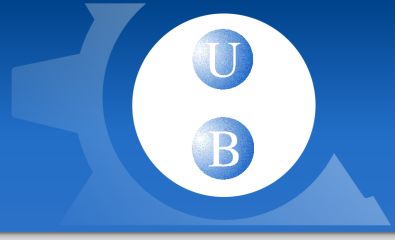

An introduction to ultra-cold gases and the exact diagonalisation technique

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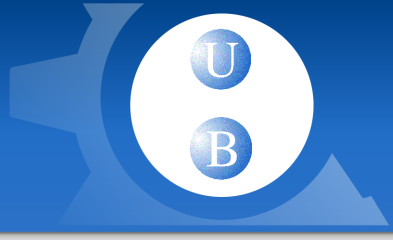
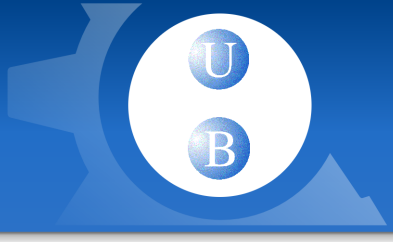
Outline



A naive idea
of a Bose gas



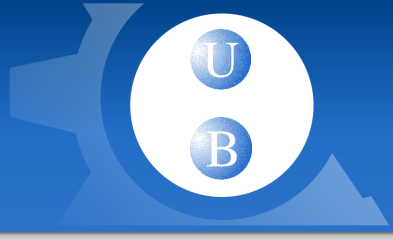
We consider a system with N **non-interacting** bosons in an harmonic trap.

$$H = \sum_{j=1}^{N} H_j^{(1)} , \tag{1}$$

where $H^{(1)} = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2$ is the one particle Hamiltonian with Schrodinger equation

$$H^{(1)} |\phi_n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |\phi_n\rangle . \tag{2}$$

A naive idea
of a Bose gas



Using the canonical ensemble, the probability to find a particle with energy ϵ_n is given by

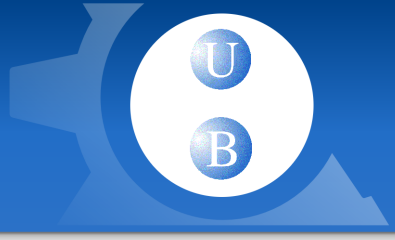
$$P(\epsilon_i) = \frac{e^{-\beta\epsilon_i}}{Z(\beta)} \tag{3}$$

where $Z(\beta) = \sum_i e^{-\beta\epsilon_i}$ is the partition function. Then, the occupation n_i of the single-particle state ϕ_i is

$$n_i = N\frac{e^{-\beta\epsilon_i}}{Z(\beta)} \ . \tag{4}$$

The condensation

The cooling process



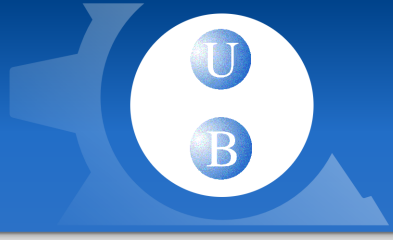
We have a gas trapped in an harmonic magnetic trap at a temperature of 3 K.

Cooling steps

1. Laser cooling ($T \sim 10^{-4} K$)
2. Magnetic evaporate ($T \sim 10^{-7} K$)

The order parameter

roughly speaking

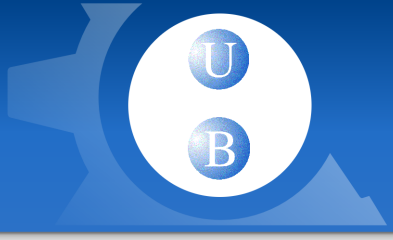


At the absolute temperature, all particles are in the ground state

$$|\Psi\rangle = |GS\rangle = |\phi_0\phi_0...\phi_0\rangle = |N, 0, ..., 0\rangle \tag{5}$$

It is intuitive to think then, that there is a monoparticle wave function that characterizes all the system. This is the **order parameter** or the wave function of the condensate, which gives us all its properties.

The OBDM
(One Body Density Matrix)



We define the OBDM as a generalization of the density function

$$n^{(1)}(r, r') = \langle \hat{\Psi}^\dagger(r)\hat{\Psi}(r') \rangle \,. \tag{6}$$

The intersting point is that its diagonalisation

$$\int \mathrm{d}^3 r n^{(1)}(r, r')\phi_i(r') = n_i\phi_i(r') \tag{7}$$

gives us a natural basis of orthonormalized **single**-particle wave functions. Its eigenvalues verify the normalization condition $\sum_i n_i = N$.
We interpret them as the occupation numbers relative to the single-particle states ϕ_i.

The OBDM
(One Body Density Matrix)

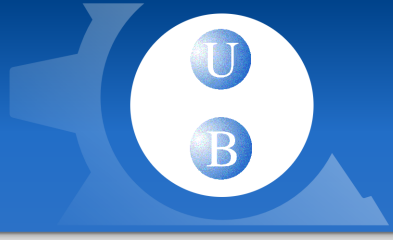
The OBDM has a simple form in this basis

$$n^{(1)}(r, r') = n_0 \phi_0^*(r)\phi_0(r) + \sum_{i \neq 0} n_i \phi_i^*(r)\phi_i(r) \qquad (8)$$

If one of the occupation numbers is much larger than the others ($n_0 >> n_i \quad \forall i > 0$), then we say that this one is macro-occupied, and condensation appears. We assign to this state the role of an order parameter.

Welcome to the real world

Considerations of a real gas



If we want a more accurate description of a bose gas, we have to consider:

- the interactions between the particles (Bogoliubov approximation)
- the system is nonuniform (generalisation of Bogoliubov, Gross-Pitaevski equation)

These considerations allow us to describe:

- vortices
- trapped condensates
- ...

The Gross-Pitevski equation

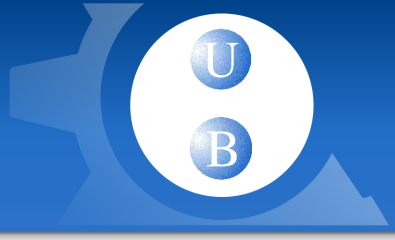
and Bogoliubov approximation

The Hamiltonian of the system in terms of the field operators Ψ is,

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \nabla \hat{\psi} \right) \mathrm{d}^3 r + \frac{1}{2} \int \hat{\psi}^\dagger \hat{\psi}^\dagger V(r - r') \hat{\psi} \hat{\psi} \mathrm{d}^3 r' \mathrm{d}^3 r \,, \tag{9}$$

where $V(r - r')$ is the two body potential.

Bogoliubov approximation



In the case that there is a macro-occupied single-particle wave function, we can write the field operator as

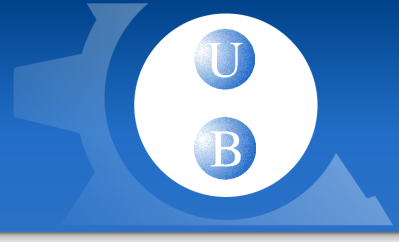
$$\hat{\Psi}(r) = \phi_0(r)a_0 + \sum_{i\neq 0} \phi_i(r)a_i \tag{10}$$

We can treat, in good aproximation, the macrospcopic component $\phi_0(r)a_0$ of the field operator as a classical field,

$$\hat{\Psi}(r) = \Psi_0(r) + \delta\hat{\Psi}(r) \tag{11}$$

If the degree of condensation is very high we can neglect the noncondensate component $\delta\hat{\Psi}$.

The Gross-Pitaevski Equation

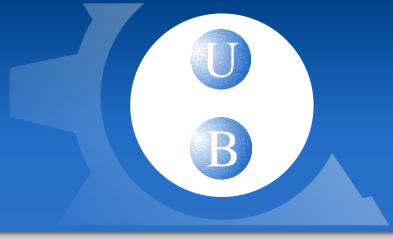


The previous approximation allows us to write the following equation as a good approximation to the behaviour of the system

$$i\hbar\frac{\partial}{\partial t}\Psi_0(r,t) = \left(\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r,t) + g|\Psi_0(r,t)|^2\right)\Psi_0(r,t) \tag{12}$$

This equation is called Gross-Pitaevski eq. and it would be equivalent to Maxwell eqns. in the field of QED.

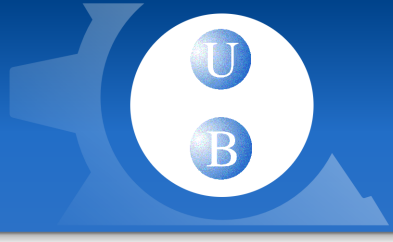
Aplicability
of the Gross-Pitaevski Equation



The hypothesis done to deduce the GPE are

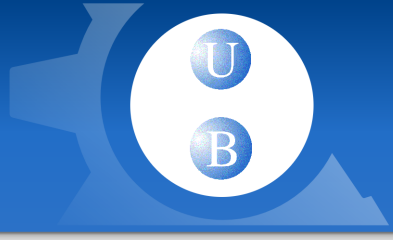
- Large number of particles to be able to use the concept of BE-condensation.
- Diluteness condition.
- Temperature is low enough. All atoms are in the condensate.

It works very well and describes a lot of phenomena.



Then, How we can study systems of few particles?

Scheme
of the exact diagonalisation technique



Exact diagonalisation:

- Allows us to solve any Hamiltonian with any statistics (numerically).
- Has a huge computational cost, which limites us to study systems with few particles.

Its algoritm consists of three steps:

1. Election of a **monoparticle** basis and construction of the **multiparticle** basis.
2. Construction the matrix of the whole Hamiltonian in the chosen basis.
3. Diagonalisation of the Hamiltonian.

Choosing a monoparticle basis

The first step

We consider a general Hamiltonian

$$H = \sum_{i=1}^{N} H_i^{(1)} + \sum_{i<j} V(r_i - r_j) \tag{13}$$

We choose the monoparticle basis such that the one body term of the Hamiltonian is diagonal. Writing the Hamiltonian in the 2nd quantization language,

$$H = \sum_{i} h_i a_i^\dagger a_i + \frac{1}{2} \sum_{jklm} V_{jklm} a_j^\dagger a_k^\dagger a_l a_m \tag{14}$$

Choosing a monoparticle basis

The first step

Example

A system of charged particles in a an harmonic trap with a transverse magnetic field is described by the Hamiltonian,

$$H^{(1)} = \frac{1}{2m}\left(\vec{p} + \frac{q}{c}\vec{A}\right) + \frac{1}{2}m\omega_{trap}^2\left(x^2 + y^2\right) , \tag{15}$$

which can be diagonalized

$$H^{(1)}|m\rangle = \epsilon_m|m\rangle , \tag{16}$$

with

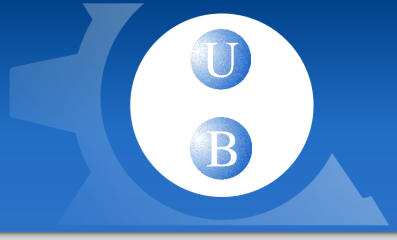
$$\epsilon_m = \hbar\left(\frac{\Omega}{2} + (\Omega - \omega_c)\frac{m}{2}\right) \tag{17}$$

$$\phi_m(r,\theta) \equiv \langle r|m\rangle = \frac{1}{\sqrt{2\pi m!}} 2^{-\frac{m}{2}} \left(\frac{r}{l_B}\right)^m e^{im\theta} e^{-\left(\frac{r}{l_B}\right)^2} , \tag{18}$$

where $\omega_c = \frac{qB}{mc}$, $\Omega = \sqrt{\omega_c^2 + 4\omega_{trap}^2}$ and $l_B = \sqrt{\frac{\hbar}{m\Omega}}$.

The multiparticle basis

Under construction



Usually, the whole Hamiltonian is block diagonal, so is much more efficient to diagonalise each block independently.

Example

In the previous example, the interaction conserves the angular momentum, so we could diagonalize for each value of the total angular momentum L.

1. We choose the subspace that will be diagonalized. In the example we fix the value of L.
2. We construct the multiparticle basis considering all the possible configurations compatible with the subspace and the statistics (fermions or bosons).

Example of a multiparticle basis

for Bosons

Example with bosons $N = 4$ $L = 5$

The multiparticle basis of a system with 4 bosons and total angular momentum 5 would be

m	0	1	2	3	4	5
$\|\psi_1\rangle =$	3	-	-	-	-	1
$\|\psi_2\rangle =$	2	1	-	-	1	-
$\|\psi_3\rangle =$	2	-	1	1	-	-
$\|\psi_4\rangle =$	1	2	-	1	-	-
$\|\psi_5\rangle =$	1	1	2	-	-	-
$\|\psi_6\rangle =$	-	3	1	-	-	-

Example of a multiparticle basis

for fermions

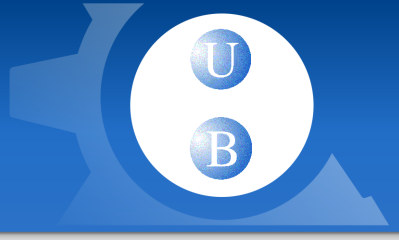
Example with fermions $N = 4$ $L = 5$

The multiparticle basis of a system with 4 fermions $\left(s = \frac{1}{2}\right)$ and total angular momentum 5 would be

m	0	1	2	3	4	5
$\|\psi_1\rangle =$	2	1	-	-	1	-
$\|\psi_2\rangle =$	2	-	1	1	-	-
$\|\psi_3\rangle =$	1	2	-	1	-	-
$\|\psi_4\rangle =$	1	1	2	-	-	-

Computation of the matrix

elements of the Hamiltonian



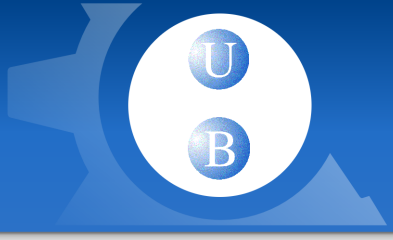
Once we have the multiparticle basis constructed, we proceed to the computation of the matrix elements.

$$H_{ij} \equiv \langle \psi_i | \hat{H} | \psi_j \rangle \tag{19}$$

The matrix elements of the one body terms are trivial due to our selection of the single particle basis. Respect to the potential, we have

$$\langle \psi_i | \hat{V} | \psi_j \rangle = \sum_{klmn} V_{klmn} \langle \psi_i | a_k^\dagger a_l^\dagger a_m a_n | \psi_j \rangle \tag{20}$$

Diagonalisation
of the Hamiltonian



Finally, we just diagonalize and we obtain the eigenvalues and the eigenvectors.
We are specially interested in the GS, since it will be the state that expermentalists expect to obtain in the laboratory.

$$|\mathrm{GS}\rangle = \sum_{i=1}^{D} \alpha_i |\Psi_i\rangle \tag{21}$$

With this expression of the GS in terms of the muliparticle basis we can compute

- the density at each point
- the OBDM
- the pair correlation function
- ...

Diagonalisation of the OBDM

Macrooccupated state

The OBDM of the GS is defined by

$$n^{(1)}(r, r') = \langle \mathrm{GS}|\hat{\Psi}^\dagger(r)\hat{\Psi}(r')|\mathrm{GS}\rangle \,. \tag{22}$$

Its diagonalisation

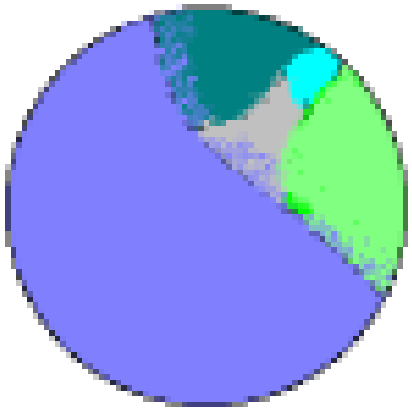
$$\int \mathrm{d}^3 r n^{(1)}(r, r')\phi_i(r') = n_i\phi_i(r') \tag{23}$$

gives us a natural basis of orthonormalized **single**-particle wave functions. Its eigenvalues verify the normalization condition $\sum_i n_i = N$.
We interpret them as the occupation numbers relative to the single-particle states ϕ_i.
If one of them is much larger than the others ($n_0 >> n_i \quad \forall i > 0$), we say that this one is macro-occupied.

Order parameter

Macro-occupied state

We assign to the macro-occupied single-particle state the role of an order parameter or the wave function of the condensate.



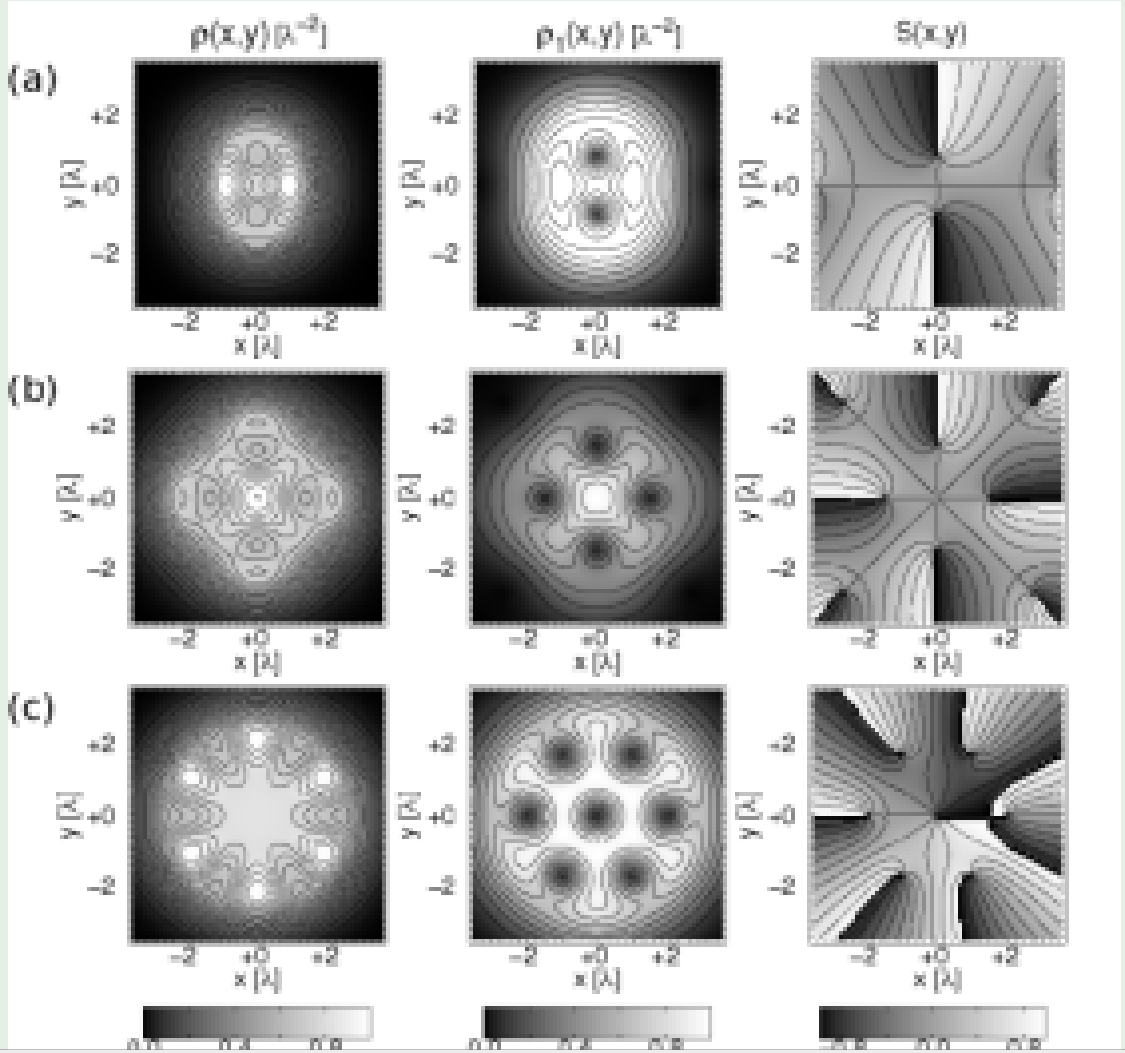
We want to characterize the properties of the condensate by the complex function

$$\phi_0(r) = \sqrt{n_0(r)} e^{iS(r)} \tag{24}$$

Order parameter

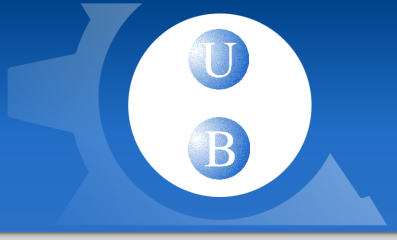
Macro-occupied state

Example



Order parameter

Macro-occupied state



Example

For $N = 6$ the first two pictures on each row show the density contour plot of the GS ($\rho(x, y)$) and the ψ_1 function ($\rho_1(x, y)$) respectively. The third picture shows tha map of the phase $S(\vec{r})$

1. shows a two vortex structure at $\Omega = 0.941$ (where degeneracy between $L = 10$ and 12 takes place).
2. shows a four vortex structure, $\Omega = 0.979$ (degeneracy between $L = 20, 22$ and 24).
3. shows a six-fold structure, $\Omega = 0.983$ (degeneracy between $L = 24, 26, 28$ and 30). In all cases $\omega_\perp = g = 1$ in units of λ and $u = \hbar\omega_\perp$.