Lecture 18

15.03.2018

Bose Einstein condensation

Bose-Einstein condensation

At a given temperature T, density ρ and chemical potential μ are related by the following equation

$$\rho(T,\mu) = \frac{1}{V}\frac{1}{\lambda^{-1}-1} + \Lambda^{-3}(T)\frac{2}{\sqrt{\pi}}\int_0^\infty dx\,\frac{x^{\frac{1}{2}}}{e^x-1}$$

$$\rho(T,\mu) = \rho_0(T,\mu) + \rho_{ex}(T,\mu) = \Lambda^{-3}(T)g_{\frac{3}{2}}(\lambda), \qquad \lambda = e^{\beta\mu}$$

Critical temperature for Bose Einstein condensation:

Determined by the density of the bose gas when $\mu = 0$

$$\boldsymbol{T_c(\rho) = \frac{h^2}{2\pi mk}\left(\frac{\rho}{\zeta\left(\frac{3}{2}\right)}\right)^{\frac{2}{3}}}$$

- $\boldsymbol{T \leq T_c}$: *Density is a mixture of condensed and normal gas*

$$\rho = \rho_0 + \rho_{ex} = \Lambda^{-3}(T_c)\zeta(3/2)$$

Below $\boldsymbol{T_c}$ **:**

A macroscopic fraction of particles condense into the ground state with the zero momentum

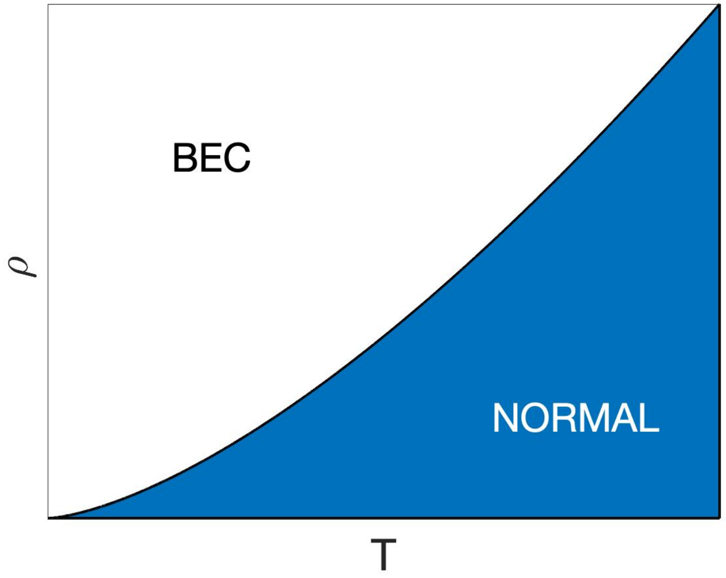
- ***Chemical potential*** $\boldsymbol{\mu = 0}$ ***remains zero for all temperatures below*** $\boldsymbol{T_c}$
- ***Excess density depends only on temperature and actually decreases with decreasing temperature***
- ***Ground state density becomes non-zero and increases with decreasing temperature***

Condensation in the momentum space means that particles becomes delocalized in space

- $\boldsymbol{T > T_c}$: *Density is that of the normal gas*

$$\rho(T,\mu) = \rho_{ex}(T,\mu) = \Lambda^{-3}(T)g_{\frac{3}{2}}(\lambda)$$

This equation determines the chemical potential $\boldsymbol{\mu(T,\rho)}$



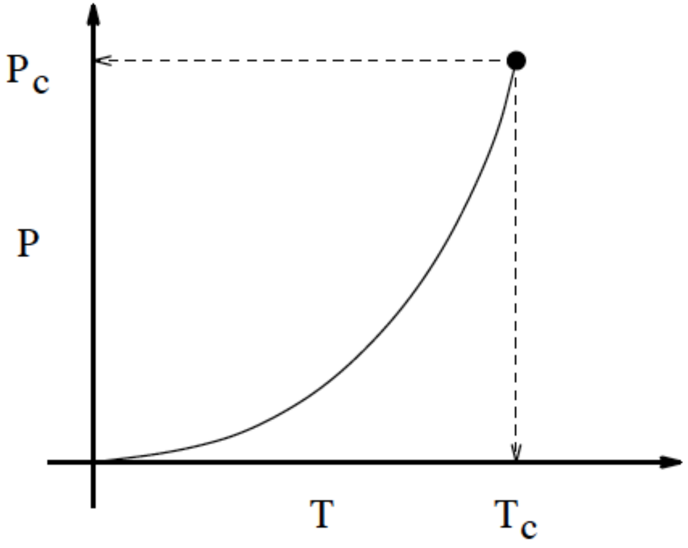
Equation of state

$$\frac{P}{kT} = -\frac{1}{V}\log(1-\lambda) - \frac{1}{\Lambda^3(T)}\frac{2}{\sqrt{\pi}}\int_0^\infty dx\, x^{\frac{1}{2}}\log(1-\lambda e^{-x})$$

$$=_{\lambda\le 1} -\frac{1}{V}\log(1-\lambda) + \frac{1}{\Lambda^3(T)}\sum_{n=1}^{\infty}\frac{\lambda^n}{n^{5/2}}$$

$$= \frac{1}{\Lambda^3(T)}g_{5/2}(\lambda) - \frac{1}{V}\log(1-\lambda)$$

$$\approx_{V\to\infty} \frac{1}{\Lambda^3(T)}g_{5/2}(\lambda)$$



$T \le T_c(\lambda = 1)$

$$\frac{P}{kT} = \frac{1}{\Lambda^3(T)}g_{5/2}(1) \to P(T) \sim T^{\frac{5}{2}}$$

The pressure becomes independent of density below T_c

Equation of state $T > T_c$

$$\frac{P}{kT} = -\frac{1}{V}\log(1-\lambda) - \frac{1}{\Lambda^3(T)}\frac{2}{\sqrt{\pi}}\int_0^\infty dx\, x^{\frac{1}{2}}\log(1-\lambda e^{-x})$$

$$=_{\lambda\leq 1} -\frac{1}{V}\log(1-\lambda) + \frac{1}{\Lambda^3(T)}\sum_{n=1}^{\infty}\frac{\lambda^n}{n^{5/2}}$$

$$= \frac{1}{\Lambda^3(T)}g_{5/2}(\lambda) - \frac{1}{V}\log(1-\lambda)$$

$$\approx \quad \frac{1}{\Lambda^3(T)}g_{5/2}(\lambda)$$

$T > T_c(\lambda < 1)$

$$\frac{P}{kT} = \frac{1}{\Lambda^3(T)}g_{5/2}(\lambda), \qquad \lambda = e^{\beta\mu(\rho,T)}$$

Classical limit: Chemical potential for $T \gg T_c$

The chemical potential is determined perturbatively from the density equation above T_c.

$$\rho = \frac{1}{\Lambda^3(T)} g_{3/2}(\lambda) \rightarrow \rho = \frac{1}{\Lambda^3(T)} \sum_{n=1}^{\infty} \frac{\lambda^n}{n^{3/2}} \rightarrow \frac{1}{\Lambda^3(T_c)} \zeta\left(\frac{3}{2}\right) = \frac{1}{\Lambda^3(T)} \sum_{n=1}^{\infty} \frac{\lambda^n}{n^{3/2}} \rightarrow$$

$$\zeta\left(\frac{3}{2}\right) = \left(\frac{T}{T_c}\right)^{3/2} \sum_{n=1}^{\infty} \frac{\lambda^n}{n^{3/2}}, \qquad T > T_c, \qquad \lambda = e^{\beta\mu}$$

Inverting the equation above we can determine the fugacity $\lambda(\rho, T)$:

$$\lambda\left(1 + 2^{-3/2}\lambda + \cdots\right) = \zeta\left(\frac{3}{2}\right)\left(\frac{T}{T_c}\right)^{-3/2},$$

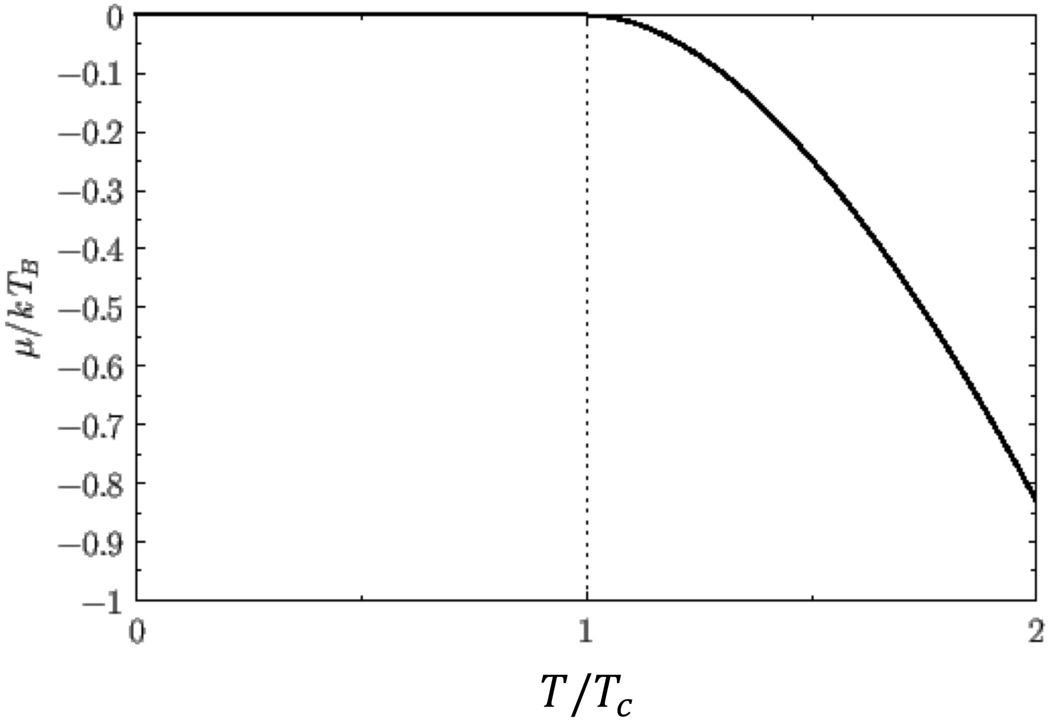
In the zeroth order, we recover the fugacity of the classical ideal gas

$$\lambda^{(0)} \approx \zeta\left(\frac{3}{2}\right)\left(\frac{T}{T_c}\right)^{-\frac{3}{2}} \rightarrow \mu = kT \ln\left[\zeta\left(\frac{3}{2}\right)\left(\frac{T}{T_c}\right)^{-\frac{3}{2}}\right]$$

Including the first correction to the classical limit

$$\lambda \approx \zeta\left(\frac{3}{2}\right)\left(\frac{T}{T_c}\right)^{-\frac{3}{2}}\left(1 - \zeta\left(\frac{3}{2}\right)\left(\frac{2T}{T_c}\right)^{-\frac{3}{2}}\right) \rightarrow$$

$$\mu = kT \ln\left[\zeta\left(\frac{3}{2}\right)\left(\frac{T}{T_c}\right)^{-\frac{3}{2}}\left(1 - \zeta\left(\frac{3}{2}\right)\left(\frac{2T}{T_c}\right)^{-\frac{3}{2}}\right)\right]$$



Equation of state for $T \gg T_c$

$$\frac{P}{kT} = \frac{1}{\Lambda^3(T)} g_{5/3}(\lambda) \approx \frac{1}{\Lambda^3(T)}\left(\lambda + 2^{-\frac{5}{2}}\lambda^2 + \cdots\right)$$

Using the expansion of the fugacity $\lambda \approx \rho\Lambda^3(T)\left(1 - 2^{-3/2}\rho\Lambda^3(T)\right)$

$$\frac{P}{kT} \approx \left(\rho - 2^{-\frac{3}{2}}\rho\Lambda^3(T) + 2^{-\frac{5}{2}}\rho\Lambda^3(T)\right)$$

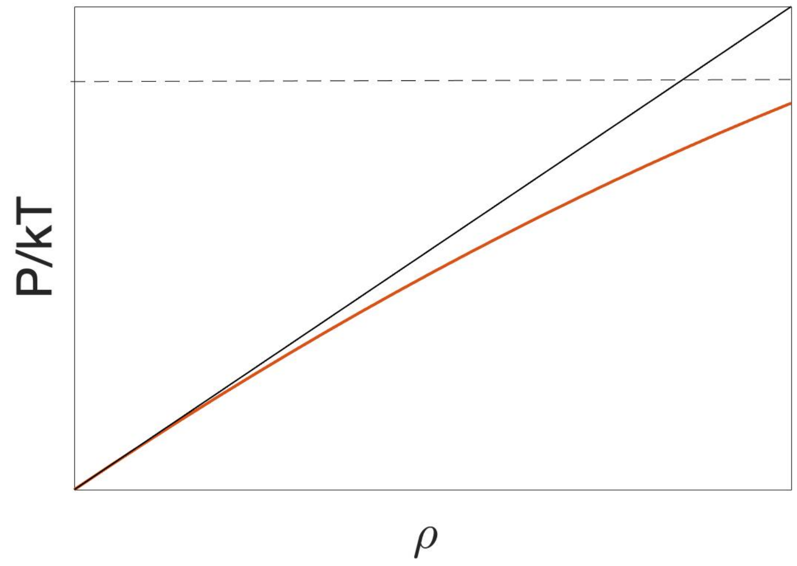
This looks like a virial expansion of the equation of state

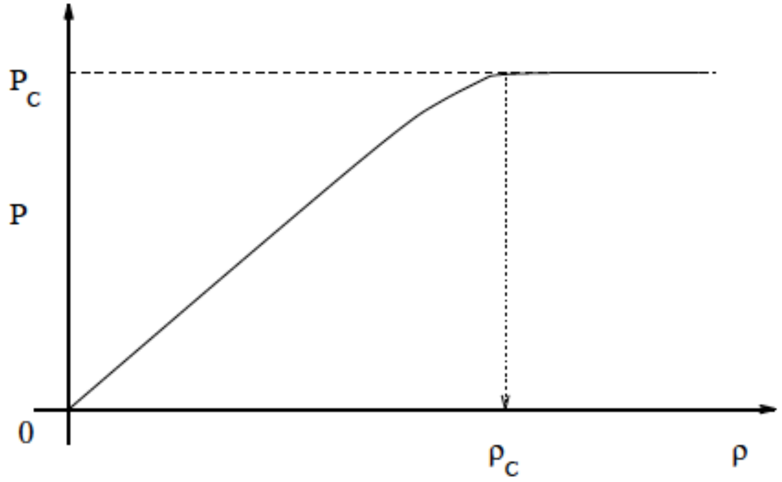
$$\frac{P}{kT} \approx \rho + B_2(T)\rho^2 + \cdots ,$$

With the second virial term

$$B_2(T) = \left(-\frac{1}{2\sqrt{2}} + \frac{1}{4\sqrt{2}}\right)\Lambda^3(T) = -\frac{1}{4\sqrt{2}}\Lambda^3(T) < 0$$

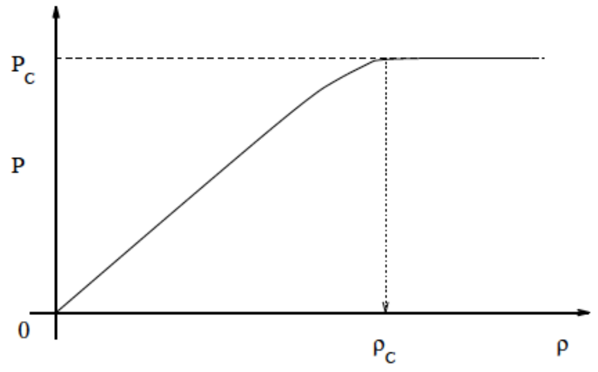
The Bose gas pressure is effectively lowered by statistical attraction forces

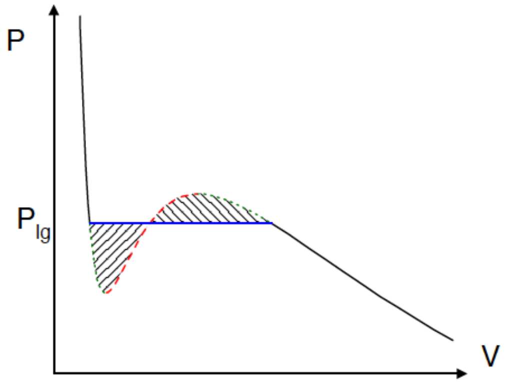




Bose Einstein condensation as a phase transition

- Classical ideal gas is reached is in the limit of very small density
- Pressure deviates from the classical law increasing the bose gas density
- At the critical point for the Bose-Einstein condensation (BEC), the gas density and the gas pressure have specific critical values
- Below the BEC, the gas pressure becomes independent of density.
- This is analogous to the liquid-gas phase transition, whereby the pressure becomes independent of the volume





Ideal Bose gases: Density of states in 2D

- Energy levels for particles on a flat domain of finite area $\mathrm{A} = L^2$:

$$\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 n^2,$$

The quantum state is given by $\psi_1 = e^{\frac{2\pi i}{L}\vec{n}\cdot\vec{r}}$, with $\vec{n} = (n_x, n_y)$

Number of quantum states between modes with n and $n + dn$:

$$D(n)dn = 2\pi n dn$$

Density of states corresponding to energy ϵ, is then

$$D_\epsilon(\epsilon) = D(n)\frac{dn}{d\epsilon} \rightarrow D(\epsilon) = \frac{Am}{2\,\pi\hbar^2}$$

In 2D, the density of states is independent of energy

Average density and chemical potential

- **In 2D:**

$$\rho^{(2D)}(\mu,T) = \frac{m}{2\,\pi\hbar^2}\int_0^\infty d\epsilon\,\frac{1}{e^{\beta(\epsilon-\mu)}-1} = -\frac{2\pi mkT}{h^2}\ln\!\left(1-e^{\beta\mu}\right)$$

$$\rho^{(2D)} = -\frac{1}{\Lambda^2(T)}\ln\!\left(1-e^{\beta\mu}\right)$$

Hence, the chemical potential as a function of density,

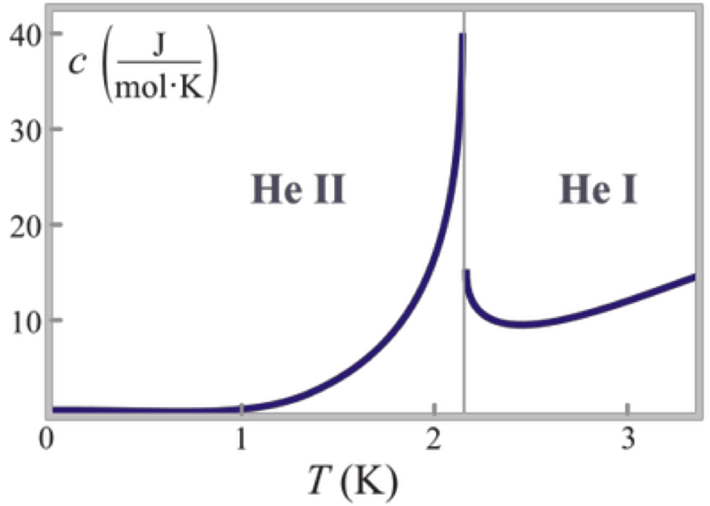
$$\mu^{(2D)}(T,\rho) = \; kT\log\left(1-e^{-\rho^{(2D)}\Lambda^2(T)}\right) < 0,$$

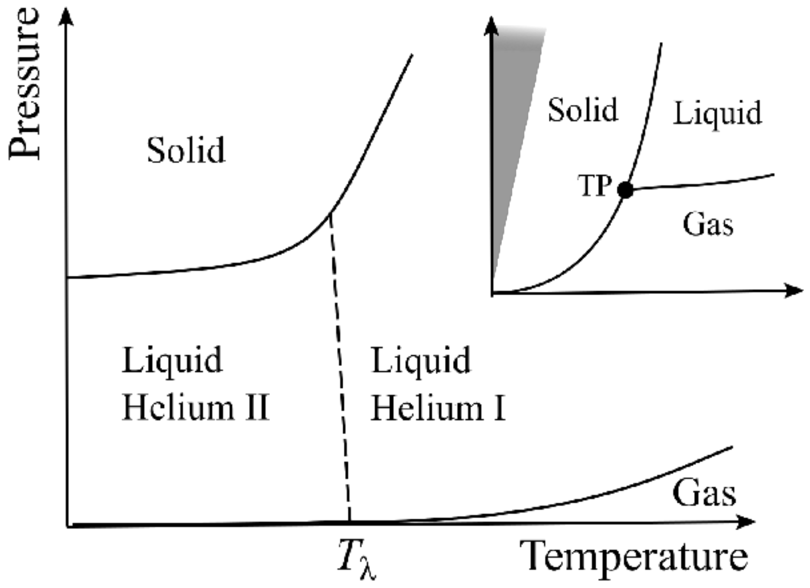
will never become zero for $T > 0$ and $\rho > 0$

This means: no Bose-Einstein condensation is expected for the *ideal* Bose gas in *two dimensions*!

Experimental realization: superfluid liquid He4

- Transition to a superfluid He4 happens at a critical temperature $T_c = 2.17K$.
- The ideal Bose gas prediction for the He^4 atoms is $T_c = 3.13K$.
- Details are however different, because the interaction potential is fairly strong, and not negligible as assumed in the ideal Bose gas.
- Superfluid He4 has a non-uniform density (higher density at the bottom of the container); ideal Bose gas predicts constant density everywhere





https://en.wikipedia.org/wiki/File:2_Helium.png

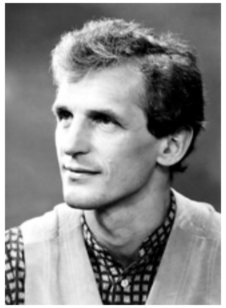
Experimental realization: atomic gases

- Using laser cooling techniues, it has been possible to cool atomic gases , e.g. Rubidium atoms in a magnetic trap ("box") to ultra-cold (nanoKelvin) temperatures.
- BEC in atomic gases was first observed in 1995 and the Nobel prize for this followed in 2001

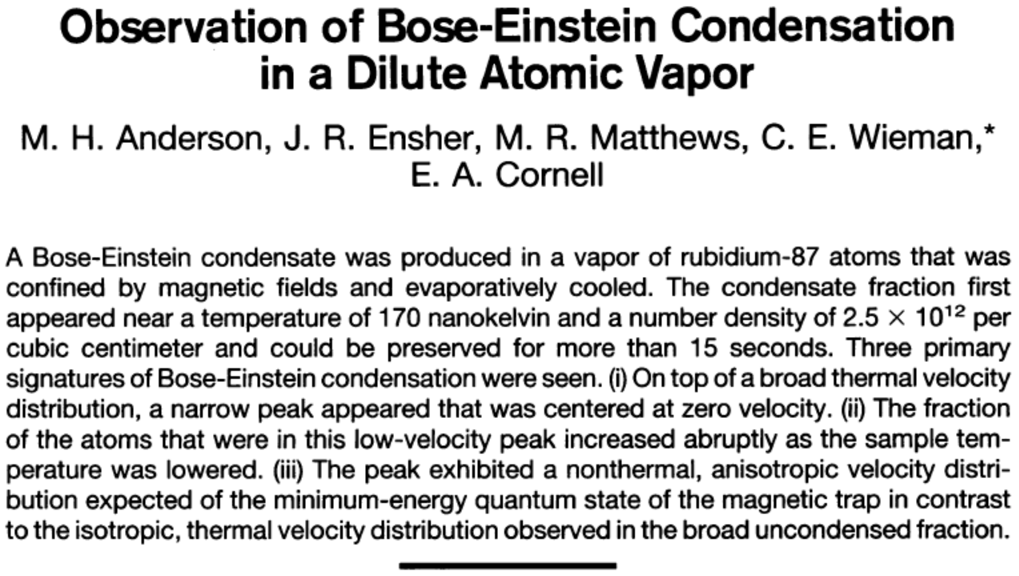
The Nobel Prize in Physics 2001


Eric A. Cornell
Prize share: 1/3


Carl E. Wieman
Prize share: 1/3

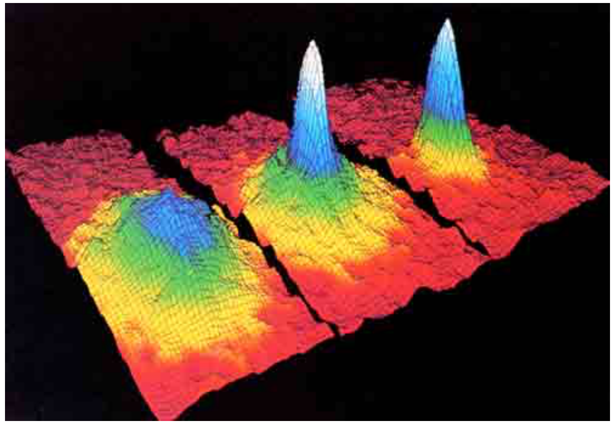

Wolfgang Ketterle
Prize share: 1/3

The Nobel Prize in Physics 2001 was awarded jointly to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman ***"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"*****.**
(Nobel Lecture)
https://www.youtube.com/watch?v=NoO7XKVmZC8


Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor

M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman,* E. A. Cornell

A Bose-Einstein condensate was produced in a vapor of rubidium-87 atoms that was confined by magnetic fields and evaporatively cooled. The condensate fraction first appeared near a temperature of 170 nanokelvin and a number density of 2.5×10^{12} per cubic centimeter and could be preserved for more than 15 seconds. Three primary signatures of Bose-Einstein condensation were seen. (i) On top of a broad thermal velocity distribution, a narrow peak appeared that was centered at zero velocity. (ii) The fraction of the atoms that were in this low-velocity peak increased abruptly as the sample temperature was lowered. (iii) The peak exhibited a nonthermal, anisotropic velocity distribution expected of the minimum-energy quantum state of the magnetic trap in contrast to the isotropic, thermal velocity distribution observed in the broad uncondensed fraction.



Weakly-interacting atomic Bose gas at 0K Gross-Pitaevskii theory

The Bose gas of condensed bosons at $T = 0K$ is described by the condensate wavefunction $\Psi_N(\boldsymbol{r}_1, \cdots \boldsymbol{r}_{\boldsymbol{N}})$

- Weak interactions in the form of 2-body collisions and short-range repulsion
- Spacially inhomogeneous gas density due to a trapping potential

$$\widehat{H}_N = \sum_{i=1}^{N} \left(-\frac{\nabla_i^2}{2m} + \frac{1}{2}\omega^2 r^2 \right) + \frac{1}{2} \sum_{i}^{N} \sum_{j \neq i}^{N} g\delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \ ,$$

The dynamics of the Bose Einstein condensate is described by the Schrödinger equation for Ψ_N

$$i\hbar \partial_t \Psi_N = \widehat{H}_N \Psi_N$$

Mean field approximation

Mean field approximation: all particles are described by the same wavefunction in the ground state $\boldsymbol{\psi}(\boldsymbol{r})$

Condensate wavefunction is determined by 1-**wavefunction** $\boldsymbol{\psi}(\boldsymbol{r})$ in the ground state (macroscopic wavefunction),

$$|\Psi_N(\boldsymbol{r}_1, \cdots \boldsymbol{r}_{\boldsymbol{N}})\rangle = |\psi(\boldsymbol{r}_1)\rangle \otimes |\psi(\boldsymbol{r}_2)\rangle \cdots \otimes |\psi(\boldsymbol{r}_N)\rangle$$

$$\Psi_N(\boldsymbol{r}_1, \cdots \boldsymbol{r}_{\boldsymbol{N}}) = \prod_i \psi(\boldsymbol{r}_i)$$

One particle probability distributions $\mathrm{P}(\mathrm{r_i}) = \psi^*(\boldsymbol{r}_i)\psi(\boldsymbol{r}_i)$ are independent and identical.

Rescale the 1-particle wavefunction $\psi(r) = \frac{1}{\sqrt{N}}\phi(r)$, such that $\int dr\, |\phi(r)|^2 = \mathrm{N}$

Gross-Pitaevskii equation

Average energy of a condensate particle

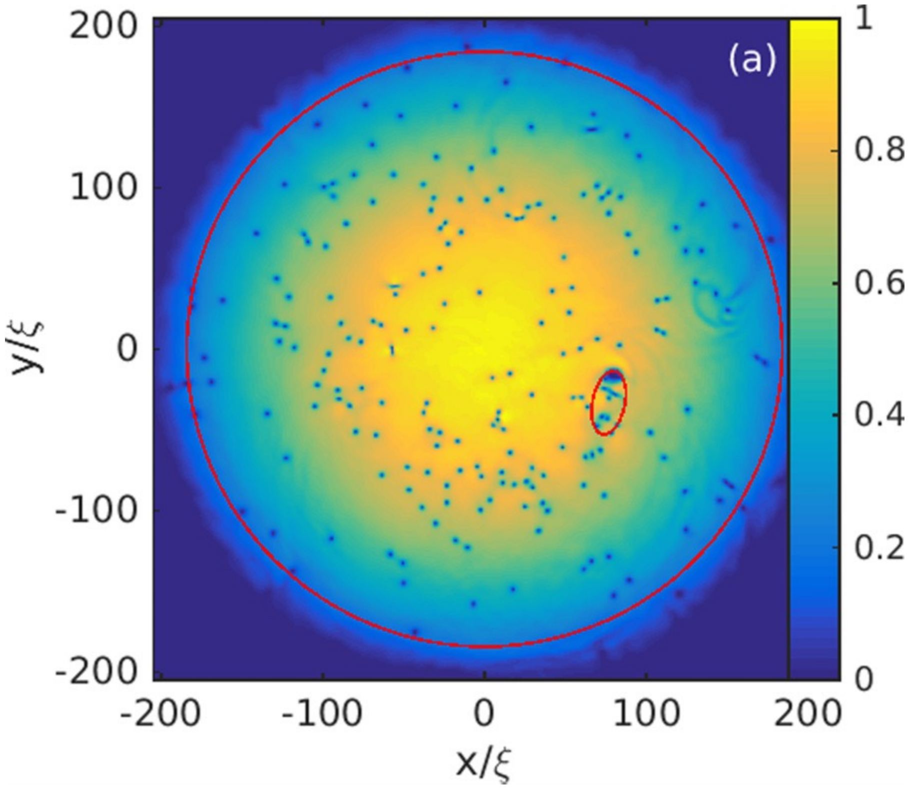
$$\Omega = \left\langle \Psi_N \middle| \hat{H} \middle| \Psi_N \right\rangle = \int dr \left[-\phi^*(r) \frac{\hbar^2}{2m} \nabla^2 \phi + \frac{1}{2} \omega^2 r^2 |\phi(r)|^2 + \frac{g}{4} |\phi(r)|^4 \right]$$

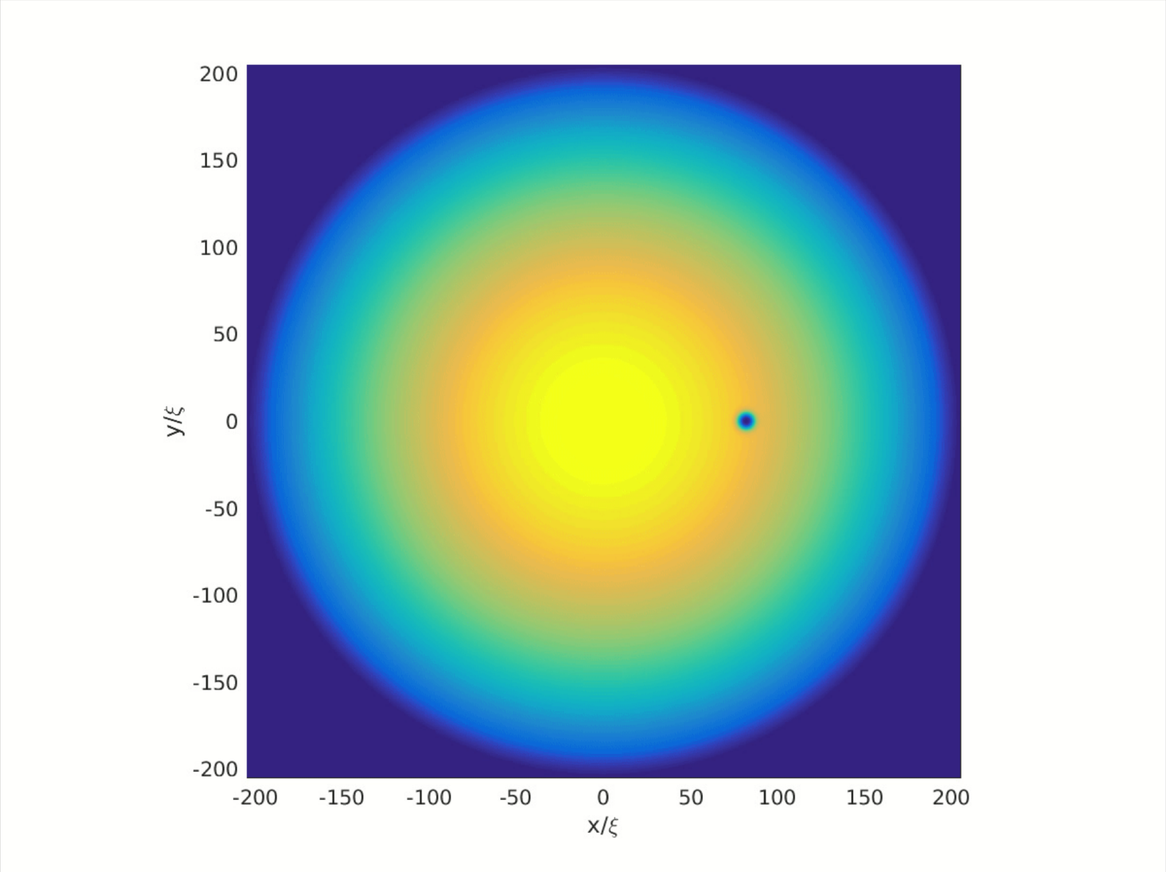
Evolution of the macroscopic wavefunction $\boldsymbol{\phi(r, t)}$

$$\langle \Psi_N | i\hbar\partial_t | \Psi_N \rangle = \left\langle \Psi_N \middle| \hat{H} \middle| \Psi_N \right\rangle \rightarrow i\hbar\partial_t \phi = \frac{\partial \Omega}{\partial \phi^*}$$

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi + \frac{1}{2} \omega^2 r^2 \phi + \mathrm{g} |\phi|^2 \phi$$

Vortex dynamics in stirred BEC





https://journals.aps.org/pre/abstract/10.1103/PhysRevE.93.032106
A. Skaugen, LA, PRE 93 (2016)

Appendix:
derivation of BEC coarsegrained energy energy $\Omega = \left\langle \Psi_N \middle| \hat{H} \middle| \Psi_N \right\rangle$

Density of particles:

$$n(r) = \langle \Psi_N \left| \sum_i \delta(r - r_i) \,|\, \Psi_N \right\rangle$$

$$= \int dr_1 \cdots dr_i \cdots dr_N \, \psi^*(r_1) \cdots \psi^*(r_N) \left(\sum_i \delta(r - r_i) \right) \psi(r_1) \cdots \psi(r_N)$$

$$= \sum_i \int dr_i \;\; \delta(r - r_i) |\psi(r_i)|^2 = \; N|\psi(r)|^2$$

Average kinetic energy

$$\left\langle \Psi_N \left| -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 \right| \Psi_N \right\rangle = \int dr_1 \cdots dr_i \cdots dr_N \, \psi^*(r_1) \cdots \psi^*(r_N) \left(-\frac{\hbar^2}{2m} \sum_i \nabla_i^2 \right) \psi(r_1) \cdots \psi(r_N)$$

$$= -\sum_i \frac{\hbar^2}{2m} \int dr_i \, \psi^*(r_i) \nabla_i^2 \psi(\mathrm{r_i}) = -N \frac{\hbar^2}{2m} \int dr \, \psi^*(r) \nabla^2 \psi(r)$$

BEC coarsegrained energy energy

Trapping potential:

$$\left\langle \Psi_N \left| \sum_i \tfrac{1}{2}\omega^2 r_i^2 \right| \Psi_N \right\rangle = \sum_i \int dr_i \, \psi^*(r_i) \left(\tfrac{1}{2}\omega^2 r_i^2\right) \psi(r_i) = N \int dr \, \tfrac{1}{2}\omega^2 r^2 |\psi(r)|^2$$

Interaction potential

$$\left\langle \Psi_N \left| \frac{g}{2} \sum_i^N \sum_{j \neq i}^N \delta(r_i - r_j) \right| \Psi_N \right\rangle =$$

$$= \frac{g}{2} \sum_i \sum_{j\neq i} \int dr_i \int dr_j \, \psi^*(r_i)\psi^*(r_j)\delta(r_i - r_j)\psi(r_i)\psi(r_j)$$

$$= g\,\frac{N(N-1\,)}{4} \int dr \, |\psi(r)|^2 |\psi(r)|^2 \approx g\,\frac{N^2}{4} \int dr \, |\psi(r)|^2 |\psi(r)|^2$$

Time evolution

$$\langle \Psi_N | i\hbar\partial_t | \Psi_N \rangle = \int dr_1 \cdots dr_N \Psi_N^* \, i\hbar \sum_i \frac{\Psi_N^*}{\psi(r_i,t)} \partial_t \psi(r_i,t) = N \int dr \, \psi^*(r,t) \, i\hbar\partial_t \psi(r,t)$$

$$\langle \Psi_N | i\hbar \partial_t | \Psi_N \rangle = \left\langle \Psi_N \middle| \hat{H} \middle| \Psi_N \right\rangle$$

$$i\hbar \int dr\, \psi^* \, \partial_t \psi = \int dr \left[-\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + \frac{\omega^2 r^2}{2} |\psi|^2 + \frac{Ng}{4} |\psi|^4 \right]$$

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi + \frac{\omega^2 r^2}{2} \phi + \mathrm{g} |\phi|^2 \phi, \qquad \phi = \frac{\psi}{\sqrt{N}}$$