Macroscopic quantum phenomena and atomic Bose-Einstein condensates

Luca Salasnich

CNR-INFM and CNISM, Research Unit of Padua
Department of Physics "Galileo Galilei", University of Padua
e-mail: luca.salasnich@cnr.it
web-page: www.padova.infm.it/salasnich/

Talk at the 7th Christmas Symposium of Physics
Maribor, December 11 2008

Summary

- Building blocks of matter: bosons and fermions
- Macroscopic quantum phenomena at ultra-low temperatures
  - Superconductivity
  - Superfluidity
  - Bose-Einstein condensation
- Gross-Pitaevskii equation
  - Derivation of the Gross-Pitaevskii equation
  - Gaussian variational approach
- Attractive BEC under anisotropic harmonic confinement
- Conclusions

Building blocks of matter: bosons and fermions

From experiments one finds that each elementary particle has an intrinsic angular momentum, that is called **spin** $\mathbf{S}$.

All particles can be divided into two groups:

– **bosons**, with spin S that is an integer multiplier of the Planck constant $\hbar$:

$$S = n\hbar\,, \quad n = 0, 1, 2, \ldots\,,$$

– **fermions**, with spin S that is a semi-integer multiplier of $\hbar$:

$$S = \frac{n}{2}\hbar\,, \quad n = 1, 2, 3, \ldots\,.$$

The reduced Planck constant reads

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34} \text{ Joule/second}\,.$$

The spin of a generic atom

$$^{A}_{Z}X$$

is the sum of the spins of its particles:
A nucleons (protons and neutrons) in the atomic nucleus and Z electrons.

Because both nucleons and electrons are fermions, the neutral atom $^{A}_{Z}\mathrm{X}$ is a boson if the numer $A + Z$ is even, while it is a fermion if $A + Z$ is odd.

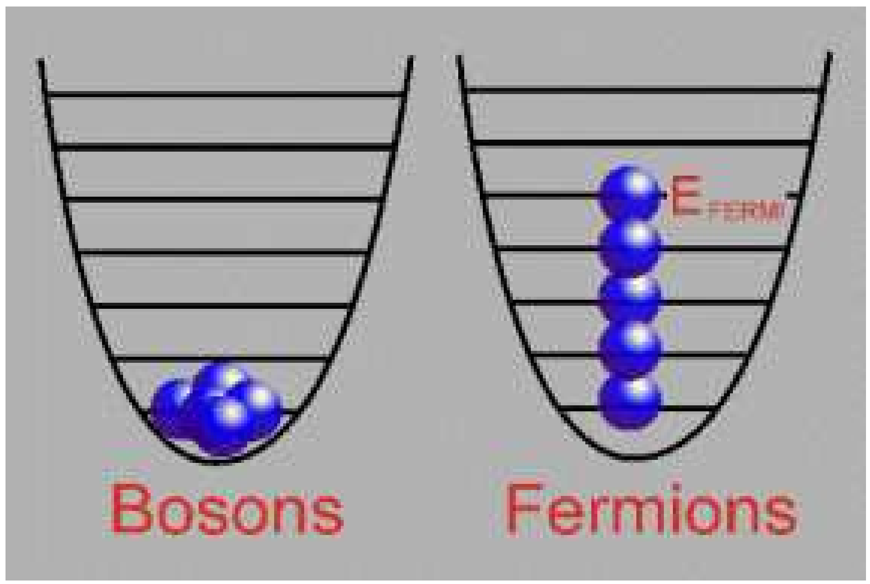
Examples: helium 4, i.e. $^{4}_{2}\mathrm{He}$, is a boson, while helium 3, i.e. $^{3}_{2}\mathrm{He}$, is fermion.

The most intresting experimental result is that
bosons and fermions have a very different behavior!!

Bosons and fermions: very different behavior

– Identical bosons can occupy the same state, i.e. they can stay very close each other; if all bosons are in the same state then there is the so-called **Bose-Einstein condensation**.

– Identical fermions CANNOT occupy the same state, i.e. they must stay far from each other: **Pauli's exclusion principle**.



Bosons and fermions in a harmonic trap.

Quantum statistical mechanics investigates the behavior of bosons and fermions as a function of temperature T. If the single-particle energy is given by

$$E(\mathbf{r},\mathbf{p}) = \frac{p^2}{2m} + U(\mathbf{r}) \; , \tag{1}$$

than ideal bosons follow the *Bose-Einstein distribution*

$$f(\mathbf{r},\mathbf{p}) = \frac{1}{\exp\left(\frac{E(\mathbf{r},\mathbf{p})-\mu}{k_B T}\right) - 1} \; , \tag{2}$$

while ideal fermions follow the *Fermi-Dirac distribution*

$$f(\mathbf{r},\mathbf{p}) = \frac{1}{\exp\left(\frac{E(\mathbf{r},\mathbf{p})-\mu}{k_B T}\right) + 1} \; , \tag{3}$$

where k_B is the Boltzmann constant. The total number of particles is

$$N = \int f(\mathbf{r},\mathbf{p}) \; \frac{d^3\mathbf{r} \; d^3\mathbf{p}}{(2\pi\hbar)^3} \; , \tag{4}$$

and this condition fixes the chemical potential μ.

Macroscopic quantum phenomena at ultra-low temperatures

When the temperature T is high, the statistical distributions of bosons and fermions reduce to the same distribution: the *Maxwell-Boltzmann distribution*

$$f(\mathbf{r},\mathbf{p}) = \exp\left(\frac{\mu}{k_B T}\right) \; \exp\left(\frac{-E(\mathbf{r},\mathbf{p})}{k_B T}\right) , \qquad (5)$$

and consequently the statistical effect of spin is not important (**classical statistical mechanics**).

To see the statistical effects of spin and the differences between bosons and fermions (quantum degeneracy) it is necessary to strongly reduce the temperature!!

For N ideal particles in a box of volume V, the critical temperature of quantum degeneracy can be estimated by equating the de Broglie wave length

$$\lambda = \frac{h}{mv} = \frac{h}{m\sqrt{\frac{3k_BT}{m}}} , \tag{6}$$

of a particle in the gas at temperature T to the inter-atomic distance

$$d = \frac{1}{n^{1/3}} , \tag{7}$$

where $n = N/V$ is the number density. In this way one finds

$$T_c \simeq \frac{\hbar^2}{mK_B} \left(\frac{N}{V}\right)^{2/3} . \tag{8}$$

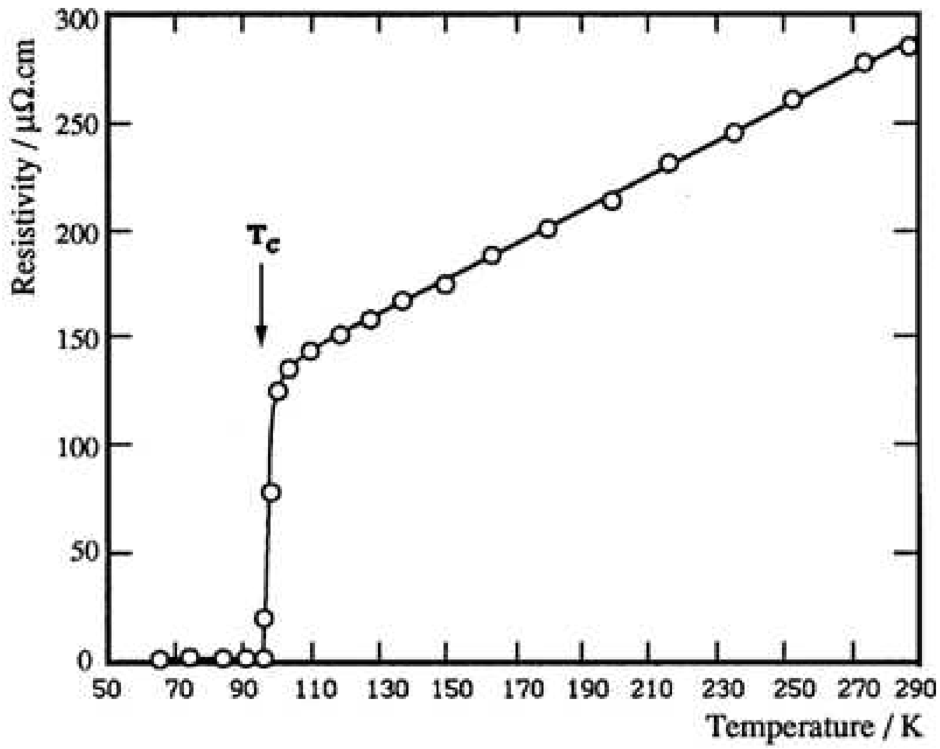
Below this critical temperature T_c the matter has a strange behavior: it can become **supermatter**, where macroscopic quantum phenomena can occur.

The **inter-particle interaction** modifies T_c and can also transform fermions in bosons (BCS theory and BCS-BEC crossover).

Superconductivity

In 1911 Heike Kamerlingh Onnes observed that in the mercury (Hg) cooled below $T_c = 4.16$ Kelvin the electrical resistence becomes zero.

Onnes called this phenomenon **superconductivity**.



Electrical resistence as a function of temperature for a superconducting material.

Many materials are superconductors below a critical temperature T_c. But others are not.

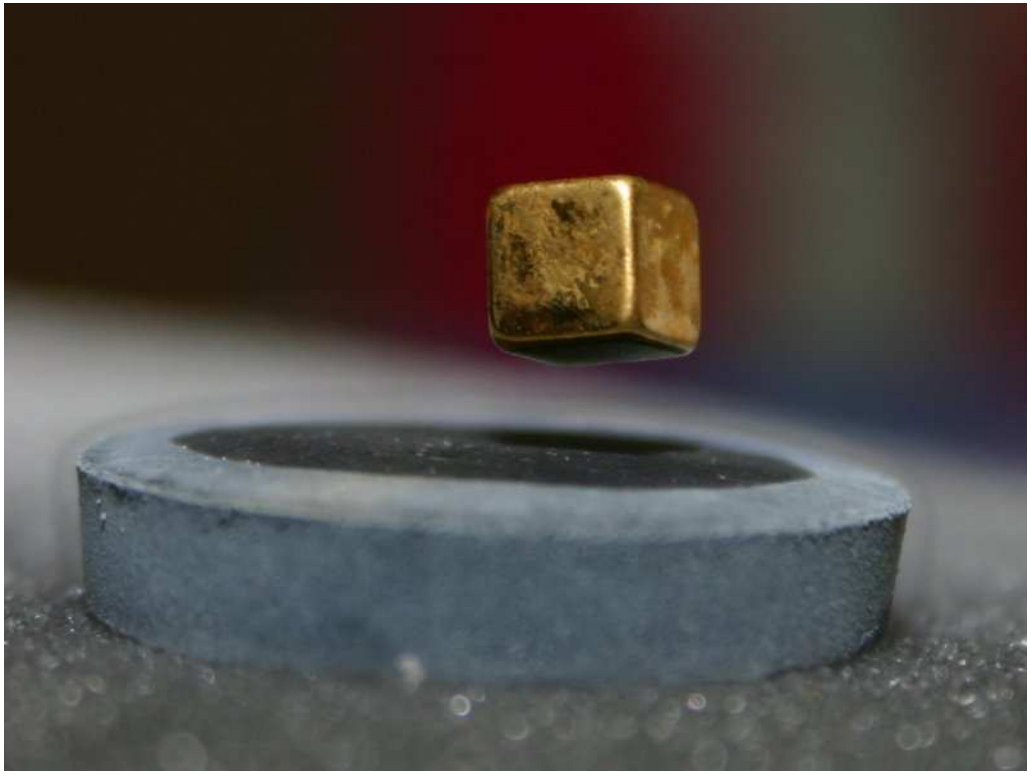
Material	**Symbol**	T_c **(Kelvin)**
Aluminium	$^{27}_{13}$Al	1.19
Tin	$^{120}_{50}$Sn	3.72
Mercury	$^{202}_{80}$Hg	4.16
Lead	$^{208}_{82}$Pb	7.20
Neodymium	$^{142}_{60}$Nb	9.30

Critical temperature T_c of some superconducting materials, at atmospheric pressure.

In 1986 Karl Alex Müller and Johannes Georg Bednorz descovered *high-temperature superconductors*.

These are *cuprates*, namely ceramic materials containing copper oxide. Their critical temperature can reach 133 Kelvin.

Superconducting materials have many interesting properties. For instance the expulsion of the magnetic field (Meissner effect).



Levitation of a magnetic material above the superconductor.

Technological applications of superconductors:

– MAGLEV trains, based on magnetic levitation (mag-lev);

– SQUIDS, which are able to measure very weak magnetic fields;

– high magnetic fields for Nuclear Magnetic Resonance (NMR) machines.

Superfluidity

In 1937 Pyotr Leonidovich Kapitza descovered that below $T_c = 2.16$ Kelvin helium 4 (^{4}He) remains liquid but it shows zero viscosity.

Kapitza called this phenomenon **superfluidity**.

Example: a macroscopic object immersed in superfluid helium moves without viscosity if its velocity v è below a critical value v_c.

In 1938 Fritz London gave a theoretical explanation of superfluidity of helium 4 on the basis of Bose-Einstein condensation.

London observed that ^{4}He is a boson and that the critical temperature T_c of Bose-Einstein condensation for an ideal Bose gas is in good agreement with the T_c of helium 4.

London introduced the idea of a "**macroscopic wave function**" $\psi(\mathbf{r}, t)$, such that

$$n(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$$

gives the density of atoms in $\mathbf{r}$ at time t, and

$$N = \int n(\mathbf{r}, t)\ d^3\mathbf{r} = \int |\psi(\mathbf{r}, t)|^2\ d^3\mathbf{r}$$

is the total number of atoms in the Bose-Einstein condensate.

In fact, all particles of the Bose-Einstein condensate are in the same quantum state; thus they are all characterized by the same quantum wave function $\psi(\mathbf{r}, t)$.

In 1950 Lev Landau and Vitaly Ginzburg proposed the idea of an "order parameter" or "macroscopic wave function" $\psi(\mathbf{r}, t)$ also for the superconductivity.

But the electrons, which transport the electric current, are fermions.

How can one explain the presence of Bose-Einstein condensation with electrons?

In 1957 John Bardeen, Leon Cooper and Robert Schrieffer (BCS theory) suggested that in superconductivity, due to the ionic cristal lattice, pairs of electrons with anti-parallel spins can couple (Cooper pairs), and each pair behaves like a bosonic particle.

BCS theory is based on Bose-Einstein condensation of Cooper pairs.

Condensate fraction f_0: fraction of particles which are in the same quantum state.

In liquid Helim 4 at zero temperature: $f_0 \simeq 10\%$.

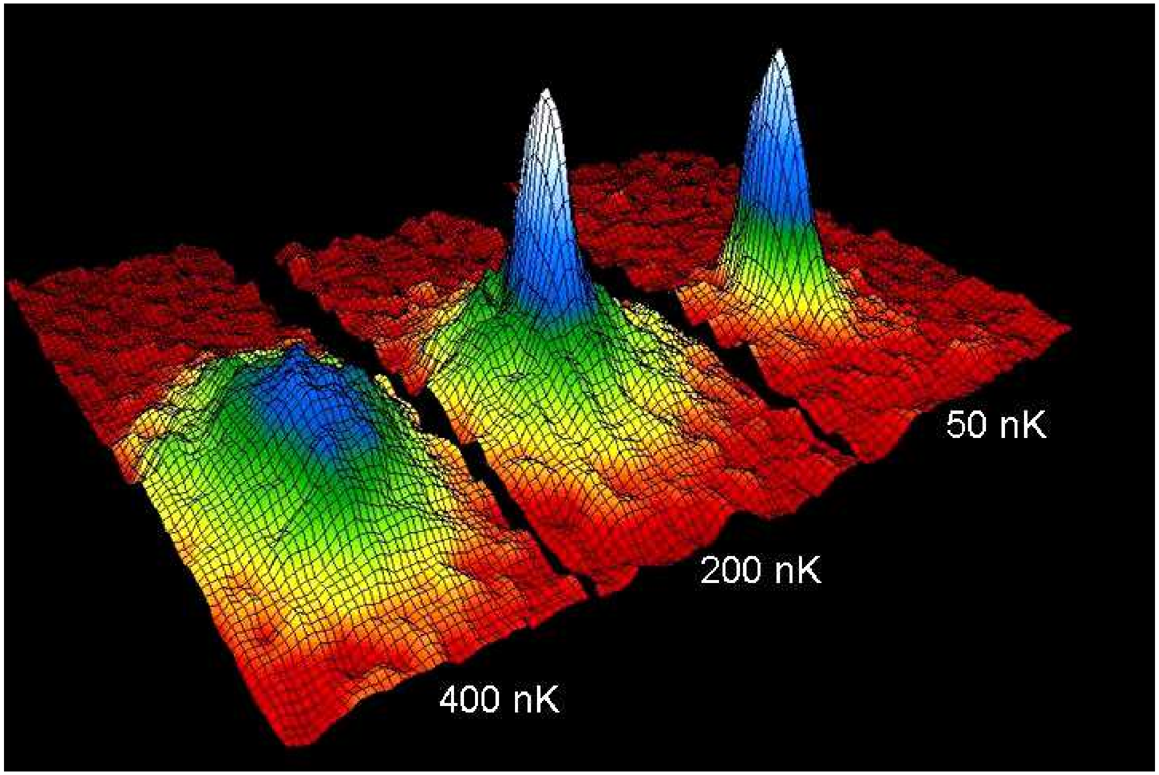
In solid superconductors at zero temperature: $f_0 \simeq 0.01\%$.

In ultra-dilute atomic gases at zero temperature: $f_0 \simeq 99\%$.

Bose-Einstein condensation in ultra-cold atoms

In 1995 Eric Cornell, Carl Wieman and Wolfgang Ketterle achieved the Bose-Einstein condensation with ultra-dilute and ultra-cold atomic vapors (^{87}Rb and ^{23}Na).

The critical temperature is about $T_c \simeq 100$ nanoKelvin.



Density profiles of the atomic gas of Rubidium.

In these experiments ultracold atoms are confined in a harmonic trap

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \tag{9}$$

produced by magnetic (magnetic-dipole-moment interaction) or electric fields (electric-dipole-moment interaction).

The critical temperature of Bose-Einstein condensation for an ideal Bose gas in a harmonic trap is

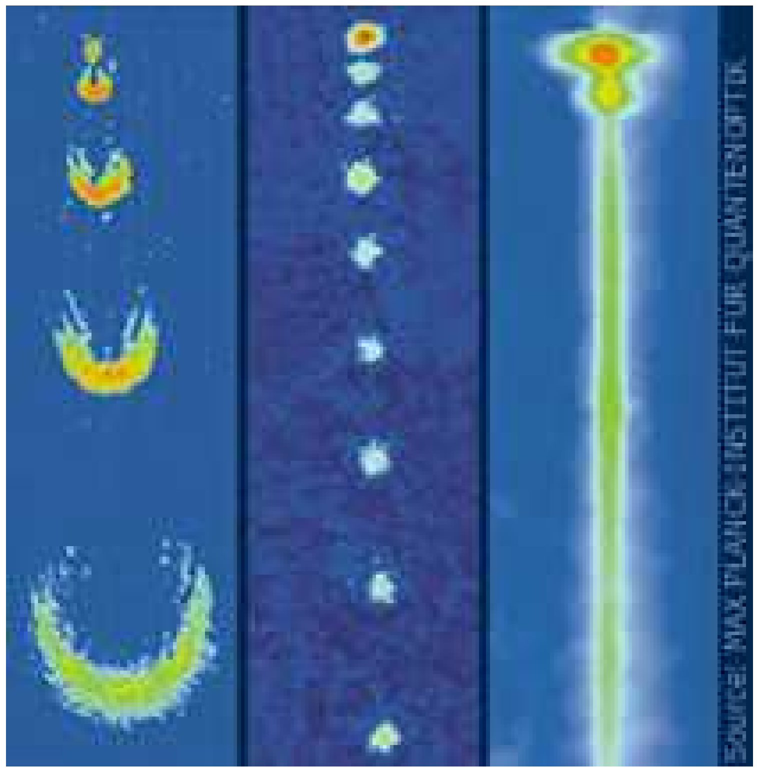
$$k_B T_c \simeq \hbar\omega \ N^{1/3} , \tag{10}$$

and the condensate fraction reads

$$f_0 = 1 - \left(\frac{T}{T_c} \right)^3 . \tag{11}$$

Bose-Einstein condensates are the atomic analog of the LASER: **coherent matter waves**.

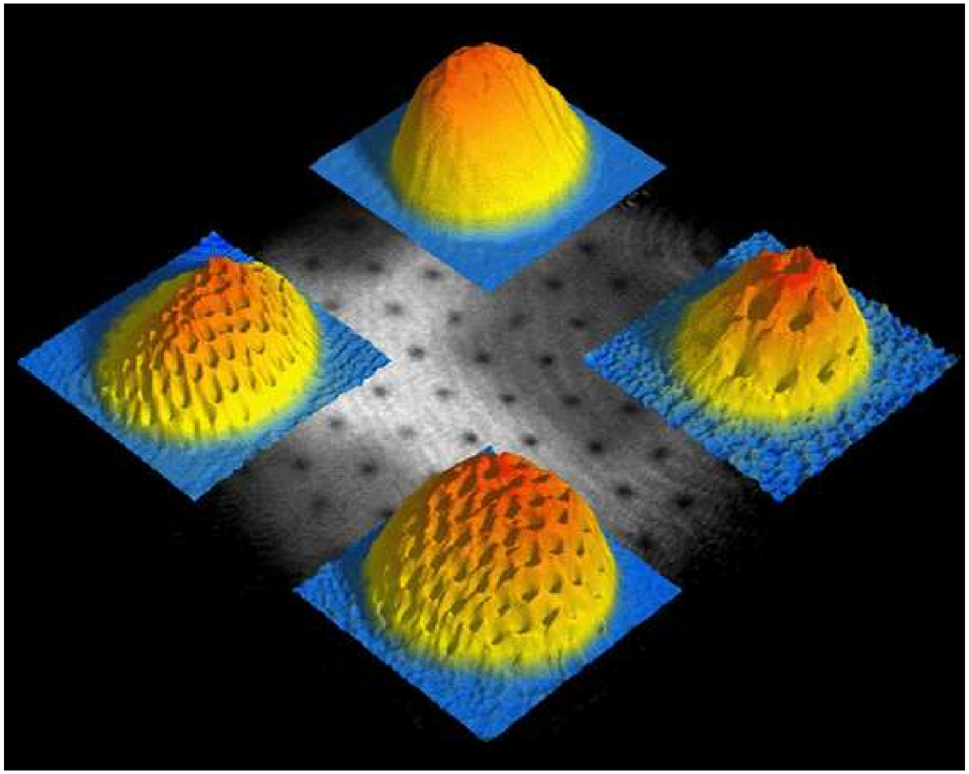
A **laser** is characterized by a beam which is collimated, monochromatic and coherent.



Esperiments to achieve an **atomic laser** with Bose-Einstein condensates.

An interesting consequence of Bose-Einstein condensation in ultra-cold atoms and helium 4 is the possibility of obtaining **quantized vortices**, where the fluid velocity follows the law

$$v = \frac{\hbar}{m} \frac{k}{r_\perp} , \qquad k = 0, 1, 2, ...$$



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

Gross-Pitaevskii equation

Bose-Einstein condensates made of ultra-cold and dilute alkali-metal atoms can be described by the following nonlinear Schrödinger equation

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

with

$\psi(\mathbf{r},t)$ the macroscopic wave function of the condensed atoms of mass m,

$U(\mathbf{r},t)$ the external confining potential

g a strength related to the inter-atomic interaction.

This equation is called *Gross-Pitaevskii equation*. It describes quite accuratele the properties of pure Bose condensates, i.e. with a condensate fraction equal to 1 (quasi-zero temperature).

Derivation of the Gross-Pitaevskii equation

The N-body stationary Schrödinger equation

$$\hat{H}\Phi(\mathbf{r}_1,...,\mathbf{r}_N) = \epsilon\ \Phi(\mathbf{r}_1,...,\mathbf{r}_N)\ , \qquad (12)$$

where

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + U(\mathbf{r}_i)\right] + \sum_{i<j} V(\mathbf{r}_i,\mathbf{r}_j) \qquad (13)$$

is the N-body Hamiltonian, can be obtained by minimizing the energy functional

$$E[\Phi] = \int \Phi^*(\mathbf{r}_1,...,\mathbf{r}_N)\hat{H}\Phi(\mathbf{r}_1,...,\mathbf{r}_N)\ d^3\mathbf{r}_1...d^3\mathbf{r}_N \qquad (14)$$

with the constraint

$$\int |\Phi(\mathbf{r}_1,...,\mathbf{r}_N)|^2\ d^3\mathbf{r}_1...d^3\mathbf{r}_N = 1\ . \qquad (15)$$

In the case of a Bose-Einstein condensate (BEC), all identical bosons are in the same single-particle quantum state $\psi(\mathbf{r})$. It is quite natural to write the N-body wave function of a BEC as

$$\Phi(\mathbf{r}_1, ..., \mathbf{r}_N) = \psi(\mathbf{r}_1) \cdot \psi(\mathbf{r}_2) \cdot \ ... \ \cdot \psi(\mathbf{r}_{N-1}) \cdot \psi(\mathbf{r}_N) \ . \tag{16}$$

By inserting this wave function in the energy functional, it becomes

$$E[\psi] \ = \ N \int \psi^*(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) \right] \psi(\mathbf{r}) \ d^3\mathbf{r} \tag{17}$$

$$+ \ \frac{1}{2} N(N-1) \int |\psi(\mathbf{r})|^2 |\psi(\mathbf{r}')|^2 V(\mathbf{r}, \mathbf{r}') \ d^3\mathbf{r} \ d^3\mathbf{r}' \tag{18}$$

In the case of a dilute BEC, the inter-atomic interaction can be taken as a contact interaction:

$$V(\mathbf{r}, \mathbf{r}') = G \ \delta(\mathbf{r} - \mathbf{r}') \ , \tag{19}$$

where

$$G = \frac{4\pi\hbar^2 a_s}{m} \tag{20}$$

is the inter-atomic strength with a_s the s-wave scattering length fixed by experiments.

Many experiments have been devoted to the study of dilute and ultra-cold Bose-Einstein condensates (BECs) with positive s-wave scattering length

$$a_s > 0 \ , \tag{21}$$

which implies an effective repulsion between atoms (^{87}Rb, ^{23}Na). There are instead few experiments with negative s-wave scattering length

$$a_s < 0 \ , \tag{22}$$

which implies an effective attraction between atoms.

^{7}Li atoms have a negative scattering length

$$a_s \simeq -14 \cdot 10^{-10} \ \mathrm{m} \ . \tag{23}$$

BECs with ^{7}Li atoms have been studied at Rice Univ.[*] and ENS[†].

Recently an attractive BEC with ^{85}Rb atoms has been investigated at JILA[‡] by using a Feshbach resonance.

[*]K.E. Strecker *et al.*, Nature **417**, 150 (2002).

[†]L. Khaykovich *et al.*, Science **296**, 1290 (2002).

[‡]S.L. Cornish *et al.*, PRL **96**, 170401 (2006).

By using the Fermi pseudo-potential, the energy functional of the BEC is further simplified and reads

$$E[\psi] = N \int \psi^*(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{1}{2} G N (N-1) |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) \; d^3\mathbf{r} \; . \tag{24}$$

By minimizing this single-particle energy functional with the constraint

$$\int |\psi(\mathbf{r})|^2 \; d^3\mathbf{r} = 1 \tag{25}$$

one obtains the so-called Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + G(N-1)|\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu \; \psi(\mathbf{r}) \; , \tag{26}$$

where μ is the Lagrange multiplier fixed by the normalization. Usually one sets N instead of $N-1$ for a large number of particles. Note that μ satisfies the equation

$$\mu = \frac{\partial E}{\partial N} \; . \tag{27}$$

Thus, μ is the chemical potential of the system.

Gaussian variational approach

The stationary properties of a dilute Bose-Einstein condensates (BEC) are well described by the Gross-Pitaevskii equation (GPE), given by

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) + \frac{4\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = \mu\ \psi(\mathbf{r})\ , \tag{28}$$

where $\psi(\mathbf{r})$ is the macroscopic wave function of the BEC, here normalized to one, i.e.

$$\int |\psi(\mathbf{r})|^2\ d^3\mathbf{r} = 1\ . \tag{29}$$

In the GPE μ is the chemical potential, $U(\mathbf{r})$ is the external trapping potential, a_s is the s-wave scattering length and N is the number of condensed atomic bosons.

The GPE can be obtained by minimizing the following energy functional

$$E = \int \left\{\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2 + U(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{2\pi\hbar^2 a_s N}{m}|\psi(\mathbf{r})|^4\right\}\ d^3\mathbf{r}\ , \tag{30}$$

with the constraint of Eq. (29).

Let us suppose that the external trap is a spherically-symmetric harmonic potential

$$U(\mathbf{r}) = \frac{1}{2} m \omega_H^2 \left(x^2 + y^2 + z^2 \right) = \frac{1}{2} m \omega_H^2 r^2 \; . \tag{31}$$

A reasonable variational ansatz for $\psi(\mathbf{r})$ is a Gaussian wave function

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4} a_H^{3/2} \sigma^{3/2}} \exp \left(\frac{-r^2}{2 a_H^2 \sigma^2} \right) , \tag{32}$$

where

$$a_H = \sqrt{\frac{\hbar}{m \omega_H}} \tag{33}$$

is the characteristic harmonic length and σ is the variational parameter, that is the scaled width of the BEC.

By inserting this trial wave function in the GPE energy functional and integrating over spatial coordinates one finds the effective energy

$$\bar{E} = \frac{2E}{\hbar \omega_H} = \frac{3}{2} \frac{1}{\sigma^2} + \frac{3}{2} \sigma^2 + \Gamma \frac{1}{\sigma^3} , \tag{34}$$

which is a function of the variational parameter σ, with $\Gamma = \sqrt{\frac{2}{\pi}} \frac{a_s N}{a_H}$ the interaction strength.

The best choice of σ is obtained by minimizing the energy $\bar{E}(\sigma)$, i.e.

$$0 = \frac{\partial \bar{E}}{\partial \sigma} = -3\frac{1}{\sigma^3} + 3\sigma^3 - 3\Gamma\frac{1}{\sigma^4} \, . \tag{35}$$

Obviously σ must also satisfy the condition

$$\frac{\partial^2 \bar{E}}{\partial \sigma^2} > 0. \tag{36}$$

It follows that

$$\sigma > 1 \quad \text{for} \quad \Gamma > 0 \, ,$$

while

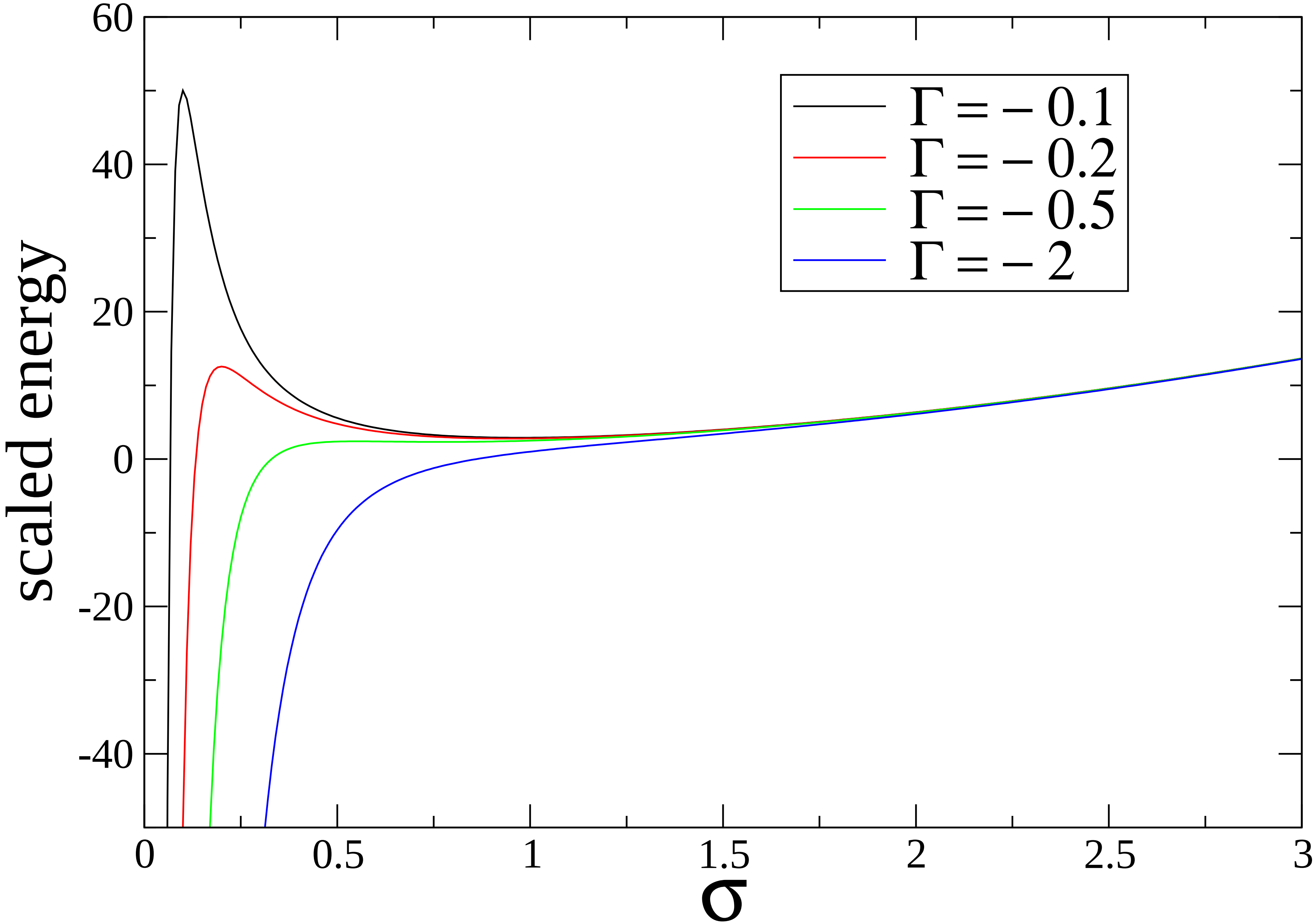
$$\sigma_c < \sigma < 1 \quad \text{for} \quad -\Gamma_c < \Gamma < 0 \, ,$$

with $\sigma_c = 1/5^{1/4} \simeq 0.67$ and $\Gamma_c = 4/5^{5/4} \simeq 0.53$.

Thus, for $a_s < 0$ it exist a critical strength

$$\frac{|a_s|N}{a_H} = \sqrt{\frac{\pi}{2}}\frac{4}{5^{5/4}} \simeq 0.67 \tag{37}$$

above which the local minumum of the energy does not exist anymore. Above this critical strength there is the so-called collapse of the condensate. For ^{7}Li atoms of Rice Univ. experiment: $N_c \simeq 1300$.



Scaled energy $\bar{E}$ as a function of the variational parameter σ for different values of the scaled interaction strength $\Gamma = \sqrt{\frac{2}{\pi}}\frac{a_s N}{a_H}$.

Attractive BEC under anisotropic harmonic confinement

Let us now consider an attractive BEC ($a_s < 0$) with an anisotropic but axially-symmetric harmonic trapping potential

$$U(\mathbf{r}) = \frac{1}{2} m \omega_\perp^2 (x^2 + y^2) + \frac{1}{2} m \omega_z^2 z^2 \; , \tag{38}$$

By using the transverse harmonic length

$$a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \; , \tag{39}$$

as unit of length, and $\hbar\omega_\perp$ as unit of energy, the scaled GPE energy functional reads

$$E = \int \left\{ \frac{1}{2} |\nabla \psi(\mathbf{r})|^2 + \left[\frac{1}{2}(x^2 + y^2) + \frac{\lambda^2}{2} z^2 \right] |\psi(\mathbf{r})|^2 + 2\pi\gamma |\psi(\mathbf{r})|^4 \right\} d^3\mathbf{r} \; , \tag{40}$$

with

$$\lambda = \frac{\omega_z}{\omega_\perp} \qquad \text{trap anisotropy}$$

$$\gamma = \frac{|a_s| N}{a_\perp} \qquad \text{interaction strength.}$$

To study this problem we use the Gaussian ansatz[§]

$$\psi(\mathbf{r}) = \frac{1}{\pi^{3/4}\sigma\eta^{1/2}} \exp\left\{-\frac{(x^2+y^2)}{2\sigma^2} - \frac{z^2}{2\eta^2}\right\}, \tag{41}$$

where σ and η are, respectively, transverse and axial widths. Inserting this ansatz into the energy functional, we obtain the effective energy

$$\bar{E} = \frac{1}{\sigma^2} + \sigma^2 + \frac{1}{2\eta^2} + \frac{\lambda^2}{2}\eta^2 - \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta}\,. \tag{42}$$

We look for values of σ and η that minimize energy $\bar{E}$ and get

$$-\frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^3\eta} = 0\,, \tag{43}$$

$$-\frac{1}{\eta^3} + \lambda^2\eta + \sqrt{\frac{2}{\pi}}\,\gamma\frac{1}{\sigma^2\eta^2} = 0\,. \tag{44}$$

These equations give local minima only if the curvature of $E(\eta,\sigma)$ is positive.

Remarkably, there is a **local minumum** also with $\lambda = 0$, i.e. also **without axial confinement**: this is the so-called bright soliton. This bright soliton collapses at a critical strength $\gamma_c \simeq 0.78$.

[§]L.S., A. Parola, and L. Reatto, PRA **66**, 043603 (2002).

We can also study the dynamics of the attractive BEC by using the Lagrangian¶

$$L = \dot{\sigma}^2 + \frac{1}{2}\dot{\eta}^2 - \bar{E}(\sigma, \eta) \; . \tag{45}$$

The equations of motion are

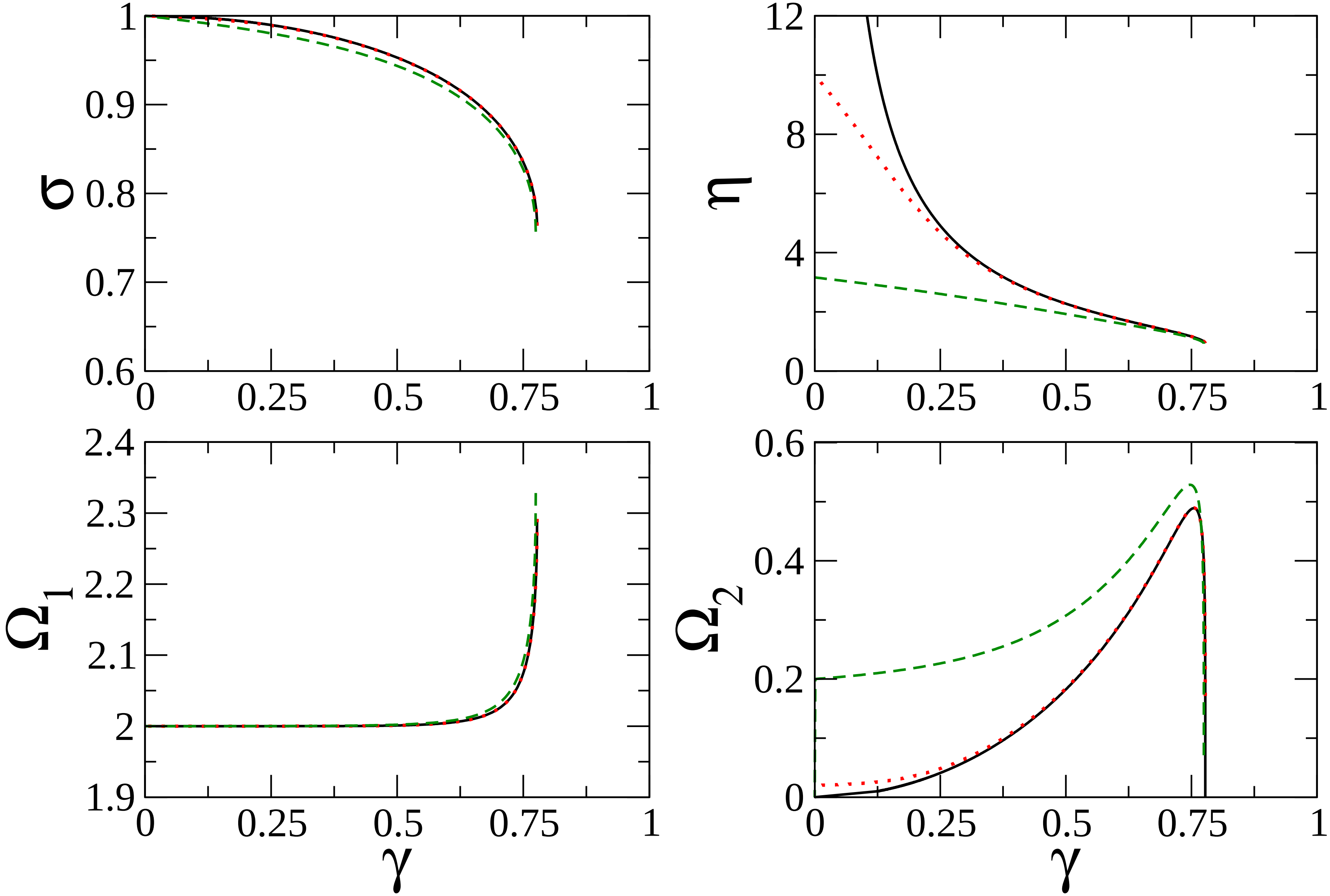
$$\ddot{\sigma} - \frac{1}{\sigma^3} + \sigma + \sqrt{\frac{2}{\pi}} \; \gamma \frac{1}{\sigma^3 \eta} = 0 \; , \tag{46}$$

$$\ddot{\eta} - \frac{1}{\eta^3} + \lambda^2 \eta + \sqrt{\frac{2}{\pi}} \; \gamma \frac{1}{\sigma^2 \eta^2} = 0 \; . \tag{47}$$

From these equations one can quite easily derive the frequencies Ω_1 and Ω_2 of small oscillations around the local minima.

Ω_1 and Ω_2 are the frequencies of **breathing modes** along radial and axial direction.

¶L.S., Int. J. Mod. Phys. B **14** 405 (2000).



Gaussian variational approach to the **attractive BEC**. Top: Widths σ and η. Bottom: Breathing frequencies ω_1 and ω_2. All *vs* interaction strength γ. Trap anisotropy: black solid line ($\lambda = 0$); red dotted line ($\lambda = 0.01$); green dashed line ($\lambda = 0.1$).

Conclusions

- Macroscopic quantum phenomena at ultra-low temperature are strongly related to Bose-Einstein condensation.

- A Bose-Einstein condensate (BEC) made of ultra-dilute and ultra-cold atomic gases can be accurately studied by using the Gross-Pitaevskii equation (GPE).

- The Gaussian variational approach is useful to study the GPE.

- BECs with negative scattering length show interesting properties:
  - collapse above a critical strength;
  - bright soliton solutions.