_0{}^{(0)} + \phi_0{}^{(2)} + o(\varepsilon^2) \tag{347}$$

where $\phi_0{}^{(0)}$, zeroth order approximation in ε, is the solution of Eq.(325). The correction $\phi_0{}^{(2)}$ is of order ε^2; its component on $\phi_0{}^{(0)}$ is purely imaginary (as both ϕ_0 and $\phi_0{}^{(0)}$ are normalized to unity) and can be considered as a (not physically relevant) change of global phase of $\phi_0{}^{(0)}$; the part of $\phi_0{}^{(2)}$ orthogonal to $\phi_0{}^{(0)}$ is given by:

$$-\mathcal{L}\left(\begin{array}{c} Q\phi_0{}^{(2)} \\ Q^*\phi_0{}^{(2)*} \end{array} \right) = \left(\begin{array}{c} QS \\ -Q^*S^* \end{array} \right) \tag{348}$$

where Q projects orthogonally to ϕ_0 and where the source term S is equal to

$$
\begin{aligned}
S(\vec{r}) = \ -\ & (1 + \langle\delta\hat{N}\rangle)g|\phi_0{}^{(0)}(\vec{r})|^2\phi_0{}^{(0)}(\vec{r}) \\
+\ & 2g\langle\hat{\Lambda}^\dagger(\vec{r})\hat{\Lambda}(\vec{r})\rangle\phi_0{}^{(0)}(\vec{r}) + g\left[\partial_s\left(s\langle\hat{\Lambda}(\vec{r}-\vec{s}/2)\hat{\Lambda}(\vec{r}+\vec{s}/2)\rangle\right)\right]_{s\to0}\phi_0{}^{(0)*}(\vec{r}) \\
-\ & g\int d^3\vec{s}\,|\phi_0{}^{(0)}(\vec{s})|^2\langle\left[\hat{\Lambda}^\dagger(\vec{s})\phi_0{}^{(0)}(\vec{s}) + \hat{\Lambda}(\vec{s})\phi_0{}^{(0)*}(\vec{s})\right]\hat{\Lambda}(\vec{r})\rangle.
\end{aligned} \tag{349}
$$

The first line of this expression contains the effect of the depletion of the condensate, the number of non-condensed particles $\langle\delta\hat{N}\rangle$ being calculated in the Bogoliubov approximation, see discussion in §7.7. The other terms are mean field terms, among which one recognizes the Hartree-Fock contribution $2g\langle\hat{\Lambda}^\dagger(\vec{r})\hat{\Lambda}(\vec{r})\rangle$ already obtained in §4.

7.6   Thermal equilibrium of the gas of quasi-particles

In the Bogoliubov approximation the quasi-particles behave as an ideal Bose gas; such a gas can reach thermal equilibrium only by contact with a thermostat. There is no such thermostat in the experiments on trapped Bose gas, relaxation to thermal equilibrium has to be provided instead by interactions between the atoms.

Fortunately the full Hamiltonian Eq.(326) contains terms cubic and quartic in $\delta\hat{\psi}$: when expressed in terms of the $\hat{b}$'s and $\hat{b}^\dagger$'s they correspond to interactions between the quasi-particles which will provide thermalization. Two situations can then be considered, depending on the sign of ϵ_k.

• "Good" case: $\epsilon_k > 0$ for all k in $+$ family. We assume for simplicity thermal equilibrium in the canonical point of view (which should be equivalent to the microcanonical point of view in the limit of large number of particles) with a N-body density matrix

$$\hat{\rho}_{1,\dots,N} = \frac{1}{Z}e^{-\beta\hat{H}} \simeq \frac{1}{Z_{\text{quad}}}e^{-\beta\hat{H}_{\text{quad}}}. \tag{350}$$

We suppose therefore that the interactions between quasi-particles, essential to ensure thermalization, have a weak effect on the thermal equilibrium state. From Eq.(350) we finally obtain the mean number of quasi-particles in mode k:

$$\langle\hat{b}_k^\dagger\hat{b}_k\rangle = \frac{1}{e^{\beta\epsilon_k} - 1}. \tag{351}$$

This good case corresponds to a thermodynamically stable condensate in state ϕ_0.

• "Bad" case: there is a mode k_0 in the $+$ family such that $\epsilon_{k_0} < 0$. In this case the quadratic Hamiltonian $\hat{H}_{\text{quad}}$ contains a harmonic oscillator of frequency $\omega_{k_0} = |\epsilon_{k_0}|/\hbar$ having formally a negative mass M:

$$-|\epsilon_{k_0}|\hat{b}_{k_0}^\dagger\hat{b}_{k_0} = \frac{1}{2M}[\hat{P}_{k_0}^2 + \omega_{k_0}^2\hat{Q}_{k_0}^2] \tag{352}$$

where $\hat{P}_{k_0}$ and $\hat{Q}_{k_0}$ correspond formally to a momentum and position operator. By collisions with the quasi-particles of positive energy the mode k_0 can loose energy which increases its own excitation; if the number of quanta in the mode can become comparable to N the process of thermalization of the gas may lead the condensate to a state different from the predicted ϕ_0.

This phenomenon of thermodynamical instability should not be confused with dynamical instability of the condensate, where ϵ_{k_0} is complex; e.g. the case of a purely imaginary ϵ_{k_0} corresponds formally to an oscillator in an expelling potential, $[\hat{P}_{k_0}^2 - |\omega_{k_0}|^2\hat{Q}_{k_0}^2]/(2M)$.

7.7 Condensate depletion and the small parameter $(\rho a^3)^{1/2}$

We assume the situation of thermodynamical stability. We calculate the mean number $\langle\delta\hat{N}\rangle$ of particles out of the condensate, that is in all the modes orthogonal to the con-

densate wavefunction ϕ_0 :

$$\langle \delta \hat{N} \rangle \equiv \int d^3\vec{r} \, \langle \delta \hat{\psi}^\dagger(\vec{r}) \delta \hat{\psi}(\vec{r}) \rangle. \tag{353}$$

In this way we can calculate explicitly the small parameter of the present theory given in Eq.(321).

To lowest order in the Bogoliubov approximation we can replace $\delta \hat{\psi}$ by $\hat{\Lambda}$ in the above expression:

$$\langle \delta \hat{N} \rangle \simeq \int d^3\vec{r} \, \langle \hat{\Lambda}^\dagger(\vec{r}) \hat{\Lambda}(\vec{r}) \rangle. \tag{354}$$

We replace $\hat{\Lambda}$ by its modal expansion; using the approximation in Eq.(350) the only terms with non-zero mean are $\langle \hat{b}_k^\dagger \hat{b}_k \rangle$ given by Eq.(351) and

$$\langle \hat{b}_k \hat{b}_k^\dagger \rangle = \langle \hat{b}_k^\dagger \hat{b}_k \rangle + 1. \tag{355}$$

We therefore obtain:

$$\begin{aligned} \langle \delta \hat{N} \rangle \quad \simeq \quad & \sum_{k \in +\text{family}} \langle \hat{b}_k^\dagger \hat{b}_k \rangle [\langle u_k | u_k \rangle + \langle v_k | v_k \rangle] \\ & + \sum_{k \in +\text{family}} \langle v_k | v_k \rangle. \end{aligned} \tag{356}$$

The contribution of the occupation numbers $\langle \hat{b}_k^\dagger \hat{b}_k \rangle$ corresponds to the so-called thermal depletion of the condensate, as it is non-zero only at finite temperature. The contribution of the $+1$ coming from the identity (355) is the so-called quantum depletion of the condensate: it expresses the fact that, even at zero temperature, there is a finite number of particles out of the condensate due to atomic interactions, contrarily to the ideal Bose gas case where all the v_k 's vanish.

It is instructive to calculate the depletion of the condensate in the homogeneous case in the thermodynamical limit, replacing the sum over the wavevector $\vec{k}$ characterizing each mode of the $+$ family by an integral. From Eq.(262) we calculate

$$\langle u_k | u_k \rangle + \langle v_k | v_k \rangle = 1 + 2\langle v_k | v_k \rangle = \frac{\frac{\hbar^2 k^2}{2m} + \rho g}{\left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\rho g \right) \right]^{1/2}}. \tag{357}$$

At zero temperature we obtained for the non-condensed fraction of particles the following integral:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T = 0) = \frac{16}{\pi^{1/2}} \left(\rho a^3 \right)^{1/2} \int_0^{+\infty} dq \, q^2 \left[\frac{q^2 + 1/2}{q \left(1 + q^2 \right)^{1/2}} - 1 \right] \tag{358}$$

where we have integrated over the solid angle in spherical coordinates and we have made the change of variable

$$\frac{\hbar^2 k^2}{2m} = 2\rho g q^2. \tag{359}$$

This integral can be calculated exactly:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T = 0) = \frac{8}{3\pi^{1/2}} \left(\rho a^3 \right)^{1/2}. \tag{360}$$

In this way we obtain a very important small parameter of the theory, $(\rho a^3)^{1/2}$, which characterizes the domain of a weakly interacting Bose gas. This small parameter is similar to the condition obtained in Eq.(95) of §3 already with a totally different point of view, a condition of Born approximation on the pseudo-potential! In the typical experimental conditions of MIT for sodium atoms we have $\rho \sim 10^{14}$ cm^{-3} and $a \sim 25$ Å, which leads to a small parameter $(\rho a^3)^{1/2} \sim 10^{-3}$. The result (360) also gives us the opportunity to recall that the number of non-condensed particles should not be confused with the number of quasi-particles for an interacting Bose gas: one notes here that the second quantity vanishes at $T = 0$ whereas the first one does not.

At finite temperature there is, in addition to the quantum depletion, a thermal depletion of the condensate:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T) - \frac{\langle \delta \hat{N} \rangle}{N}(0) = \frac{32}{\pi^{1/2}} \int_0^{+\infty} dq \, \frac{q(q^2 + 1/2)}{(q^2 + 1)^{1/2}} \left[\exp \left(2\beta \rho g q (q^2 + 1)^{1/2} \right) - 1 \right]^{-1}. \tag{361}$$

The integral over q depends only on the parameter $\rho g / (k_B T)$. At low temperature $k_B T \ll \rho g$ this parameter is large so that the modes with a $q \sim 1$ have a very low occupation number: one can neglect q as compared to one and one-half (which amounts to restricting to the linear part of the Bogoliubov spectrum) and one obtains a small correction to the zero temperature case:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T) = \frac{\langle \delta \hat{N} \rangle}{N}(0) \left[1 + \left(\frac{\pi k_B T}{2\rho g} \right)^2 + \ldots \right]. \tag{362}$$

At high temperature $k_B T \gg \rho g$ the major fraction of the populated Bogoliubov modes have a q much larger than unity, so that we can now neglect one and one-half as compared to q^2 (which amounts to restricting to the quadratic part of the Bogoliubov spectrum).

To this approximation we recover the ideal Bose gas result

$$\frac{\langle \delta \hat{N} \rangle}{N}(T) \simeq \frac{\zeta(3/2)}{\rho \lambda_{\mathrm{dB}}^3} \tag{363}$$

where λ_{dB} is the thermal de Broglie wavelength and ζ stands for the Riemann Zeta function (see §2). For a given temperature indeed the density of non-condensed particles in presence of a condensate saturates to its maximal value $\zeta(3/2)\lambda_{\mathrm{dB}}^{-3}$ for the ideal Bose gas in a box (see Eq.(5) and Eq.(2)).

In the high temperature regime $k_B T \gg \rho g$ our Bogoliubov approach can therefore be valid only if $\rho \lambda_{\mathrm{dB}}^3 \gg \zeta(3/2)$. Both inequalities on ρ can be satisfied simultaneously only if $2\zeta(3/2)a/\lambda_{\mathrm{dB}} \ll 1$. Amusingly this condition is similar to the condition $a\Delta k \ll 1$ obtained in §3 (see Eq.(96)) for the validity condition of the Born approximation for the pseudo-potential.

7.8 Fluctuations in the number of condensate particles

The Bogoliubov theory that we have presented also allows a calculation of the fluctuations of N_0 in the canonical ensemble. This has the advantage of removing the effect of fluctuations in the total number of particles present in the grand-canonical ensemble, a "trivial" contribution to the fluctuations of N_0.

As the total number of particles is fixed to N the variance of N_0 is exactly equal to the variance of $\delta \hat{N}$, number of non-condensed particles. The mean value of $\delta \hat{N}$ has been given in the previous section, we now have to calculate the mean value of its square:

$$\langle (\delta \hat{N})^2 \rangle = \int d\vec{r}_1 \int d\vec{r}_2 \, \langle \delta\hat{\psi}^\dagger(\vec{r}_1)\delta\hat{\psi}(\vec{r}_1)\delta\hat{\psi}^\dagger(\vec{r}_2)\delta\hat{\psi}(\vec{r}_2) \rangle \tag{364}$$

$$= \langle \delta \hat{N} \rangle + \int d\vec{r}_1 \int d\vec{r}_2 \, \langle \delta\hat{\psi}^\dagger(\vec{r}_1)\delta\hat{\psi}^\dagger(\vec{r}_2)\delta\hat{\psi}(\vec{r}_1)\delta\hat{\psi}(\vec{r}_2) \rangle \tag{365}$$

where we have used the commutation relation Eq.(323) and the fact Eq.(322) that ϕ is orthogonal to $\delta\hat{\psi}$. To lowest order in the Bogoliubov approximation we can replace $\delta\hat{\psi}$ by $\hat{\Lambda}$ in the above expression and take the approximation Eq.(350) for the equilibrium density operator. As $\hat{H}_{\mathrm{quad}}$ is quadratic in the field $\hat{\Lambda}$, Wick's theorem can be used. We finally find for the variance of the number of non-condensed particles:

$$\mathrm{Var}(\delta \hat{N}) \simeq \langle \delta \hat{N} \rangle + \int d\vec{r}_1 \int d\vec{r}_2 \left[\left| \langle \hat{\Lambda}^\dagger(\vec{r}_1)\hat{\Lambda}(\vec{r}_2) \rangle \right|^2 + \left| \langle \hat{\Lambda}(\vec{r}_1)\hat{\Lambda}(\vec{r}_2) \rangle \right|^2 \right]. \tag{366}$$

The variance in Eq.(366) is simple to calculate in the homogeneous case of a gas in a cubic box of size L with periodic boundary conditions. The eigenmodes (u, v) are simply plane waves Eq.(259) with real coefficients U_k, V_k given in Eq.(262) and depending only on the modulus k of the wavevector $\vec{k}$. We find for the two correlation functions appearing in Eq.(366) the simple expression:

$$\langle \hat{\Lambda}^\dagger(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle = \frac{1}{L^3} \sum_{\vec{k} \neq \vec{0}} \left[(U_k^2 + V_k^2)n_k + V_k^2 \right] e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} \tag{367}$$

$$\langle \hat{\Lambda}(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle = \frac{1}{L^3} \sum_{\vec{k} \neq \vec{0}} U_k V_k (1 + 2n_k) e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} \tag{368}$$

where we have introduced the mean occupation numbers $n_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle$. After spatial integration of the square modulus of these quantities we obtain

$$\text{Var}(\delta \hat{N}) = \langle \delta \hat{N} \rangle + \sum_{\vec{k} \neq \vec{0}} \left[\left(U_k^2 + V_k^2 \right) n_k + V_k^2 \right]^2 + U_k^2 V_k^2 (1 + 2n_k)^2 \tag{369}$$

where the mean number of non-condensed particles $\langle \delta \hat{N} \rangle$ is already given in Eq.(356):

$$\langle \delta \hat{N} \rangle = \sum_{\vec{k} \neq \vec{0}} \left(U_k^2 + V_k^2 \right) n_k + V_k^2. \tag{370}$$

We first apply formula (369) to the limiting case of zero temperature. All the occupation numbers n_k vanish. For the ideal Bose gas ($g = 0$) all the V_k's are zero and the variance of $\delta \hat{N}$ vanishes as expected, since all the particles are in the ground state of the box. For the interacting Bose gas we find

$$\text{Var}(\delta \hat{N})(T = 0) = \frac{1}{8} \sum_{\vec{k} \neq \vec{0}} \frac{1}{q^2 (1 + q^2)} \tag{371}$$

where q is given as function of k by Eq.(359). In the thermodynamical limit we replace the discrete sum by an integral and this leads to a variance scaling as the number of particles for a fixed density:

$$\frac{\text{Var}(\delta \hat{N})(T = 0)}{N} = 2\pi^{1/2} \left(\rho a^3 \right)^{1/2}. \tag{372}$$

In the regime of validity of the Bogoliubov approach one has $\rho a^3 \ll 1$ so that the fluctuations of N_0 are sub-poissonian.

The situation can be totally different at finite temperature. Consider first the case of the ideal Bose gas [54]:

$$\begin{aligned}
\text{Var}(\delta \hat{N}) &= \sum_{\vec{k} \neq \vec{0}} n_k (1 + n_k) \\
&= \sum_{\vec{k} \neq \vec{0}} \frac{1}{4 \sinh^2(\beta \epsilon_k / 2)}
\end{aligned} \tag{373}$$

with $\epsilon_k = \hbar^2 k^2 / (2m)$. In the thermodynamical limit one may be tempted to replace in the usual manner the sum over $\vec{k}$ by an integral. This leads however to an integral divergent in $k = 0$: the integrand scales as $1/k^4$, which is not compensated by the Jacobian k^2 of three-dimensional integration in spherical coordinates. In this case the contribution of the sum in the thermodynamical limit is dominated by the terms close to $k = 0$ where $\beta \epsilon_k \ll 1$ and the function $\sinh$ can be linearized. We then obtain

$$\text{Var}(\delta \hat{N})_{g=0} \simeq \left(\frac{k_B T}{\Delta} \right)^2 \sum_{\vec{n} \neq \vec{0}} \frac{1}{n^4}. \tag{374}$$

In this expression we have introduced the kinetic energy difference between the ground state and the first excited state for a single particle in the box:

$$\Delta = \frac{h^2}{2mL^2} \tag{375}$$

and the sum ranges over all the vectors $\vec{n}$ with integer components and a non-vanishing norm n. By a numerical calculation we obtain

$$\sum_{\vec{n} \neq \vec{0}} \frac{1}{n^4} = 16.53 \ldots \tag{376}$$

A remarkable feature is that the variance of N_0 scales as L^4 that is as the volume of the box to the power $4/3$, or equivalently as the number of particles to the power $4/3$ in the thermodynamical limit. This is much larger than N in the thermodynamical limit.

Do the fluctuations of N_0 remain large in presence of interactions? As the spectrum ϵ_k is linear at small k the divergence of n_k^2 is only as $1/k^2$, which has a finite integral in three dimensions. However the mode functions U_k, V_k are also diverging in $k = 0$, each as $1/k^{1/2}$, so that one recovers the $1/k^4$ dependence of the summand close to $k = 0$.

As in the ideal Bose gas case we replace in the thermodynamical limit the summand by its low k approximation:

$$n_k \sim \frac{k_B T}{\hbar k c} \tag{377}$$

$$U_k \sim \frac{1}{2q^{1/2}} \tag{378}$$

$$V_k \sim -\frac{1}{2q^{1/2}} \tag{379}$$

and we keep in the summation the most diverging terms. We finally obtain [55, 56]

$$\mathrm{Var}(\delta\hat{N})_{g>0} \simeq \frac{1}{2}\left(\frac{k_B T}{\Delta}\right)^2 \sum_{\vec{n}\neq\vec{0}} \frac{1}{n^4}. \tag{380}$$

Remarkably this result differs from the ideal Bose gas case Eq.(374) by a factor $1/2$ only: fluctuations of N_0 remain large. The fact that Eq.(380) does not depend on the strength g of the interaction is valid only at the thermodynamical limit and indicates that the limit $g \to 0$ and the thermodynamical limit do not commute.

7.9   A simple reformulation of thermodynamical stability condition

The thermodynamical stability condition simply requires that the Bogoliubov Hamiltonian $\hat{H}_{\mathrm{quad}}$ is the sum of a constant (function of $\hat{N}$) and of a *positive* quadratic operator in the field variables. In the diagonal form (344) positivity is clearly equivalent to the requirement ϵ_k positive for all k in the $+$ family. How to express this condition from the non-diagonal form (339)? We simply have to rewrite Eq.(339) as

$$\hat{H}_{\mathrm{quad}} = f(\hat{N}) + \frac{1}{2}\int d^3\vec{r}\,(\hat{\Lambda}^\dagger, \hat{\Lambda})\eta\mathcal{L}\begin{pmatrix} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{pmatrix} \tag{381}$$

where η is the operator

$$\eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{382}$$

so that $\eta\mathcal{L}$ is an Hermitian operator.

The thermodynamical stability condition is therefore equivalent to the requirement that $\eta\mathcal{L}$ is positive:

$$\eta\mathcal{L} \geq 0. \tag{383}$$

More precisely, as $\hat{\Lambda}$ is orthogonal to ϕ_0, $\eta\mathcal{L}$ has to be strictly positive in the subspace orthogonal to $(|\phi_0\rangle, 0)$ and $(0, |\phi_0{}^*\rangle)$.

We can give a simple physical interpretation of this condition: ϕ_0 has to be a local minimum of the Gross-Pitaevskii energy functional

$$E[\phi, \phi^*] = N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\text{grad}}\, \phi|^2 + U(\vec{r})|\phi(\vec{r})|^2 + \frac{1}{2} Ng|\phi(\vec{r})|^4 \right], \tag{384}$$

which is the expression of §5 with the approximation $N_0 \simeq N$. Let us consider indeed the variation δE of E from $E_0 \equiv E[\phi_0, \phi_0{}^*]$ up to second order in a small deviation $\delta\phi$ of ϕ from ϕ_0.

The terms linear in $\delta\phi$ are given by:

$$\delta E^{(1)} = N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} \vec{\text{grad}}\, \phi_0{}^* \cdot \vec{\text{grad}}\, \delta\phi + U(\vec{r})\phi_0{}^*\delta\phi + Ng\phi_0{}^{*2}\phi_0\delta\phi + \text{c.c.} \right]. \tag{385}$$

By integration by parts and using the fact that ϕ_0 solves the Gross-Pitaevskii equation Eq.(325) we rewrite this expression as

$$\delta E^{(1)} = N\mu[\langle\phi_0|\delta\phi\rangle + \langle\delta\phi|\phi_0\rangle]. \tag{386}$$

As both ϕ and ϕ_0 are normalized to unity $\delta\phi$ actually fulfills the identity

$$\langle\phi_0|\delta\phi\rangle + \langle\delta\phi|\phi_0\rangle = -\langle\delta\phi|\delta\phi\rangle. \tag{387}$$

The *a priori* first order energy change is *a posteriori* of second order:

$$\delta E^{(1)} = -N\mu\langle\delta\phi|\delta\phi\rangle! \tag{388}$$

The terms *a priori* quadratic in $\delta\phi$ are given by:

$$\delta E^{(2)} = N \int d^3\vec{r} \quad \left[\frac{\hbar^2}{2m} \vec{\text{grad}}\, \delta\phi^* \cdot \vec{\text{grad}}\, \delta\phi + U(\vec{r})\delta\phi^*\delta\phi + 2Ng|\phi_0|^2\delta\phi^*\delta\phi \right.$$
$$\left. + \frac{1}{2} Ng\phi_0{}^{*2}\delta\phi^2 + \frac{1}{2} Ng\phi_0{}^2\delta\phi^{*2} \right]. \tag{389}$$

We transform this expression by splitting $\delta\phi$ in a part parallel to ϕ_0 and a part orthogonal to ϕ_0 :

$$\delta\phi(\vec{r}) = \gamma\phi_0(\vec{r}) + \delta\phi_\perp(\vec{r}). \tag{390}$$

Using integration by parts, the Gross-Pitaevskii equation and the fact that operator $\mathcal{L}$ contains projectors orthogonally to ϕ_0, ϕ_0^* we are able to write $\delta E^{(2)}$ as

$$
\begin{aligned}
\delta E^{(2)} &= |\gamma|^2 N\mu + \frac{1}{2}(\gamma+\gamma^*)^2 N^2 g \int d^3\vec{r}\,|\phi_0|^4 + (\gamma+\gamma^*)N^2 g \int d^3\vec{r}\,|\phi_0|^2(\phi_0^*\delta\phi_\perp + \text{c.c.}) \\
&\quad + \frac{1}{2}N \int d^3\vec{r}\,(\delta\phi_\perp^*, \delta\phi_\perp)(\eta\mathcal{L} + \mu\,\text{Id})\begin{pmatrix}\delta\phi_\perp \\ \delta\phi_\perp^*\end{pmatrix}.
\end{aligned}
\tag{391}
$$

Note that we had to add μ times the identity matrix Id to $\eta\mathcal{L}$ as Eq.(389), contrarily to $\eta\mathcal{L}$, does not contain any term proportional to μ . From Eq.(387) we see that $\gamma + \gamma^*$ is actually of second order in $\delta\phi_\perp$ so that it can be set to zero in Eq.(391).

Summing the *a priori* first and second order energy changes we see that $\delta E^{(1)}$ exactly cancels the terms involving explicitly μ in Eq.(391) so that we arrive at

$$\delta E \simeq \frac{1}{2}N \int d^3\vec{r}\,(\delta\phi_\perp^*, \delta\phi_\perp)\eta\mathcal{L}\begin{pmatrix}\delta\phi_\perp \\ \delta\phi_\perp^*\end{pmatrix}. \tag{392}$$

Thermodynamical stability that is positivity of $\eta\mathcal{L}$ is therefore equivalent to the Gross-Pitaevskii energy functional having a local minimum in ϕ_0 .

7.10 Thermodynamical stability implies dynamical stability

As we show now the positivity of $\eta\mathcal{L}$ automatically leads to a purely real spectrum for $\mathcal{L}$, that is to dynamical stability. Consider an eigenvector (u, v) of $\mathcal{L}$ with the eigenvalue ϵ . Contracting the operator $\eta\mathcal{L}$ between the ket $(|u\rangle, |v\rangle)$ and the bra $(\langle u|, \langle v|)$ we get

$$(\langle u|, \langle v|)\eta\mathcal{L}\begin{pmatrix}|u\rangle \\ |v\rangle\end{pmatrix} = \epsilon\left[\langle u|u\rangle - \langle v|v\rangle\right]. \tag{393}$$

The matrix element of $\eta\mathcal{L}$ is real positive as $\eta\mathcal{L}$ is supposed to be a positive hermitian operator. We now face two possible cases for the real quantity $\langle u|u\rangle - \langle v|v\rangle$:

- $\langle u|u\rangle - \langle v|v\rangle = 0$. In this case $\eta\mathcal{L}$ has a vanishing expectation value in $(|u\rangle, |v\rangle)$; as $\eta\mathcal{L}$ is positive, $(|u\rangle, |v\rangle)$ has to be an eigenvector of $\eta\mathcal{L}$ with the eigenvalue zero; as η is invertible we find that $(|u\rangle, |v\rangle)$ is an eigenvalue of $\mathcal{L}$ with the eigenvalue 0, so that $\epsilon = 0$ is a real number.

- $\langle u|u \rangle - \langle v|v \rangle > 0$: we get ϵ as the ratio of two real numbers, so that ϵ is real.

7.11 Examples of thermodynamical instability

7.11.1 Real condensate wavefunction with a node

Let us assume that the solution of the Gross-Pitaevskii equation is a real function $\phi_0(\vec{r})$. To decide if this solution is thermodynamically stable one has to check the positivity of the operator $\eta\mathcal{L}$. Consider an eigenvector of $\eta\mathcal{L}$ with eigenvalue ε :

$$\eta\mathcal{L}\begin{pmatrix} u \\ v \end{pmatrix} = \varepsilon \begin{pmatrix} u \\ v \end{pmatrix}. \tag{394}$$

This ε should not be confused with the quasi-particle energies as $\eta\mathcal{L}$ and $\mathcal{L}$ have different spectra. By performing the sum and the difference of the two lines of Eq.(394) we get decoupled equations for the sum $\psi_s = u + v$ and the difference $\psi_d = u - v$:

$$\varepsilon|\psi_s\rangle = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) + 2NgQ\phi_0^2(\vec{r})Q - \mu\right]|\psi_s\rangle \tag{395}$$

$$\varepsilon|\psi_d\rangle = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) - \mu\right]|\psi_d\rangle. \tag{396}$$

Both operators involved in these equations have to be positive to achieve thermodynamical stability. Note that for $g > 0$ the positivity of the second operator Eq.(396) implies the positivity of the first one Eq.(395) as $gQ\phi_0^2(\vec{r})Q$ is positive.

We therefore concentrate on Eq.(396). It involves the Gross-Pitaevskii Hamiltonian

$$\mathcal{H}_{GP} = \frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) - \mu. \tag{397}$$

An obvious eigenvector of this Hamiltonian is $\psi_d = \phi_0$ with eigenvalue $\varepsilon = 0$, as ϕ_0 solves the Gross-Pitaevskii equation! The condition of a positive ε in Eq.(396) simply means that ϕ_0 should be the ground state of $\mathcal{H}_{GP}$!

We can then invoke a theorem claiming that the ground state of a potential has no node [58]. If $\phi_0(\vec{r})$ has a node it cannot be the ground state of $\mathcal{H}_{GP}$. The ground state of $\mathcal{H}_{GP}$ has therefore an eigenenergy ε lower than the one of ϕ_0 , that is lower than zero, so that the operator $\eta\mathcal{L}$ is not positive and there is no thermodynamical stability.

As an example consider in a harmonic trap with eigenaxis z , a solution of the Gross-Pitaevskii equation even along x and y but odd along z , so that it vanishes in the plane $z = 0$. Such a solution exists, for $g > 0$: within the class of *real* functions ϕ odd along z and even along x , y , the Gross-Pitaevskii energy $E[\phi, \phi]$, bounded from below, has a minimum, reached in ϕ_0 , and this ϕ_0 then solves the Gross-Pitaevskii equation. This solution however is no longer a local minimum of $E[\phi, \phi^*]$ when one includes all possible deviations of ϕ from ϕ_0 (complex and with no well defined parity along z).

7.11.2 Condensate with a vortex

Can we get a thermodynamically stable condensate wavefunction with a node? To beat the results of the previous subsection we now assume ϕ_0 to be complex.

A particular class of complex wavefunctions with a node are condensate wavefunctions with vortices. A vortex is characterized (i) by a nodal, not necessarily straight, line in ϕ_0 (the center of the so-called vortex core) and (ii) by the fact that the phase of ϕ_0 changes by $2q\pi$, q non-zero integer, along a closed path around the vortex core (q is the so-called charge of the vortex). This second property means that the circulation of the local velocity field (defined in §5.3.3) around the vortex core is $2\pi\hbar q/m$.

A condensate wavefunction can have several vortices; the change of the phase of ϕ_0 along a closed path is now $2\pi q_{\mathrm{sum}}$ where q_{sum} is the algebraic sum of the charges of the vortex lines enclosed by the path.

It has been shown that a condensate wavefunction with a vortex in a harmonic trap is not thermodynamically stable [59]. In the limit of vanishing interaction between the particles ($g = 0$) this is clear indeed. Suppose that the trap is cylindrically symmetric with respect to z . $|\phi_0\rangle$ can be chosen as $(|n_x = 1, n_y = 0, n_z = 0\rangle + i|n_x = 0, n_y = 1, n_z = 0\rangle)/\sqrt{2}$ where $|n_x, n_y, n_z\rangle$ is the eigenstate of the harmonic oscillator with quantum number n_α along axis α ($\alpha = x, y, z$). The chemical potential is simply $2\hbar\omega_{x,y} + \frac{1}{2}\hbar\omega_z$ where ω_α is the atomic oscillation frequency along axis α . One then finds that $(|u\rangle = |n_x = 0, n_y = 0, n_z = 0\rangle, |v\rangle = 0)$ is an eigenvector of $\eta\mathcal{L}$ with the strictly negative energy $\varepsilon = -\hbar\omega_{x,y}$.

What happens in the opposite Thomas-Fermi regime of strong interactions? An intuitive answer can be obtained in a 2D model of the Gross-Pitaevskii equation, assuming for simplicity a quasi-isotropic trapping potential and restricting to the following class of

condensate wavefunctions:

$$\phi_0(x, y) = \phi_{\text{slow}}(x, y) \tanh[\kappa|\vec{r} - \vec{\alpha}R|]e^{i\theta_{\vec{\alpha}R}}. \tag{398}$$

In this ansatz $\phi_{\text{slow}}(x, y)$ is the usual square root of inverted parabola Thomas-Fermi approximation for a condensate wavefunction without vortex, with a radius R; the $\tanh[\,]$ represents the correction to the modulus of ϕ_0 due to the vortex core (of adjustable position $\vec{\alpha}R$ and inverse width κ); $\theta_{\vec{\alpha}R}$ is the polar angle of a system of Cartesian coordinates (X, Y) centered on the vortex core, and represents (approximately for $\vec{\alpha} \neq \vec{0}$) the phase of the unit-charge vortex.

One then calculates the mean energy of ϕ_0, with the simplification that $\phi_{\text{slow}}(x, y)$ varies very slow at the scale of κ^{-1}, and one minimizes this energy over κ. This leads to the inverse size of the vortex core on the order of the local healing length of the condensate:

$$\frac{\hbar^2\kappa^2}{m} = 0.59 \left[\mu - \frac{1}{2}m\omega^2(\alpha R)^2\right]. \tag{399}$$

The mean energy of ϕ_0 (384) is now a function of the position of the vortex core only,

$$E = E_{\text{no vortex}} + W(\vec{\alpha}) \tag{400}$$

where $E_{\text{no vortex}}$ is the energy of the condensate with no vortex and

$$W(\vec{\alpha}) = N\frac{(\hbar\omega)^2}{\mu_0}\left\{\frac{1}{2} + (1 - \alpha^2)\left[\frac{2\ln 2 + 1}{3} + \ln\frac{\nu\mu_0}{\hbar\omega} + \ln(1 - \alpha^2)\right]\right\} \tag{401}$$

with $\nu = 0.49312$ and μ_0 the chemical potential in the absence of vortex. This function W represents an effective potential seen by the vortex core. As shown in Fig.14a this potential is maximal at the center of the trap so that it is actually an expelling potential for the vortex core: shifting the vortex core away from the center of the trap lowers the condensate energy.

A method to stabilize the vortex is to rotate the harmonic trap around z at a frequency Ω (the trap is anisotropic in the $x - y$ plane otherwise rotation would have no effect). Thermodynamical equilibrium will now be obtained in the frame rotating at the frequency Ω, where the harmonic trap is time independent. As this frame is non Galilean the Hamiltonian and therefore the Gross-Pitaevskii energy functional have to

be supplemented by the inertial energy term $-\Omega L_z$ per atom, where L_z is the angular momentum operator along z. The effective potential $W(\vec{\alpha})$ gets an extra term:

$$W_\Omega(\vec{\alpha}) = W_{\Omega=0}(\vec{\alpha}) - N\hbar\Omega(1 - \alpha^2)^2 \qquad (402)$$

where $W_{\Omega=0}$ is the result (401) in the absence of rotation. As shown in Fig.14b this extra term can trap the vortex core at the center of the harmonic trap if Ω is large enough.

What happens if Ω is increased significantly ? It becomes favorable to put more vorticity in the condensate. As the vortices with charge larger than one are unstable the way out is to create several vortices with unit charge. This can be analyzed along the previous lines by a generalized multi-vortex ansatz, as discussed in [60]. A condensate with vortices has been recently obtained at the ENS in a rotating trap [61].

Another philosophy was followed at JILA: rather than relying on thermal equilibrium in a rotating trap to produce a vortex they used a "quantum engineering " technique [62] to directly induce the vortex by giving angular momentum to the atoms through coupling to electromagnetic fields [63]. It has also been suggested to imprint the phase of the vortex on the condensate through a lightshift induced by a laser beam whose spatial intensity profile has been conveniently tailored [64]. Such an imprinting technique has successfully led to the observation of dark and gray solitons in atomic condensates with repulsive interactions in Hannover [65] and in the group of W. Phillips at NIST. All these techniques illustrate again the powerfulness of atomic physics in its ability to manipulate a condensate.

8 Phase coherence properties of Bose-Einstein condensates

Consider two Bose-Einstein condensates prepared in spatially well separated traps and that have 'never seen each other' (e.g. one rubidium condensate at JILA and one rubidium condensate at ENS). It is 'natural' to assume that these two condensates do not have a well defined relative phase. However the trend in the literature on Bose condensates is to assume that the two condensates are in a *coherent* state with a well defined relative phase, the so-called 'symmetry-breaking' point of view. So imagine that one lets the two condensates spatially overlap. Will interference fringes appear on the resulting atomic
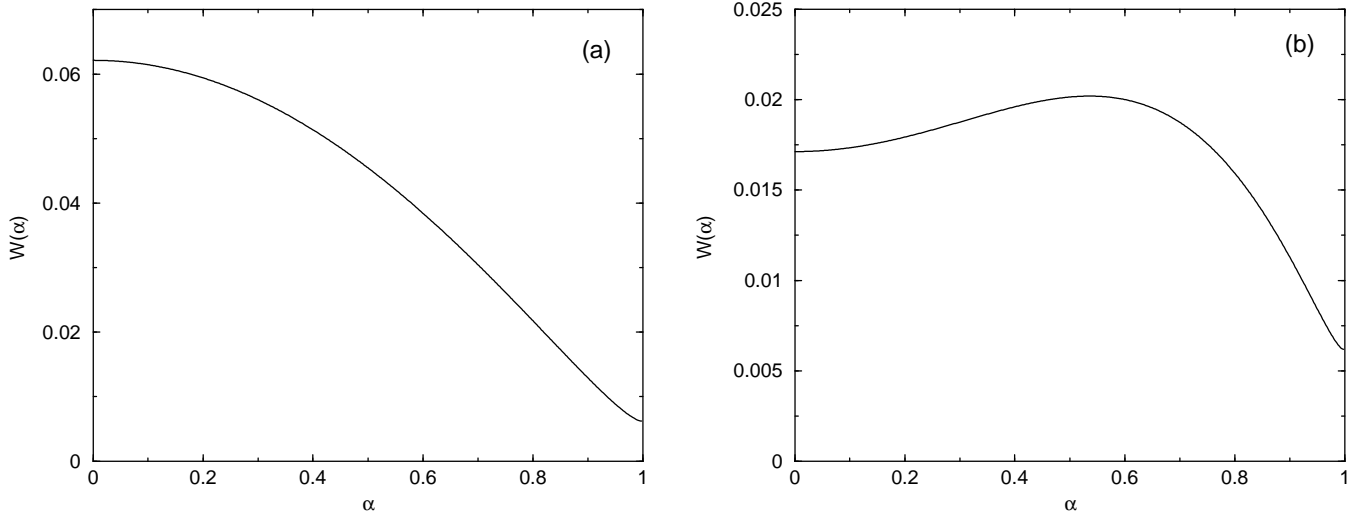
Figure 14: In a 2D model, effective potential energy W of a vortex in a quasi-axisymmetric harmonic trap as function of the distance αR of the core from the trap center, for $\mu_0 = 80\hbar\omega$. (a) $\Omega = 0$ and (b) $\Omega = 0.045\omega$. The unit of energy is $N\hbar\omega$ where ω is the oscillation frequency of the atoms in the trap.

density or not ?

One of the goals of this chapter is to answer this question and to reconcile the symmetry breaking point of view with the 'natural' point of view.

8.1   Interference between two BECs

At MIT a double well trapping potential was obtained by superimposing a sharp barrier induced with laser light on top of the usual harmonic trap produced with a magnetic field. In this way one can produce two Bose-Einstein condensates, one on each side of the barrier. The height of the barrier can be made much larger than the chemical potential of the gas so that coupling between the two condensates *via* tunneling through the wall is very small. In this way one can consider the two condensates as independent.

One can then switch off the barrier and magnetic trap, let the two condensates ballistically expand and spatially overlap. One then measures the spatial density of the cloud by absorption imaging. This spatial density exhibits clearly fringes [66] (see figure 15). These fringes have to be interference fringes, as hydrodynamic effects (such as sound

waves) are excluded at the very low densities of the ballistically expanded condensates. We show here on a simple model that we indeed expect to see interference fringes in such an experiment, even if the two condensates have initially no well defined relative phase.
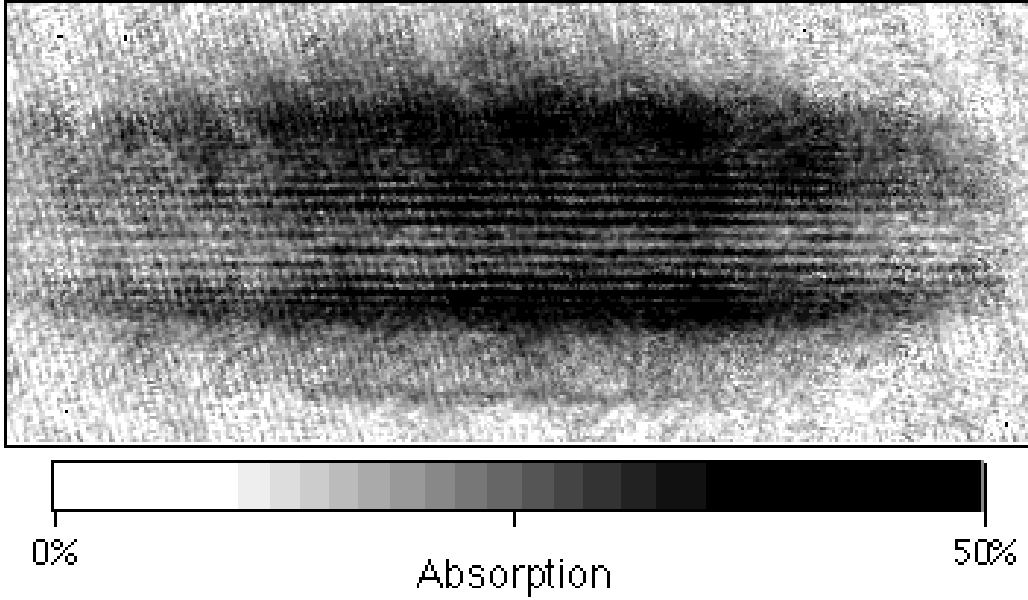

Figure 15: Interference fringes between two condensates observed at MIT [66].

8.1.1 A very simple model

In our simple modelization of an MIT-type interference experiment we will concentrate on the positions of the particles on an axis x connecting the two condensates so that we use a one-dimensional model enclosed in a box of size L with periodic boundary conditions. We assume that the system is initially in the Fock state

$$|\Psi\rangle = |\frac{N}{2} : k_a, \frac{N}{2} : k_b\rangle \tag{403}$$

with $N/2$ particles in the plane wave of momentum $\hbar k_a$ and $N/2$ particles in the plane wave of momentum $\hbar k_b$:

$$\langle x|k_{a,b}\rangle = \frac{1}{\sqrt{L}} \exp\left[ik_{a,b}x\right] . \tag{404}$$

We assume that one detects the position of all the particles. What will be the outcome ? As the numbers of particles are exactly defined in the two modes a and b the relative phase between the atomic fields in the two modes is totally undefined.

8.1.2   A trap to avoid

If we calculate the *mean density* in the state given by (403) we find a uniform result

$$\langle \hat{\psi}^{\dagger}(x)\hat{\psi}(x)\rangle = N/L \tag{405}$$

and we may be tempted to conclude that no interference fringes will appear in the beating of two Fock state condensates.

Actually this naive statement is wrong. Interference fringes appeared in a *single realization* of the experiment at MIT. We have therefore to consider the probability of the outcome of a particular density profile in a single realization of the measurement and not the average of the density profile over many realizations of the experiment. Indeed we will see that by interfering two independent Bose-Einstein condensates we get interference fringes on the density profile in each single realization of the experiment but the position of the interference pattern is random so that by averaging the density profile over many realizations we wash out the fringes.

We wish to emphasize the following crucial point of the quantum theory: Whatever single-time measurement is performed on the system all the information about the outcomes of a single realization of the measurement procedure is contained in the $N-$ body density matrix, here

$$\hat{\rho} = |\Psi\rangle\langle\Psi|. \tag{406}$$

Indeed the only information we can get from quantum mechanics on a single realization outcome is its probability P, which can be obtained from $\hat{\rho}$ by

$$P = \mathrm{Tr}[\hat{O}\hat{\rho}] \tag{407}$$

where the operator $\hat{O}$ depends on the considered outcome. E.g. in our gedanken experiment P is the probability density of finding the N particles at positions $x_1, x_2, ...x_N$ and the operator $\hat{O}$ is expressed in terms of the field operator as

$$\hat{O} = \frac{1}{N!}\hat{\psi}^{\dagger}(x_1)....\hat{\psi}^{\dagger}(x_N)\hat{\psi}(x_N)....\hat{\psi}(x_1). \tag{408}$$

In a first quantized picture this corresponds to the fact that the probability density P is equal to the modulus squared of the $N-$ body wavefunction.

The complete calculation of the $N-$ body distribution function $P(x_1, \ldots, x_N)$ for the state $|\Psi\rangle$ in Eq.(403) is involved and we will see in the coming subsections how to circumvent the difficulty. But we can do a simple calculation of the pair distribution function of the atoms in state $|\Psi\rangle$:

$$
\begin{align}
\rho(x_1, x_2) &= \langle\Psi|\hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2)\hat{\psi}(x_1)|\Psi\rangle \tag{409} \\
&= ||\hat{\psi}(x_2)\hat{\psi}(x_1)|\Psi\rangle||^2. \tag{410}
\end{align}
$$

We expand the field operator on the two modes $\phi_{a,b}$ and on other arbitrary orthogonal modes not relevant here as they are not populated in $|\Psi\rangle$:

$$
\hat{\psi}(x) = \hat{a}\langle x|k_a\rangle + \hat{b}\langle x|k_b\rangle + \ldots \tag{411}
$$

where $\hat{a}$ and $\hat{b}$ annihilate a particle in state k_a and k_b respectively. We obtain

$$
\begin{align}
\hat{\psi}(x_2)\hat{\psi}(x_1)|\Psi\rangle &= \left[\frac{N}{2}\left(\frac{N}{2}-1\right)\right]^{1/2}\langle x_2|k_a\rangle\langle x_1|k_a\rangle|\frac{N}{2}-2:k_a, \frac{N}{2}:k_b\rangle \\
&+ \left[\frac{N}{2}\left(\frac{N}{2}-1\right)\right]^{1/2}\langle x_2|k_b\rangle\langle x_1|k_b\rangle|\frac{N}{2}:k_a, \frac{N}{2}-2:k_b\rangle \\
&+ \frac{N}{2}\left[\langle x_2|k_a\rangle\langle x_1|k_b\rangle + \langle x_2|k_b\rangle\langle x_1|k_a\rangle\right]|\frac{N}{2}-1:k_a, \frac{N}{2}-1:k_b\rangle. \tag{412}
\end{align}
$$

The last line of this expression exhibits an interference effect between two amplitudes, that could not appear in the previous naive reasoning on the one-body density operator Eq.(405)! In the limit $N \gg 1$ and using the fact that the populated modes are plane waves the pair distribution function simplifies to

$$
\rho(x_1, x_2) \simeq \left(\frac{N}{L}\right)^2\left\{1 + \frac{1}{2}\cos\left[(k_a - k_b)(x_1 - x_2)\right]\right\}. \tag{413}
$$

This function exhibits oscillations around an average value equal to the square of the mean density. The oscillations are due to the interference effect in Eq.(412): they favor detections of pairs of particles with a distance $|x_1 - x_2|$ equal to $2n\pi/|k_a - k_b|$ (n integer) and they rarefy detections of pairs of particles with a distance $(2n+1)\pi/|k_a - k_b|$. We therefore see on the pair distribution function a precursor of the interference fringes observed when the positions of all the particles are measured!

8.1.3 A Monte Carlo simulation

By sampling the $N-$ body distribution function P with a Monte Carlo technique, Javanainen and Sung Mi Yoo in [67] made a numerical experiment with $N = 10^3$ particles and $k_b = -k_a$. By distributing the measured positions in a given realization $x_1, x_2, ...x_N$ among 30 position bins they obtained histograms like the ones in figure 16. It turns out that the density in the outcome of each realization of the numerical experiment can be fitted by a cosine:

$$\frac{N}{2L} \left| e^{ik_a x} e^{i\theta_a} + e^{ik_b x} e^{i\theta_b} \right|^2 \tag{414}$$

where θ_a and θ_b are phases varying randomly from one realization to the other. In other words one has the impression that for each realization the system is in the state

$$|\theta\rangle_N = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{2}} \left(a_{k_a}^\dagger e^{i\theta} + a_{k_b}^\dagger e^{-i\theta} \right) \right]^N |0\rangle \tag{415}$$

with the angle $\theta = (\theta_a - \theta_b)/2$ randomly distributed in $[-\pi/2, \pi/2]$. Such a state, corresponding to a well defined phase between the two modes a and b , is called a phase state [68].

8.1.4 Analytical solution

We wish to explain the result of the numerical experiment with an analytical argument. This has been done with slightly different points of view in [6, 69]. We give here what we think is the simplest possible presentation.

Let us allow Poissonian fluctuations in the number of particles N_a and N_b , corresponding to the distribution probabilities:

$$\mathcal{P}_\epsilon(N_\epsilon) = \frac{(\bar{N}_\epsilon)^{N_\epsilon}}{N_\epsilon!} e^{-\bar{N}_\epsilon} \qquad \epsilon = a, b \tag{416}$$

with mean number of particles $\bar{N}_a = \bar{N}_b = \bar{N}/2$. These fluctuations become very small as compared to $\bar{N}$ when the number of particles becomes large:

$$\frac{\Delta N_\epsilon}{\bar{N}_\epsilon} = \frac{1}{\sqrt{\bar{N}_\epsilon}} \to 0 \quad \text{for} \quad \bar{N}_\epsilon \to \infty. \tag{417}$$

The corresponding density operator is a statistical mixture of Fock states:

$$\hat{\rho} = \sum_{N_a, N_b = 0}^{\infty} \mathcal{P}_a(N_a) \mathcal{P}_b(N_b) |N_a : k_a, N_b : k_b\rangle \langle N_a : k_a, N_b : k_b|. \tag{418}$$
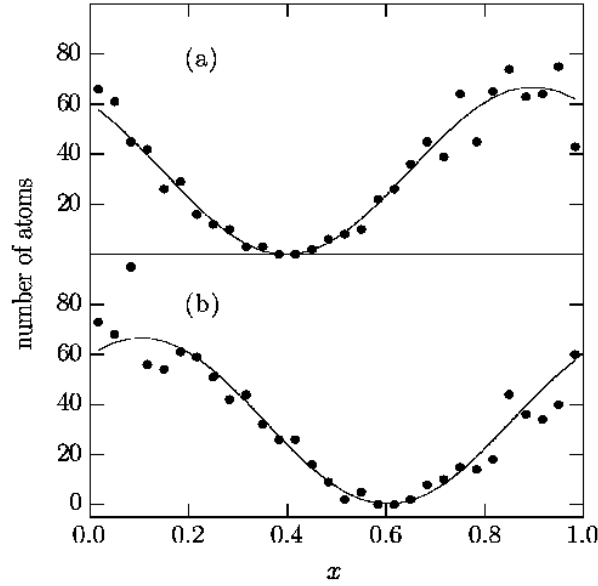
Figure 16: For two different Monte Carlo realizations (a) and (b) of the gedanken experiment, histogram of the measured positions of $N = 1000$ particles for an initial Fock state with $N/2$ particles in plane wave k_a and $N/2$ particles in plane wave $k_b = -k_a$ [67]. The positions of the particles are expressed in units of $2\pi/(k_a - k_b)$ and are considered modulo $2\pi/(k_a - k_b)$.

From this form one can *imagine* that a single realization of the experiment is in a Fock state, provided that one keeps in mind that N_a and N_b vary in an impredictable way from one experimental realization to the other. We known from the work [67] that there will be interference fringes in each experimental realization, but this fact is not intuitive.

The same density operator can also be written in terms of a statistical mixture of phase states:

$$\hat{\rho} = \sum_{N=0}^{\infty} \frac{(\bar{N})^N}{N!} e^{-\bar{N}} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} |\theta\rangle_{NN}\langle\theta|. \tag{419}$$

From this form one can *imagine* that a single realization of the experiment is in a phase state, provided that one keeps in mind that the total number of particles N and the relative phase θ vary in an impredictable way from one realization to the other. This last form leads to the following algorithm to generate the positions of the particles according to the correct probability distribution:

1. generate an integer N according to the Poisson distribution of parameter $\bar{N}$

2. generate θ according to a uniform probability distribution within $-\pi/2$ and $\pi/2$

3. generate the positions $x_1, ...x_N$ *as if* the system was in the state $|\theta\rangle_N$, in which case all the particles are in the same single particle-state and the probability density $P(x_1, ...x_N)$ is factorized:

$$P(x_1, ...x_N) = \prod_{j=1}^{N} p(x_j) \tag{420}$$

where

$$p(x) = \frac{1}{2L} \left| e^{ik_a x} e^{i\theta} + e^{ik_b x} e^{-i\theta} \right|^2. \tag{421}$$

One then obtains interference fringes in each experimental realization, in a very explicit way.

One could also use a third form of the same density operator $\hat{\rho}$, that is a statistical mixture of Glauber coherent states:

$$\hat{\rho} = \int_0^{2\pi} \frac{d\theta_a}{2\pi} \int_0^{2\pi} \frac{d\theta_b}{2\pi} |\text{coh} : \bar{N}_a^{1/2} e^{i\theta_a}, \text{coh} : \bar{N}_b^{1/2} e^{i\theta_b}\rangle\langle\text{coh} : \bar{N}_a^{1/2} e^{i\theta_a}, \text{coh} : \bar{N}_b^{1/2} e^{i\theta_b}|. \tag{422}$$

This mathematical form is at the origin of the popular belief that condensates are in coherent states. From this form one can only *imagine* that a single realization of the experiment is in a coherent state, keeping in mind that the phases θ_a and θ_b vary in an impredictable way from one realization to the other. In this representation the occurrence of interference fringes is straightforward.

There is an important difference between the coherent states and the Fock or phase states: as the number of particles is a conserved quantity in the non-relativistic Hamiltonian used to describe the experiments on atomic gases it seems difficult to produce a condensate in a coherent state in some mode ψ, that is with $\hat{\rho}$ being a pure state $|\text{coh} : \alpha\rangle\langle\text{coh} : \alpha|$ where α is a complex number.

On the contrary one could imagine producing a condensate in a Fock state by measuring the number of particles in the condensate. One could then obtain a phase state by applying a $\pi/2$ Rabi pulse on the Fock state changing the internal atomic state a to a superposition $(|a\rangle + |b\rangle)/\sqrt{2}$ where b is another atomic internal state; such a Rabi pulse has been demonstrated at JILA and has allowed the measurement of the coherence time of the relative phase between the a and b condensates [70].

8.1.5 Moral of the story

- there is in general no unique way of writing the density operator $\hat{\rho}$ as a statistical mixture. The canonical form corresponding to the diagonalization of $\hat{\rho}$ is always a possibility but not always the most convenient one. E.g. in our simple model the eigenbasis (Fock states) is less convenient than the non-orthogonal family of phase states (symmetry breaking states).

- no measurement or no set of measurements performed *on the system* can distinguish between two different mathematical forms of the same density matrix as a statistical mixture.

- the symmetry breaking point of view consists in writing (usually in an approximate way) the $N-$ body density operator as a statistical mixture of Hartree-Fock states. One can then imagine that a given experimental realization of the system is a Hartree-Fock state, whose physical properties are immediate to understand as all the particles are in the same quantum state.

- If the system is not in a state that is as simple as a Hartree-Fock state (e.g. in a Fock state for our simple model) it is dangerous to make reasonings on the single particle density operator (that is on the first order correlation function of the atomic field operator) to predict outcomes of single measurements on the system: the relevant information may be stored in higher order correlation functions of the field.

8.2 What is the time evolution of an initial phase state ?

8.2.1 Physical motivation

Consider an interference experiment between two condensates A and B either in spatially separated traps or in different internal states (JILA-type configuration [70]). Assume that the two condensates have been prepared initially in a state with a well defined relative phase θ ; this has actually been achieved at JILA. Let the system evolve freely for some time t . How long will the relative phase remain well defined ? This question is probably not an easy one to answer. We present here a simple model including only two modes of the field. In real life the other modes of the field are not negligible (see for example [71] for a discussion of finite temperature effects) and phenomena neglected here

such as losses of particles from the trap and fluctuations in the total number of particles may be important in a real experiment [7, 29].

We assume that the state of the system at time $t = 0$ is a phase state. More specifically, expanding the $N-$ th power in Eq.(415) with the binomial formula, we take as initial state:

$$|\Psi(t = 0)\rangle = 2^{-N/2} \sum_{N_a=0}^{N} \left(\frac{N!}{N_a!N_b!}\right)^{1/2} e^{i(N_a - N_b)\theta}|N_a : \phi_a, N_b : \phi_b\rangle \qquad (423)$$

where $N_b = N - N_a$ and $\phi_{a,b}$ are the steady state condensate wavefunctions with $N_{a,b}$ particles in condensates A, B respectively. The time evolution during t is simple for each individual Fock states, as the system is then in a steady state with total energy $E(N_a, N_b)$:

$$|N_a : \phi_a, N_b : \phi_b\rangle \rightarrow e^{-iE(N_a,N_b)t/\hbar}|N_a : \phi_a, N_b : \phi_b\rangle. \qquad (424)$$

The time evolution of the phase state Eq.(423) is much more complicated: the state vector $|\Psi(t)\rangle$ is a sum of many oscillating functions of time.

8.2.2 A quadratic approximation for the energy

The discussion can be greatly simplified if one uses the fact that the binomial factor in Eq.(423) for large N is a function of N_a and N_b sharply peaked around $N_a = N_b = N/2$ with a width $\sqrt{N}$: from Stirling's formula $n! \simeq (n/e)^n\sqrt{2\pi n}$ we obtain indeed

$$\frac{1}{2^N}\frac{N!}{N_a!N_b!} \simeq \frac{1}{\sqrt{2\pi}2^N}\left(\frac{N}{N_aN_b}\right)^{1/2} e^{-N_a\log(N_a/N)-N_b\log(N_b/N)} \simeq \left(\frac{2}{\pi N}\right)^{1/2} e^{-(N_a-N_b)^2/(2N)}. \qquad (425)$$

We therefore expand the energy E in powers of $N_a - N/2$ and $N_b - N/2$ up to second order.

$$\begin{aligned}
E(N_a, N_b) &= E(N/2, N/2) + (N_a - N/2)\partial_{N_a}E + (N_b - N/2)\partial_{N_b}E \\
&\quad + \frac{1}{2}(N_a - N/2)^2\partial_{N_a}^2 E + \frac{1}{2}(N_b - N/2)^2\partial_{N_b}^2 E \\
&\quad + (N_a - N/2)(N_b - N/2)\partial_{N_a}\partial_{N_b}E + \dots, \qquad (426)
\end{aligned}$$

all the derivatives being taken in $(N_a, N_b) = (N/2, N/2)$. Note that the first derivatives of the energy are the chemical potentials $\mu_{a,b}$ of the two condensates; as the condensates

are independent condensates (there is no mechanism locking the relative phase of the condensates) one has in general $\mu_a \neq \mu_b$. As we restrict to the set of occupation numbers such that $N_a + N_b = N$ we can rewrite the expansion of the energy using $N_a - N/2 = -(N_b - N/2) = (N_a - N_b)/2$:

$$E(N_a, N_b) \simeq E(N/2, N/2) + \frac{1}{2}(N_a - N_b)(\mu_a - \mu_b) + \frac{\hbar}{4}(N_a - N_b)^2 \chi \qquad (427)$$

where we have introduced the quantity

$$\chi = \frac{1}{2\hbar} \left[(\partial_{N_a} - \partial_{N_b})^2 E \right]_{N_a = N_b = N/2}. \qquad (428)$$

8.2.3 State vector at time t

If one uses the quadratic approximation of the energy the system evolves from the initial state Eq.(423) to the state

$$|\Psi(t)\rangle = 2^{-N/2} \sum_{N_a=0}^{N} \left(\frac{N!}{N_a! N_b!} \right)^{1/2} e^{i(N_a - N_b)(\theta + vt)} e^{-i(N_a - N_b)^2 \chi t/4} |N_a : \phi_a, N_b : \phi_b\rangle \qquad (429)$$

The contribution of the term linear in $N_a - N_b$ in Eq.(427) is contained in the quantity

$$v = \frac{1}{2\hbar}(\mu_b - \mu_a). \qquad (430)$$

The resulting effect on the time evolution is simply to shift the relative phase between the condensate from θ to $\theta + vt$: this is a mere phase drift with a velocity v. This phase drift takes place only if the 'frequencies' $\mu_a/\hbar$ and $\mu_b/\hbar$ of the atomic fields in A and in B are different.

The effect of the quadratic term in Eq.(427) is to spread the relative phase of the two condensates. This effect is formalized in [6], we give here the intuitive result. The spreading of the phase can be understood in analogy with the spreading of the wavepacket of a fictitious massive particle, with the relative phase θ being the position x of the particle and the occupation number difference $N_b - N_a$ being the wavevector k of the particle. The energy term proportional to χ plays the role of the kinetic energy of the particle responsible for the spreading in position. The effective mass of the fictitious particle is M such that

$$\frac{1}{4}(N_a - N_b)^2 \chi \longleftrightarrow \frac{\hbar k^2}{2M} \qquad (431)$$

so that

$$M = \frac{2\hbar}{|\chi|}. \tag{432}$$

Replacing the discrete sum in Eq.(429) by an integral we formally obtain the expansion of the time dependent state vector of the fictitious particle over the plane waves in free space. In this case the variance of the position of the fictitious particle spreads as

$$\Delta x^2(t) = \Delta x^2(0) + \left(\frac{\hbar \Delta k}{M}\right)^2 t^2. \tag{433}$$

Within the approximation (425) the wavepacket of the fictitious particle is a Gaussian in momentum space, with a standard deviation $\Delta k = (N/2)^{1/2}$. Initially the position x is well defined with a spread $\sim 1/\Delta k \ll 1$. The relative phase of the condensates will start becoming undefined when the position spread Δx of the fictitious particle becomes on the order of unity. This happens after a time

$$t_{\text{spread}} \sim \frac{M}{\hbar \Delta k} = \frac{2\sqrt{2}}{|\chi| N^{1/2}}. \tag{434}$$

At times much longer than t_{spread} it is not correct to replace the discrete sum over $(N_a - N_b)/2$ by an integral. The discreteness of $N_a - N_b$ leads to reconstructions of a phase state (the so-called revivals) at times $t_q = q\pi/\chi$, q integer: one can check indeed from Eq.(429) that a phase state is reconstructed with a relative phase $\theta + vt_q + q\pi/2$ for N even and $\theta + vt_q$ for N odd. The observability of even the first revival at time t_1 is a non trivial question: the revivals are easily destroyed by decoherence phenomena such as the loss of a few particles out of the condensate due to inelastic atomic collisions [7], and effects of the non-condensed fraction also need to be investigated. This fragility of the revivals is not surprising if one realizes that the state vector $|\Psi(t)\rangle$ in Eq.(429) is a Schrödinger cat at time $t_1/2$, that is a coherent superposition of the N particles in some state ϕ_1 and of the N particles in some state ϕ_2 orthogonal to ϕ_1 : the revival at time t_1 is suppressed if the Schrödinger cat at time $t_1/2$ is transformed by decoherence into a statistical mixture of the states $|N : \phi_{1,2}\rangle$, which is difficult to avoid for large values of N (see the lecture notes of Michel Brune in this volume).

8.2.4 An indicator of phase coherence

To characterize the degree of phase correlation between the two condensates it is natural to consider the average of $\langle \hat{a}^\dagger \hat{b} \rangle$ where $\hat{a}, \hat{b}$ annihilate a particle in condensates A and

B respectively. Consider indeed the average over many experimental realizations of some one-body observable $\hat{O}$ sensitive to the relative phase of the two condensates. This observable necessarily has a non-vanishing matrix element between the modes ϕ_a and ϕ_b so that in second quantized form the part of $\langle\hat{O}\rangle$ sensitive to the relative phase involves $\langle\hat{a}^\dagger\hat{b}\rangle$. E.g. in the case of spatially separated condensates one can beat on a $50-50$ matter waves beam splitter atoms leaking out of the condensates and detect the atoms in the output channels of the beam splitter [6]; the number of counts in the $+$ output channel averaged of many experimental realizations is proportional to the expectation value of

$$\hat{O} = \frac{\hat{a}^\dagger + \hat{b}^\dagger}{\sqrt{2}} \frac{\hat{a} + \hat{b}}{\sqrt{2}}. \tag{435}$$

Expanding this product of operators we get 'diagonal' terms such as $\hat{a}^\dagger\hat{a}$ not sensitive to the relative phase, and crossed terms (actually interference terms!) such as $\hat{a}^\dagger\hat{b}$ sensitive to the phase. In the JILA-type configuration, where the condensates A and B are in different internal atomic states, an observable $\hat{O}$ similar to Eq.(435) has been achieved by mixing the internal states of the two condensates by a $\pi/2$ electromagnetic pulse and by measuring the mean density of atoms in A and B [70].

From the Schwartz inequality $|\langle u|v\rangle| \leq ||u||\,||v||$ and setting $|u\rangle = \hat{a}|\Psi\rangle$, $|v\rangle = \hat{b}|\Psi\rangle$ we obtain an upper bound for the expectation value of $\hat{a}^\dagger\hat{b}$:

$$|\langle\Psi|\hat{a}^\dagger\hat{b}|\Psi\rangle| \leq \langle\Psi|\hat{a}^\dagger\hat{a}|\Psi\rangle^{1/2}\langle\Psi|\hat{b}^\dagger\hat{b}|\Psi\rangle^{1/2}. \tag{436}$$

The case of a maximally well defined relative phase corresponds to an equality in this inequality, obtained if $|u\rangle$ and $|v\rangle$ are proportional. In the present situation of equal mean numbers of particles $N/2$ in A and in B this corresponds to $|\Psi\rangle$ being a phase state.

For an initial phase state it is possible to calculate the expectation value of $\hat{a}^\dagger\hat{b}$ as function of time from the expansion (429). One obtains after simple transformations the sum

$$\langle\hat{a}^\dagger\hat{b}\rangle(t) = \frac{N}{2^N}e^{-2i(\theta+vt)}\sum_{N_a=0}^{N-1}\frac{(N-1)!}{N_a!(N_b-1)!}e^{i\chi t[N_a-(N_b-1)]} \tag{437}$$

with $N_b = N - N_a$ as in Eq.(429). After inspection one realizes that this sum is the binomial expansion of a $(N-1)-$th power so that the final result is [72]:

$$\langle\hat{a}^\dagger\hat{b}\rangle(t) = \frac{N}{2}e^{-2i(\theta+vt)}\cos^{N-1}\chi t. \tag{438}$$

From this very simple expression one can calculate the time t_c after which the relative phase has experienced a significant spread. For short times $\chi t \ll 1$ one can expand the cosine function in Eq.(438) to second order in t:

$$\cos^N \chi t = e^{N \log \cos \chi t} \simeq e^{-N(\chi t)^2/2}.$$ (439)

One obtains a Gaussian decay of phase coherence with a collapse time

$$t_c = \frac{1}{|\chi| N^{1/2}}$$ (440)

equivalent to the rougher estimate Eq.(434) up to a numerical factor. One can also easily see the revivals (reconstruction of $|\Psi\rangle$ to a phase state) at times $t_q = q\pi/\chi$ when the cosine function is equal to ± 1 in Eq.(438).

Formula (440) can be used to calculate the coherence time of the relative phase of the condensates in the present zero-temperature model. As an interesting application of this formula we now show that the spreading time of the relative phase can be significantly different for mutually interacting and non-mutually interacting condensates. Assume for simplicity that the two condensates are stored in cubic boxes of identical size L and with periodic boundary conditions. In the MIT-type configuration the two boxes are spatially separated and the atoms are in the same internal state; the energy of a configuration with N_a, N_b atoms in the condensates A, B is then

$$E = \frac{g}{2L^3} \left[N_a^2 + N_b^2 \right].$$ (441)

From Eq.(428) this form of E leads for an initial phase state to a collapse time of the relative phase

$$t_c = N^{1/2} \frac{\hbar}{2\rho g}$$ (442)

where $\rho = N/(2L^3)$ is the mean spatial density in each of the condensates. In the JILA-type configuration the atoms are in the same spatial box but in different internal states; the energy of a configuration with N_a, N_b atoms in the condensates A, B is given now by Eq.(294) if the two internal states are subject to spatial demixing, or by Eq.(295) if there is no demixing instability. The collapse time is then given by

$$t_c = N^{1/2} \frac{\hbar}{\rho[g_{aa} + g_{bb} - 2(g_{aa}g_{bb})^{1/2}]}$$ (443)

for a demixed condensates and by

$$t_c = N^{1/2} \frac{\hbar}{\rho[g_{aa} + g_{bb} - 2g_{ab}]} \tag{444}$$

for fully overlapping condensates. When the coupling constants among the various internal states are close to each other the denominator in Eqs.(443,444) can become small, which results in a relative phase coherence time t_c much larger than in the MIT-configuration Eq.(442). This fortunate feature of close coupling constants is present for rubidium in the JILA experiment [70]!

In real life the condensates are usually stored in harmonic traps; the simple formulas obtained for a cubic box have to be revisited. This has been done analytically for spatially separated condensates [73, 74] and numerically for mutually interacting condensates [29, 75].

9 Symmetry breaking description of condensates

We have already seen in chapter 8 that it is very convenient, physically, to introduce phase states to understand the phenomenon of interference between two Bose-Einstein condensates: rather than assuming that two Bose-Einstein condensates that "have never seen each other" are in Fock states, one assumes that they are in a phase state with a relative phase varying in an unpredictable way for any new experimental realization. One can even suppose that the condensates are in coherent states of the atomic field; this description is said to 'break the symmetry', here the $U(1)$ symmetry associated to the invariance of the Hamiltonian by a change of the phase of the atomic field operator.

In this chapter we consider other examples of symmetry breaking descriptions: $SO(3)$ symmetry breaking (case of spinor condensates) and spatial translational symmetry breaking (case of one dimensional condensates with attractive interactions). In both cases the procedure is the same: the ground state of the system is symmetric, its mean-field approximation by Hartree-Fock states breaks the symmetry. In both cases we will consider Gedanken experiments whose single outcomes can be predicted from the exact ground state and from the Hartree-Fock state. This will illustrate the ability of the mean-field approximation to allow physical predictions in an easy and transparent way, correct in the limit of a large number of particles.

9.1 The ground state of spinor condensates

The alkali atoms used in the Bose-Einstein condensation experiments have an hyperfine structure in the ground state, each hyperfine level having several Zeeman sublevels. We have up to now ignored this structure in the lecture, as we were implicitly assuming that the atoms were polarized in a well defined Zeeman sublevel.

Consider for example ^{23} Na atoms used at MIT in the group of Wolfgang Ketterle. The ground state has an hyperfine splitting between the lower multiplicity of angular momentum $F = 1$ and the higher multiplicity of angular momentum $F = 2$. All the three Zeeman sublevels $m_F = 0, \pm 1$ of the lower multiplicity $F = 1$ cannot be trapped in a magnetic trap (if $m_F = -1$ is trapped than $m_F = +1$ which experiences an opposite Zeeman shift is antitrapped). But they can all be trapped in an optical dipole trap, produced with a far off-resonance laser beam, as the Zeeman sublevels experience then all the same lightshift. This optical trapping was performed at MIT [76], opening the way to a series of interesting experiments with condensates of particles of spin one [77].

We concentrate here on a specific aspect, the ground state of the spinor condensate, assuming for simplicity that the atoms are stored in a cubic box with periodic boundary conditions.

9.1.1 A model interaction potential

We have to generalize the model scalar pseudo-potential of Eq.(73) to the case of particles having a spin different from zero. As we want to keep the simplicity of a contact interaction potential we choose the simple form

$$V(1,2) \equiv \mathcal{V}_{\text{spin}}(1,2)\delta(\vec{r_1} - \vec{r_2}) \left[\frac{\partial}{\partial r_{12}} \left(r_{12} \cdot \right) \right] \tag{445}$$

that is the product of an operator acting only on the spin of the particles 1 and 2, and of the usual regularized contact interaction acting only on the relative motion of the two particles. The interaction potential $V(1, 2)$ has to be invariant by a simultaneous rotation of the spin variables and of the position variables of the two particles. As the contact interaction is already rotationally invariant, the spin part of the interaction $\mathcal{V}_{\text{spin}}(1, 2)$ has to be invariant by any simultaneous rotation of the two spins.

This condition of rotational invariance of $\mathcal{V}_{\text{spin}}(1,2)$ is easy to express in the coupled basis obtained by the addition of the two spins of particle 1 and particle 2: within each subspace of well defined total angular momentum $\mathcal{V}_{\text{spin}}(1,2)$ has to be a scalar. Let us restrict to the case studied at MIT, with spin one particles. By addition of $F = 1$ and $F = 1$ we obtain a total angular momentum $F_{\text{tot}} = 2$, 1 or 0, so that one can write

$$\mathcal{V}_{\text{spin}}(1,2) = g_2 P_{F_{\text{tot}}=2}(1,2) + g_1 P_{F_{\text{tot}}=1}(1,2) + g_0 P_{F_{\text{tot}}=0}(1,2) \tag{446}$$

where the g's are coupling constants and the $P(1,2)$'s are projectors on the subspace of particles 1 and 2 with a well defined total angular momentum F_{tot}. At this stage we can play a little trick, using the fact that the states of $F_{\text{tot}} = 1$ are antisymmetric by the exchange of particles 1 and 2 (whereas the other subspaces are symmetric). The regularized contact interaction scatters only in the s-wave, where the external wavefunction of atoms 1 and 2 is even by the exchange of the positions $\vec{r}_1$ and $\vec{r}_2$; as our atoms are bosons, the spin part has also to be symmetric by exchange of the spins of atoms 1 and 2 so that the 'fermionic' part of $\mathcal{V}_{\text{spin}}(1,2)$, that is in the subspace $F_{\text{tot}} = 1$, has no effect. We can therefore change g_1 at will without affecting the interactions between bosons. The most convenient choice is to set $g_1 = g_2$ so that we obtain

$$\mathcal{V}_{\text{spin}}(1,2) = g_2 \text{Id}(1,2) + (g_0 - g_2)P_{F_{\text{tot}}=0}(1,2) \tag{447}$$

where Id is the identity. The subspace $F_{\text{tot}} = 0$ is actually of dimension one, and it is spanned by the vanishing total angular momentum state $|\psi_0(1,2)\rangle$. Using the standard basis $|m = -1, 0, +1\rangle$ of single particle angular momentum with z as quantization axis, one can write

$$|\psi_0(1,2)\rangle = -\frac{1}{\sqrt{3}} \left[| + 1, -1\rangle + | - 1, +1\rangle - |0,0\rangle\right]. \tag{448}$$

A more symmetric writing is obtained in the single particle angular momentum basis $|x, y, z\rangle$ used in chemistry, defined by

$$| + 1\rangle = -\frac{1}{\sqrt{2}} (|x\rangle + i|y\rangle) \tag{449}$$

$$| - 1\rangle = +\frac{1}{\sqrt{2}} (|x\rangle - i|y\rangle) \tag{450}$$

$$|0\rangle = |z\rangle. \tag{451}$$

The vector $|\alpha\rangle$ in this basis $(\alpha = x, y, z)$ is an eigenvector of angular momentum along axis α with the eigenvalue zero. One then obtains

$$|\psi_0(1,2)\rangle = \frac{1}{\sqrt{3}} \left[|x, x\rangle + |y, y\rangle + |z, z\rangle \right]. \tag{452}$$

To summarize the part of the Hamiltonian describing the interactions between the particles can be written, if one forgets for simplicity the regularizing operator in the pseudo-potential:

$$
\begin{aligned}
H_{\text{int}} &= \frac{g_2}{2} \int d^3\vec{r} \sum_{\alpha,\beta=x,y,z} \hat{\psi}_\alpha^\dagger \hat{\psi}_\beta^\dagger \hat{\psi}_\beta \hat{\psi}_\alpha \\
&\quad + \frac{g_0 - g_2}{6} \int d^3\vec{r} \sum_{\alpha,\beta=x,y,z} \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha^\dagger \hat{\psi}_\beta \hat{\psi}_\beta.
\end{aligned} \tag{453}
$$

where $\hat{\psi}_\alpha(\vec{r})$ is the atomic field operator for the spin state $|\alpha\rangle$. This model Hamiltonian has also been proposed by [78, 79, 80].

9.1.2 Ground state in the Hartree-Fock approximation

As we are mainly interested in the spin contribution to the energy we assume for simplicity that the condensate is in a cubic box of size L with periodic boundary conditions. We assume that the interactions between the atoms are repulsive ($g_2, g_0 \geq 0$) and we suppose that there is no magnetic field applied to the sample.

We now minimize the energy of the condensate within the Hartree-Fock trial statevectors $|N_0 : \phi\rangle$ with the constraint that the number of particles N_0 is fixed ($|\phi\rangle$ is normalized to unity) but without any constraint on the total angular momentum of the spins. The external part of the condensate wavefunction is simply the plane wave with momentum $\vec{k} = \vec{0}$ whereas the spinor part of the wavefunction remains to be determined:

$$\langle \vec{r} | \phi \rangle = \frac{1}{L^{3/2}} \sum_{\alpha=x,y,z} c_\alpha |\alpha\rangle \quad \text{with} \quad \sum_\alpha |c_\alpha|^2 = 1. \tag{454}$$

Using the model interaction Hamiltonian Eq.(453) we find for the mean energy per particle in the condensate

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2 + \frac{N_0 - 1}{6L^3}(g_0 - g_2)|A|^2 \tag{455}$$

where we have introduced the complex quantity

$$A = \sum_{\alpha=x,y,z} c_\alpha^2 = \vec{c}^2 \tag{456}$$

where $\vec{c}$ is the vector of components (c_x, c_y, c_z). We have to minimize the mean energy over the state of the spinor.

- Case $g_2 > g_0$

This is the case of sodium [77]. As the coefficient $g_0 - g_2$ is negative in Eq.(455) we have to maximize the modulus of the complex quantity A. As the modulus of a sum is less than the sum of the moduli we immediately get the upper bound

$$|A| \leq \sum_{\alpha=x,y,z} |c_\alpha|^2 = 1 \tag{457}$$

leading to the minimal energy per particle

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2 + \frac{N_0 - 1}{6L^3}(g_0 - g_2). \tag{458}$$

The upper bound for $|A|$ is reached only if all complex numbers c_α^2 have the same phase modulo 2π. This means that one can write

$$c_\alpha = e^{i\theta} n_\alpha \tag{459}$$

where θ is a constant phase and $\vec{n} = (n_x, n_y, n_z)$ is any unit vector with real components. Physically this corresponds to a spinor condensate wavefunction being the zero angular momentum state for a quantization axis pointing in the direction of $\vec{n}$. The direction of $\vec{n}$ is well defined in the Hartree-Fock ansatz, but it is arbitrary as no spin direction is privileged by the Hamiltonian. We are facing symmetry breaking, here a rotational $SO(3)$ symmetry breaking, as we shall see.

- Case $g_2 < g_0$

In this case we have to minimize $|A|$ to get the minimum of energy. The minimal value of $|A|$ is simply zero, corresponding to spin configurations such that

$$\vec{c}^2 \equiv \sum_{\alpha=x,y,z} c_\alpha^2 = 0 \tag{460}$$

with an energy per condensate particle

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2. \tag{461}$$

To get more physical understanding we split the vector $\vec{c}$ as

$$\vec{c} = \vec{R} + i\vec{I} \tag{462}$$

where the vectors $\vec{R}$ and $\vec{I}$ have purely real components. Expressing the fact that the real part and imaginary part of $\vec{c}^2$ vanish, and using the normalization condition $\vec{c} \cdot \vec{c}^* = 1$ in Eq.(454) we finally obtain

$$\vec{R} \cdot \vec{I} = 0 \tag{463}$$

$$\vec{R}^2 = \vec{I}^2 = \frac{1}{2}. \tag{464}$$

This means that the complex vector $\vec{c}$ is circularly polarized with respect to the axis Z orthogonal to $\vec{I}$ and $\vec{R}$. Physically this corresponds to a spinor condensate wavefunction having an angular momentum $\pm\hbar$ along the axis Z. The direction of axis Z is well defined in the Hartree-Fock ansatz but it is arbitrary.

9.1.3 Exact ground state of the spinor part of the problem

Imagine that we perform some intermediate approximation, assuming that the particles are all in the ground state $\vec{k} = \vec{0}$ of the box but not assuming that they are all in the same spin state. We then have to diagonalize the model Hamiltonian

$$H_{\text{spin}} = \frac{g_2}{2L^3} \sum_{\alpha,\beta=x,y,z} \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\beta \hat{a}_\alpha + \frac{1}{6L^3}(g_0 - g_2)\hat{A}^\dagger \hat{A} \tag{465}$$

where $\hat{a}_\alpha$ annihilates a particle in state $|\vec{k} = 0\rangle|\alpha\rangle$ ($\alpha = x, y, z$) and where we have introduced

$$\hat{A} = \hat{a}_x^2 + \hat{a}_y^2 + \hat{a}_z^2. \tag{466}$$

Up to a numerical factor $\hat{A}$ annihilates a pair of particles in the two-particle spin state $|\psi_0(1,2)\rangle$ of vanishing total angular momentum, as shown by Eq.(452).

The Hamiltonian Eq.(465) can be diagonalized exactly [81]. This is not surprising as (i) it is rotationally invariant and (ii) the bosonic N_0- particle states with a well defined

total angular momentum S_{N_0} can be calculated: one finds that $S_{N_0} = N_0, N_0 - 2, \ldots,$ leading to degenerate multiplicities of H_{spin} of degeneracy $2S_{N_0} + 1$.

In practice one may use the following tricks: The double sum proportional to g_2 in Eq.(465) can be expressed in terms of the operator number $\hat{N}_0$ of condensate particles only,

$$\hat{N}_0 = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha. \tag{467}$$

So diagonalizing H_{spin} amounts to diagonalizing $\hat{A}^\dagger \hat{A}$!

Second the total momentum operator $\hat{\vec{S}}$ of the N_0 spins, defined as the sum of all the spin operators of the individual atoms in units of $\hbar$, can be checked to satisfy the identity

$$\hat{\vec{S}} \cdot \hat{\vec{S}} + \hat{A}^\dagger \hat{A} = \hat{N}_0(\hat{N}_0 + 1) \tag{468}$$

so that the Hamiltonian for N_0 particles becomes a function of $\hat{\vec{S}}$ [81]:

$$H_{\text{spin}} = \frac{g_2}{2L^3}\hat{N}_0(\hat{N}_0 - 1) + \frac{1}{6L^3}(g_0 - g_2)\left[\hat{N}_0(\hat{N}_0 + 1) - \hat{\vec{S}} \cdot \hat{\vec{S}}\right]. \tag{469}$$

We recall that $\hat{\vec{S}} \cdot \hat{\vec{S}} = S_{N_0}(S_{N_0} + 1)$ within the subspace of total spin S_{N_0}.

When $g_2 < g_0$ the ground state of H_{spin} corresponds to the multiplicity $S_{N_0} = N_0$, containing *e.g.* the state with all the spins in the state $|+\rangle$. In this case the N_0- particle states obtained with the Hartree-Fock approximation are exact eigenstates of H_{spin}.

When $g_2 > g_0$ the ground state of H_{spin} corresponds to the multiplicity of minimal total angular momentum, $S_{N_0} = 1$ for N_0 odd or $S_{N_0} = 0$ for N_0 even. In this case the Hartree-Fock state is a symmetry breaking approximation of the exact ground state of H_{spin}. The error on the energy per particle tends to zero in the thermodynamical limit; for N_0 even one finds indeed

$$\frac{\delta E}{N_0} = -\frac{1}{3L^3}(g_0 - g_2). \tag{470}$$

But what happens if one restores the broken symmetry by summing up the Hartree-Fock ansatz over the direction $\vec{n}$ defined in Eq.(459)? Assume that N_0 is even; one has then to reconstruct from the Hartree-Fock ansatz a rotationally invariant state. This amounts to considering the following normalized state for the N_0 spins:

$$|\Psi\rangle = \sqrt{N_0 + 1} \int \frac{d^2\vec{n}}{4\pi} |N_0 : \vec{n}\,\rangle \tag{471}$$

where $d^2\vec{n}$ indicates the integration over the unit sphere (that is over all solid angles) and $|N_0 : \vec{n}\rangle$ is the state with N_0 particles in the single particle state

$$|\vec{n}\rangle = n_x|x\rangle + n_y|y\rangle + n_z|z\rangle. \tag{472}$$

The state vector $|\Psi\rangle$, being non zero and having a vanishing total angular momentum, is equal to the exact ground state of H_{spin}!

The expression (471) can be used as a starting point to obtain various forms of $|\Psi\rangle$. If one expresses the Hartree-Fock state as the N_0-th power of the creation operator $\sum_\alpha \hat{a}_\alpha^\dagger n_\alpha$ acting on the vacuum $|\text{vac}\rangle$, and if one expands this power with the usual binomial formula, the integral over $\vec{n}$ can be calculated explicitly term by term and one obtains:

$$|\Psi\rangle = \mathcal{N}\left(\hat{A}^\dagger\right)^{N_0/2}|\text{vac}\rangle \tag{473}$$

where $\mathcal{N}$ is a normalization factor and the operator $\hat{A}$ is defined in Eq.(466). Formula (473) indicates that $|\Psi\rangle$ is simply a 'condensate' of pairs in the pair state $|\psi_0(1,2)\rangle$. It can be used to expand $|\Psi\rangle$ over Fock states with a well defined number of particles in the modes $m = 0, m = \pm 1$, reproducing Eq.(13) of [81].

To be complete we mention another way of constructing the exact eigenvectors and energy spectrum of H_{spin}. The idea is to diagonalize $\hat{A}^\dagger \hat{A}$ using the fact that $\hat{A}$ obeys a commutation relation that is reminiscent of that of an annihilation operator:

$$[\hat{A}, \hat{A}^\dagger] = 4\hat{N}_0 + 6. \tag{474}$$

In this way $\hat{A}^\dagger$ acts as a raising operator: acting on an eigenstate of $\hat{A}^\dagger \hat{A}$ with eigenvalue λ and N_0 particles, it gives an eigenstate of $\hat{A}^\dagger \hat{A}$ with eigenvalue $\lambda + 4N_0 + 6$ and with $N_0 + 2$ particles. One can also check from the identity (468) that the action of $\hat{A}^\dagger$ does not change the total spin:

$$[\hat{A}^\dagger, \hat{\vec{S}} \cdot \hat{\vec{S}}] = 0. \tag{475}$$

By repeated actions of $\hat{A}^\dagger$ starting from the vacuum one arrives at Eq.(473), creating the eigenstates with N_0 even and vanishing total spin $S = 0$. By repeated actions of $\hat{A}^\dagger$ starting from the eigenstates with $N_0 = 2$ and total spin $S = 2$ (e.g. the state $|++\rangle$) one obtains all the states with N_0 even and total spin $S = 2$. More generally the eigenstate of H_{spin} with total spin S, a spin component $m = S$ along z and N_0 particles is:

$$||N_0, S, m = S\rangle \propto \left(\hat{A}^\dagger\right)^{(N_0-S)/2}|S : +1\rangle \tag{476}$$

where $|S : +1\rangle$ represents S particles in the state $|+1\rangle$. From Eq.(476) one can generate the states with spin components $m = S - 1, \ldots, -S$ by repeated actions of the spin-lowering operator $\hat{S}_- = \hat{S}_x - i\hat{S}_y$ in the usual way. We note that formula (476) was derived independently in [82].

9.1.4 Advantage of a symmetry breaking description

Imagine that we have prepared a condensate of sodium atoms ($g_2 > g_0$) in the collective ground spin state, and that we let the atoms leak one by one out of the trap, in a way that does not perturb their spin. We then measure the spin component along z of the outgoing atoms. Suppose that we have performed this measurement on k atoms, with $k \ll N_0$. We then raise the simple question: what is the probability p_k that all the k detections give a vanishing angular momentum along z ?

Let us start with a naive reasoning based on the one-body density matrix of the condensate (even if the reader has been warned already in §8.1.2 on the dangers of such an approach!). The mean occupation numbers of the single particle spin states $|m = -1\rangle$, $|m = 0\rangle$ and $|m = +1\rangle$ in the initial condensate are obviously all equal to $N_0/3$, as the condensate is initially in a rotationally symmetric state. The probability of detecting the first leaking atom in $|m = 0\rangle$ is therefore $1/3$. Naively we assume that since $k \ll N_0$ the detections have a very weak effect on the state of the condensate and the probability of detecting the n-th atom ($n \leq k$) in the $m = 0$ channel is nearly independent of the $n-1$ previous detection results. The probability for k detections in the $m = 0$ channel should then be

$$p_k^{\text{naive}} = \frac{1}{3^k}. \tag{477}$$

Actually this naive reasoning is wrong (and by far) as soon as $k \geq 2$. The first detection of an atom in the $m = 0$ channel projects the spin state of the remaining atoms in

$$|\Psi_1\rangle = \mathcal{N}_1 \hat{a}_0 |\Psi\rangle \tag{478}$$

where $\hat{a}_0$ annihilates an atom in spin state $m = 0$, $|\Psi\rangle$ is the collective spin ground state (471) and $\mathcal{N}_1$ is a normalization factor. The probability of detecting the second atom in $m = 0$ (knowing that the first atom was detected in $m = 0$) is then given by

$$\frac{p_2}{p_1} = \frac{\langle \Psi_1 | \hat{a}_0^\dagger \hat{a}_0 | \Psi_1 \rangle}{\langle \Psi_1 | \sum_{m=-1}^{+1} \hat{a}_m^\dagger \hat{a}_m | \Psi_1 \rangle}. \tag{479}$$

The denominator is simply equal to $N_0 - 1$ as $|\Psi_1\rangle$ is a state with $N_0 - 1$ particles. Using the integral form (471) and the simple effect of an annihilation operator on a Hartree-Fock state, *e.g.*

$$\hat{a}_0^2 |N_0 : \vec{n}\rangle = [N_0(N_0 - 1)]^{1/2} \, n_z^2 |N_0 - 2 : \vec{n}\rangle \tag{480}$$

we are able to express the probability in terms of integrals over solid angles:

$$\frac{p_2}{p_1} = \frac{\displaystyle\int d^2\vec{n} \int d^2\vec{n}' \; n_z^2 n_z'^2 (\vec{n} \cdot \vec{n}')^{N_0 - 2}}{\displaystyle\int d^2\vec{n} \int d^2\vec{n}' \; n_z n_z' (\vec{n} \cdot \vec{n}')^{N_0 - 1}}. \tag{481}$$

We suggest the following procedure to calculate these integrals. One first integrates over $\vec{n}'$ for a fixed $\vec{n}$, using spherical coordinates relative to the 'vertical' axis directed along $\vec{n}$: the polar angle θ' is then the angle between $\vec{n}'$ and $\vec{n}$ so that one has simply $\vec{n} \cdot \vec{n}' = \cos\theta'$. The integral over θ' and over the azimuthal angle ϕ' can be performed, giving a result involving only n_z. The remaining integral over $\vec{n}$ is performed with the spherical coordinates of vertical axis z. This leads to

$$\frac{p_2}{p_1} = \frac{3}{5} + \frac{2}{5(N_0 - 1)}. \tag{482}$$

The ratio p_2/p_1 is therefore different from the naive (and wrong!) prediction (477). For $N_0 = 2$ one finds $p_2/p_1 = 1$ so that the second atom is surely in $m = 0$ if the first atom was detected in $m = 0$. As the two atoms were initially in the state with total angular momentum zero, this result could be expected from the expression (448) of the two-particle spin state. In the limit of large N_0 we find that once the first atom has been detected in the $m = 0$ channel, the probability for detecting the second atom in the same channel $m = 0$ is $3/5$. This somehow counter-intuitive result shows that the successive detection probabilities are strongly correlated in the case of the spin state (471).

The exact calculation of the ratio

$$\frac{p_{k+1}}{p_k} = \frac{\displaystyle\int d^2\vec{n} \int d^2\vec{n}' \; n_z^{k+1} n_z'^{k+1} (\vec{n} \cdot \vec{n}')^{N_0 - (k+1)}}{\displaystyle\int d^2\vec{n} \int d^2\vec{n}' \; n_z^k n_z'^k (\vec{n} \cdot \vec{n}')^{N_0 - k}} \tag{483}$$

is getting more difficult when k increases. The large N_0 limit for a fixed k is easier to obtain: in the integral over $\vec{n}'$ the function $(\vec{n} \cdot \vec{n}')^{N_0 - (k+1)}$ is extremely peaked around

$\vec{n}' = \vec{n}$ so that we can replace $n_z'^{k+1}$ by n_z^{k+1}. This leads to

$$\lim_{N_0 \to +\infty} \frac{p_{k+1}}{p_k} = \frac{2k+1}{2k+3}.\tag{484}$$

We now give the reasoning in the symmetry breaking point of view, which assumes that a single experimental realization of the condensate corresponds to a Hartree-Fock state $|N_0 : \vec{n}\rangle$ with the direction $\vec{n}$ being an impredictable random variable with uniform distribution over the sphere. If the system is initially in the spin state $|N_0 : \vec{n}\rangle$ there is no correlation between the spins, and the probability of having k detections in the channel $m = 0$ is simply $(n_z^2)^k$. One has to average over the unknown direction $\vec{n}$ to obtain

$$p_k^{\text{sb}} = \int \frac{d^2\vec{n}}{4\pi} n_z^{2k} = \frac{1}{2k+1}.\tag{485}$$

One recovers in an easy calculation the large N_0 limit of the exact result, Eq.(484)! We note that the result (485) is much larger than the naive (and wrong) result (477) as soon as $k \gg 1$.

9.2   Solitonic condensates

We consider in this section a Bose-Einstein condensate with effective attractive interactions subject to a strong confinement in the $x - y$ plane so that it constitutes an approximate one-dimensional interacting Bose gas along z. Such a situation is interesting physically as it gives rise in free space to the formation of 'bright' solitons well known in optics but not yet observed with atoms. Also the model of a one-dimensional Bose gas with a δ interaction potential has known exact solutions in free space, that can be used to test the translational symmetry breaking Hartree-Fock approximation.

9.2.1   How to make a solitonic condensate ?

Consider a steady state condensate with effective attractive interactions in a three dimensional harmonic trap. The confinement in the $x - y$ plane is such that the transverse quanta of oscillation $\hbar\omega_{x,y}$ are much larger than the typical mean field energy per particle $N_0|g||\phi|^2$, where ϕ is the condensate wavefunction with N_0 particles. This confinement prevents the occurrence of a spatial collapse of the condensate (see §5.2.1).

The confinement is however not strong enough to violate the validity condition of the Born approximation for the pseudo-potential, $k|a| \ll 1$ with $k \simeq (m\omega_{x,y}/\hbar)^{1/2}$.

In this case we face a quasi one-dimensional situation, where the condensate wavefunction is approximately factorized as

$$\phi(x, y, z) = \psi(z)\chi_x(x)\chi_y(y) \tag{486}$$

where χ_x and χ_y are the normalized ground states of the harmonic oscillator along x and along y respectively. By inserting the factorized form (486) in the Gross-Pitaevskii energy functional Eq.(139) and by integrating over the directions x and y we obtain an energy functional for ψ :

$$E[\psi, \psi^*] = N_0 \int dz \left[\frac{\hbar^2}{2m} \left| \frac{d\psi}{dz} \right|^2 + \frac{1}{2}m\omega_z^2 z^2 |\psi(z)|^2 + \frac{1}{2}N_0 g_{1d}|\psi(z)|^4 \right] \tag{487}$$

where we have dropped the zero-point energy of the transverse motion and we have called g_{1d} the quantity

$$g_{1d} = g \int dx \int dy \ |\chi_x(x)|^4 |\chi_y(y)|^4 = g\frac{m(\omega_x\omega_y)^{1/2}}{2\pi\hbar}. \tag{488}$$

The corresponding time independent Gross-Pitaevskii equation for ψ is

$$\mu\psi(z) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dz^2} + \left[\frac{1}{2}m\omega_z^2 z^2 + N_0 g_{1d}|\psi(z)|^2 \right] \psi(z). \tag{489}$$

The energy functional Eq.(487) corresponds to a one-dimensional interacting Bose gas with an effective coupling constant between the atoms equal to g_{1d} , that is one can imagine that the particles have a binary contact interaction

$$V(z_1, z_2) = g_{1d}\delta(z_1 - z_2). \tag{490}$$

Note that such a Dirac interaction potential leads to a perfectly well defined scattering problem in one dimension, contrarily to the three dimensional case.

Imagine now that we slowly decrease the trap frequency along z while keeping intact the transverse trap frequencies, until ω_z vanishes. What will happen then? If g was positive the cloud would simply expand without limit along z . With attractive interaction the situation is dramatically different: due to the slow evolution of ω_z the condensate

wavefunction will follow adiabatically the minimal energy solution of the Gross-Pitaevskii equation. For $\omega_z = 0$ this minimal energy solution is the so-called bright soliton, well known in non-linear optics. We recall the analytic form of the solitonic wavefunction:

$$\psi(z) = \frac{1}{(2l)^{1/2}} \frac{1}{\cosh(z/l)} \tag{491}$$

where l is the spatial radius of the soliton:

$$l = -\frac{2\hbar^2}{N_0 m g_{1d}}. \tag{492}$$

Note that this size l results of a compromise between minimization of kinetic energy by an increase of the size and minimization of interaction energy by a decrease of the size, so that the typical kinetic energy per particle $\hbar^2/(ml^2)$ is roughly opposite to the interaction energy per particle $N_0 g_{1d}/l$. We also give the corresponding chemical potential:

$$\mu = -\frac{1}{8} N_0^2 \frac{m g_{1d}^2}{\hbar^2}. \tag{493}$$

We briefly address the validity of the Gross-Pitaevskii solution (491). As we have pointed out in the three dimensional case (see for example §3.2.1) we wish that the Born approximation for the interaction potential be valid. In one dimension the δ interaction potential can be treated in the Born approximation only if the relative wavevector of the colliding particles is **high** enough (in contrast to the three-dimensional case):

$$\left| \frac{\hbar^2 k}{m g_{1d}} \right| \gg 1. \tag{494}$$

This condition can be obtained of course from a direct calculation, but also from a dimensionality argument ($m g_{1d}/\hbar^2$ is the **inverse** of a length) and from the fact that the Born approximation should apply in the limit $g_{1d} \to 0$ for a fixed k. If we use the estimate $k \simeq 1/l$ we obtain the condition

$$-\frac{\hbar^2}{m g_{1d} l} \simeq N_0 \gg 1, \tag{495}$$

implicitly valid here as we started from a condensate!

Another phenomenon neglected in the prediction (491) is the spreading of the center of mass coordinate during the switch-off of the trapping potential along z. Whereas

Eq.(491) assumes that the abscissa of the center of the soliton z_0 is exactly 0 the spreading of the center of mass leads in real life to a finite width probability distribution for z_0. This spreading can be calculated simply for an almost pure condensate $N_0 \simeq N$, using the fact that the center of mass coordinate operator $\hat{Z}$ and the total momentum operator $\hat{P}$ of the gas along z axis are decoupled from the relative coordinates of the particles in a harmonic potential, in presence of interactions depending only on the relative coordinates. To prove this assertion one expresses the operators $\hat{Z}$ and $\hat{P}$ in terms of the position and momentum operators of each particle i of the gas:

$$\hat{Z} = \frac{1}{N} \sum_{i=1}^{N} z_i \tag{496}$$

$$\hat{P} = \sum_{i=1}^{N} p_i \tag{497}$$

and one derives the following equations of motion in Heisenberg point of view:

$$\frac{d\hat{Z}}{dt} = \frac{\hat{P}}{Nm} \tag{498}$$

$$\frac{d\hat{P}}{dt} = -Nm\omega_z^2(t)\hat{Z}. \tag{499}$$

The spreading acquired by $\hat{Z}$ is not negligible when it becomes comparable to the size l of the soliton.

The spreading of $\hat{Z}$ is interesting to calculate in the absence of harmonic confinement along z, $\omega_z \equiv 0$, with the simple assumption that all the particles of the gas are at time $t = 0$ in the soliton state $|\psi\rangle$ of Eq.(491). As $\hat{P}$ is a constant of motion for $\omega_z = 0$ one has simply

$$\hat{Z}(t) = \hat{Z}(0) + \frac{\hat{P}t}{Nm} \tag{500}$$

so that the variance of the center of mass coordinate at time t is

$$\mathrm{Var}(\hat{Z})(t) = \mathrm{Var}(\hat{Z})(0) + \frac{t}{Nm}\langle \hat{Z}(0)\hat{P} + \hat{P}\hat{Z}(0)\rangle + \frac{t^2}{N^2m^2}\mathrm{Var}(\hat{P}). \tag{501}$$

One then replaces $\hat{Z}(0)$ and $\hat{P}$ by the sums (496, 497). As the single particle wave-function ψ has vanishing mean position and mean momentum all the 'crossed terms'

expectation values involving two different particles vanish. As $\psi(z)$ is a real wavefunction one finds also $\langle \psi | zp + pz | \psi \rangle = 0$ so that the contribution linear in time vanishes. One is left with

$$\mathrm{Var}(\hat{Z})(t) = \frac{1}{N} \langle \psi | z^2 | \psi \rangle + \frac{t^2}{Nm^2} \langle \psi | p^2 | \psi \rangle. \tag{502}$$

The variance of $\hat{Z}$, initially N times smaller than the single particle variance $\langle \psi | z^2 | \psi \rangle$, becomes equal to the single particle variance after a time

$$t_c = \left(\frac{Nm^2 \langle \psi | z^2 | \psi \rangle}{\langle \psi | p^2 | \psi \rangle} \right)^{1/2} = N^{1/2} \frac{\pi m l^2}{2\hbar} \tag{503}$$

where we used the explicit expressions

$$\langle \psi | z^2 | \psi \rangle = \frac{\pi^2 l^2}{12} \tag{504}$$

$$\langle \psi | p^2 | \psi \rangle = \frac{\hbar^2}{3l^2}. \tag{505}$$

The spreading phenomenon of the position of the soliton is formally equivalent to the spreading of the relative phase of two condensates initially prepared in a phase state (see §8.2). The critical time t_c in (503) scales as $N^{1/2} \hbar / |\mu|$ as in Eq.(442).

9.2.2 Ground state of the one-dimensional attractive Bose gas

We consider here the model of the one-dimensional gas of N bosonic particles interacting with the contact potential Eq.(490) and in the absence of any confining potential.

It turns out that in this model with $g_{1d} > 0$ one can calculate exactly the eigenenergies and eigenstates of the Hamiltonian for N particles using the Bethe ansatz [83]. We consider here the less studied attractive case $g_{1d} < 0$, where several exact results are also available. In particular the exact expression for the ground state energy is known [84]:

$$\hat{E}_0(N) = -\frac{1}{24} \frac{m g_{1d}^2}{\hbar^2} N(N^2 - 1) \tag{506}$$

and the corresponding $N-$ particle wavefunction of the ground state is [85]:

$$\Psi(z_1, \ldots, z_N) = \mathcal{N} \exp \left[\frac{m g_{1d}}{2\hbar^2} \sum_{1 \leq i < j \leq N} |z_i - z_j| \right]. \tag{507}$$

To determine the normalization factor $\mathcal{N}$ we enclose the gas in a fictitious box of size L tending to $+\infty$: [5]

$$|\mathcal{N}|^2 = \frac{(N-1)!}{NL}\left(\frac{m|g_{1d}|}{\hbar^2}\right)^{N-1}. \tag{508}$$

To what extent can we recover these results using a Hartree-Fock ansatz $|N:\psi\rangle$ for the ground state wavefunction? As discussed around Eq.(151) we get a mean energy for the Hartree-Fock state very similar to Eq.(487):

$$E[\psi,\psi^*] = N\int dz\left[\frac{\hbar^2}{2m}\left|\frac{d\psi}{dz}\right|^2 + \frac{1}{2}(N-1)g_{1d}|\psi(z)|^4\right]. \tag{509}$$

We minimize this functional using the results of §9.2.1, replacing N_0 by $N-1$, and we obtain

$$E_0^{\mathrm{hf}}(N) = -\frac{1}{24}\frac{mg_{1d}^2}{\hbar^2}N(N-1)^2. \tag{510}$$

The deviation of the Hartree-Fock result from the exact result is a fraction $1/N$ of the energy and is small indeed in the large N limit, as expected from the validity condition (495)!

There is a notable difference of translational properties however. Whereas the exact ground state (507) is invariant by a global translation of the positions of the particles, as it should be, the Hartree-Fock ansatz leads to condensate wavefunctions ψ localized within the length l around some arbitrary point z_0 (around $z_0 = 0$ in Eq.(491)):

$$\psi_{z_0}(z) = \frac{1}{(2l)^{1/2}}\frac{1}{\cosh[(z-z_0)/l]} \tag{511}$$

with a spatial radius

$$l = -\frac{2\hbar^2}{(N-1)mg_{1d}}. \tag{512}$$

The Hartree-Fock ansatz $|N:\psi\rangle$ therefore breaks the translational symmetry of the system.

---

[5]The center of mass of the gas corresponds to a fictitious particle of wavevector K, where $\hbar K$ is the total momentum of the gas, and of position Z, where Z is the centroid of the gas. In the ground state $|\Psi\rangle$ the center of mass is completely delocalized with $K=0$. The factor $1/L$ in $|\mathcal{N}|^2$ originates from the normalization of the fictitious particle plane wave in the fictitious box of size L, $\langle Z|K\rangle = e^{iKZ}/\sqrt{L}$. The more correct mathematical way (not used here) is to normalize in free space (no box) using the closure relation $\int dK|K\rangle\langle K| = \mathrm{Id}$, which amounts to replace L by 2π.

Breaking a symmetry of the system costs energy, and this can be checked for the present translational symmetry breaking. As the center of mass coordinates Z, P of the N particles are decoupled from the relative coordinates of the particles we can write the total energy of the gas as the sum of the kinetic energy of the center of mass and an 'internal' energy including the kinetic energy of the relative motion of the particles and the interaction energy. Whereas the exact ground state wavefunction has a vanishing center of mass kinetic energy, the symmetry breaking ansatz $|N : \psi\rangle$ contains a center of mass kinetic energy:

$$E_{\text{c.o.m.}} = \langle N : \psi | \frac{\hat{P}^2}{2mN} | N : \psi \rangle \tag{513}$$

where mN is the total mass of the gas and $\hat{P}$ is the total momentum operator. Using the definition (497), expanding the square of $\hat{P}$, and using the fact that the soliton wavefunction ψ has a vanishing mean momentum we obtain

$$E_{\text{c.o.m.}} = \langle \psi | \frac{p^2}{2m} | \psi \rangle \tag{514}$$

$$= \frac{1}{24} \frac{m g_{1d}^2}{\hbar^2} (N - 1)^2. \tag{515}$$

We see that $E_{\text{c.o.m.}}$ accounts for half the energy difference between the exact ground state energy (506) and the Hartree-Fock energy (510).

9.2.3 Physical advantage of the symmetry breaking description

We now raise the question: is there a Bose-Einstein condensate in the one-dimensional free Bose gas with attractive interaction? To make things simple we assume that the gas is at zero temperature so that the $N-$ particle wavefunction is known exactly, see Eq.(507).

We start with a reasoning in terms of the one-body density operator (even if we know from the previous physical examples that this may be dangerous). Paraphrasing the usual three dimensional definition of a Bose-Einstein condensate in free space we put the one-dimensional gas in a fictitious box of size L and we calculate the mean number of particles n_0 in the plane wave with vanishing momentum $p = 0$ in the limit $L \to +\infty$.

The calculation with the exact ground state wavefunction has been done [85]. One

finds that n_0 is going to zero as $1/L$:

$$\lim_{L\to+\infty} n_0 L = C(N)\frac{2\hbar^2}{m|g_{1d}|}. \tag{516}$$

The factor $C(N)$ is given by

$$C(N) = \sum_{i=1}^{N}\sum_{j=i}^{N}\frac{(j-1)!}{(i-1)!}\frac{(N-i)!}{(N-j)!}\prod_{k=i}^{j}\left[k(N+1-k)-\frac{1}{2}(N+1)\right]^{-1} \tag{517}$$

and converges to $\pi^2/2$ in the large N limit, so that n_0 no longer depends on N in this limit. There is therefore no macroscopic population in the $p=0$ momentum state. One may then be tempted to conclude that there is no Bose-Einstein condensate, even at zero temperature, in the one-dimensional Bose gas with attractive contact interactions. However we have learned that a reasoning based on the one-body density matrix may miss crucial correlations between the particles, and that the symmetry breaking point of view may be illuminating in this respect.

The translational symmetry breaking point of view approximates the state of the gas by the N-body density operator:

$$\hat{\rho}^{\text{sb}} = \lim_{L\to+\infty}\int_{-L/2}^{L/2}\frac{dz_0}{L}|N:\psi_{z_0}\rangle\langle N:\psi_{z_0}|. \tag{518}$$

In the large N limit we expect this prescription to be valid for few-body observables. Of course for a $N-$ body observable such as the kinetic energy of the center of mass of the gas, the results will be different, Eq.(515) for the symmetry breaking point of view vs. a vanishing value for the exact result.

Let us test this expectation by calculating in the Hartree-Fock approximation the mean number of particles in the plane wave $\langle z|k\rangle = \exp(ikz)/L^{1/2}$. Using the following action of the annihilation operator $\hat{a}_k$ of a particle with wavevector k on the Hartree-Fock state:

$$\hat{a}_k|N:\psi_{z_0}\rangle = N^{1/2}\langle k|\psi_{z_0}\rangle|N-1:\psi_{z_0}\rangle \tag{519}$$

we obtain

$$n_k^{\text{hf}} = N|\langle k|\psi\rangle|^2. \tag{520}$$

The momentum distribution of the particles in the gas in this approximation is simply proportional to the momentum distribution of a single particle in the solitonic wavefunction ψ ! It turns out that the Fourier transform of the $1/\cosh$ function can be calculated

exactly, and it is also a $1/\cosh$ function. We finally obtain:

$$n_k^{\text{hf}} \simeq \frac{1}{L} \frac{\pi^2 \hbar^2}{m|g_{1d}|} \frac{1}{\cosh^2\left(\frac{\pi k l}{2}\right)} \tag{521}$$

where l is the soliton size given in Eq.(512). For $k = 0$ one recovers the large N limit of the exact result (516).

In more physical terms, one can imagine from Eq.(518) that a given experimental realization of the Bose gas corresponds to a condensate of N particles in the solitonic wavefunction (511), with a central position z_0 being a random variable varying in an unpredictable way for any new realization of the experiment. There is therefore a Bose-Einstein condensate in the one-dimensional attractive Bose gas!

An illustrative gedanken experiment would be to measure the positions along z of all the particles of the gas. In the symmetry breaking point of view the positions $z_1, \ldots, z_N$ obtained in a single measurement are randomly distributed according to the density $|\psi_{z_0}^2|(z) = |\psi(z - z_0)|^2$ where z_0 varies from shot to shot as the relative phase of the two condensates did in the MIT interference experiment. As we know the exact ground state (507) we also know the exact $N-$ body distribution function, $|\Psi(z_1, \ldots, z_N)|^2$. This is however not so easy to use!

So we suggest instead to consider the mean spatial density of the particles *knowing* that the center of mass of the cloud has a position Z. In the exact formalism this gives [85]:

$$
\begin{aligned}
\rho(z|Z) &= \int dz_1 \ldots \int dz_N |\Psi(z_1, \ldots, z_N)|^2 \left(\sum_{j=1}^{N} \delta(z - z_j)\right) L\delta\left(Z - \frac{1}{N}\sum_{n=1}^{N} z_n\right) \quad (522) \\
&= \frac{2N}{l} \sum_{k=0}^{N-2} \frac{(N-2)!}{(N-k-2)!} \frac{N!}{(N+k)!}(-1)^k (k+1) \exp\left[-(k+1)\frac{2N}{N-1}\frac{|z-Z|}{l}\right]
\end{aligned}
$$

where l is the N-dependent length of the soliton (512), the integrals are taken in the range $[-L/2, L/2]$ and $L \to +\infty$; the factor L, compensating the one in the normalization factor of Ψ, ensures that the integral of $\rho(z|Z)$ over z is equal to N.

In the symmetry breaking point of view the definition of $\rho(z|Z)$ is similar to Eq.(522); the factor L cancels with the $1/L$ factor of Eq.(518). This leads to

$$\rho^{\text{sb}}(z|Z) = \int dz_0 \int dz_1 \ldots \int dz_N \left(\prod_{k=1}^{N} |\psi(z_k - z_0)|^2\right) \left(\sum_{j=1}^{N} \delta(z - z_j)\right) \delta\left(Z - \frac{1}{N}\sum_{n=1}^{N} z_n\right)$$

$$= N \int dz_1 \ldots \int dz_N \left(\prod_{k=1}^{N} |\psi(z_k)|^2 \right) \delta \left(Z - z + z_1 - \frac{1}{N} \sum_{n=1}^{N} z_n \right) \tag{523}$$

where we have made the change of variables $z_k \to z_k + z_0$ (which allows to integrate over z_0) and we have replaced the sum over the indiscernible particles j by N times the contribution of particle $j = 1$. The multiple integral over the positions $z_1, \ldots, z_N$ can be turned into a single integral over a wavevector q by using the identity $\delta(X) = \int dq/(2\pi) \exp(iqX)$, allowing a numerical calculation of $\rho^{\mathrm{sb}}(z|Z)$.

Does the approximate result (523) get close to the exact result for large N? We compare numerically in figure 17 the exact density $\rho(z|Z)$ to the symmetry breaking mean-field prediction $\rho^{\mathrm{sb}}(z|Z)$: modestly large values of N give already good agreement between the two densities. This validates the symmetry breaking approach for the considered gedanken experiment.

What happens in the large N limit? In Eq.(523) each variable z_k explores an interval of size $\sim l$ so that the quantity $(z_1 + \ldots + z_N)/N$ has a standard deviation $\sim l/\sqrt{N}$ much smaller than l and can be neglected as compared to z_1 inside the δ distribution. This leads to

$$\rho^{\mathrm{sb}}(z|Z) \simeq N|\psi_{z_0=Z}(z)|^2 \quad \text{for} \quad \sqrt{N} \gg 1 \tag{524}$$

where the solitonic wavefunction $\psi_{z_0=Z}$ is given in Eq.(511). Numerical calculation of $\rho^{\mathrm{sb}}(z|Z)$ shows that Eq.(524) is a good approximation over the range $|z - Z| \simeq l$ for $N = 10$ already!
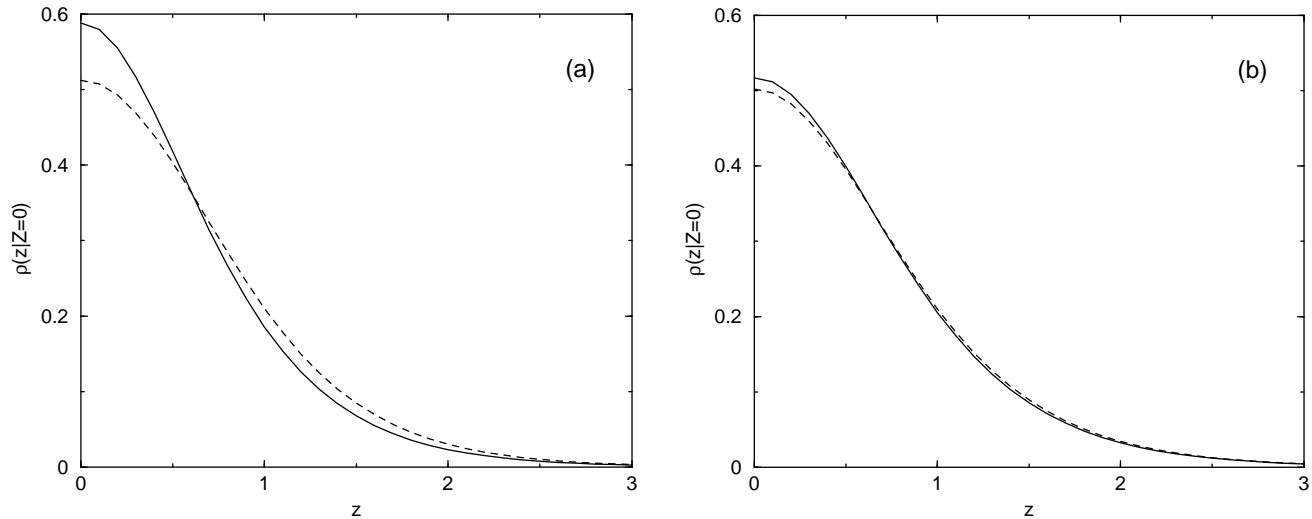
Acknowledgments

Figure 17: For the ground state of the one-dimensional attractive Bose gas, position dependence of the mean density of particles knowing that the center-of-mass of the gas is in $Z = 0$. Solid line: exact result $\rho(z|Z = 0)$. Dashed line: mean-field approximation $\rho^{\text{sb}}(z|Z = 0)$. The position z is expressed in units of the 'soliton' radius l given in Eq.(512), and the linear density in units of N/l. The number of particles is (a) $N = 10$ and (b) $N = 45$.

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