Quantum Statistical Physics with Ultracold Atoms

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Summary

- Historical introduction
- Bose-Einstein condensation
- **Tutoring: Problem 1**
- Bose gas on the surface of a sphere
- **Tutoring: Problem 2**
- BEC dynamics and Gross-Pitaevskii equation
- **Tutoring: Problem 3**
- From 3D GPE to 1D GPE and 1D NPSE
- **Tutoring: Problem 4**
- Conclusions

Historical introduction (I)

In 1924 Wolfgang Pauli introduced the concept of spin. Now we know that any particle has an intrinsic angular momentum, called spin $\vec{S} = (S_x, S_y, S_z)$, characterized by two quantum numbers s ed m_s, where for s fixed one has $m_s = -s, -s+1, ..., s-1, s$, and in addition

$$S_z = m_s \hbar \ ,$$

with $\hbar$ ($1.054 \cdot 10^{-34}$ Joule$\times$seconds) the reduced Planck constant.
In honour of Satyendra Nath Bose and Enrico Fermi all the particles are now divided into two groups:
– **bosons**, characterized by an integer s:

$$s = 0, 1, 2, 3, ...$$

– **fermions**, characterized by a half-integer s:

$$s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, ...$$

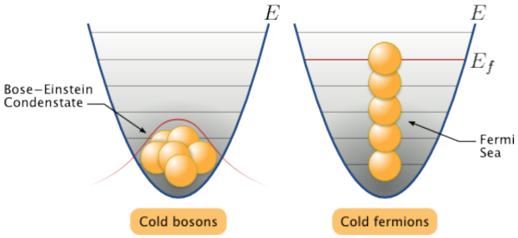
<u>Examples</u>: the photon is a boson ($s = 1$, $m_s = -1, 1$), while the electron is a fermion ($s = \frac{1}{2}$, $m_s = -\frac{1}{2}, \frac{1}{2}$).
Among "not elementary particles": helium ${}^4_2$He is a boson ($s = 0$, $m_s = 0$), while helium ${}^3_2$He is a fermion ($s = \frac{1}{2}$, $m_s = -\frac{1}{2}, \frac{1}{2}$).

Historical introduction (II)

A fundamental experimental and theoretical[1] result: identical bosons and identical fermions have a very different behavior!!

– Identical bosons can occupy the same single-particle quantum state, i.e. thay can stay together; if all bosons are in the same single-particle quantum state one has Bose-Einstein condensation.

– Identical fermions CANNOT occupy the same single-particle quantum state, i.e. they somehow repel each other: Pauli exclusion principle.

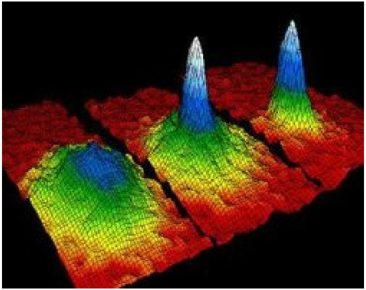


Identical bosons (a) and identical spin-polarized fermions (b) in a harmonic trap at very low temperature.

[1] Spin-statistics theorem [Markus Friez 1939; Wolfgang Pauli 1940].

Historical introduction (III)

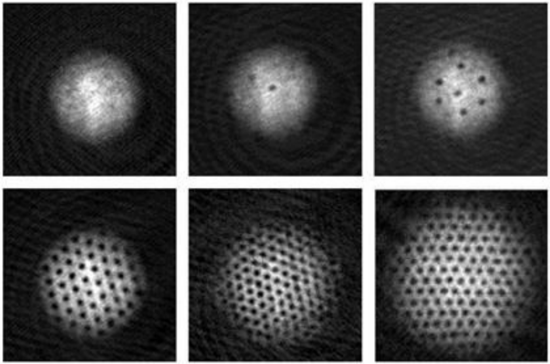
In 1995 Eric Cornell, Carl Wieman e Wolfgang Ketterle [Nobel Prize in Physics 2001] achieved Bose-Einstein condensation (BEC) cooling gases of ^{87}Rb and ^{23}Na atoms.
For these bosonic systems, which are very dilute and ultracold, the critical temperature to reach the BEC is about $T_{BEC} \simeq 100$ nanoKelvin.



Density profiles of a gas of Rubidium atoms: formation of the Bose-Einstein condensate. For an atom of ^{87}Rb the total nuclear spin is $I = \frac{3}{2}$, the total electronic spin is $S = \frac{1}{2}$, and the total atomic spin is $F = 1$ o $F = 2$: the neutral ^{87}Rb atom is a boson.

Historical introduction (IV)

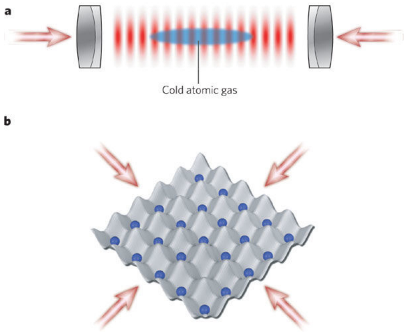
An interesting consequence of Bose-Einstein condensation with ultracold atoms is the possibility to generate quantized vortices.



Formation of quantized vortices in a condensed gas of ^{87}Rb atoms. The number of vortices increases by increasing the rotational frequency of the system.

Historical introduction (V)

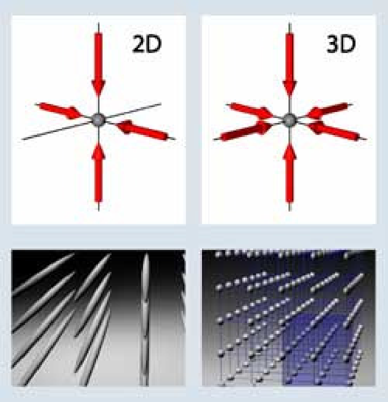
NeI 2002 the group of Immanuel Block at Munich obtained, with the intereference of counterpropagating laser beams inside an optical cavity delimitated by mirrors, a stationary optical lattice. Quite remarkably, this optical lattice traps ultracold atoms.



Due to the coupling between the electric field $\mathbf{E}(\mathbf{r}, t)$ of the laser beams and dipolar electric moment $\mathbf{d}$ of each atom, the resulting periodic potential traps neutral atoms in the minuma of the the optical lattice.

Historical introduction (VI)

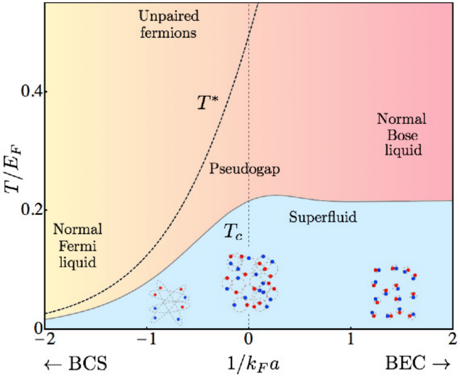
In the last years the studies of atoms trapped with light (atoms in optical lattices) have been refined.



Tuning the intensity and the shape of the optical lattice it is now possible to trap atoms in very different configurations, and also very different numbers of atoms: from many atoms per site to a single atom per site.

Historical introduction (VII)

In 2004 the 3D BCS-BEC crossover has been observed with **ultracold gases made of two-component fermionic ^{40}K or ^{6}Li atoms.**[2]



This crossover is obtained using a Fano-Feshbach resonance to change the 3D s-wave scattering length a_F of the inter-atomic potential.

[2] C.A. Regal et al., PRL **92**, 040403 (2004); M.W. Zwierlein et al., PRL **92**, 120403 (2004); J. Kinast et al., PRL **92**, 150402 (2004).

Historical introduction (VIII)

In 2018 Bose-Einstein condensates (BECs) made of ultracold alkali-metal atoms under microgravity were achieved dropping the BEC down a 146-meter-long drop chamber[3], but also rocketing the BEC and conducting experiments during in-space flight.[4]

In 2020 a BEC in harmonic trap[5] has been observed with the NASA's Cold Atom Laboratory onboard of the International Space Station. Moreover, in 2022 the same team has reported the observation of ultracold atomic bubbles.[6]

[3] T. van Zoest, et al., Science **328**, 1540 (2010)
[4] D. Becker et al., Nature **562**, 391 (2018).
[5] D.C. Aveline et al., Nature **582**, 193 (2020).
[6] R.A. Carollo et al., Nature **606**, 281 (2022).

Bose-Einstein condensation (I)

For a gas of non-interacting bosons, which can occupy the single-particle energy levels ϵ_α of the single-particle quantum states $|\alpha\rangle$, we have found that the thermal average of the internal energy is given by

$$E = \sum_\alpha \epsilon_\alpha N_\alpha \ , \tag{1}$$

where

$$N_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1} \tag{2}$$

is the termal average of the number of bosons in the single-particle quantum state $|\alpha\rangle$. That is the Bose-Einstein distribution.
The thermal average of the total number of bosons then reads

$$N = \sum_\alpha N_\alpha = \sum_\alpha \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1} \ . \tag{3}$$

At fixed temperature $T = \frac{1}{k_B \beta}$, N is fully determined by the chemical potential μ.

Bose-Einstein condensation (II)

Let us suppose for simplicity that the set of single-particle energy levels ϵ_α is given by

$$\epsilon_0 \,,\ \epsilon_1 \,,\ \epsilon_2 \,,\ \epsilon_3 \ ,\ \dots \tag{4}$$

where

$$\epsilon_0 < \epsilon_1 \leq \epsilon_2 \leq \epsilon_3 \leq \ \dots \, . \tag{5}$$

Clearly it must be

$$\mu < \epsilon_0 \tag{6}$$

to avoid divergences in the Bose-Einstein distributions of each

$$N_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1} \ . \tag{7}$$

Moreover, as $\mu \to \epsilon_0$ the distribution

$$N_0 = \frac{1}{e^{\beta(\epsilon_0 - \mu)} - 1} \tag{8}$$

becomes very large: under this condition we have Bose-Einstein condensation, i.e. a macrosopic number of bosons in the lowest single-particle energy level ϵ_0.

Bose-Einstein condensation (III)

In the presence of Bose-Einstein condensation (BEC) it is useful to write the total number of bosons as follows

$$N = N_0 + \sum_{\alpha \neq 0} N_\alpha = \frac{1}{e^{\beta(\epsilon_0 - \mu)} - 1} + \sum_{\alpha \neq 0} \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1} \ . \tag{9}$$

The exact condensate fraction is defined as

$$\frac{N_0}{N} = 1 - \frac{\sum_{\alpha \neq 0} \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1}}{\sum_{\alpha} \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - 1}} \ . \tag{10}$$

Following Einstein (1924), instead of using the exact formula of N_0 we assume that N_0 is unknown but we also set

$$\mu = \epsilon_0 \tag{11}$$

in the BEC phase (i.e. when $N_0 > 0$). In this way, in the BEC phase we find

$$N = N_0 + \sum_{\alpha \neq 0} \frac{1}{e^{\beta(\epsilon_\alpha - \epsilon_0)} - 1} \ . \tag{12}$$

Bose-Einstein condensation (IV)

At the critical temperature T_{BEC} we have $N_0 = 0$ and consequently

$$N = \sum_{\alpha \neq 0} \frac{1}{e^{(\epsilon_\alpha - \epsilon_0)/(k_B T_{BEC})} - 1} \ , \tag{13}$$

while for $T < T_{BEC}$ we have

$$N = N_0 + \sum_{\alpha \neq 0} \frac{1}{e^{(\epsilon_\alpha - \epsilon_0)/(k_B T)} - 1} \ . \tag{14}$$

Then the condensate fraction reads

$$\frac{N_0}{N} = 1 - \frac{\sum_{\alpha \neq 0} \frac{1}{e^{(\epsilon_\alpha - \mu)/(k_B T)} - 1}}{\sum_{\alpha \neq 0} \frac{1}{e^{(\epsilon_\alpha - \mu)/(k_B T_{BEC})} - 1}} \ . \tag{15}$$

Bose-Einstein condensation (V)

Let us now consider a Bose gas of atoms with mass m in a hypercubic box of volume L^D. The single-particle energy spectrum is

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} \; . \tag{16}$$

In the continuum limit

$$\sum_{\mathbf{k}} \to L^D \int \frac{d^D\mathbf{k}}{(2\pi)^D} \tag{17}$$

and the total number density $n = \frac{N}{L^D}$ in the BEC phase is given by

$$n = n_0 + \int \frac{d^D\mathbf{k}}{(2\pi)^D} \frac{1}{e^{\frac{\hbar^2 q^2}{2mk_B T}} - 1} \; , \tag{18}$$

where $n_0 = N_0/L^D$ is the condensate number density.

Bose-Einstein condensation (VI)

The critical temperature T_{BEC} of Bose-Einstein condensation is obtained setting $n_0 = 0$ in the previous equation. In this way one finds

$$k_B \, T_{BEC} = \begin{cases} \frac{1}{2\pi\zeta(3/2)^{2/3}} \frac{\hbar^2}{m} n^{2/3} & \text{for } D = 3 \\ 0 & \text{for } D = 2 \\ \text{no solution} & \text{for } D = 1 \end{cases} \tag{19}$$

where $\zeta(x)$ is the Riemann zeta function.

This result was extended to interacting systems by David Mermin and Herbert Wagner in 1966. The so-called Mermin-Wagner theorem, applied to our context, states that there is no Bose-Einstein condensation at finite temperature in homogeneous systems with sufficiently short-range interactions in dimensions $D \leq 2$.

Tutoring: Problem 1 (I)

Problem
Consider a three-dimensional uniform bosonic gas of non-interacting spinless particles in a box. Calculate the critical temperature T_{BEC} of Bose-Einstein condensation as a function of the number density n of bosons and the condensate fraction n_0/n as a function of the temperature T.

Solution
In the three-dimensional case $(D = 3)$ from the equation

$$n = n_0 + \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\frac{\hbar^2 q^2}{2mk_B T}} - 1} ,$$

we find

$$n = n_0 + \zeta(3/2) \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} .$$

Tutoring: Problem 1 (II)

It follows that

$$\frac{n_0}{n} = 1 - \frac{\zeta(3/2)\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2} T^{3/2}}{n} = 1 - \frac{\zeta(3/2)\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2} T^{3/2}}{\zeta(3/2)\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2} T_{BEC}^{3/2}} .$$

Thus, the condensate fraction reads

$$\frac{n_0}{n} = 1 - \left(\frac{T}{T_{BEC}}\right)^{3/2} .$$

The critical temperature of Eq. (19) and this formula for the condensate fraction of non-interacting massive bosons were obtained in 1925 by Albert Einstein extending previous results derived by Satyendra Nath Bose for a gas a photons (massless bosons).

Bose gas on the surface of a sphere (I)

The theoretical study of a Bose gas on the surface of a sphere is triggered by the experimental confinement the atoms on a bubble trap,[7] which needs microgravity conditions.[8]
The energy of a particle of mass m moving on the surface of a sphere of radius R is quantized according to the formula

$$\epsilon_l = \frac{\hbar^2}{2mR^2} l(l+1) \; , \tag{20}$$

where $\hbar$ is the reduced Planck constant and $l = 0, 1, 2, ...$ is the **integer quantum number** of the angular momentum. This energy level has the degeneracy $2l + 1$ due to the magnetic quantum number $m_l = -l, -l+1, ..., l-1, l$ of the third component of the angular momentum.

[7] B. M. Garraway and H. Perrin, J. Phys. B **49**, 172001 (2016).
[8] E.R. Elliott et al., npj Microgravity **4**, 16 (2018); R.A. Carollo et al., R.A. Carollo et al., Nature **606**, 281 (2022).

Bose gas on the surface of a sphere (II)

In quantum statistical mechanics the total number N of non-interacting bosons moving on the surface of a sphere and at equilibrium with a thermal bath of absolute temperature T is given by

$$N = \sum_{l=0}^{+\infty} \frac{2l+1}{e^{(\epsilon_l - \mu)/(k_B T)} - 1} \,, \tag{21}$$

where k_B is the Boltzmann constant and μ is the chemical potential. In the Bose-condensed phase, we can set[9] $\mu = 0$ and

$$N = N_0 + \sum_{l=1}^{+\infty} \frac{2l+1}{e^{\epsilon_l/(k_B T)} - 1} \,, \tag{22}$$

where N_0 is the number of bosons in the lowest single-particle energy state, i.e. the number of bosons in the Bose-Einstein condensate (BEC).

[9] For details, see Martina Russo, BSc thesis, Supervisor: LS, Univ. of Padova (2019).

Bose gas on the surface of a sphere (III)

Within the semiclassical approximation, where $\sum_{l=1}^{+\infty} \to \int_1^{+\infty} dl$, the previous equation becomes

$$n = n_0 + \frac{mk_B T}{2\pi\hbar^2}\left(\frac{\hbar^2}{mR^2 k_B T} - \ln\left(e^{\hbar^2/(mR^2 k_B T)} - 1\right)\right) , \qquad (23)$$

where $n = N/(4\pi R^2)$ is the 2D number density and $n_0 = N_0/(4\pi R^2)$ is the 2D condensate density.

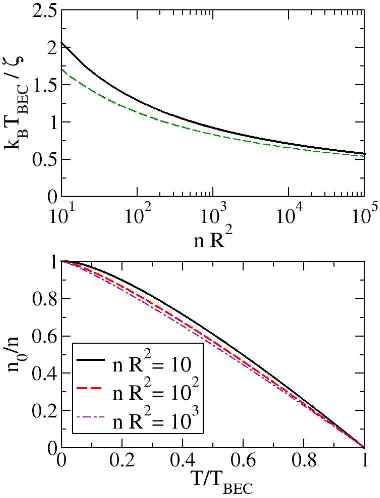
At the critical temperature T_{BEC}, where $n_0 = 0$, one then finds[10]

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2}{m} n}{\frac{\hbar^2}{mR^2 k_B T_{BEC}} - \ln\left(e^{\hbar^2/(mR^2 k_B T_{BEC})} - 1\right)} . \qquad (24)$$

As expected, in the limit $R \to +\infty$ one gets $T_{BEC} \to 0$, in agreement with the Mermin-Wagner theorem.[11] However, for any finite value of R the critical temperature T_{BEC} is larger than zero.

[10] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).
[11] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

Bose gas on the surface of a sphere (IV)



Top panel: T_{BEC} vs nR^2, with $\zeta = \hbar^2 n/m$. Solid line: semiclassical approximation (solid line); dashed line: numerical evaluation of the sum.
Bottom panel: condensate fraction n_0/n vs temperature T/T_{BEC}.

Bose gas on the surface of a sphere (IV)

We now consider a system of interacting bosons on the surface of a sphere of radius R and contact interaction of strength g.[12]
Within a perturbative scheme[13] generalizing the previous equations we obtain the BEC critical temperature

$$k_B T_{BEC} = \frac{\frac{2\pi\hbar^2 n}{m} - \frac{gn}{2}}{\frac{\hbar^2}{2mR^2 k_B T_{BEC}}\left(1+\sqrt{1+\frac{2gmnR^2}{\hbar^2}}\right) - \ln\left(e^{\frac{\hbar^2}{mR^2 k_B T_{BEC}}\sqrt{1+\frac{2gmnR^2}{\hbar^2}}} - 1\right)}, \quad (25)$$

where the condensate density n_0 is zero.

[12] A. Tononi and LS, Phys. Rev. Lett. **123**, 160403 (2019).
[13] H. Kleinert, S. Schmidt, and A. Pelster, Phys. Rev. Lett. **93**, 160402 (2004).

Tutoring: Problem 2 (I)

Problem

Consider a bosonic gas of N non-interacting spinless particles under harmonic confinement given by the external trapping potential

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \ .$$

Calculate the critical temperature T_{BEC} of Bose-Einstein condensation as a function of the number N of bosons and the condensate fraction N_0/N as a function of the temperature T.

Solution

One must generalize previous results taking into account the external potential $U(\mathbf{r})$ acting on bosons. This can be done introducing the shifted single-particle energy

$$\xi_k(\mathbf{r}) = \frac{\hbar^2 k^2}{2m} + U(\mathbf{r}) - \mu \ .$$

Tutoring: Problem 2 (II)

In this way one can write the local number density as

$$n(\mathbf{r}) = n_0(\mathbf{r}) + \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\frac{\xi_q(\mathbf{r})}{k_B T}} - 1} ,$$

where $n_0(\mathbf{r})$ is the local condensate density. Below T_{BEC} one can set $\mu = 0$. Moreover, at T_{BEC} by definition $n_0(\mathbf{r}) = 0$ and consequently

$$n(\mathbf{r}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\frac{\frac{\hbar^2 k^2}{2m} + U(\mathbf{r})}{k_B T_{BEC}}} - 1} .$$

After integration over momenta one obtains

$$n(\mathbf{r}) = \frac{1}{\lambda^3_{T_{BEC}}} g_{3/2}(e^{-\frac{U(\mathbf{r})}{k_B T_{BEC}}}) ,$$

where

$$\lambda_{T_{BEC}} = \left(\frac{2\pi\hbar^2}{m k_B T_{BEC}} \right)^{1/2}$$

is the de Broglie wavelength at the critical temperature T_{BEC}

Tutoring: Problem 2 (III)

and $g_n(x)$ is the Bose function, defined as

$$g_n(x) = \frac{1}{\Gamma(n)} \int_0^{+\infty} dy \; \frac{x \; y^{n-1} \; e^{-y}}{1 - x \; e^{-y}} = \sum_{i=1}^{+\infty} \frac{x^i}{i^n} \; ,$$

with $\Gamma(n)$ the Euler gamma function, and the last equality holds only if $|x| < 1$. Moreover, integrating over coordinates one gets

$$N = \int d^3\mathbf{r} \; n(\mathbf{r}) = g_3(1) \left(\frac{\hbar\omega}{k_B T_{BEC}} \right)^3 \; ,$$

from which

$$T_{BEC} = \frac{\hbar\omega}{g_3(1) \; k_B} N^{1/3} \; .$$

Tutoring: Problem 2 (IV)

For $T \leq T_{BEC}$ one can write

$$N = N_0 + \int \frac{d^3\mathbf{r} d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\frac{\frac{\hbar^2 k^2}{2m} + U(\mathbf{r})}{k_B T}} - 1}$$

and consequently

$$\frac{N_0}{N} = 1 - \frac{1}{N} \int \frac{d^3\mathbf{r} d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\frac{\frac{\hbar^2 q^2}{2m} + U(\mathbf{r})}{k_B T}} - 1} .$$

After integration over coordinates and momenta, and taking into account the formula of T_{BEC}, one finally gets

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_{BEC}} \right)^3 .$$

BEC dynamics and Gross-Pitaevskii equation (I)

At zero temperature static and dynamical properties of a pure **Bose-Einstein condensate** made of weakly-interacting dilute and ultracold atoms are very well described by the Gross-Pitaevskii equation[14]

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) + (N-1) \frac{4\pi\hbar^2 a_s}{m} |\psi(\mathbf{r}, t)|^2 \right] \psi(\mathbf{r}, t) \ , \tag{26}$$

where $U(\mathbf{r})$ is the external trapping potential and a_s is the s-wave scattering length of the inter-atomic potential.
Here $\psi(\mathbf{r}, t)$ is the wavefunction of the **Bose-Einstein condensate** normalized to one, i.e.

$$\int |\psi(\mathbf{r}, t)|^2 \, d^3\mathbf{r} = 1 \ , \tag{27}$$

and such that $n(\mathbf{r}) = N |\psi(\mathbf{r}, t)|^2$ is the local number density of the N condensed atoms.

[14] E.P. Gross, Nuovo Cimento **20**, 454 (1961); L.P. Pitaevskii, Sov. Phys. JETP. **13**, 451 (1961).

BEC dynamics and Gross-Pitaevskii equation (II)

The Gross-Pitaevskii equation, that is a nonlinear Schrödinger equation with cubic nonlinearity, can be deduced from the many-body quantum Hamiltonian of N identical spinless particles

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} V(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{28}$$

where $U(\mathbf{r})$ is the external potential and $V(\mathbf{r} - \mathbf{r}')$ is the inter-atomic potential.

The time-dependent Schrödinger equation of this many-body system is given by

$$i\hbar \frac{\partial}{\partial t} \boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \hat{H} \boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t), \tag{29}$$

where $\boldsymbol{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t)$ is the time-dependent many-body wavefuction.

BEC dynamics and Gross-Pitaevskii equation (III)

The time-dependent many-body Schrödinger equation is the Euler-Lagrange equation of the following many-body action functional

$$S = \int dt \; d^3\mathbf{r}_1 \; ... \; d^3\mathbf{r}_N \; \mathbf{\Psi}^*(\mathbf{r}_1, ..., \mathbf{r}_N, t) \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \mathbf{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) \; . \tag{30}$$

In the case of a pure Bose-Einstein condensate one assumes all bosons in the same time-dependent single-particle orbital (Hartree approximation)

$$\mathbf{\Psi}(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \prod_{i=1}^{N} \psi(\mathbf{r}_i, t) \; . \tag{31}$$

Inserting this ansatz into the many-body action functional one gets

$$\begin{aligned} S \;\; = \;\; & N \int dt \; d^3\mathbf{r} \; \psi^*(\mathbf{r}, t) \Big(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - U(\mathbf{r}) \\ - \;\; & \frac{N-1}{2} \int d^3\mathbf{r}' \; |\psi(\mathbf{r}', t)|^2 V(\mathbf{r} - \mathbf{r}') \Big) \psi(\mathbf{r}, t) \; . \end{aligned} \tag{32}$$

BEC dynamics and Gross-Pitaevskii equation (IV)

The Euler-Lagrange equation of the previous action functional reads

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)\int d^3\mathbf{r}' \; |\psi(\mathbf{r}',t)|^2 V(\mathbf{r}-\mathbf{r}')\right]\psi(\mathbf{r},t) \; . \tag{33}$$

This is the time-dependent Hartree equation for N identical bosons in the same single-particle state $\psi(\mathbf{r},t)$.
In the case of dilute gases we assume (Fermi pseudo-potential) that

$$V(\mathbf{r}) \simeq g \; \delta^{(3)}(\mathbf{r}) \tag{34}$$

with $\delta^{(3)}(\mathbf{r})$ the Dirac delta function and, by construction,

$$g = \int V(\mathbf{r}) \; d^3\mathbf{r} \; . \tag{35}$$

From 3D scattering theory, the s-wave scatering length a_s of the inter-atomic potential can be written (Born approximation) as

$$a_s = \frac{m}{4\pi\hbar^2}\int V(\mathbf{r}) \; d^3\mathbf{r} \; . \tag{36}$$

BEC dynamics and Gross-Pitaevskii equation (V)

From the Hartree equation we have obtained the Gross-Pitaevskii (GP) equation

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + (N-1)g|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t) \ , \quad (37)$$

with

$$g = \frac{4\pi\hbar^2}{m} a_s \ . \quad (38)$$

Clearly, this is the Euler-Lagrange equation of the GP action functional

$$S = N \int dt\, d^3\mathbf{r}\ \psi^*(\mathbf{r},t)\Big(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 - U(\mathbf{r}) - \frac{N-1}{2}g|\psi(\mathbf{r},t)|^2\Big)\psi(\mathbf{r},t) \ . \quad (39)$$

Tutoring: Problem 3 (I)

Problem

By using the Gaussian variational method on the Gross-Pitaevskii functional calculate the energy per particle of a Bose-Einstein condensate under harmonic confinement, given by

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \; .$$

Solution

We start from the Gaussian variational wave function

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4} a_H^{3/2} \sigma^{3/2}} \, e^{-(x^2+y^2+z^2)/(2a_H^2\sigma^2)} \; ,$$

where $a_H = \sqrt{\hbar/(m\omega)}$ is the characteristic length of the harmonic confinement and σ is the dimensionless variational parameter.

Tutoring: Problem 3 (II)

Inserting this wave function in the Gross-Pitaevskii energy functional

$$E = N \int d^3\mathbf{r} \left\{ \psi^*(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \right] \psi(\mathbf{r}) + \frac{1}{2} N g |\psi(\mathbf{r})|^4 \right\} ,$$

after integration we obtain the energy E as a function of σ, namely

$$E = N\hbar\omega \left(\frac{3}{4}\frac{1}{\sigma^2} + \frac{3}{4}\sigma^2 + \frac{\gamma}{2}\frac{1}{\sigma^3} \right) ,$$

where $\gamma = \sqrt{2/\pi} N a_s / a_H$ is the dimensionless strength of the inter-particle interaction with $g = 4\pi\hbar^2 a_s / m$ and a_s the s-wave scattering length.

Tutoring: Problem 3 (III)

The best choice for σ is obtained by extremizing the energy function:

$$\frac{dE}{d\sigma} = 0 \ ,$$

from which we obtain

$$\sigma(\sigma^4 - 1) = \gamma \ .$$

It is clear that σ grows with γ, if $\gamma > 0$. Instead, if $\gamma < 0$ there are two possible values of σ: one value corresponds to a minimum of the energy E (meta-stable solution) and the other corresponds to a maximum of the energy E (unstable solution). It is straightforward to show that these two solutions exists only if $\gamma > -4/5^{5/4}$.

From 3D GPE to 1D GPE and 1D NPSE (I)

Let us now consider a very strong harmonic confinement of frequency $\omega_\perp$ along x and y and a generic confinement $\mathcal{U}(z)$ along z, namely

$$U(\mathbf{r}) = \frac{1}{2} m {\omega_\perp}^2 (x^2 + y^2) + \mathcal{U}(z) \; . \tag{40}$$

On the basis of the chosen external confinement, we adopt the ansatz

$$\psi(\mathbf{r}, t) = f(z,t) \frac{1}{\pi^{1/2} a_\perp} \exp\left(\frac{x^2 + y^2}{2{a_\perp}^2} \right) \; , \tag{41}$$

where $f(z,t)$ is the axial wave function and $a_\perp = \sqrt{\hbar/(m\omega_\perp)}$ is the characteristic length of the transverse harmonic confinement.

From 3D GPE to 1D GPE and 1D NPSE (II)

By inserting Eq. (41) into the GP action (39) and integrating along x and y, the resulting effective action functional depends only on the field $f(z,t)$.
One easily finds that the Euler-Lagrange equation of the axial wavefunction $f(z,t)$ reads

$$i\hbar\frac{\partial}{\partial t}f(z,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \mathcal{U}(z) + \gamma|f(z,t)|^2\right] f(z,t) \ , \qquad (42)$$

where

$$\gamma = \frac{(N-1)g}{2\pi {a_\perp}^2} \qquad (43)$$

is the effective one-dimensional interaction strength and the additive constant $\hbar\omega_\perp$ has been omitted because it does not affect the dynamics.

From 3D GPE to 1D GPE and 1D NPSE (III)

The 1D GPE is derived from the 3D GPE assuming a transverse Gaussian with a constant transverse width $a_\perp$.
A more general assumption,[15] is based on a space-time dependent transverse width

$$\psi(\mathbf{r}, t) = f(z,t) \frac{1}{\pi^{1/2} a_\perp \sigma(z,t)} \exp\left(\frac{x^2 + y^2}{2 a_\perp{}^2 \sigma(z,t)^2} \right) , \tag{44}$$

where $f(z,t)$ is the axial wave function and $\sigma(z,t)$ is the adimensional transverse width in units of $a_\perp$.
From this ansatz one gets the **1D nonpolynomial Schrödinger equation** (1D NPSE)

$$i\hbar \frac{\partial}{\partial t} f = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \mathcal{U}(z) + \frac{\gamma |f|^2}{\sigma^2} + \frac{\hbar \omega_\perp}{2} \left(\frac{1}{\sigma^2} + \sigma^2 \right) \right] f , \tag{45}$$

$$\sigma = \left(1 + \gamma |f|^2\right)^{1/4} . \tag{46}$$

[15] LS, A. Parola, L. Reatto, Phys. Rev. A **66**, 043603 (2002); Phys. Rev. Lett. **91**, 080405 (2003).

Tutoring: Problem 4 (I)

Problem

Show that, in the absence of axial confinement, i.e. $\mathcal{U}(z) = 0$, the stationary 1D GPE

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \gamma|\phi(z)|^2 \right] \phi(z) = \mu \; \phi(z) \; ,$$

with $\gamma < 0$ (self-focusing) admits the bright soliton solution

$$\phi(z) = \sqrt{\frac{m|\gamma|}{8\hbar^2}} \; Sech\left[\frac{m|\gamma|}{4\hbar^2}\zeta \right]$$

with $Sech[x] = \frac{2}{e^x + e^{-x}}$ and

$$\mu = -\frac{m \; \gamma^2}{16 \; \hbar^2} \; .$$

Solution

Let us assume that $\phi(z)$ is real. Then the stationary 1D GPE can be rewritten as

$$\phi''(z) = -\frac{\partial W(\phi)}{\partial \phi} \; ,$$

Tutoring: Problem 4 (II)

where

$$W(\phi) = \frac{1}{2}\frac{m|\gamma|}{\hbar^2}\phi^4 + \frac{m\mu}{\hbar^2}\phi^2 \,.$$

Thus, $\phi(z)$ can be seen as the "coordinate" for a fictitious particle at "time" z. The constant of motion of the problem reads

$$K = \frac{1}{2}\phi'(z)^2 + W(\phi) \,,$$

from which one finds

$$\frac{d\phi}{dz} = \sqrt{2(K - W(\phi))} \,.$$

Tutoring: Problem 4 (III)

Imposing that $\phi(z) \to 0$ as $|z| \to \infty$ one gets $K = 0$ and consequently

$$\frac{d\phi}{\sqrt{-2W(\phi)}} = dz \ ,$$

or explicity

$$\frac{d\phi}{\sqrt{-\frac{m|\gamma|}{\hbar^2}\phi^4 + \frac{2m|\mu|}{\hbar^2}\phi^2}} = dz \ ,$$

with $\mu < 0$. Inserting the integrals one obtains

$$\int_{\phi(0)}^{\phi(z)} \frac{d\phi}{\phi\sqrt{-\frac{m|\gamma|}{\hbar^2}\phi^2 + \frac{2m|\mu|}{\hbar^2}}} = z \ .$$

Setting $\phi'(0) = 0$, from the definition of K and using $K = 0$ one finds $W(\phi(0)) = 0$ and therefore

$$\phi(0) = \sqrt{\frac{2|\mu|}{|\gamma|}} \ .$$

Tutoring: Problem 4 (IV)

After solving the integral equation one gets

$$\frac{1}{\sqrt{\frac{m|\mu|}{\hbar}}} ArcSech\left[\sqrt{\frac{|\gamma|}{2|\mu|}}\phi(z)\right] = z$$

from which

$$\phi(z) = \sqrt{\frac{2|\mu|}{|\gamma|}} Sech\left[\sqrt{\frac{m|\mu|}{\hbar^2}} z\right] \ .$$

Finally, imposing the normalization condition

$$\int dz \ \phi(z)^2 = 1 \ ,$$

one obtains

$$\mu = -\frac{m \ \gamma^2}{16 \ \hbar^2} \ .$$

Conclusions

At the end of these lectures I hope you may comment using the words of Enrico Fermi:

"Before I came here I was confused about this subject.
Having listened to your lectures I am still confused.
But on a higher level."

THANK YOU VERY MUCH FOR YOUR ATTENTION!