ECT* Workshop
January 2015

Basic concepts of cold atomic gases

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Plan for the lectures:

- Cold gases and BEC
- Order parameter and Gross-Pitaevskii theory
- Order parameter and superfluidity
- Fermions

Bibliography:

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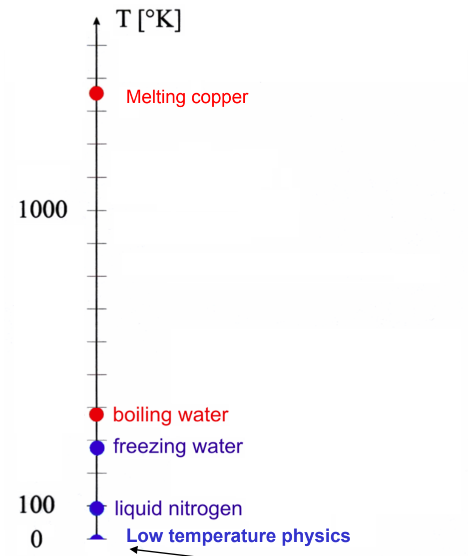
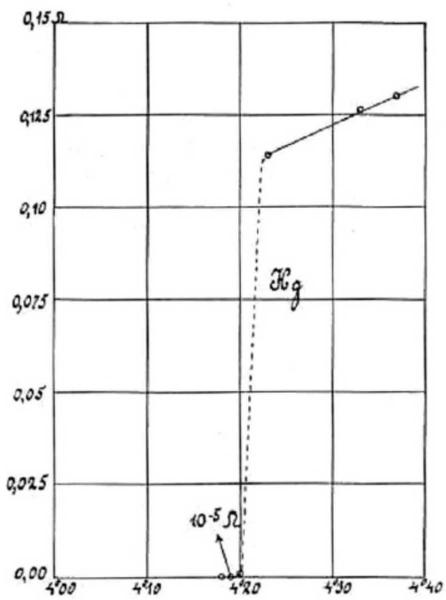
Cold gases and BEC

Hot and cold

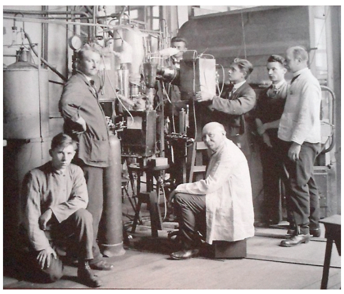


Just a boring little corner?

Superconductivity

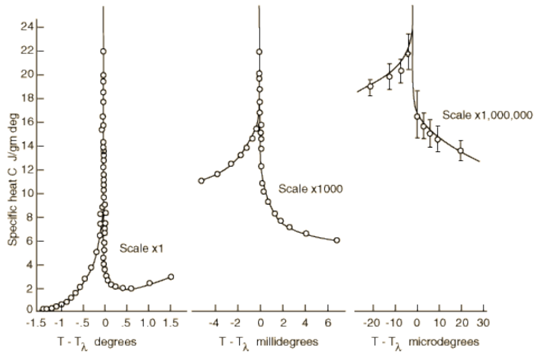


Leiden, 1905



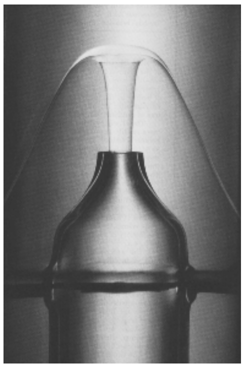
Superfluidity

anomaly in the specific heat
(Leiden, 1927)



[taken from Buckingham, M.J., and Fairbank, W.M. (1961)]

anomaly in the viscosity
(Allen and Misener, Kapitza,1938)



In 1938 Fritz London had the intuition: is superfluidity a manifestation of Bose-Einstein condensation ?

644 NATURE APRIL 9, 1938, VOL. 141

the effective mass m^* being of the order of magnitude of the mass of the atoms. But in the present case we are obliged to apply Bose-Einstein statistics instead of Fermi statistics.

(3) In his well-known papers, Einstein has already discussed a peculiar condensation phenomenon of the 'Bose-Einstein' gas; but in the course of time the degeneracy of the Bose-Einstein gas has rather got the reputation of having only a purely imaginary existence. Thus it is perhaps not generally known that this condensation phenomenon actually represents a discontinuity of the derivative of the specific heat (phase transition of third order). In the accompanying figure the specific heat (C_v) of an *ideal* Bose-Einstein gas is represented as a function of T/T_0 where

$$T_0 = \frac{h^2}{2\pi m^* k}\left(\frac{n}{2{,}615}\right)^{2/3}.$$

With m^* = the mass of a He atom and with the mol. volume $\frac{N_l}{n} = 27{\cdot}6$ cm.^{3} one obtains $T_0 = 3{\cdot}09°$. For

expected to furnish quantitative insight into the properties of liquid helium.

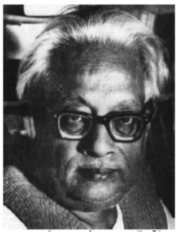
The conception here proposed might also throw a light on the peculiar transport phenomena observed with He II (enormous conductivity of heat[5], extremely small viscosity[6] and also the strange fountain phenomenon recently discovered by Allen and Jones[2]).

A detailed discussion of these questions will be published in the *Journal de Physique*.

F. LONDON.

Institut Henri Poincaré,
Paris.
March 5.

[1] Fröhlich, H., *Physica*, **4**, 639 (1937).
[2] Allen, J. F., and Jones, H., NATURE, **141**, 243 (1938).
[3] Simon, F., NATURE, **133**, 529 (1934).
[4] London, F., *Proc. Roy. Soc.*, A, **153**, 576 (1936).
[5] Rollin, *Physica*, **2**, 557 (1935); Keesom, W. H., and Keesom, H. P., *Physica*, **3**, 359 (1936); Allen, J. F., Peierls, R., and Zaki Uddin, M., NATURE, **140**, 62 (1937).
[6] Burton, E. F., NATURE, **135**, 265 (1935); Kapitza, P., NATURE, **141**, 74 (1938); Allen, J. F. and Misener, A. D., NATURE, **141**, 75 (1938).



Bose

Plancks Gesetz und Lichtquantenhypothese.

Von Bose (Dacca-University, Indien).

(Eingegangen am 2. Juli 1924.)

Der Phasenraum eines Lichtquants in bezug auf ein gegebenes Volumen wird in „Zellen" von der Größe h^3 aufgeteilt. Die Zahl der möglichen Verteilungen der Lichtquanten einer makroskopisch definierten Strahlung unter diese Zellen liefert die Entropie und damit alle thermodynamischen Eigenschaften der Strahlung.

Plancks Formel für die Verteilung der Energie in der Strahlung des schwarzen Körpers bildet den Ausgangspunkt für die Quantentheorie, welche in den letzten 20 Jahren entwickelt worden ist und in allen Gebieten der Physik reiche Früchte getragen hat. Seit der Publikation im Jahre 1901 sind viele Arten der Ableitung dieses Gesetzes vorgeschlagen worden. Es ist anerkannt, daß die fundamentalen Voraussetzungen der Quantentheorie unvereinbar sind mit den Gesetzen der klassischen Elektrodynamik. Alle bisherigen Ableitungen machen Gebrauch von der Relation

$$\varrho_\nu d\nu = \frac{8\pi\nu^2 d\nu}{c^3} E,$$

Mit Rücksicht auf den oben gefundenen Wert von A^s ist also

$$E = \sum_s \frac{8\pi h \nu^{s^3} d\nu^s}{c^3} V \frac{e^{-\frac{h\nu^s}{\beta}}}{1 - e^{-\frac{h\nu^s}{\beta}}}.$$

Mit Benutzung der bisherigen Resultate findet man ferner

$$S = k\left[\frac{E}{\beta} - \sum_s A^s \lg\left(1 - e^{\frac{h\nu^s}{\beta}}\right)\right],$$

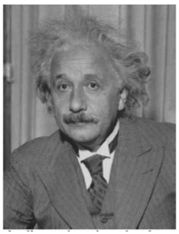
woraus mit Rücksicht darauf, daß $\frac{\partial S}{\partial E} = \frac{1}{T}$, folgt, daß $\beta = kT$. Setzt man dies in obige Gleichung für E ein, so erhält man

$$E = \sum_s \frac{8\pi h \nu^{s^3}}{c^3} V \frac{1}{e^{\frac{h\nu^s}{kT}} - 1} d\nu^s,$$

welche Gleichung Plancks Formel äquivalent ist.

(Übersetzt von A. Einstein.)

Anmerkung des Übersetzers. Boses Ableitung der Planckschen Formel bedeutet nach meiner Meinung einen wichtigen Fortschritt. Die hier benutzte Methode liefert auch die Quantentheorie des idealen Gases, wie ich an anderer Stelle ausführen will.



Einstein

Quantentheorie des einatomigen idealen Gases.

Zweite Abhandlung.

Von A. Einstein.

In einer neulich in diesen Berichten (XXII 1924, S. 261) erschienenen Abhandlung wurde unter Anwendung einer von Hrn. D. Bose zur Ableitung der Planckschen Strahlungsformel erdachten Methode eine Theorie der »Entartung« idealer Gase angegeben. Das Interesse dieser Theorie liegt darin, daß sie auf die Hypothese einer weitgehenden formalen Verwandtschaft zwischen Strahlung und Gas gegründet ist. Nach dieser Theorie weicht das entartete Gas von dem Gas der mechanischen Statistik in analoger Weise ab wie die Strahlung gemäß dem Planckschen Gesetze von der Strahlung gemäß dem Wienschen Gesetze. Wenn die Bosesche Ableitung der Planckschen Strahlungsformel ernst genommen wird, so wird man auch an dieser Theorie des idealen Gases nicht vorbeigehen dürfen; denn wenn es gerechtfertigt ist, die Strahlung als Quantengas aufzufassen, so muß die Analogie zwischen Quantengas und Molekülgas eine vollständige sein. Im folgenden sollen die früheren Überlegungen durch einige neue ergänzt werden, die mir das Interesse an dem Gegenstande zu steigern scheinen. Der Bequemlichkeit halber schreibe ich das Folgende formal als Fortsetzung der zitierten Abhandlung.

4 Sitzung der physikalisch-mathematischen Klasse vom 8. Januar 1925

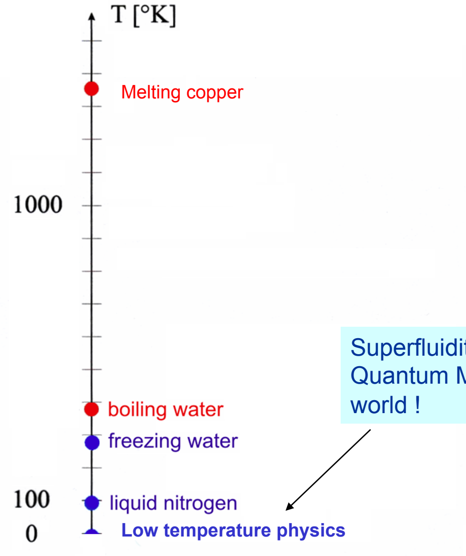
Was geschieht nun aber, wenn ich bei dieser Temperatur $\frac{n}{V}$ (z. B. durch isothermische Kompression) die Dichte der Substanz noch mehr wachsen lasse?

Ich behaupte, daß in diesem Falle eine mit der Gesamtdichte stets wachsende Zahl von Molekülen in den 1. Quantenzustand (Zustand ohne kinetische Energie) übergeht, während die übrigen Moleküle sich gemäß dem Parameterwert $\lambda = 1$ verteilen. Die Behauptung geht also dahin, daß etwas Ähnliches eintritt wie beim isothermen Komprimieren eines Dampfes über das Sättigungsvolumen. Es tritt eine Scheidung ein; ein Teil »kondensiert«, der Rest bleibt ein »gesättigtes ideales Gas« ($A = 0$ $\lambda = 1$).

Daß die beiden Teile in der Tat ein thermodynamisches Gleichgewicht bilden, sieht man ein, indem man zeigt, daß die »kondensierte« Substanz und das gesättigte ideale Gas pro Mol dieselbe Plancksche Funktion $\Phi = S - \frac{E + pV}{T}$ haben. Für die »kondensierte« Substanz verschwindet Φ, weil S, E und V einzeln verschwinden[1]. Für das »gesättigte Gas« hat man nach (12) und (13) für $A = 0$ zunächst

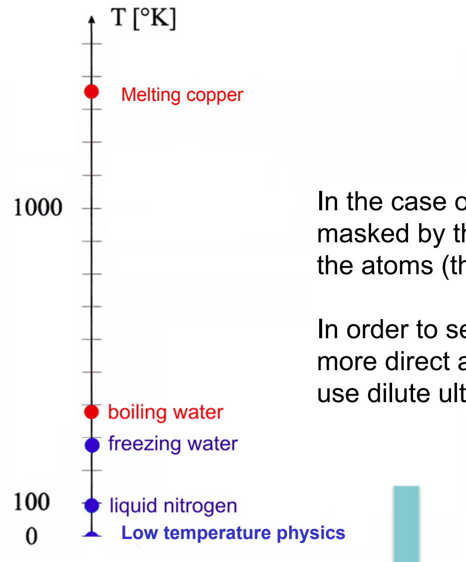
$$S = -\varkappa \sum_s \lg(1 - e^{-\alpha^s}) + \frac{E}{T}. \qquad (25)$$

Hot and cold



Superfluidity and superconductivity: Quantum Mechanics in the macroscopic world !

Hot and cold

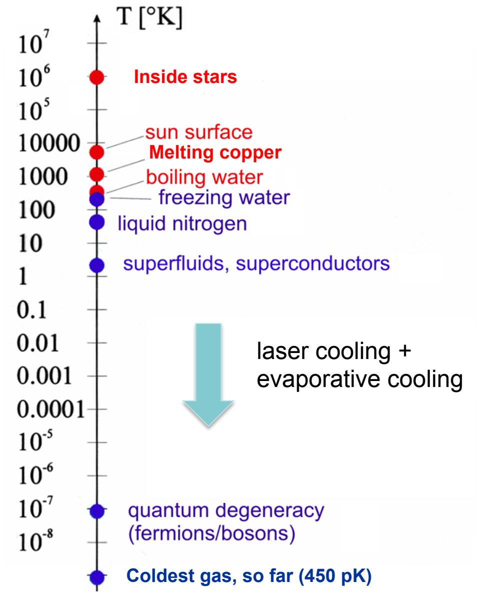


In the case of superfluid helium, BEC is masked by the strong interaction among the atoms (the system is dense).

In order to see the effects of BEC in a more direct and clean way, one has to use dilute ultracold (metastable) gases.

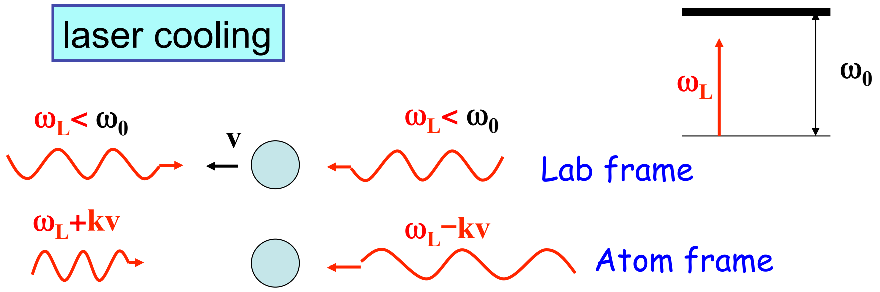
One must cool down further

Cold, very cold



An amazingly interesting new frontier !!

laser cooling



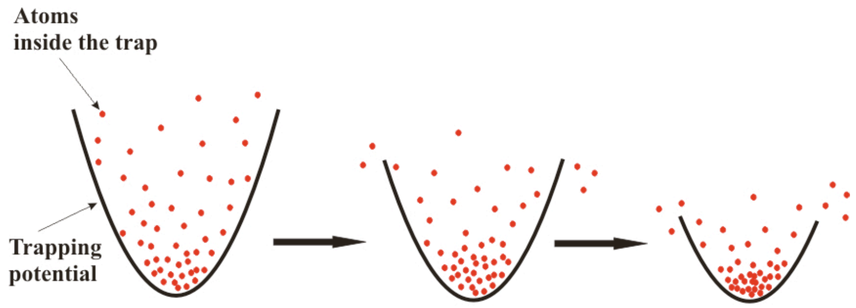
Red detuned laser.

An atom moving against the beam sees the “right” frequency due to Doppler effect. It absorbs a photon, thus decreasing its momentum. Then the photon is re-emitted with isotropic probability.

Using beams in all directions, the net effect is a cooling of the gas.

Evaporative cooling

The hottest atoms are forced to escape by means of suitable radio frequency transitions



Important remark: these cold gases are metastable !

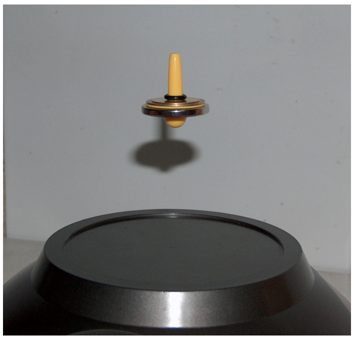
The stable configuration is a solid phase.

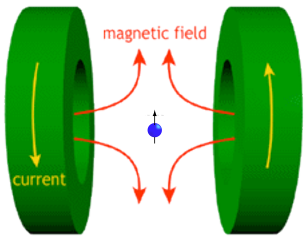
But, in order to reach the solid phase, inelastic collisions between atoms (at least three-body) must occur. Such collisions are **rare** if the gas is **dilute**.

Of course, one cannot confine the gas within a box with solid surfaces: collisions with material walls would quickly kill the gas phase.

Confinement without walls: **magnetic** and/or **optical trapping** inside ultrahigh vacuum chambers.

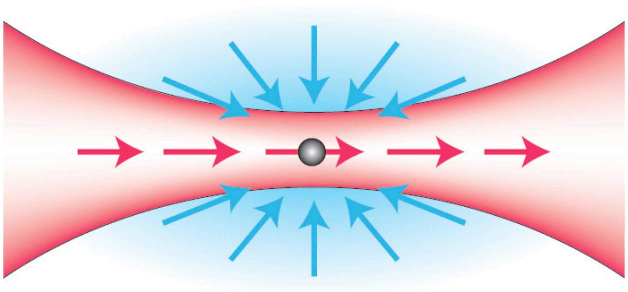
Magnetic confinement





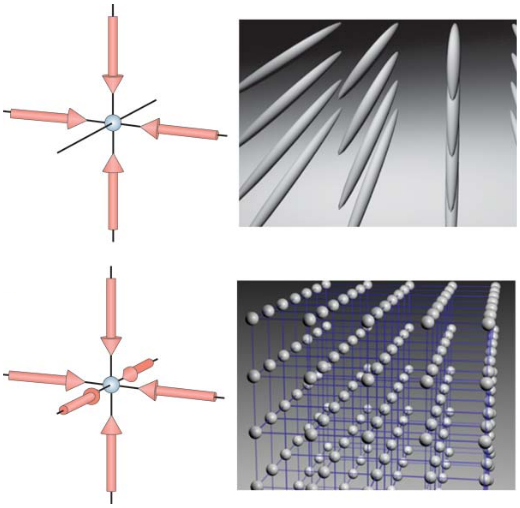
Atoms have magnetic moment and hence they feel an external magnetic field.
The field can be designed such to produce harmonic confinement around a minimum.

Optical confinement

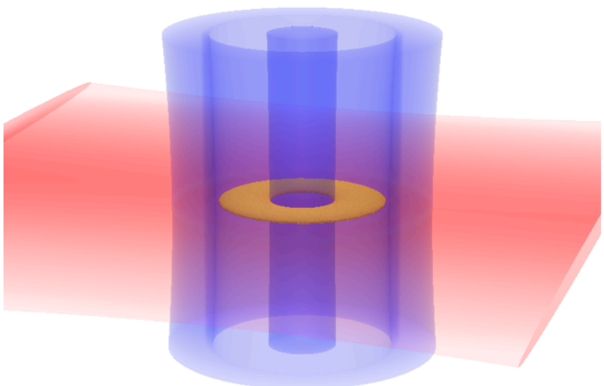


The dipole force between atoms and a light field (interaction of the induced atomic dipole moment with the intensity gradient of the light field) can be used to produce attractive or repulsive optical dipole potentials for atoms in a *far-detuned* light.

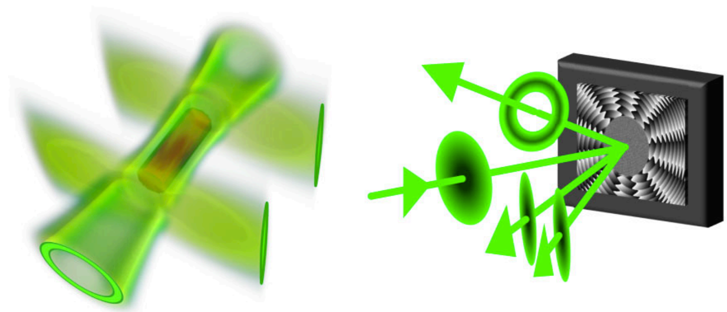
Most traps are harmonic, but laser beams of various shapes and geometries can be used to produce different confining potentials, like **optical lattices**



Most traps are harmonic, but laser beams of various shapes and geometries can be used to produce different confining potentials, like **optical lattices**, **toroidal traps**



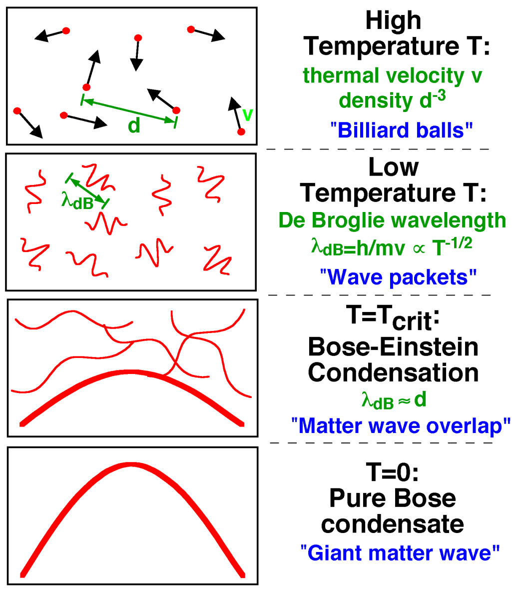
Most traps are harmonic, but laser beams of various shapes and geometries can be used to produce different confining potentials, like **optical lattices**, **toroidal traps**, **square-like boxes**, etc.



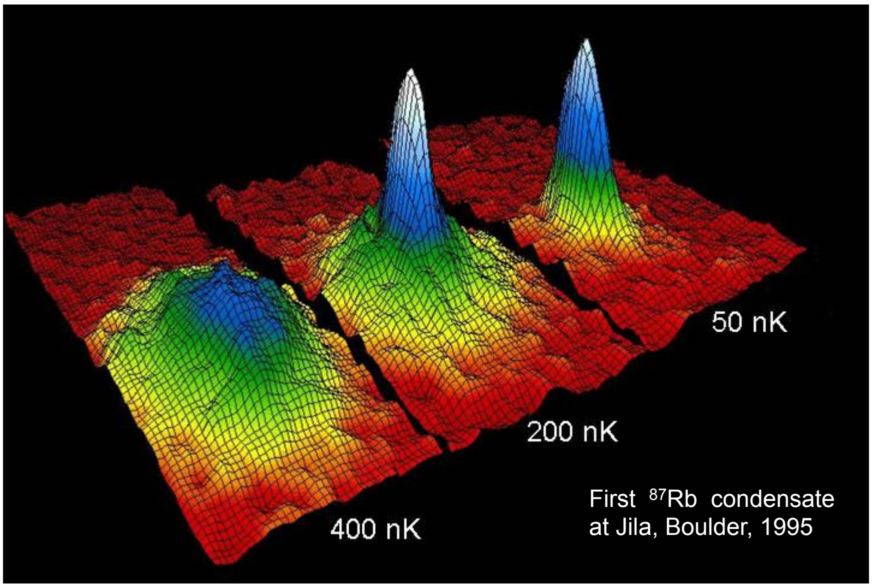
So, trap the (bosonic) atoms and cool them down to BEC

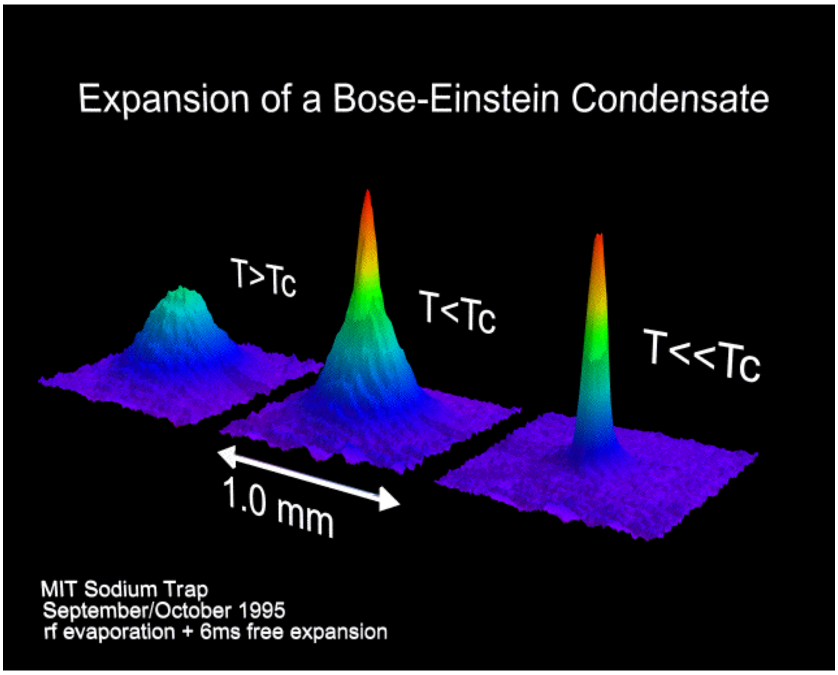
…

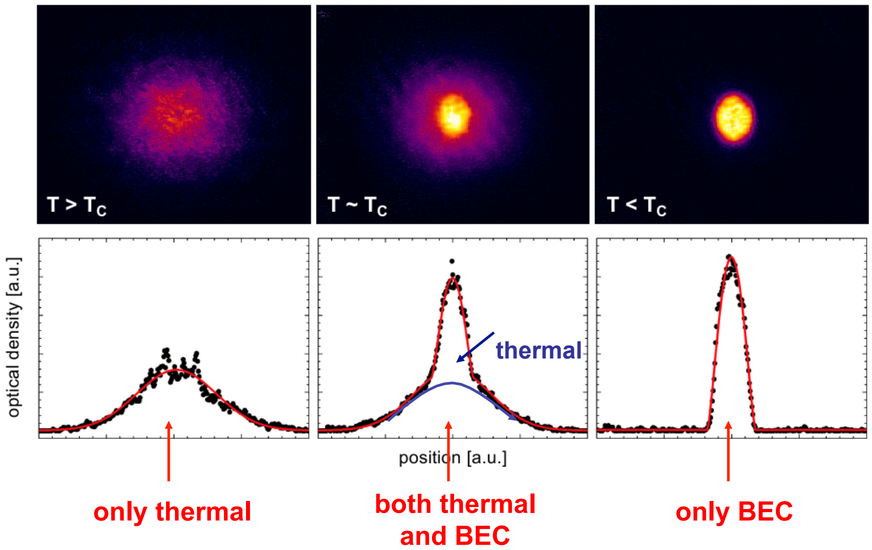
from classical particles to **matter waves**



(Taken from W. Ketterle)


50 nK
200 nK
400 nK
First ^{87}Rb condensate
at Jila, Boulder, 1995


Expansion of a Bose-Einstein Condensate
T>Tc
T<Tc
T<<Tc
1.0 mm
MIT Sodium Trap
September/October 1995
rf evaporation + 6ms free expansion



Temperature is measured by fitting the tails of the thermal component !

Many more condensates

1996: ^{7}Li (Rice)
1997: ^{87}Rb (Texas, Stanford, Konstanz), ^{23}Na (Rowland Inst),
1998: ^{87}Rb (Munich, Hannover, Sussex, Kyoto, Paris, Paris, Otago), H (MIT), ^{23}Na (NIST)
1999: ^{87}Rb (Firenze, Oxford, Pisa, Amsterdam)
2000: ^{87}Rb (Tokyo)
2001: ^{87}Rb (2 in USA, Germany, Munich, Tokyo, Camberra, Tuebingen, Paris, Weizmann), ^{7}Li (Paris), ^{41}K (Firenze), He* (Paris)
…

then ^{85}Rb, Cs, Yb, Cr, Dy, Er, Sr, Li_2, Na_2, Cs_2 and mixtures.

and fermions too…

Why alkali atoms first?

Goal: increase the phase space density to reach a regime of quantum degeneracy.

Steps: Laser cooling (pre-cooling stage) + evaporative cooling

Efficent laser cooling with: hydrogen, helium, alkali atoms, metastable rare gases, earth-alkali atoms, etc.

Efficent evaporative cooling if “good” collisions (elastic collisions necessary for evaporation and thermalization) dominates over “bad” collisions (atom losses due to two- and three-body inelastic collisions). Alkali atoms are the best **!!**

Why BEC is important ?

Paradigm of statistical mechanics (phase transition in the absence of interactions).

Exact description of the effects of interactions for dilute gases.

Fundamental concepts (long range order; spontaneous symmetry breaking; etc.) which play an important role in many areas of physics.

… and moreover

the observation of BEC opened new prospects in Physics: cold atoms as a tool for new advances in atomic physics, quantum optics, quantum technologies, quantum simulations, …

BEC shows up in condensed matter, nuclear physics, elementary particle physics, astrophysics, and atomic physics.

- Cooper pairs of electrons in superconductors
- ^{4}He atoms in superfluid liquid He
- Excitons, biexcitons in semiconductors
- Alkali atoms in ultracold atom gases
- ^{3}He atom pairs in superfluid ^{3}He-A,B
- Neutron pairs, protron pairs in nuclei And neutron stars
- Mesons in neutron star matter

(taken from Debbie Jin)

and also exciton-polariton condensates, of course!

Some relevant properties of BEC

Those due to interaction:
- **sound propagation and collective oscillations**
- **solitary waves**

Those due to phase coherence:
- **interference**
- **atom laser**

Superfluid properties (interaction + coherence):
- **viscousless motion**
- **quantized vortices**
- **Josephson effect**
- **second sound**

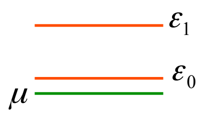
Quantum phase transitions:
- **Superfluid - Mott insulator**
- **Berezinskii-Kosterlitz-Thouless**
- **...**

BEC in noninteracting gases

Occupation number of single-particle states: $$n_i = \frac{1}{\exp[(\varepsilon_i - \mu)/k_B T] - 1}$$

where $$H_0 \phi_i = \varepsilon_i \phi_i$$

The value of μ is fixed by normalization condition $$\sum_i n_i = N$$



BEC starts when the chemical potential is so close to ε_0 that $(\varepsilon_0 - \mu) << k_B T$ *and* the occupation number of $i=0$ state $(n_0 \equiv N_0)$ becomes large and comparable to N:

$$N_0 \approx \frac{k_B T}{\varepsilon_0 - \mu} >> 1$$

BEC in noninteracting gases

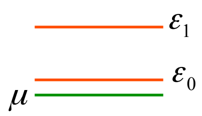
Occupation number of single-particle states: $$n_i = \frac{1}{\exp[(\varepsilon_i - \mu)/k_B T] - 1}$$

where $$H_0 \phi_i = \varepsilon_i \phi_i$$

The value of μ is fixed by normalization condition $$\sum_i n_i = N$$

If $\varepsilon_i - \mu >> \varepsilon_0 - \mu$

for $i>0$, one can replace μ with ε_0 in the above expression and the occupation number of i-state **does not depend** any more on **N !**

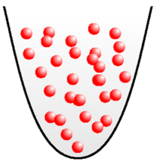


Mechanism of BEC: $$N = N_0 + \sum_{i \neq 0} \frac{1}{\exp[(\varepsilon_i - \varepsilon_0)/k_B T] - 1}$$

number of atoms N_T out of the condensate depends only on T, not on N.

The condition **N_T=N** fixes the value of critical temperature

BEC in noninteracting gases in 3D harmonic potential



$$H_0\phi_i = \varepsilon_i\phi_i$$

Single-particle hamiltonian: $H_0 = p^2/2m + V_{ext}$

Confining potential: $V_{ext} = \frac{1}{2}m\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right]$

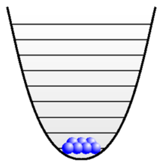
Spectrum of eigenstates:

$$\varepsilon(n_x,n_y,n_z) = (n_x+\frac{1}{2})\hbar\omega_x + (n_y+\frac{1}{2})\hbar\omega_y + (n_z+\frac{1}{2})\hbar\omega_z$$

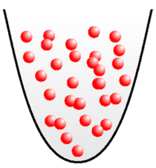
Condition for BEC:

$$\mu = \varepsilon(0,0,0)$$

$$N_T = \sum_{n_x,n_y,n_z \neq 0} \frac{1}{\exp[\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)] - 1}$$



BEC in noninteracting gases in 3D harmonic potential



$$N_T = \sum_{n_x,n_y,n_z \neq 0} \frac{1}{\exp[\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)] - 1}$$

If $k_B T >> \hbar\omega_i$

then one can transform the discrete sum into an integral (semiclassical approximation).

The integration gives

$$N_T = \left(\frac{k_B T}{\hbar\omega_{ho}}\right)^3 g_3(1)$$

where $\omega_{ho} = (\omega_x\omega_y\omega_z)^{1/3}$

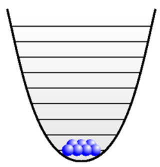
and $g_3(1)=\varsigma(3)$, with $\varsigma(n)$ Riemann ς function

Critical temperature when $N_T=N$, which implies:

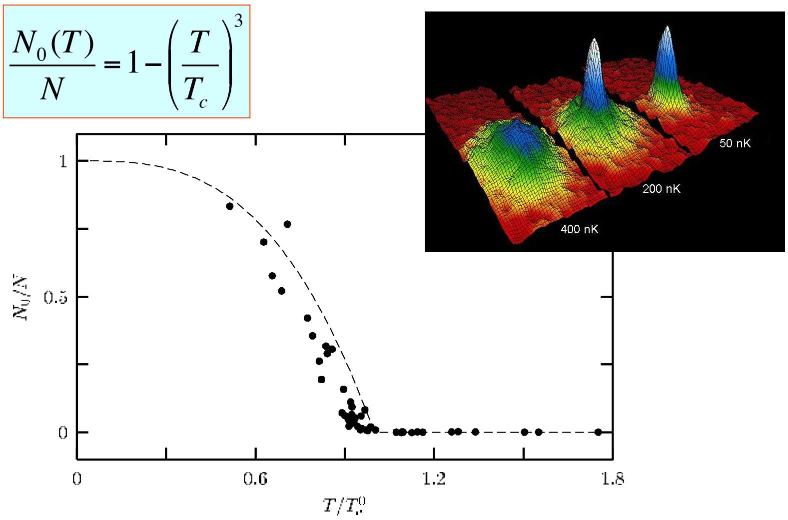
$$k_B T_c = 0.94\hbar\omega_{ho}N^{1/3}$$

and

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



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



Condensate fraction measured at JILA (1996)
EXPERIMENTAL EVIDENCE
OF PHASE TRANSITION

BEC in interacting gases

Many-body Hamiltonian:

$$\hat{H} = \int d\mathbf{r}\,\hat{\Psi}^+(\mathbf{r})\left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r}) + \frac{1}{2}\iint d\mathbf{r}\,d\mathbf{r}'\,\hat{\Psi}^+(\mathbf{r})\hat{\Psi}^+(\mathbf{r}')V(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})$$

where $\hat{\Psi}(\mathbf{r})$ and $\hat{\Psi}^+(\mathbf{r})$ are bosonic field operators.

one-body density matrix: $n^{(1)}(\mathbf{r},\mathbf{r}') = \left\langle \hat{\Psi}^+(\mathbf{r})\hat{\Psi}(\mathbf{r}')\right\rangle$

Relevant observables directly related to the one-body density matrix:

particle density: $n(\mathbf{r}) = \left\langle \hat{\Psi}^+(\mathbf{r})\hat{\Psi}(\mathbf{r})\right\rangle = n^{(1)}(\mathbf{r},\mathbf{r})$

momentum distribution:

$$n(\mathbf{p}) = \left\langle \hat{\Psi}^+(\mathbf{p})\hat{\Psi}(\mathbf{p})\right\rangle = (2\pi\hbar)^{-3}\int d\mathbf{R}\,d\mathbf{s}\;n^{(1)}(\mathbf{R}+\mathbf{s}/2,\mathbf{R}-\mathbf{s}/2)\,e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}$$

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momentum distribution:

$$n(\mathbf{p}) = (2\pi\hbar)^{-3}\int d\mathbf{R}d\mathbf{s}\; n^{(1)}(\mathbf{R}+\mathbf{s}/2,\mathbf{R}-\mathbf{s}/2)e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}$$

In uniform systems $n^{(1)}(\mathbf{r},\mathbf{r}') = n^{(1)}(s) = \frac{1}{V}\int dp\, n(p)e^{ips/\hbar}$

Usual situation: *n(p)* is smooth function $\Rightarrow$ $n^{(1)}(s)_{s\to\infty} = 0$

However, the occurrence of BEC in noninteracting gases suggests that the *p=0* state (lowest single-particle state in the uniform system) can be macroscopically occupied below a given critical temperature T_c.
In terms of momentum distribution this means:

$$n(p) = N_0\delta(p) + \tilde{n}(p)$$

BEC **Smooth function**

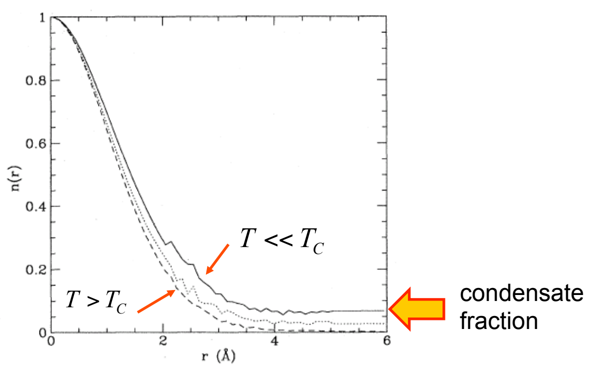
BEC in interacting gases

$$n(p) = N_0\delta(p) + \tilde{n}(p) \Rightarrow n^{(1)}(s)_{s\to\infty} = n_0 = \frac{N_0}{V}$$

Off-diagonal long range order
(Landau, Lifschitz, Penrose, Onsager)

Example of calculation of density matrix in highly correlated many-body system: liquid He4

(Ceperley, Pollock 1987)



BEC in interacting gases

nonuniform systems: same concept, but in a more general form.
Starting from the eigenvalues and eigenfunctions of the one-body density matrix.

$$\int d\mathbf{r}' n^{(1)}(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}') = n_i \phi_i(\mathbf{r})$$

$$n^{(1)}(\mathbf{r},\mathbf{r}') = \sum_i n_i \phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')$$

Single-particle occupation numbers

BEC occurs when $n_o \equiv N_0 >> 1$

If this happens, then it is convenient to rewrite the density matrix by separating the contribution arising from the condensate:

$$n^{(1)}(\mathbf{r},\mathbf{r}') = N_0 \phi_0^*(\mathbf{r})\phi_0(\mathbf{r}') + \sum_{i\neq 0} n_i \phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')$$

For large N the sum tends to zero at large distances.
Conversely, the first term remains finite even at large |***r-r'***|, where one recovers the concept of long range order.
But the diagonalization of the density matrix works even for finite systems!!
The condensate can be identified with the eigenfunction having the largest eigenvalue (of order N).

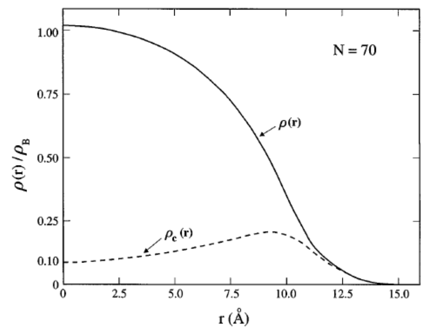
BEC in interacting gases

Example of diagonalization of the one-body density matrix: ^{4}He droplets.

[Lewart, Pandharipande and Pieper, Phys. Rev. B (1988)]

TABLE III. Number of particles having a given angular momentum for the 70-atom ^{4}He drop. The number of particles in the condensate is shown separately.

l	N_l	
Condensate	25.33	26.46
0	1.13	
1	3.74	
2	5.06	
3	5.51	
4	5.55	
5	4.92	
6	4.20	
7	3.63	
8	2.98	
9	1.97	
10	1.32	
Total	65.34	



Note: In bulk superfluid helium the condensate fraction is of the order of 0.1.
In the droplet, the condensate fractions is locally larger near the surface, where the system is more dilute.

Order parameter and Gross-Pitaevskii equation

Order parameter

Starting from the definition of $n^{(1)}$ $$n^{(1)}(\mathbf{r},\mathbf{r}') = \left\langle \hat{\Psi}^{+}(\mathbf{r})\hat{\Psi}(\mathbf{r}')\right\rangle$$

and using its eigenfunctions

$$\int d\mathbf{r}' n^{(1)}(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}') = n_i\phi_i(\mathbf{r}) \qquad n^{(1)}(\mathbf{r},\mathbf{r}') = \sum_i n_i\phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')$$

one can define annihilation and creation operators $\hat{a}_i,\, \hat{a}_i^+$

such that $[\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$ $\quad [\hat{a}_i, \hat{a}_j] = 0$ $\quad \left\langle \hat{a}_j^+\hat{a}_i\right\rangle = \delta_{ij}n_i$

and $$\hat{\Psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{a}_i \qquad \hat{\Psi}^+(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r})\hat{a}_i^+$$

Order parameter

Separating the condensate in $n^{(1)}$

$$n^{(1)}(\mathbf{r},\mathbf{r}') = N_0\phi_0^*(\mathbf{r})\phi_0(\mathbf{r}') + \sum_{i\neq 0} n_i\phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')$$

is equivalent to writing

$$\hat{\Psi}(\mathbf{r}) = \phi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0}\phi_i(\mathbf{r})\hat{a}_i$$

into the definition $n^{(1)}(\mathbf{r},\mathbf{r}') = \left\langle \hat{\Psi}^+(\mathbf{r})\hat{\Psi}(\mathbf{r}')\right\rangle$

Key point !

If the system exhibits BEC, then $\left\langle \hat{a}_0^+\hat{a}_0\right\rangle = n_0 = N_0 >> 1$

while $[\hat{a}_0, \hat{a}_0^+] = 1$

This means that the noncommutativity of these operators is inessential for most physical properties.

$\hat{a}_0, \hat{a}_0^+$ can be replaced by *c*-numbers $\rightarrow \sqrt{N_0}$

Order parameter

$$\hat{\Psi}(\mathbf{r}) = \phi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0}\phi_i(\mathbf{r})\hat{a}_i$$

becomes

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

with

$$\Psi_0(\mathbf{r}) = \sqrt{N_0}\,\phi_0(\mathbf{r})$$ Condensate wave function (order parameter)

$$\delta\hat{\Psi}(\mathbf{r}) = \sum_{i\neq 0}\phi_i(\mathbf{r})\hat{a}_i$$ non-condensed part (operator)

Under certain conditions the non-condensed part is small and the **field operator** can be approximated with a **classical field.**

One can also write $\Psi_0(\mathbf{r}) = \left\langle \hat{\Psi}\right\rangle$

Order parameter

The order parameter is $\Psi_0(\mathbf{r}) = \sqrt{N_0}\,\phi_0(\mathbf{r})$

It can be written as $\Psi_0 = |\Psi_0| e^{iS}$

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Is it a solution of a Schrödinger-like equation ?

Starting point: equation of motion for the field operator $\left\langle i\hbar \frac{\partial}{\partial t} \hat{\Psi} \right\rangle = \left\langle [\hat{\Psi}, \hat{H}] \right\rangle$

$$\left\langle i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r},t) \right\rangle = \left\langle \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) + \int d\mathbf{r}' \hat{\Psi}^+(\mathbf{r}',t) V(|\mathbf{r}-\mathbf{r}'|) \hat{\Psi}(\mathbf{r}',t) \right] \hat{\Psi}(\mathbf{r},t) \right\rangle$$

Equation for the order parameter

$$\left\langle i\hbar \frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)\right\rangle = \left\langle \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\hat{\Psi}^{+}(\mathbf{r}',t)V(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}',t)\right]\hat{\Psi}(\mathbf{r},t)\right\rangle$$

This is an equation for the field operator. But we want something for the classical field

$$\Psi_0(\mathbf{r},t) = \left\langle \hat{\Psi}(\mathbf{r},t)\right\rangle$$

Delicate issue: replacing the field operator with the classical field (order parameter) in the interaction term requires a proper procedure.

Equation for the order parameter

$$\left\langle i\hbar \frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)\right\rangle = \left\langle \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\hat{\Psi}^{+}(\mathbf{r}',t)V(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}',t)\right]\hat{\Psi}(\mathbf{r},t)\right\rangle$$

A simple and correct procedure is applicable (in 3D) if

- The **range** of interaction and ***s*-wave scattering length *a*** are much **smaller** than the average **distance d** between particles
- **Temperature** is sufficiently **low.**
- **Macroscopic variations** of the order parameter are considered (variations over distances much larger than *a*).

Only low energy two-body scattering properties are relevant for describing the many-body problem.

Equation for the order parameter

$$\left\langle i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t)\right\rangle = \left\langle \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + \int d\mathbf{r}'\hat{\Psi}^+(\mathbf{r}',t)V(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}(\mathbf{r}',t)\right]\hat{\Psi}(\mathbf{r},t)\right\rangle$$

Only low energy two-body scattering properties are relevant for describing the many-body problem.

The scattering length ***a*** is the only relevant interaction parameter !!

The equation for order parameter is obtained by substituting

$$\Psi_0(\mathbf{r},t) = \left\langle \hat{\Psi}(\mathbf{r},t)\right\rangle$$

and by replacing V with the **effective potential**

$$V_{eff} = g\delta(r-r') \quad \text{with} \quad g = 4\pi\hbar^2 a/m$$

Equation for the order parameter

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

Gross-Pitaevskii equation

density: $n(\mathbf{r},t) = |\Psi_0(\mathbf{r},t)|^2$

It requires that:

✓ The gas is dilute (quantum fluctuations are negligible) → $na^3 << 1$

✓ The temperature is low (thermal fluctuations are negligible) → $T << T_C$

It is equivalent to:

✓treating the field operator like a classical field $\hat{\Psi}(\mathbf{r}) = \Psi_0(\mathbf{r}) + \cancel{\delta\hat{\Psi}(\mathbf{r})}$

Equation for the order parameter

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

Gross-Pitaevskii equation

For non dilute gases and/or finite T one has

$$n(\mathbf{r},t)\neq n_0(\mathbf{r},t)=\left|\Psi_0(\mathbf{r},t)\right|^2$$

and the problem becomes harder

GP $$i\hbar\frac{\partial}{\partial t}\Psi_0(\mathbf{r},t)=\left[-\frac{\hbar^2\nabla^2}{2m}+V_{ext}(\mathbf{r})+g\left|\Psi_0(\mathbf{r},t)\right|^2\right]\Psi_0(\mathbf{r},t)$$

Now, some remarks on this equation…

GP $i\hbar\frac{\partial}{\partial t}\Psi_0(\mathbf{r},t)=\left[-\frac{\hbar^2\nabla^2}{2m}+V_{ext}(\mathbf{r})+g|\Psi_0(\mathbf{r},t)|^2\right]\Psi_0(\mathbf{r},t)$

Remark #1

GP equation for order parameter is analog to **Maxwell** equations in classical electrodynamics.

Condensate wave function represents **classical limit of de Broglie wave** (corpuscolar nature of matter no longer important).

Difference : GP contains Planck constant explicitly, Maxwell doesn't.
This follows from the **different dispersion laws** of photons and atoms:

from particles to waves: $p \to \hbar k, E \to \hbar\omega$

	particles (energy)		waves (frequency)
photons	$E = cp$	→	$\omega = ck$
atoms	$E = p^2/2m$	→	$\omega = \hbar k^2/2m$

GP $i\hbar\frac{\partial}{\partial t}\Psi_0(\mathbf{r},t)=\left[-\frac{\hbar^2\nabla^2}{2m}+V_{ext}(\mathbf{r})+g|\Psi_0(\mathbf{r},t)|^2\right]\Psi_0(\mathbf{r},t)$

Remark #2

GP equation is **nonlinear**.

It is a special case of **nonlinear Schrödinger equation (NLSE)** widely used in many fields.

It shares many analogies with the physics of **nonlinear optics**.

The equation for the order parameter is **not** an equation for a **wave function** and the solution is **not** a wave function in the usual QM sense (e.g., no linear superposition) . It is sometimes called **macroscopic wave function** or **condensate wave function**. It must not be confused with the many-body wave function $\Psi_N(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N;t)$

The nonlinearity comes from interparticle interactions, which are represented by a **mean-field** potential energy in the effective hamiltonian.

GP

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

Remark #3

The solution is a complex function, with **modulus** and **phase**.

The energy of the system does not depend on phases, but the condensate has a well defined phase. This can be viewed as an example of **broken gauge symmetry**.

Be careful: in **finite systems** neither Long Range Order or Broken Gauge Symmetry are applicable concepts, strictly speaking, but the order parameter of the condensate is still well defined (eigenfunction of the one-body density matrix).

The **phase** of the order parameter is crucial for **superfluidity**.

GP

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

Remark #4

The GP equation can be also obtained from the least action principle

$$\delta\left[-i\hbar\int\Psi_0^*\frac{\partial}{\partial t}\Psi_0\,d\mathbf{r}\,dt+\int E dt\right]=0$$

which yields

$$i\hbar\frac{\partial}{\partial t}\Psi_0=\frac{\delta E}{\delta\Psi_0^*}$$

where

$$E=\int d\mathbf{r}\left(\frac{\hbar^2}{2m}|\nabla\Psi_0(\mathbf{r})|^2+V_{ext}(\mathbf{r})|\Psi_0(\mathbf{r})|^2+\frac{g}{2}|\Psi_0(\mathbf{r})|^4\right)$$

Gross-Pitaevskii energy functional

I emphasized the basic physics of GP equation because:

- The GP theory is exact in some limits
- The GP equation has been widely and successfully used for BECs
- Several generalizations of GP equations are currently used in different contexts: finite T, strongly interacting bosons, mixtures, and even fermions! [But take care of ckecking what is supposed to be exact, approximate or just qualitative !]

What next:

Statics and dynamics of BECs with GP equation