Cold atoms

Lecture 1.

20. September 2006

Low temperature physics
(borrowed from an undergraduate course)

Existence absolutní nuly

• Absolutní nula teploty pro ideální plyn

definována vztahem

$$\tfrac{1}{2} m \left\langle v^2 \right\rangle = \tfrac{3}{2} k_B T$$

a podmínkou nulové kinetické energie

• Pro všechny další systémy se použije transitivnosti teploty pro tělesa v kontaktu (nultý zákon termodynamiky)

• Absolutní nula není dostižitelná konečným procesem (3. zákon termodyn.)

$$S \to 0, \quad C_v \to 0, \quad \ldots$$

• Zvláštní jevy, makroskopické kvantové jevy, jako supravodivost, v blízkosti nuly. Ovšem co je „blízkost“ ? Vysokoteplotní supravodivost, život, …

Teploty ve vesmíru

Stupnice	nitra hvězd	10^6 - 10^8 K
	hvězdné atmosféry	10^3 - 10^4 K
	komety, planety …	10^1 - 10^2 K
	….	
	reliktní záření jako minimum	~ 2,72 K
	mlhovina Bumerang (souhvězdí Kentaura)	1,15 K

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	důvod: rychlá expanse plynů z centrální hvězdy	

Pozemský rekord

-89,3°C↔183.75 K

1983 Antarktida
stanice Vostok

Nízké teploty v laboratoři (jen výběr !!)

K	Teplotní rekordy	Objevy	Teorie
	1877 *Pictet* kapalný kyslík?		
77	1895 *von Linde* kap. vzduch		
22	1898 *Dewar* kapalný vodík		
	1905 *von Linde* kap. dusík		
4,2	1908 *Kamerlingh-Onnes* kapalné helium	1911 *Kamerlingh-Onnes* supravodivost kovů	
			1924 *Einstein* Bose-Einsteinova kondensace
0,3	odsávané helium		
mK	1933 paramagn. demagnet.	1937 *Kapica* supratekutost Helia-4	1939 *Landau* teorie supratekutosti
	1951 *H. London* rozpouštěcí refrigerátor		1947 *Bogoljubov* teorie supratekutosti
μK	1956 *Kurti* NDR (jaderná …)	1972 *Osheroff* supratekutost Helia-3	
	1985 *Hänsch* laserové chlazení (princip)	1986 *Müller a Bednorz* vysokoteplot. supravodivost	1956 *BCS* * teorie supravodivosti
			1975 *Leggett* teorie supratekutosti Helia-3
nK		1995 *Wieman, … Ketterle* BEC v atomových parách	
pK			

**Bardeen, Cooper a Schrieffer*

Naše hlavní téma

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pokrok na logaritmické škále

**Bardeen, Cooper a Schrieffer*

Chlazení jadernou adiabatickou demagnetisací

NDR nuclear demagnetization refrigeration

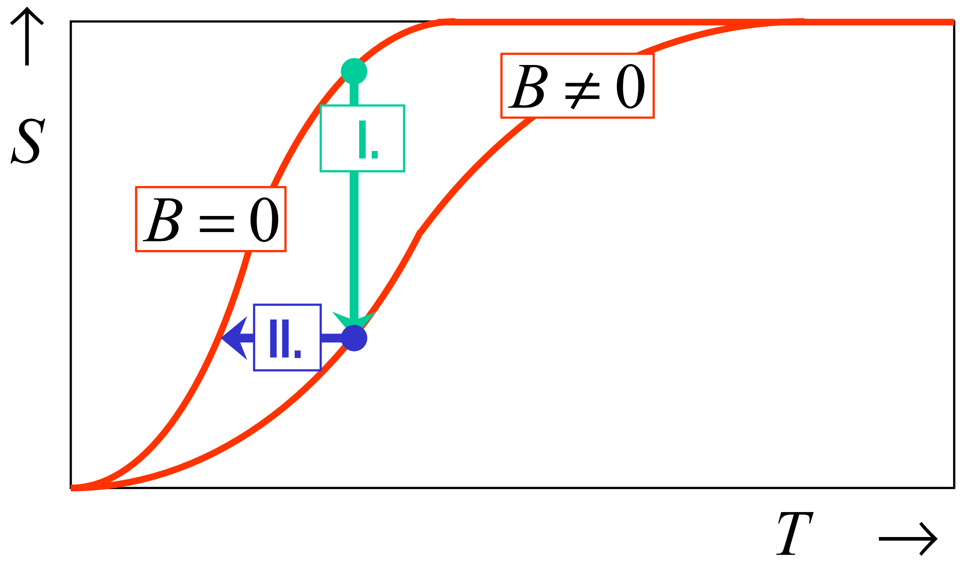
<u>pevná látka</u>	elektrony		T_e	
	jádra	mřížkové kmity	T_L	τ_L
				τ_{LS}
		jaderné spiny	T_S	τ_S

V rovnováze se teploty všech podsystémů vyrovnají.

Spin-mřížková relaxace je pomalá!

Můžeme proto generovat nerovnovážnou velmi nízkou spinovou teplotu

Princip NDR



I. KROK ***izotermická magnetizace***

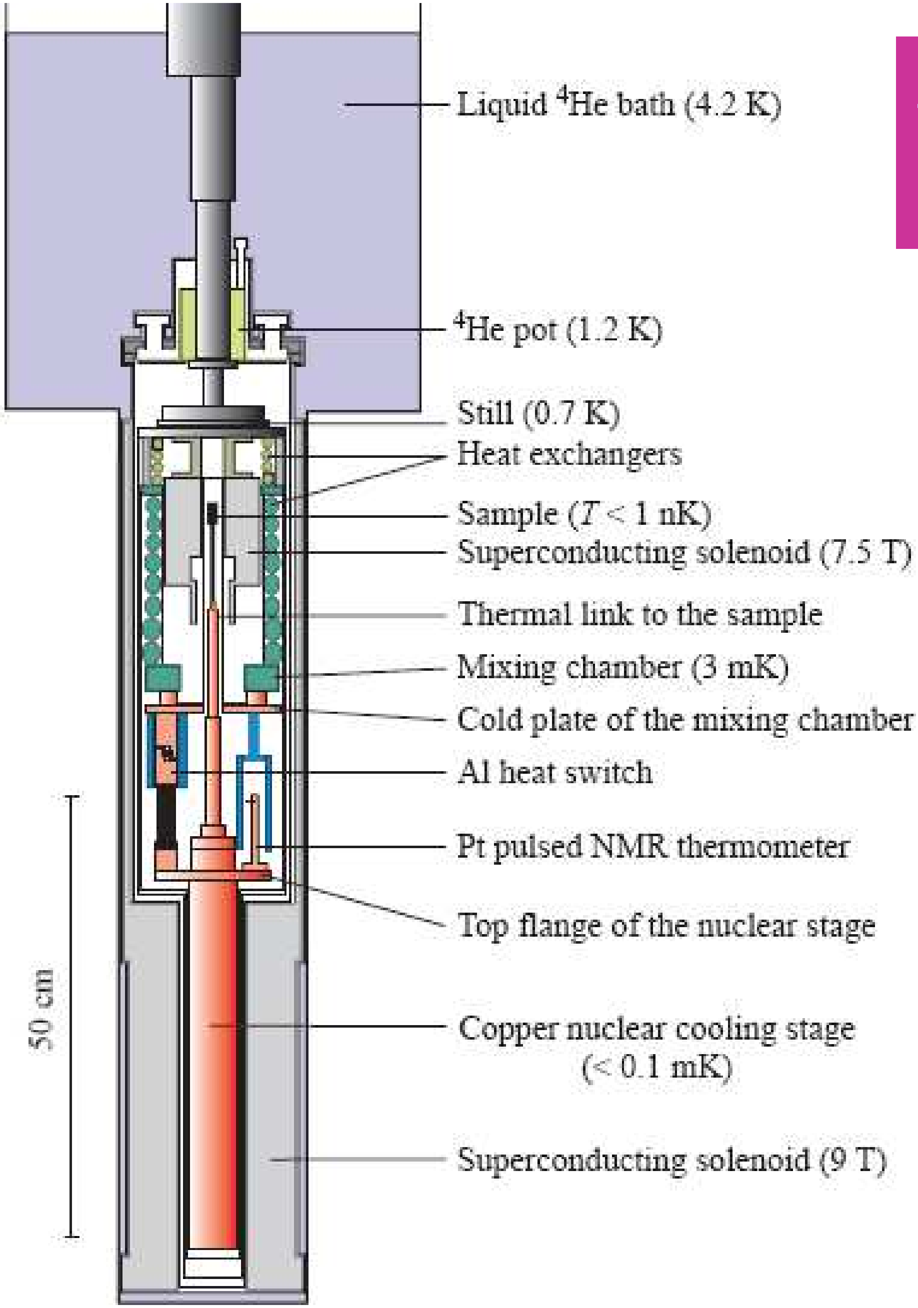
Entropie s magnetickým polem klesá

≡ snižuje se orientační neuspořádanost

II. KROK ***adiabatická demagnetizace***

Teplota a vnitřní energie klesají

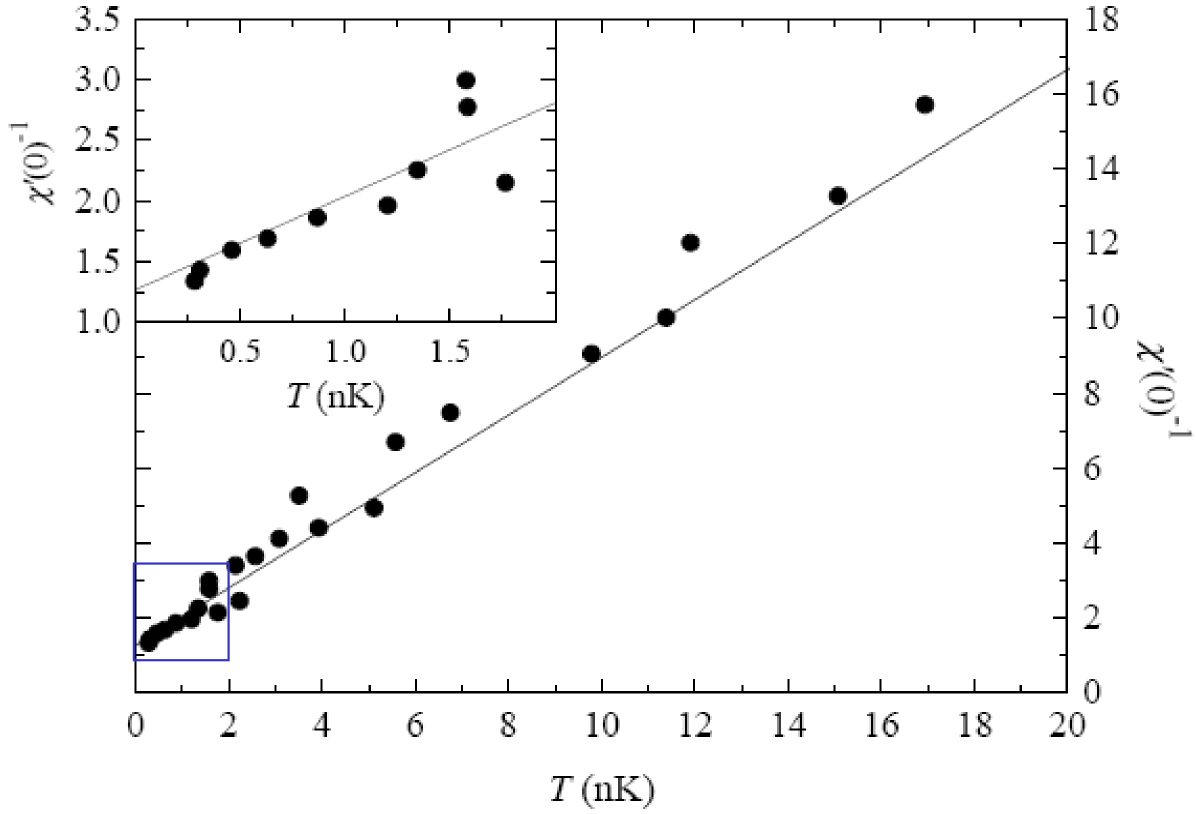
Kryostat, kde byla dosažena rekordní teplota 100 pK



Helsinki University of Technology
YKI, Low Temperature Group
2000

1. Předchlazení čerpáním helia 0,7 K
2. První stupeň: rozpouštěcí refrigerátor 3 mK
3. Druhý stupeň: NDR v mědi <0,1 mK
4. Třetí stupeň: NDR v samotném vzorku: monokrystal Rh <1 nK

Spinová magnetická susceptibilita monokrystalu rhodia



$$\chi'(0) = \frac{\lambda}{T-\theta},$$

$$\theta = -1.65 \text{ nK}$$

Curie-Weissův zákon jaderné spiny v rhodiu … antiferomagnetické uspořádání

↑↓↑↓↑↓↑↓↑↓↑↓↑↓


MILAN ODEHNAL
Supravodivost
a jiné
kvantové
jevy
CV
CESTA
K VĚDĚNÍ

Introductory matter on bosons

Bosons and Fermions (capsule reminder)

independent quantum postulate

Identical particles are indistinguishable

Bosons and Fermions (capsule reminder)

independent quantum postulate

Identical particles are **indistinguishable**

Bosons and Fermions (capsule reminder)

independent quantum postulate

Identical particles are **indistinguishable**

Permuting particles does not lead to a different state

Two particles

$$\Psi(x_1, x_2) \rightarrow \Psi(x_2, x_1) = \lambda \Psi(x_1, x_2)$$

Bosons and Fermions (capsule reminder)

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$$\boxed{\lambda^2 = 1}$$

$\lambda = -1$	$\lambda = +1$
fermions	**bosons**
antisymmetric Ψ	symmetric Ψ
half-integer spin	integer spin

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comes from nowhere "empirical fact"

everybody knows *our present concern*

Bosons and Fermions (capsule reminder)

Independent particles (… non-interacting)

basis of single-particle states (α complete set of quantum numbers)

$$\{|\alpha\rangle\} \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta} \quad |\psi\rangle = \sum |\alpha\rangle\langle\alpha|\psi\rangle$$

$$\langle x|\alpha\rangle = \varphi_\alpha(x)$$

Bosons and Fermions (capsule reminder)

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FOCK SPACE space of many particle states

basis states … symmetrized products of single-particle states for bosons

… antisymmetrized products of single-particle states for fermions

specified by the set of **occupation numbers** **0, 1, 2, 3, …** for bosons

0, 1 **…** for fermions

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$$\{\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_p, \ldots\}$$

$$\Psi_{\{n_\alpha\}} = \left| n_1, n_2, n_3, \ldots, n_p, \ldots \right\rangle \quad n\text{-particle state} \quad n = \Sigma n_p$$

Bosons and Fermions (capsule reminder)

Representation of occupation numbers (basically, *second quantization*)

…. for **fermions**

Pauli principle

fermions keep apart – as sea-gulls

$$\{\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_p, \ldots\}$$

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$$| 0 \rangle = | 0, 0, 0, \ldots, 0, \ldots \rangle \quad 0\text{-particle state} \quad \textbf{vacuum}$$

$$| 1_p \rangle = | 0, 0, 0, \ldots, 1, \ldots \rangle \quad 1\text{-particle} \quad \varphi_{\alpha_p}(x)$$

$$| \cdots \rangle = | 0, 1, 1, \ldots, 0, \ldots \rangle \quad 2\text{-particle} \quad \left(\varphi_{\alpha_1}(x)\varphi_{\alpha_2}(x') - \varphi_{\alpha_1}(x')\varphi_{\alpha_2}(x)\right)/\sqrt{2}$$

$$| \cdots \rangle = | 0, 2, 0, \ldots, 0, \ldots \rangle \quad 2\text{-particle} \quad \varphi_{\alpha_1}(x)\varphi_{\alpha_1}(x') \text{ (crossed out) not allowed}$$

$$| F \rangle = | \underbrace{1, 1, \ldots, 1}_{N}, 0, \ldots \rangle \quad N\text{-particle ground state}$$

…

Bosons and Fermions (capsule reminder)

Representation of occupation numbers (basically, *second quantization*)
…. for **bosons**

princip identity

bosons prefer to keep close – like monkeys

$$\{\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_p, \ldots\}$$

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$$\left| \cdots \right\rangle = \left| 0, 1, 1, \ldots, 0, \ldots \right\rangle \quad 2\text{-particle} \quad \left(\varphi_{\alpha_1}(x)\varphi_{\alpha_2}(x') + \varphi_{\alpha_1}(x')\varphi_{\alpha_2}(x) \right) / \sqrt{2}$$

$$\left| \cdots \right\rangle = \left| 0, 2, 0, \ldots, 0, \ldots \right\rangle \quad 2\text{-particle} \quad \varphi_{\alpha_1}(x)\varphi_{\alpha_1}(x')$$

$$\left| B \right\rangle = \left| N, 0, 0, \ldots, 0, \ldots \right\rangle \quad N\text{-částicový základní stav}$$

all on a single orbital

$$\varphi_{\alpha_1}(x_1)\varphi_{\alpha_1}(x_2)\cdots\varphi_{\alpha_1}(x_N)$$

Examples of bosons

bosons

simple particles
N not conserved

elementary particles

photons

quasi particles

phonons
magnons

complex particles
N conserved

atoms

^{4}He, $\underbrace{^{7}Li,\ ^{23}Na,\ ^{87}Rb}_{\text{alkali metals}}$

excited atoms

Examples of bosons (extension of the table)

bosons

simple particles
N not conserved

elementary particles

photons

quasi particles

phonons
magnons

composite quasi particles

excitons
Cooper pairs

complex particles
N conserved

atoms

^{4}He, $\underbrace{^{7}\text{Li},\ ^{23}\text{Na},\ ^{87}\text{Rb}}_{\text{alkali metals}}$

excited atoms

ions

molecules

Digression: How a complex particle, like an atom, can behave as a single whole, a boson

ESSENTIAL CONDITION

the identity includes characteristics like mass of charge, but also the values of observables corresponding to internal degrees of freedom, which **are not allowed to vary during the dynamical processes in question.**

Digression: How a complex particle, like an atom, can behave as a single whole, a boson

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$^{23}_{11}\text{Na}$	$^{87}_{37}\text{Rb}$
$[\mathrm{Ne}]3s^1$	$[\mathrm{Kr}]5s^1$
$\boldsymbol{^2S_{\frac{1}{2}}}$	$\boldsymbol{^2S_{\frac{1}{2}}}$
$I=\frac{3}{2}$	$I=\frac{3}{2}$

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$^2\boldsymbol{S}_{\frac{1}{2}}$	$^2\boldsymbol{S}_{\frac{1}{2}}$
$I = \frac{3}{2}$	$I = \frac{3}{2}$

Rubidium

37 electrons — *total electron spin* $S = \frac{1}{2}$

37 protons, 50 neutrons — *total nuclear spin* $I = \frac{3}{2}$

total spin of the atom

$$\vec{F} = \vec{S} + \vec{I}$$

$$F = |S - I|, \ldots, S + I = 1, 2$$

Two distinguishable species coexist; can be separated by joint effect of the hyperfine interaction and of the Zeeman splitting in a magnetic field

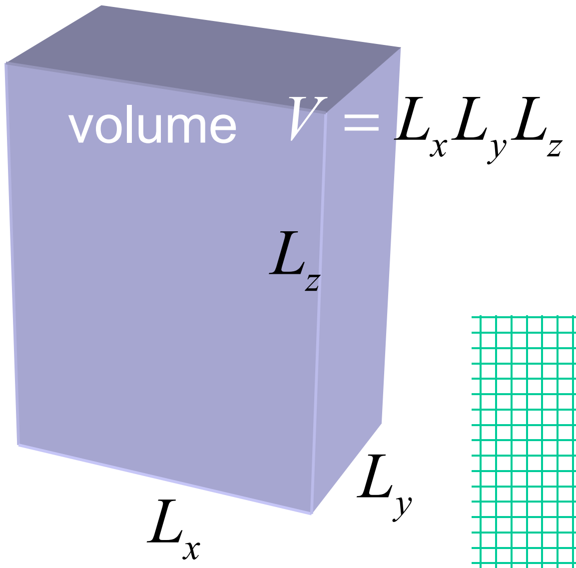
Plane waves in a cavity

Plane wave in classical terms and its quantum transcription

$$X = X_0 \mathrm{e}^{-\mathrm{i}(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})}, \quad \omega = \omega(k), \quad \lambda = 2\pi / k$$

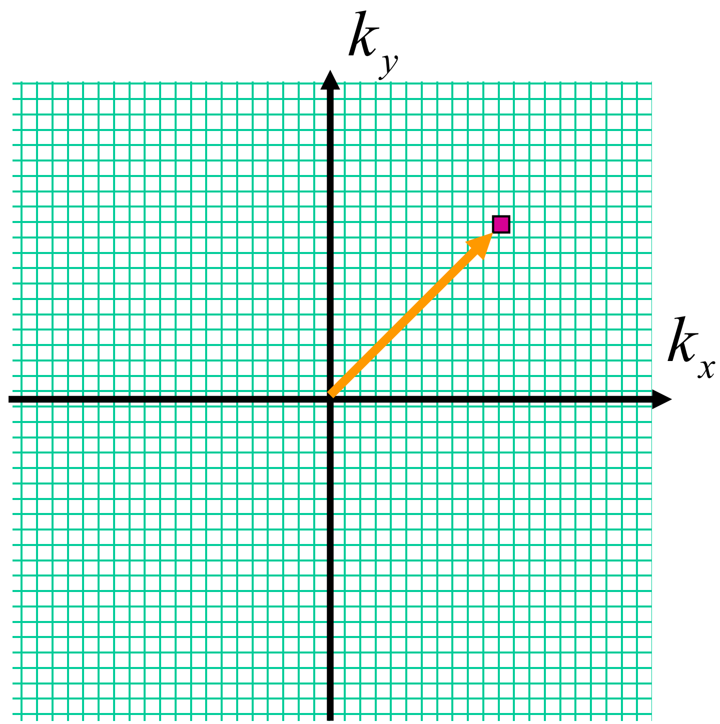
$$\varepsilon = \hbar\omega, \quad \boldsymbol{p} = \hbar\boldsymbol{k}, \quad \varepsilon = \varepsilon(p), \quad \lambda = h/p$$ de Broglie wavelength

Discretization ("quantization") of wave vectors in the cavity



periodic boundary conditions

$$\begin{cases} k_{x\ell} = \dfrac{2\pi}{L_x}\cdot \ell, \\ k_{ym} = \dfrac{2\pi}{L_x}\cdot m, \\ k_{zn} = \dfrac{2\pi}{L_x}\cdot n \end{cases}$$



Cell size (per ***k*** vector)

$$\Omega_k = (2\pi)^d / V$$

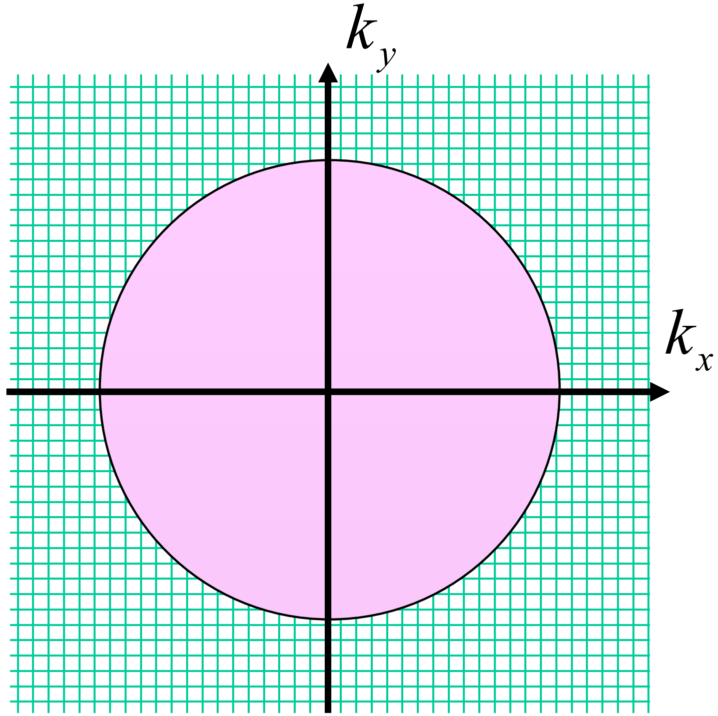
Cell size (per ***p*** vector)

$$\Omega_p = h^d / V$$

In the (***r, p***)-phase space

$$\hbar^d \Omega_k V = h^d$$

Density of states



IDOS Integrated Density Of States:

How many states have energy less than ε

Invert the dispersion law

$$\varepsilon(p) \quad \square \quad p(\varepsilon)$$

Find the volume of the *d*-sphere in the *p*-space

$$\Omega_d(p) = C_d \cdot p^d$$

Divide by the volume of the cell

$$\Gamma(\varepsilon) = \Omega_d(p(\varepsilon)) / \Omega_p = V \cdot \Omega_d(p(\varepsilon)) / h^d$$

DOS Density Of States:

How many states are around ε per unit energy per unit volume

$$\boxed{\mathcal{D}(\varepsilon) = \frac{1}{V}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Gamma(\varepsilon)}$$

$$= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Omega_d(p(\varepsilon)/h)^d = dC_d h^{-1} \cdot (p(\varepsilon)/h)^{d-1} \frac{\mathrm{d}\,p(\varepsilon)}{\mathrm{d}\varepsilon}$$

Ideal quantum gases at a finite temperature

$$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$$ Boltzmann distribution

high temperatures, dilute gases

Ideal quantum gases at a finite temperature

$$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$$ Boltzmann distribution

high temperatures, dilute gases

fermions

bosons

N

N

FD

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1}$$

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}-1}$$

BE

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta\varepsilon}-1}$$

Ideal quantum gases at a finite temperature

$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$ Boltzmann distribution

high temperatures, dilute gases

fermions — N — FD

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1}$$

$T \to 0$

$$|F\rangle = |1, 1, \ldots, 1, 0, \ldots\rangle$$

bosons — N — BE

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}-1}$$

$T \to 0$

$$|B\rangle = |N, 0, 0, \ldots, 0, \ldots\rangle$$

bosons

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta\varepsilon}-1}$$

$T \to 0$

$$|\mathrm{vac}\rangle$$

Ideal quantum gases at a finite temperature

$$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$$ Boltzmann distribution

high temperatures, dilute gases

fermions

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N

N

FD

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)} + 1}$$

BE

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)} - 1}$$

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta\varepsilon} - 1}$$

$T \to 0$

$T \to 0$

$T \to 0$

freezing out

$$|F\rangle = |1\,,1\,,\ldots,1\,,\,0\,,\ldots\rangle$$

$$|B\rangle = |N\,,0\,,0\,,\ldots,0\,,\ldots\rangle$$

$$|\mathrm{vac}\rangle$$

Ideal quantum gases at a finite temperature

$$\langle n \rangle = \mathrm{e}^{-\beta(\varepsilon-\mu)}$$ Boltzmann distribution

high temperatures, dilute gases

fermions

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FD

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1}$$

$T \to 0$

$$|F\rangle = |1, 1, \ldots, 1, 0, \ldots\rangle$$

bosons

N

BE

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu)}-1}$$

$T \to 0$

?

$$|B\rangle = |N, 0, 0, \ldots, 0, \ldots\rangle$$

$$\langle n \rangle = \frac{1}{\mathrm{e}^{\beta\varepsilon}-1}$$

$T \to 0$

freezing out

$$|\mathrm{vac}\rangle$$

The Planck formula for black-body radiation

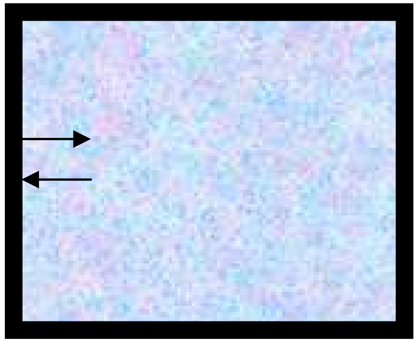
Equilibrium radiation in a cavity

Plane electromagnetic wave and its "photon" transcription

two polarizations

$$\boldsymbol{E} = E_0 \boldsymbol{s}\,\mathrm{e}^{-\mathrm{i}(\omega t - \boldsymbol{k}\boldsymbol{r})}, \quad \omega = ck, \quad \lambda = 2\pi / k$$

$$\varepsilon = \hbar\omega, \ \boldsymbol{p} = \hbar\boldsymbol{k}, \quad \varepsilon = cp, \quad \lambda = h/p = hc/\varepsilon$$



CAVITY

walls at temperature *T*

emit and absorb radiation

inside the cavity an equilibrium distribution of radiation … depends only on the temperature

ENERGY DENSITY PER UNIT VOLUME

$$\rho(T,\varepsilon) = 2 \cdot \varepsilon \cdot \langle n_\varepsilon \rangle \cdot \mathcal{D}(\varepsilon)$$

polarization photon energy population of a mode DOS

Planck formula

ENERGY DENSITY PER UNIT VOLUME

$$\rho(T,\varepsilon) = 2 \cdot \varepsilon \cdot \langle n_\varepsilon \rangle \cdot \mathcal{D}(\varepsilon)$$

polarization — photon energy — population of a mode — DOS

$$\langle n \rangle = \frac{1}{e^{\beta\varepsilon} - 1}$$

$$\mathcal{D}(\varepsilon) = \frac{4\pi}{c^3 h^3} \cdot \varepsilon^2$$

$$\frac{d}{d\varepsilon} W = \rho(T,\varepsilon) = \frac{8\pi}{c^3 h^3} \cdot \frac{\varepsilon^3}{e^{\beta\varepsilon} - 1}$$

PLANCK FOMULA IN THE STANDARD FORM:

$$\frac{d}{d\nu} W = \rho(T,\nu) = \frac{8\pi h}{c^3} \cdot \frac{\nu^3}{e^{\frac{h\nu}{k_B T}} - 1}$$

our final result

Stephan-Boltzmann law

ENERGY DENSITY PER UNIT VOLUME

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}W = \rho(T,\varepsilon) = \frac{8\pi}{c^3 h^3}\cdot\frac{\varepsilon^3}{\mathrm{e}^{\beta\varepsilon}-1}$$

TOTAL ENERGY PER UNIT VOLUME

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$W = \sigma T^4$ Stefan-Boltzmann law

$\sigma = \dfrac{8\pi^5 k_B^4}{15 c^3 h^3}$ universal constant

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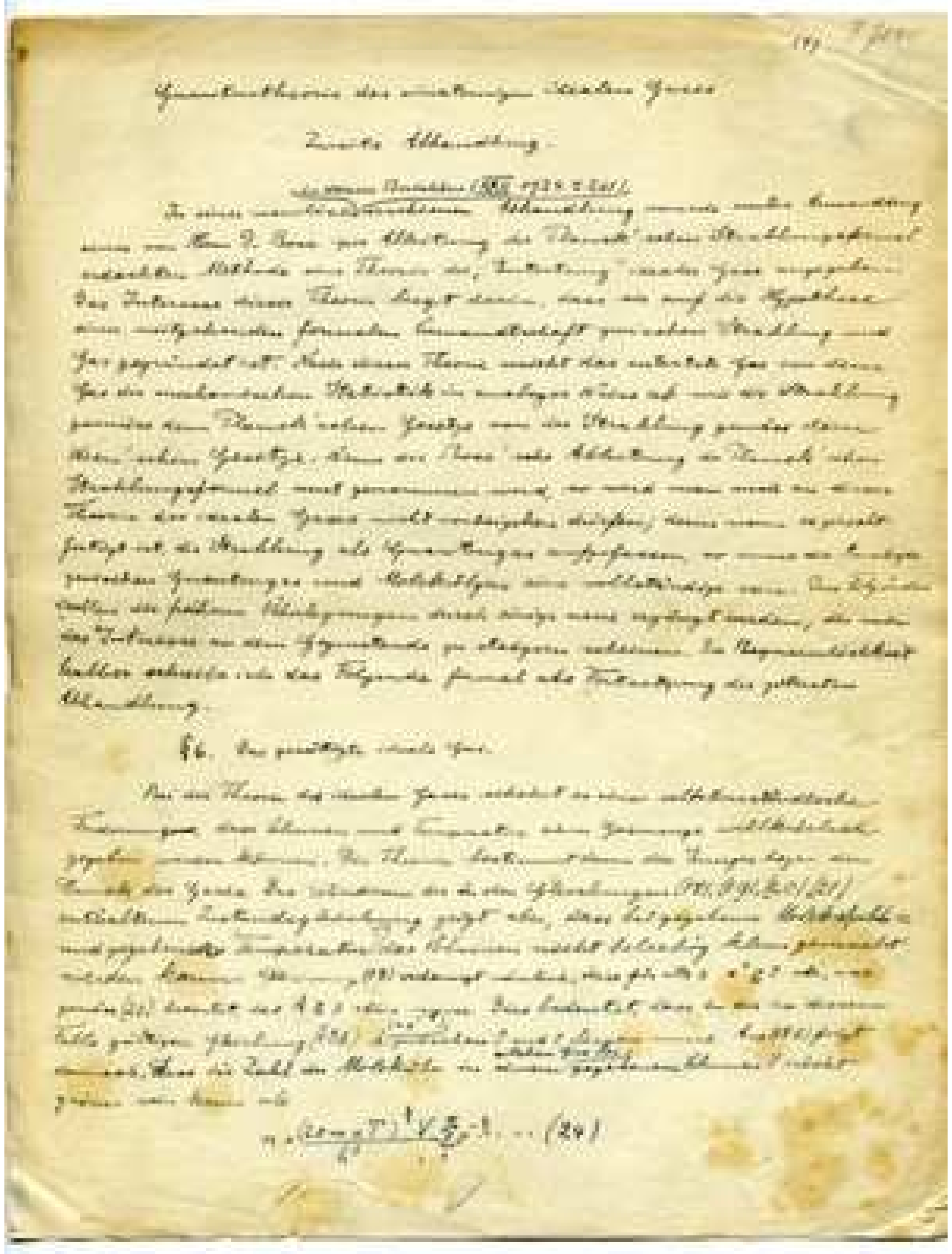
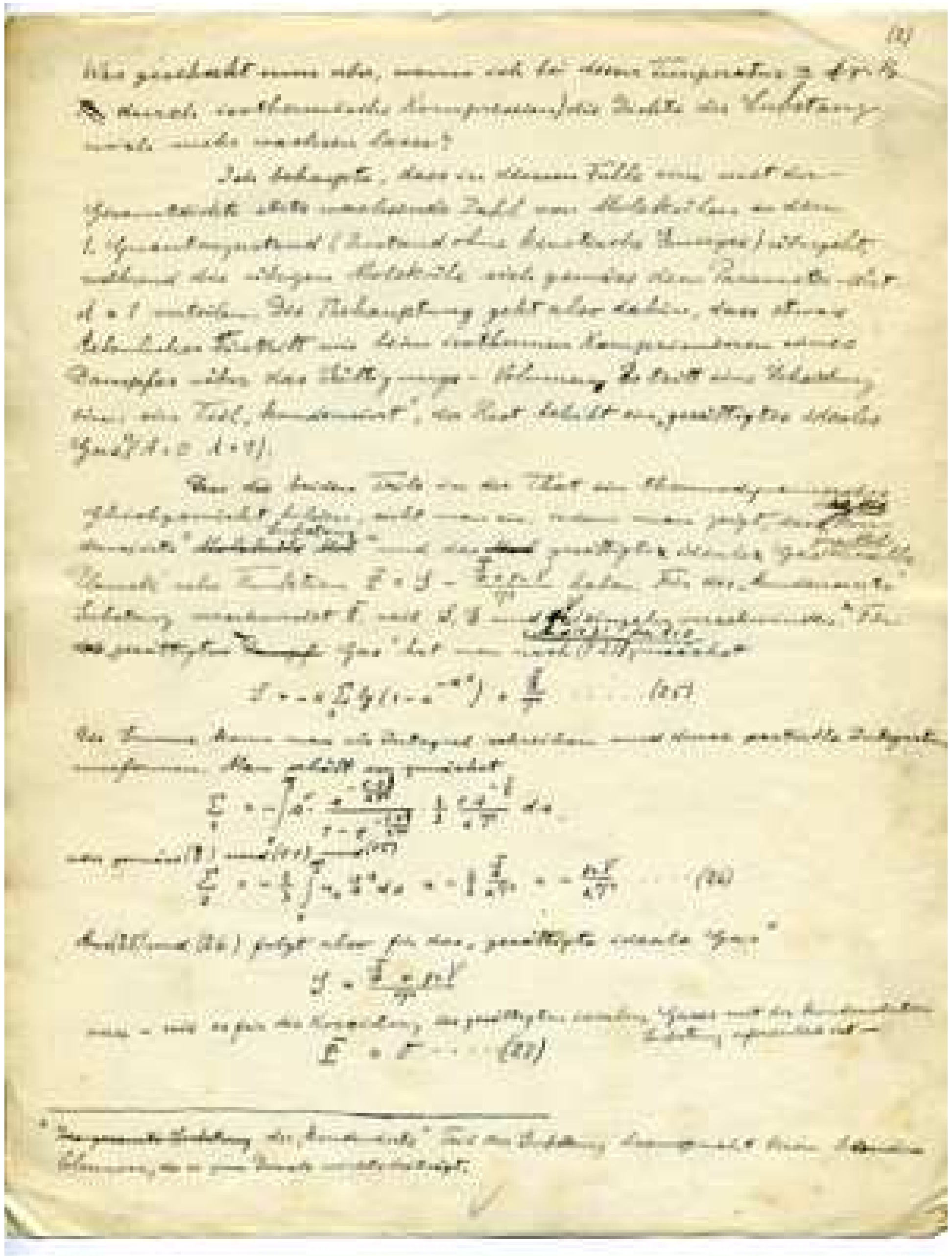
Black body radiation is at the cross-section of all three basic theories of modern physics

Bose-Einstein condensation: elementary approach

Einstein's manuscript with the derivation of BEC





What is the nature of BEC?

With lowering the temperature, the atoms of the gas lose their energy and drain down to the lowest energy states. There is less and less of these:

$$\mathcal{N}(E < k_B T) = \text{const} \times T^{3/2}$$

A given amount N of the atoms becomes too large starting from a critical temperature.

Their excess precipitates to the lowest level, which becomes *macroscopically occupied,* i.e., it holds a finite fraction of all atoms.

This is the BE condensate.

At the zero temperature, all atoms are in the condensate.

Einstein was the first to realize that and to make an exact calculation of the integrals involved.

$$\boxed{\tilde{\mathcal{N}}_{\mathrm{G}}(T) = V \times 4\pi \left(\frac{2mk_B T}{h^2} \right)^{\frac{3}{2}} \Gamma(\tfrac{3}{2}) \zeta(\tfrac{3}{2}) \equiv B T^{\frac{3}{2}}}$$

A gas with a fixed average number of atoms

Ideal boson gas (macroscopic system)

atoms: mass m, dispersion law $\varepsilon(p) = \dfrac{p^2}{2m}$

system as a whole:

volume V, particle number N, density $n=N/V$, temperature T.

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Always $\mu < 0$. At high temperatures, in the thermodynamic limit, the continuum approximation can be used:

$$N \approx V \int_0^\infty d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon) \equiv \tilde{\mathcal{N}}(T, \mu)$$

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It holds

$$\tilde{\mathcal{N}}(T,\mu<0) < \tilde{\mathcal{N}}(T,0) < \infty$$

For each temperature, we get a critical number of atoms the gas can accommodate. Where will go the rest?

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For each temperature, we get a critical number of atoms the gas can accommodate. Where will go the rest? To the condensate

Condensate concentration

The integral is doable:

$$\tilde{\mathcal{N}}(T,0) = V\int_0^\infty \mathrm{d}\varepsilon \frac{1}{\mathrm{e}^{\beta\varepsilon}-1}\mathcal{D}(\varepsilon)$$

use the general formula

$$= V\,4\pi\left(\frac{2mk_BT}{h^2}\right)^{\frac{3}{2}}\Gamma(\tfrac{3}{2})\zeta(\tfrac{3}{2})$$

$\sqrt{\pi}/2$

Riemann function

$$= V\left(2\pi\frac{2mk_BT}{h^2}\right)^{\frac{3}{2}}\cdot 2{,}612$$

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CRITICAL TEMPERATURE

the lowest temperature at which all atoms are still accomodated in the gas:

$$\tilde{\mathcal{N}}(T_c,0) = N$$

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atomic mass

$$T_c = \frac{h^2}{4\pi mk_B}\cdot\left(\frac{N}{2,612V}\right)^{\frac{2}{3}} = 0,52725\frac{h^2}{4\pi uk_B}\cdot\frac{n^{\frac{2}{3}}}{M} = 8,0306\times10^{-19}\cdot\frac{n^{\frac{2}{3}}}{M}$$

Condensate concentration

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A few estimates:

system	M	n	T_C
He liquid	4	2×10^{28}	1.47 K
Na trap	23	2×10^{20}	1.19 μK
Rb trap	87	2×10^{17}	3.16 nK

Digression: simple interpretation of T_C

Rearranging the formula for critical temperature

$$T_c = \frac{h^2}{4\pi m k_B} \cdot \left(\frac{N}{2,612 V} \right)^{\frac{2}{3}}$$

we get

$$\left(\frac{V}{N} \right)^{\frac{1}{3}} \approx \frac{h}{\sqrt{m k_B T_c}}$$

mean interatomic distance

thermal de Broglie wavelength

The quantum breakdown sets on when

the wave clouds of the atoms start overlapping

de Broglie wave length for atoms and molekules

$$\lambda = \frac{2\pi\hbar}{p}$$

Thermal energies small … NR formulae valid:

$$\lambda = \frac{2\pi\hbar}{\sqrt{2mE_{\text{kin}}}}$$

$m = A\text{u}$

… at. (mol.) mass

At thermal equilibrium

$$\langle E_{\text{kin}} \rangle = \tfrac{3}{2} k_B T$$

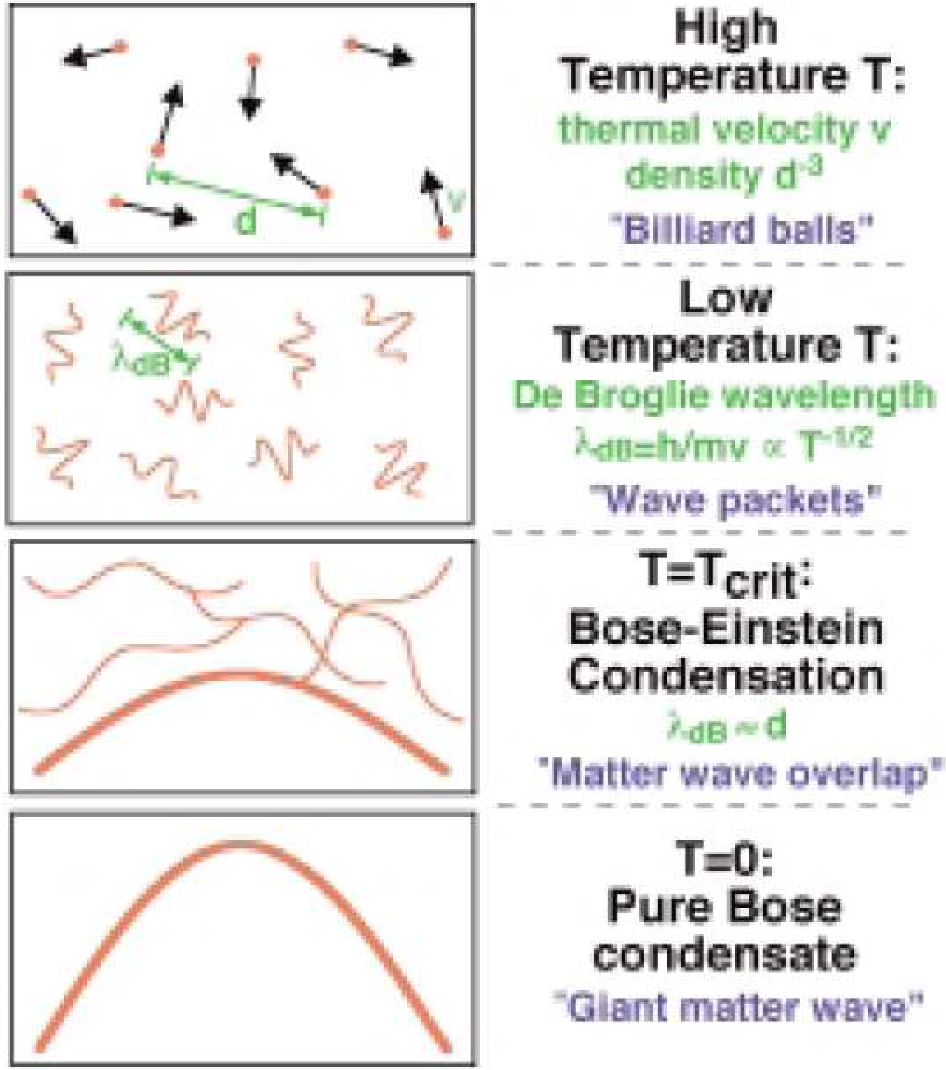
thermal wave length

$$\lambda = \frac{2\pi\hbar}{\sqrt{3\text{u}\, k_B}} \cdot \frac{1}{\sqrt{AT}} = 2{,}5\times 10^{-9} \cdot \frac{1}{\sqrt{AT}}$$

Two useful equations

$$E_{\text{kin}} = \tfrac{3}{2} T / 11600 \quad \text{eV} \quad \text{K} \qquad \bar{v} = \sqrt{\langle v^2 \rangle} = 158\sqrt{\frac{T}{A}}$$

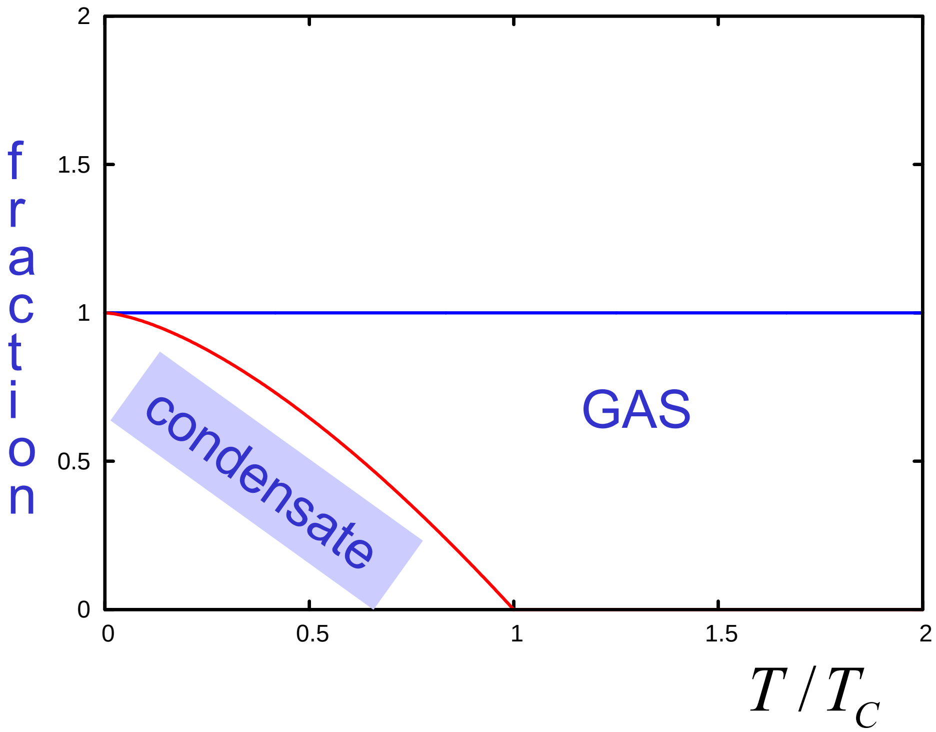
Ketterle explains BEC to the King of Sweden



Condensate concentration

$$n_G = \frac{\tilde{\mathcal{N}}(T_C,0)}{V} = B\,T^{\frac{3}{2}} = n\left(\frac{T}{T_C}\right)^{\frac{3}{2}} \quad \text{for} \quad T < T_C$$

$$n \equiv n_G + n_{BE} = n\left(\frac{T}{T_C}\right)^{\frac{3}{2}} + n\left[1-\left(\frac{T}{T_C}\right)^{\frac{3}{2}}\right]$$



Where are the condensate atoms?

ANSWER: On the lowest one-particle energy level

For understanding, return to the discrete levels.

$$N = \mathcal{N}(T, \mu) = \sum_j \langle n(\varepsilon_j) \rangle = \sum_j \frac{1}{e^{\beta(\varepsilon_j - \mu)} - 1}$$

There is a sequence of energies

$$\mu < \varepsilon_0 = \varepsilon(\vec{0}) = 0 < \varepsilon_1 < \varepsilon_2 \cdots$$

For very low temperatures, $\beta(\varepsilon_1 - \varepsilon_0) \gg 1$

all atoms are on the lowest level, so that

$$n_0 = N - O(e^{-\beta(\varepsilon_1 - \varepsilon_0)})$$ all atoms are in the condensate

$$N \approx \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1}$$ connecting equation

$$\mu \approx \varepsilon_0 - \frac{k_B T}{N}$$ chemical potential is zero on the gross energy scale

Where are the condensate atoms? Continuation

ANSWER: On the lowest one-particle energy level

For temperatures below T_C

all condensate atoms are on the lowest level, so that

$$n_0 = N_{BE}$$ all condensate atoms remain on the lowest level

$$N_{BE} \approx \frac{1}{\mathrm{e}^{\beta(\varepsilon_0 - \mu)} - 1}$$ connecting equation

$$\mu \approx \varepsilon_0 - \frac{k_B T}{N_{BE}}$$ chemical potential keeps zero on the gross energy scale

question … what happens with the occupancy of the next level now?

Estimate:

$$\varepsilon_1 - \varepsilon_0 \sim \left(h^2 / m\right) \cdot V^{-\frac{2}{3}}$$

$$n_0 = \frac{k_B T}{\varepsilon_0 - \mu} = O(V), \quad n_1 = \frac{k_B T}{\varepsilon_1 - \mu} = O(V^{\frac{2}{3}})$$ .... much slower growth

Where are the condensate atoms? Summary

ANSWER: On the lowest one-particle energy level

The final balance equation for $T < T_C$ is

$$N = \mathcal{N}(T, \mu) = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} + V \int_0^\infty d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon)$$

LESSON:

be slow with making the thermodynamic limit (or any other limits)

Closer look at BEC

- Thermodynamically, this is a real phase transition, although unsual

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- BEC is a "condensation in the momentum space", unlike the usual liquefaction of classical gases, which gives rise to droplets in the coordinate space.
- This is somewhat doubtful, especially now, that the best observed BEC takes place in traps, where the atoms are significantly localized
- What is valid on the "momentum condensation": BEC gives rise to quantum coherence between very distant places, just like the usual plane wave

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- What is valid on the "momentum condensation": BEC gives rise to quantum coherence between very distant places, just like the usual plane wave
- BEC is a **macroscopic quantum phenomenon** in two respects:

  ♠ it leads to a correlation between a macroscopic fraction of atoms

  ♠ the resulting coherence pervades the whole macroscopic sample

Off-Diagonal Long Range Order

Analysis on the one-particle level

Coherence in BEC: ODLRO

***O**ff-**D**iagonal Long Range Order*

Without field-theoretical means, the coherence of the condensate may be studied using the **one-particle density matrix.**

Definition of OPDM for non-interacting particles: Take an additive observable, like local density, or current density. Its average value for the whole assembly of atoms in a given equilibrium state:

$$\langle X \rangle = \sum_{\alpha} \langle \alpha | X | \alpha \rangle \langle n_{\alpha} \rangle \quad \text{double average, quantum and thermal}$$

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$$= \operatorname{Tr} \rho X \qquad \rho = \sum_{\alpha} | \alpha \rangle \langle n_{\alpha} \rangle \langle \alpha |$$

OPDM for homogeneous systems

In coordinate representation

$$\rho(\boldsymbol{r},\boldsymbol{r}') = \sum_{\boldsymbol{k}} \langle \boldsymbol{r} | \boldsymbol{k} \rangle \langle n_{\boldsymbol{k}} \rangle \langle \boldsymbol{k} | \boldsymbol{r}' \rangle$$

$$= \frac{1}{V} \sum_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')} \langle n_{\boldsymbol{k}} \rangle$$

- depends only on the relative position (transl. invariance)
- Fourier transform of the occupation numbers
- isotropic … provided thermodynamic limit is allowed
- in systems without condensate, the *momentum distribution* is smooth and the density matrix has a finite range.

CONDENSATE lowest orbital with $\boldsymbol{k}_0$

OPDM for homogeneous systems: ODLRO

CONDENSATE   lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')}\langle n_0\rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle}_{FT\text{ of a smooth function has a finite range}}$$

$$\equiv \rho_{\mathrm{BE}}(\boldsymbol{r}-\boldsymbol{r}') + \rho_{\mathrm{G}}(\boldsymbol{r}-\boldsymbol{r}')$$

OPDM for homogeneous systems: ODLRO

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DIAGONAL ELEMENT $\boldsymbol{r}=\boldsymbol{r}'$

$$\rho(\boldsymbol{0}) = \rho_{\mathrm{BE}}(\boldsymbol{0}) + \rho_{\mathrm{G}}(\boldsymbol{0})$$

$$= n_{\mathrm{BE}} + n_{\mathrm{G}}$$

OPDM for homogeneous systems: ODLRO

CONDENSATE lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')}\langle n_0\rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle}_{FT \text{ of a smooth function has a finite range}}$$

$$\equiv \rho_{\mathrm{BE}}(\boldsymbol{r}-\boldsymbol{r}') \quad + \rho_{\mathrm{G}}(\boldsymbol{r}-\boldsymbol{r}')$$

DIAGONAL ELEMENT $\boldsymbol{r} = \boldsymbol{r}'$

$$\rho(\boldsymbol{0}) = \rho_{\mathrm{BE}}(\boldsymbol{0}) \quad + \rho_{\mathrm{G}}(\boldsymbol{0})$$

$$= n_{\mathrm{BE}} \quad + n_{\mathrm{G}}$$

DISTANT OFF-DIAGONAL ELEMENT $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$

$$\rho_{\mathrm{BE}}(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} n_{\mathrm{BE}}$$

$$\rho_{\mathrm{G}}(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} 0$$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') \xrightarrow{|\boldsymbol{r}-\boldsymbol{r}'|\to\infty} n_{\mathrm{BE}}$$

Off-Diagonal Long Range Order

ODLRO

From OPDM towards the macroscopic wave function

CONDENSATE lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')} \langle n_0 \rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V} \sum_{\boldsymbol{k} \neq \boldsymbol{k}_0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')} \langle n_{\boldsymbol{k}} \rangle}_{FT \text{ of a smooth function has a finite range}}$$

$$= \underbrace{\Psi(\boldsymbol{r})\Psi^*(\boldsymbol{r}')}_{\text{dyadic}} + \frac{1}{V} \sum_{\boldsymbol{k} \neq \boldsymbol{k}_0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')} \langle n_{\boldsymbol{k}} \rangle$$

MACROSCOPIC WAVE FUNCTION

$\Psi(\boldsymbol{r}) = \sqrt{n_{BE}} \cdot \mathrm{e}^{\mathrm{i}(\boldsymbol{k}_0 \boldsymbol{r} + \varphi)}$, $\varphi \ldots$ an arbitrary phase

- expresses ODLRO in the density matrix
- measures the condensate density
- appears like a pure state in the density matrix, but macroscopic
- expresses the notion that the condensate atoms are in the same state
- is the order parameter for the BEC transition

From OPDM towards the macroscopic wave function

CONDENSATE lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')}\langle n_0\rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle}_{FT \text{ of a smooth function has a finite range}}$$

$$= \underbrace{\Psi(\boldsymbol{r})\Psi^*(\boldsymbol{r}')}_{\text{dyadic}} + \frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle$$

MACROSCOPIC WAVE FUNCTION

$$\Psi(\boldsymbol{r}) = \sqrt{n_{BE}}\cdot\mathrm{e}^{\mathrm{i}(\boldsymbol{k}_0\boldsymbol{r}+\varphi)}, \quad \varphi \ldots \text{ an arbitrary phase}$$

- expresses ODLRO in the density matrix ✓
- measures the condensate density ✓
- appears like a pure state in the density matrix, but macroscopic ✓
- expresses the notion that the condensate atoms are in the same state
- is the order parameter for the BEC transition

From OPDM towards the macroscopic wave function

CONDENSATE lowest orbital with $\boldsymbol{k}_0 = O(V^{-\frac{1}{3}}) \approx 0$

$$\rho(\boldsymbol{r}-\boldsymbol{r}') = \underbrace{\frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_0(\boldsymbol{r}-\boldsymbol{r}')}\langle n_0\rangle}_{\text{coherent across the sample}} + \underbrace{\frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle}_{FT\text{ of a smooth function has a finite range}}$$

$$= \underbrace{\Psi(\boldsymbol{r})\Psi^*(\boldsymbol{r}')}_{\text{dyadic}} + \frac{1}{V}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}\langle n_{\boldsymbol{k}}\rangle$$

MACROSCOPIC WAVE FUNCTION

$\Psi(\boldsymbol{r}) = \sqrt{n_{BE}}\cdot\mathrm{e}^{\mathrm{i}(\boldsymbol{k}_0\boldsymbol{r}+\varphi)},\quad \varphi\ldots$ an arbitrary phase ? **why bother?**

- expresses ODLRO in the density matrix ✓
- measures the condensate density ✓
- appears like a pure state in the density matrix, but macroscopic ✓
- expresses the notion that the condensate atoms are in the same state ? **how?**
- is the order parameter for the BEC transition ? **what is it?**

F.Laloë: Do we really understand Quantum mechanics, Am.J.Phys.**69**, 655 (2001)

In passing, and as a side remark, it is amusing to notice that the recent observation of the phenomenon of Bose–Einstein condensation in dilute gases (Ref. 25) can be seen, in a sense, as a sort of realization of the initial hope of Schrödinger: This condensation provides a case where the many-particle matter wave does propagate in ordinary space. Before condensation takes place, we have the usual situation: The atoms belong to a degenerate quantum gas, which has to be described by wave functions defined in a huge configuration space. But, when they are completely condensed, they are restricted to a much simpler many-particle state that can be described by the same wave function, exactly as a single particle. In other words, the matter wave becomes similar to a classical field with two components (the real part and the imaginary part of the wave function), resembling an ordinary sound wave for instance. This illustrates why, somewhat paradoxically, the ''exciting new states of matter'' provided by Bose–Einstein condensates are not an example of an extreme quantum situation; they are actually more classical than the gases from which they originate (in terms of quantum description, interparticle correlations, etc.). Conceptually, of course, this remains a very special case and does not solve the general problem associated with a naive view of the Schrödinger waves as real waves.

The end

Problems

Some problems are expanding on the presented subject matter and are voluntary… (*)

The other ones are directly related to the theme of the class and are to be worked out within a week. The solutions will be presented on the next seminar and posted on the web.

(1.1*) Problems with metastable states and quasi-equilibria in defining the temperature and applying the 3rd law of thermodynamics

(1.2*) Relict radiation and the Boomerang Nebula

(1.3) Work out in detail the integral defining T_c

(1.4) Extend the resulting series expansion to the full balance equation (BE integral)

(1.5) Modify for a 2D gas and show that the BE condensation takes never place

(1.6) Obtain an explicit procedure for calculating the one-particle density matrix for an ideal boson gas [*difficult*]