

Cold atoms

Lecture 4.

31st October, 2007

Preliminary plan/reality in the fall term

Lecture 1	Something about everything (see next slide)	Oct 4
...	The textbook version of BEC in extended systems	
Lecture 2	thermodynamics, grand canonical ensemble, extended gas; atomic clouds in the traps – independent bosons.	Oct 11
...		
Lecture 3	atomic clouds in the traps – interactions, GP equation at zero temperature, variational prop., chem. potential	Oct 17
...		
Lecture 4	Infinite systems: Bogolyubov theory	Oct 31
...		

Recapitulation

BEC in atomic clouds

Nobelists I. Laser cooling and trapping of atoms



The Nobel Prize in Physics 1997

"for development of methods to cool and trap atoms with laser light"



Steven Chu

1/3 of the prize

USA

Stanford University
Stanford, CA, USA

b. 1948



Claude Cohen-Tannoudji

1/3 of the prize

France

Collège de France; École
Normale Supérieure
Paris, France

b. 1933
(in Constantine, Algeria)



William D. Phillips

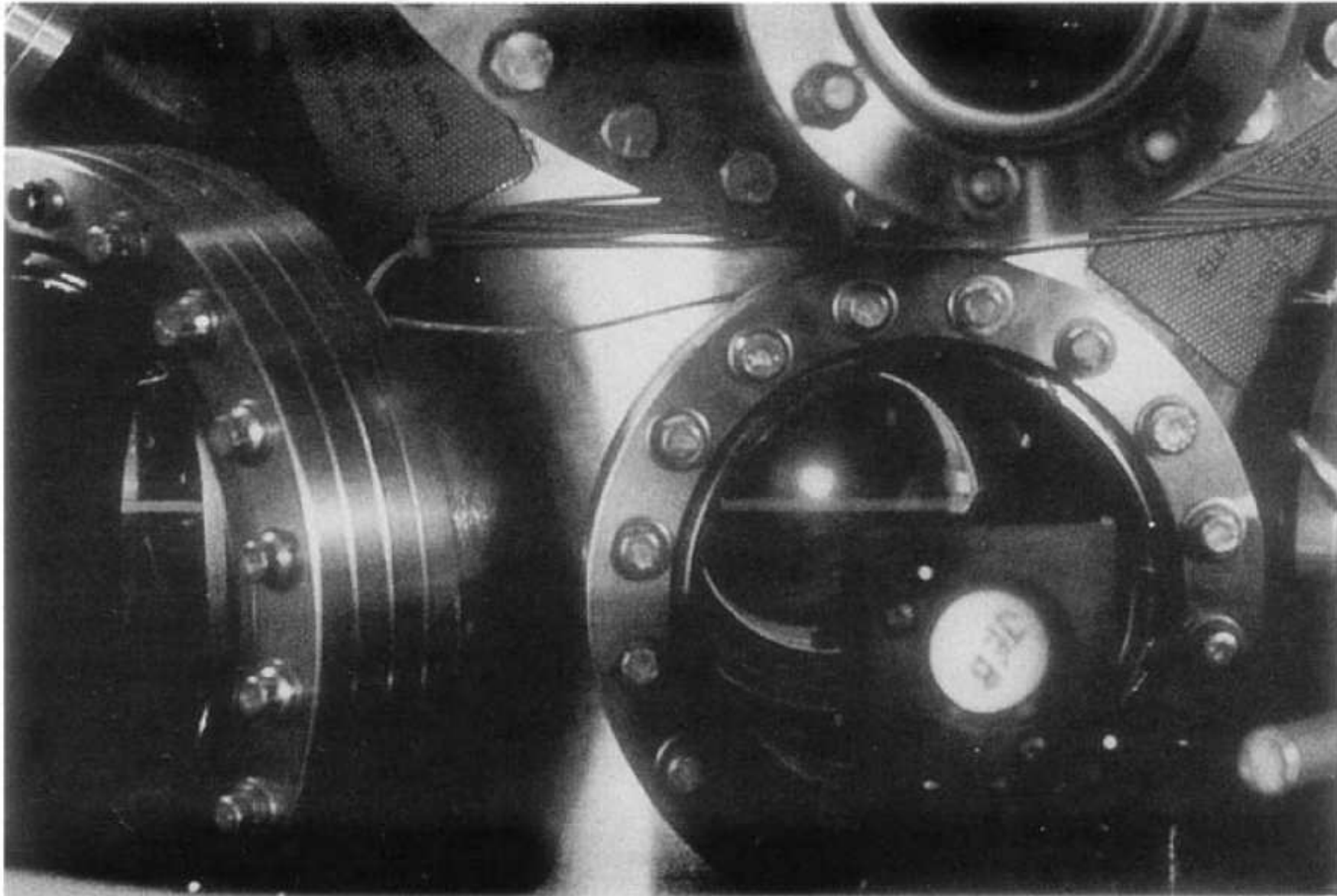
1/3 of the prize

USA

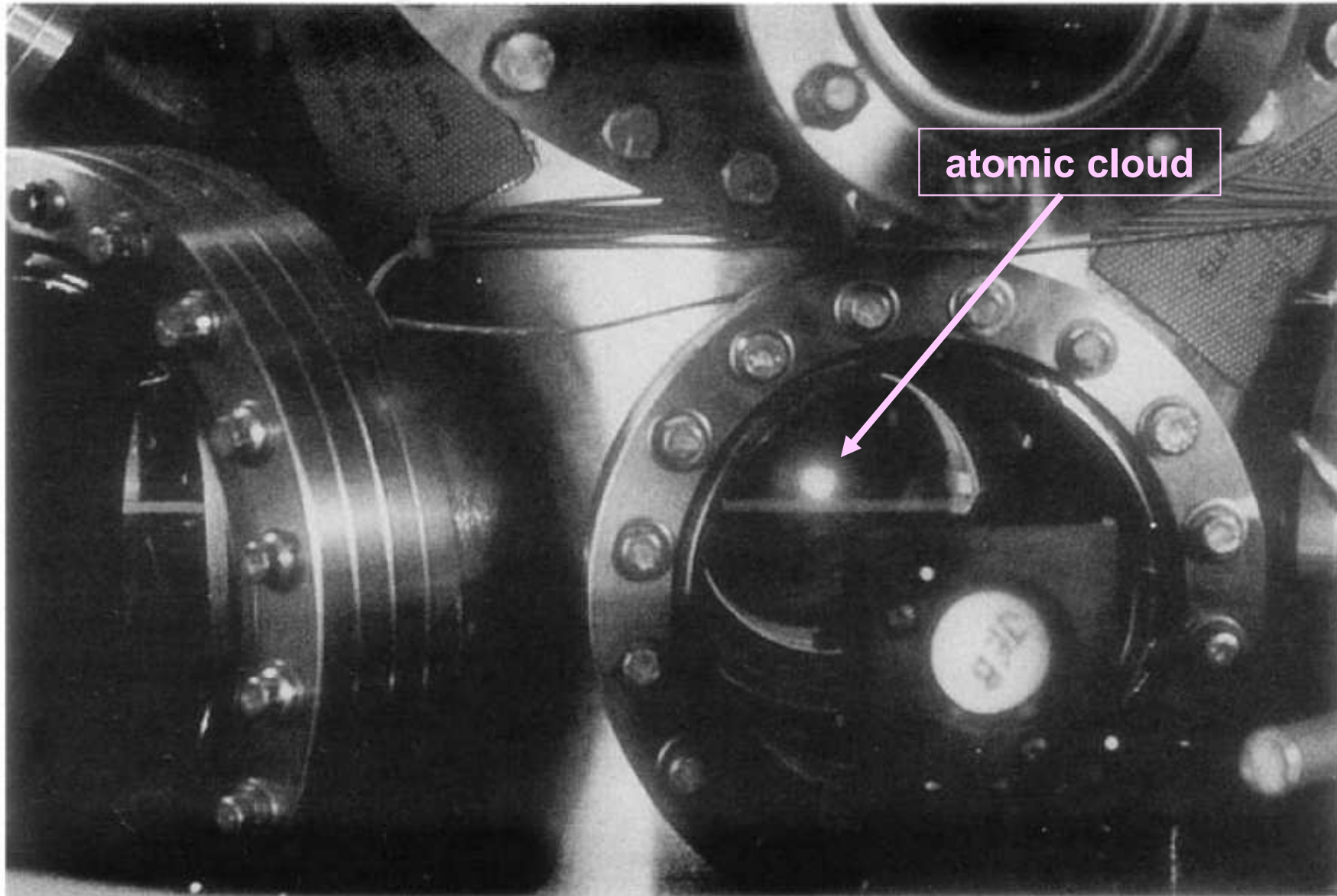
National Institute of
Standards and
Technology
Gaithersburg, MD, USA

b. 1948

Doppler cooling in the Chu lab



Doppler cooling in the Chu lab



Nobelists II. BEC in atomic clouds



The Nobel Prize in Physics 2001

"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"



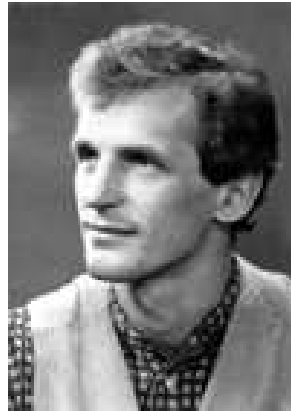
Eric A. Cornell

1/3 of the prize

USA

University of Colorado, JILA
Boulder, CO, USA

b. 1961



Wolfgang Ketterle

1/3 of the prize

Federal Republic of Germany

Massachusetts Institute of
Technology (MIT)
Cambridge, MA, USA

b. 1957



Carl E. Wieman

1/3 of the prize

USA

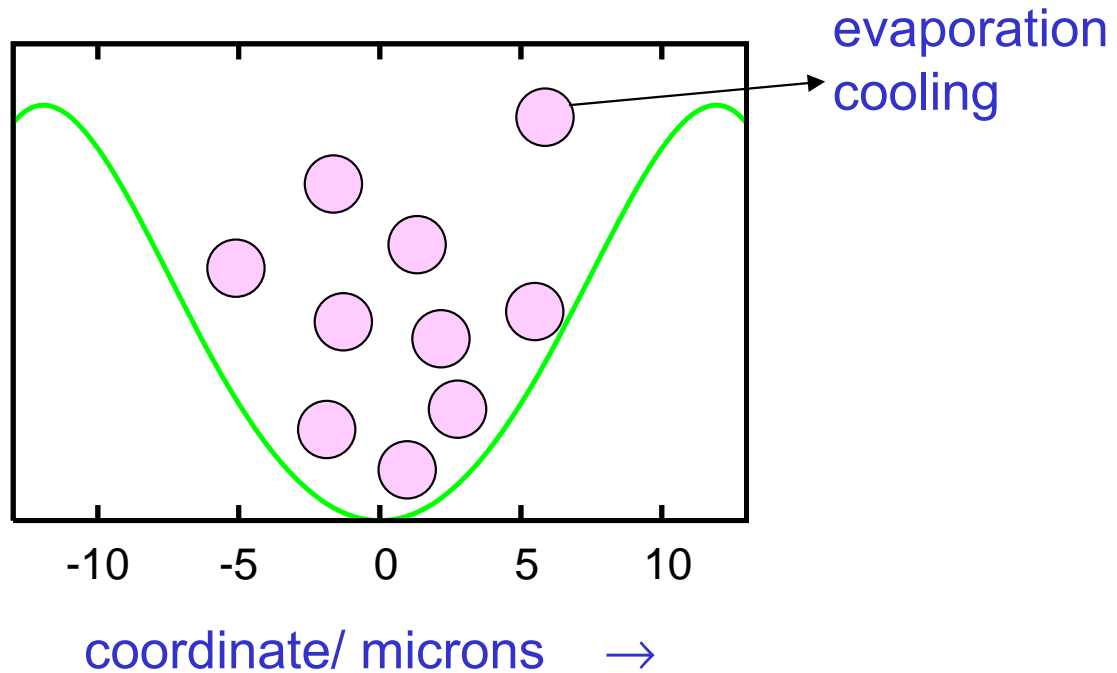
University of Colorado, JILA
Boulder, CO, USA

b. 1951

Trap potential

Typical profile

?

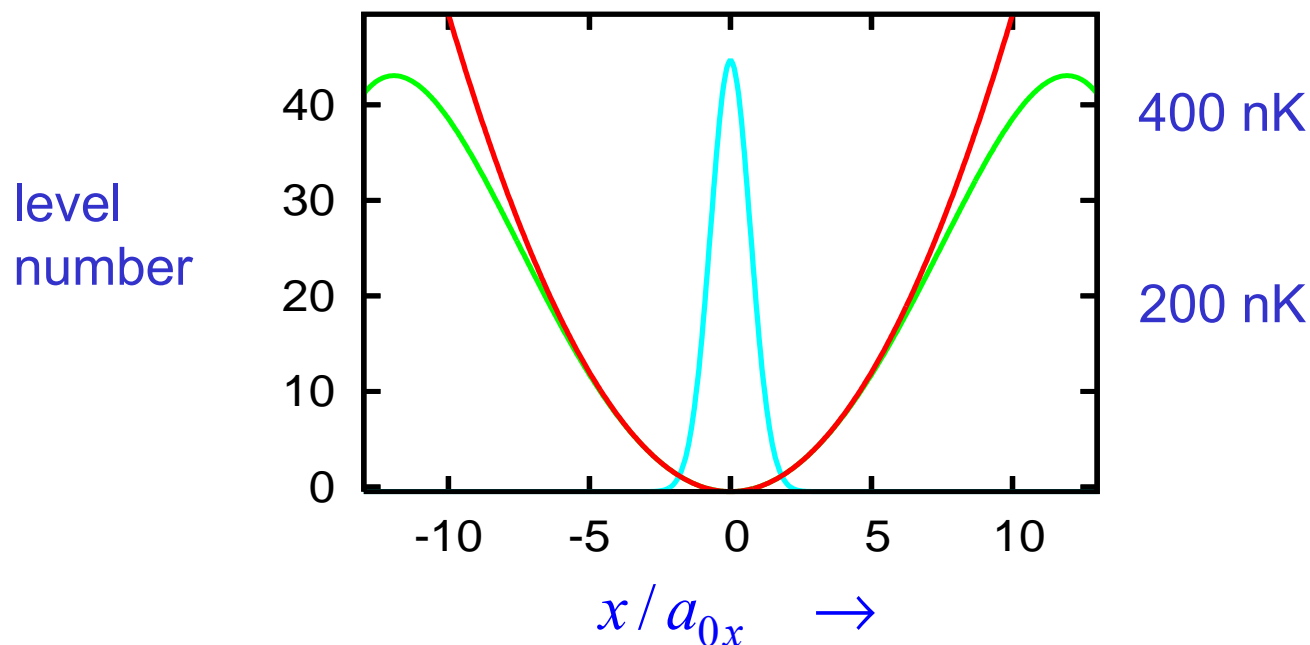


This is just one direction

Presently, the traps are mostly 3D

The trap is clearly from the real world, the atomic cloud is visible almost by a naked eye

Ground state orbital and the trap potential



$$\psi_0(x, y, z) = \phi_{0x}(x) \phi_{0y}(y) \phi_{0z}(z)$$

$$\phi_0(u) = \frac{1}{\sqrt{a_0 \pi}} e^{-\frac{u^2}{2a_0^2}}, \quad a_0 = \sqrt{\frac{\hbar}{m\omega}}, \quad E_0 = \frac{1}{2} \hbar \omega = \frac{1}{2} \cdot \frac{\hbar^2}{ma_0^2} = \frac{1}{2} \cdot \frac{\hbar^2}{Mu_m a_0^2}$$

$$V(u) = \frac{1}{2} m \omega^2 u^2 = \frac{1}{2} \hbar \omega \left(\frac{u}{a_0} \right)^2$$

- characteristic energy
- characteristic length

BEC observed by TOF in the velocity distribution

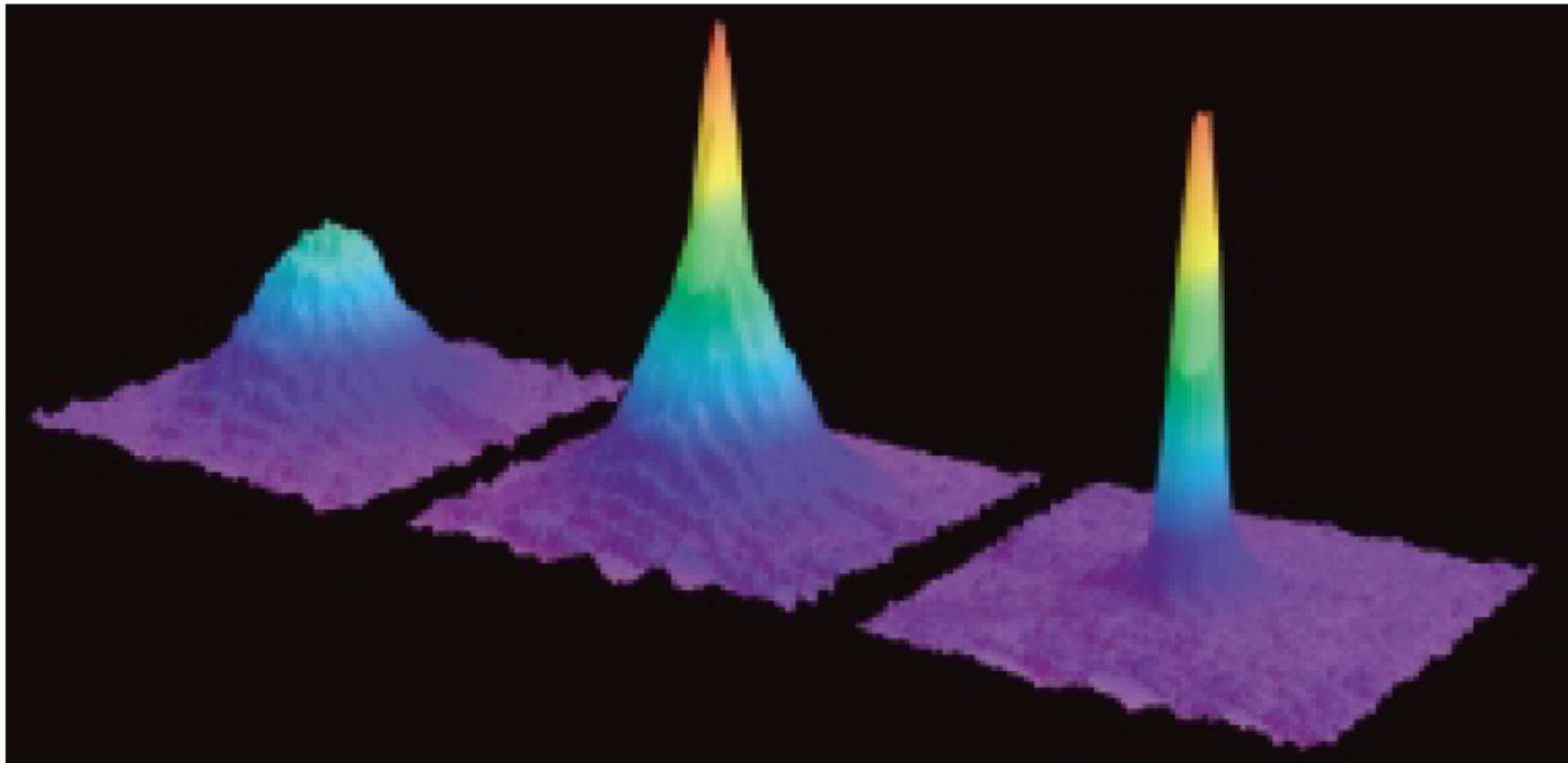
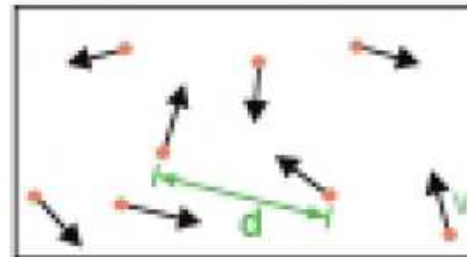


Figure 7. Observation of Bose-Einstein condensation by absorption imaging. Shown is absorption vs. two spatial dimensions. The Bose-Einstein condensate is characterized by its slow expansion observed after 6 ms time-of-flight. The left picture shows an expanding cloud cooled to just above the transition point; middle: just after the condensate appeared; right: after further evaporative cooling has left an almost pure condensate. The total number of atoms at the phase transition is about 7×10^5 , the temperature at the transition point is $2 \mu\text{K}$.

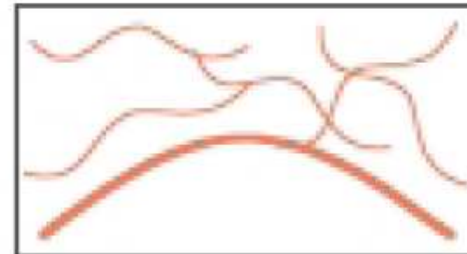
Ketterle explains BEC to the King of Sweden



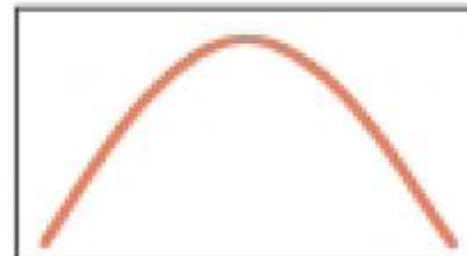
High Temperature T:
thermal velocity v
density d^{-3}
"Billiard balls"



Low Temperature T:
De Broglie wavelength
 $\lambda_{dB} = h/mv \propto T^{-1/2}$
"Wave packets"



T = T_{crit}:
Bose-Einstein Condensation
 $\lambda_{dB} \sim d$
"Matter wave overlap"

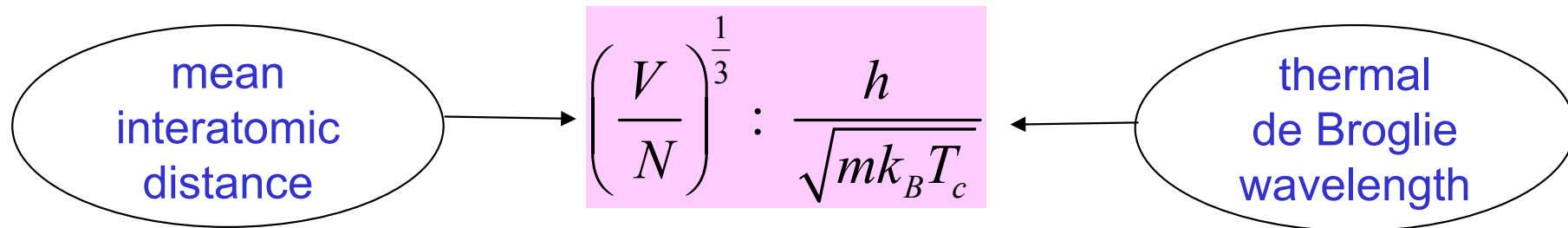


T = 0:
Pure Bose condensate
"Giant matter wave"

Simple estimate of T_c (following the Ketterle slide)

The quantum breakdown sets on when

the wave clouds of the atoms start overlapping



Critical temperature

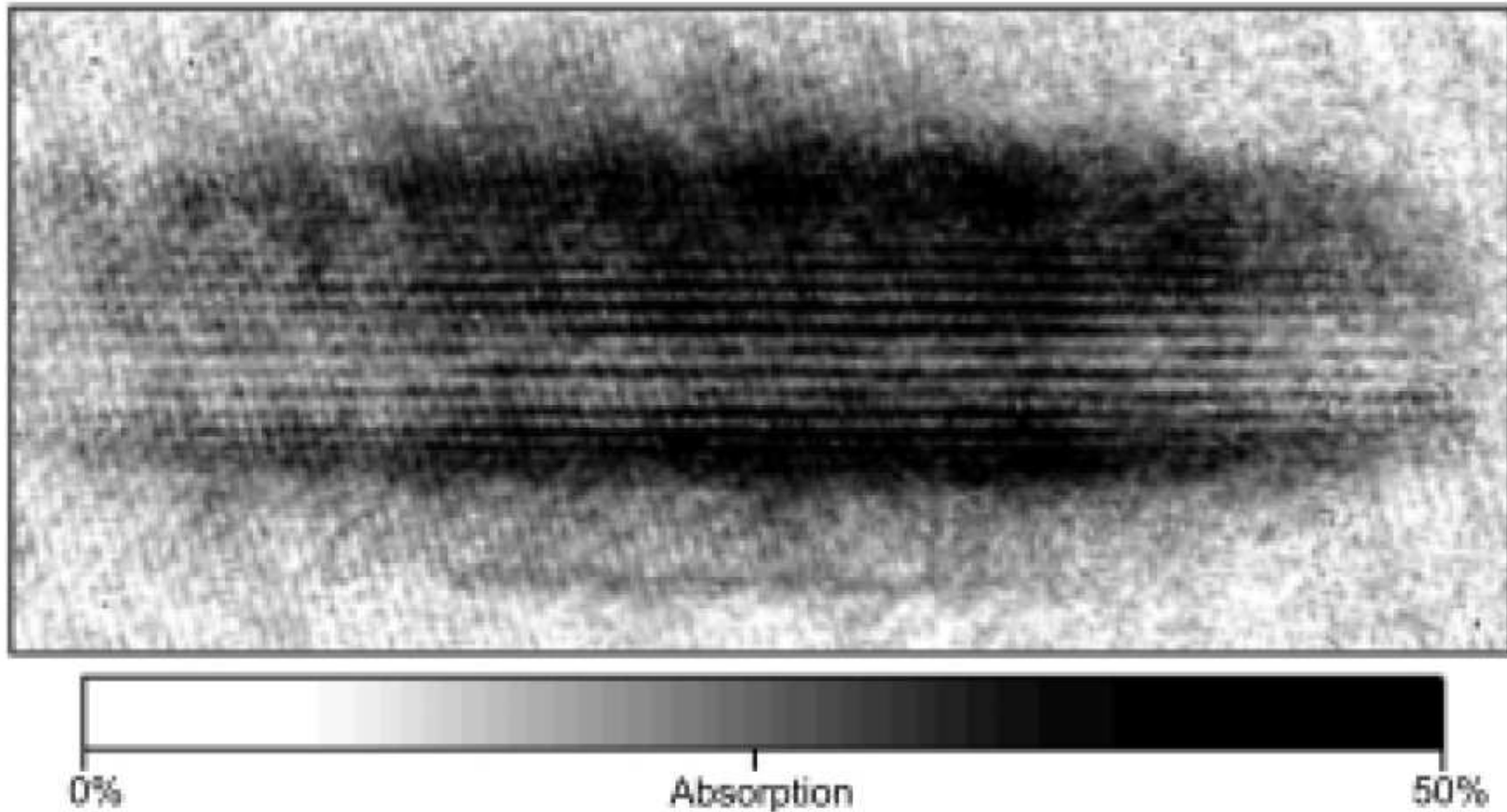
ESTIMATE

$$T_c : \frac{h^2}{mk_B} \cdot \left(\frac{N}{V}\right)^{\frac{2}{3}}$$

TRUE EXPRESSION

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

Interference of atoms



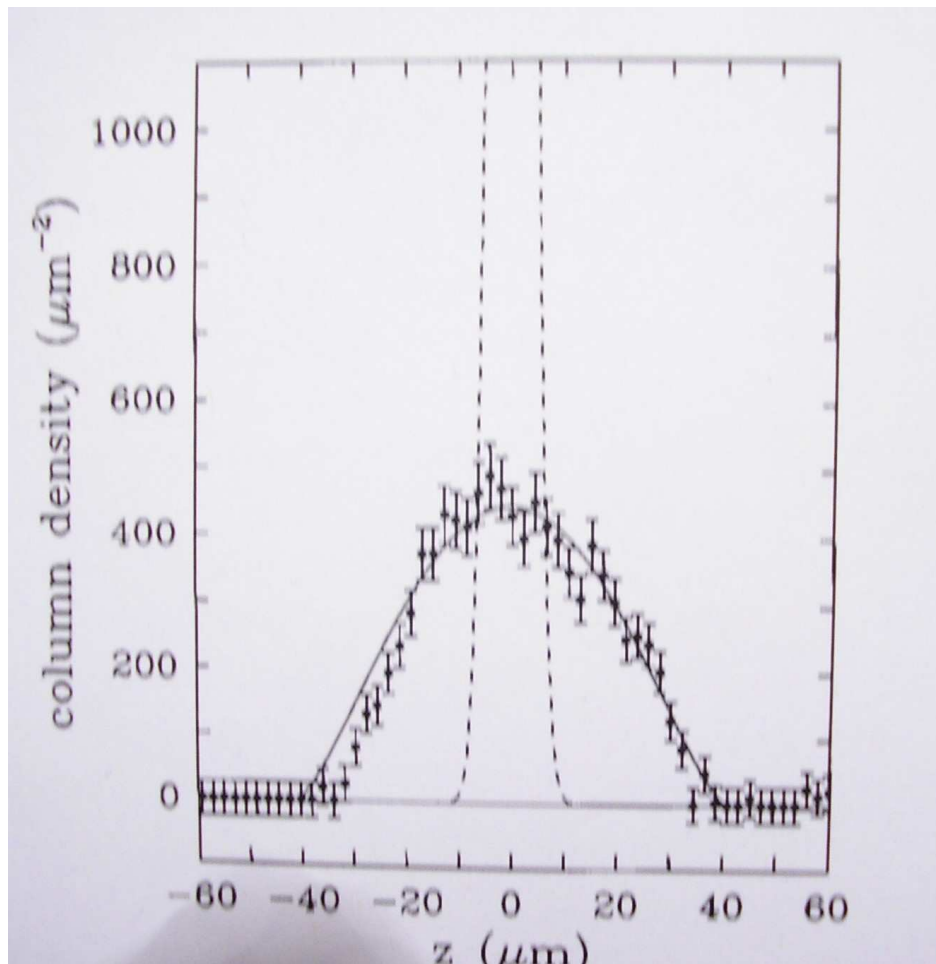
Two coherent condensates are interpenetrating and interfering.
Vertical stripe width $15\ \mu\text{m}$
Horizontal extension of the cloud $1,5\text{mm}$

*Today, we will be mostly concerned with
the extended ("infinite") BE gas/liquid*

Microscopic theory well developed
over nearly 60 past years

Interacting atoms

Importance of the interaction – synopsis



Without interaction, the condensate would occupy the ground state of the oscillator (dashed - - - -)

In fact, there is a significant broadening of the condensate of 80 000 sodium atoms in the experiment by *Hau et al.* (1998), perfectly reproduced by the solution of the GP equation

Many-body Hamiltonian

$$\hat{H} = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b)$$

True interaction potential at low energies (micro-kelvin range)

replaced by an effective potential, Fermi pseudopotential

$$U(r) = g \cdot \delta(\mathbf{r})$$

$$g = \frac{4\pi a_s \hbar^2}{m},$$

a_s ... the scattering length

Experimental data

	C_6 (a.u.)	β_6 (a.u.)	a_0 (a.u.)
${}^7\text{Li}_2$	1388 ^a	65	-27.3 ^b
${}^{23}\text{Na}_2$	1472 ^c	89	77.3 ^d
${}^{39}\text{K}_2$	3897 ^e	129	-33 ^f
${}^{85}\text{Rb}_2$	4700 ^g	164	-369 ^g
${}^{87}\text{Rb}_2$	4700 ^g	165	106 ^g
${}^{133}\text{Cs}_2$	6890 ^h	197	2400 ^h

Mean-field treatment of interacting atoms

Many-body Hamiltonian and the Hartree approximation

$$\hat{H} = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + \frac{1}{2} \sum_{a \neq b} \sum_b U(\mathbf{r}_a - \mathbf{r}_b)$$

We start from the **mean field approximation**.

This is an educated way, similar to (almost identical with) the **HARTREE APPROXIMATION** we know for many electron systems.

Most of the interactions is indeed absorbed into the mean field and what remains are explicit quantum correlation corrections

$$\hat{H}_{\text{GP}} = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + V_H(\mathbf{r}_a)$$

$$V_H(\mathbf{r}_a) = \int d\mathbf{r}_b U(\mathbf{r}_a - \mathbf{r}_b) n(\mathbf{r}_b) = g \cdot n(\mathbf{r}_a)$$

$$n(\mathbf{r}) = \sum_{\alpha} n_{\alpha} |\varphi_{\alpha}(\mathbf{r})|^2$$

$$\left(\frac{1}{2m} p^2 + V(\mathbf{r}) + V_H(\mathbf{r}) \right) \varphi_{\alpha}(\mathbf{r}) = E_{\alpha} \varphi_{\alpha}(\mathbf{r})$$

self-consistent
system

Gross-Pitaevskii equation at zero temperature

Consider a condensate. Then **all occupied orbitals are the same** and we have a single self-consistent equation for a single orbital

$$\left(\frac{1}{2m} p^2 + V(\mathbf{r}) + gN |\varphi_0(\mathbf{r})|^2 \right) \varphi_0(\mathbf{r}) = E_0 \varphi_0(\mathbf{r})$$

Putting

$$\Psi(\mathbf{r}) = \sqrt{N} \cdot \varphi_0(\mathbf{r})$$

we obtain a closed equation for the **order parameter**:

$$\left(\frac{1}{2m} p^2 + V(\mathbf{r}) + g |\Psi(\mathbf{r})|^2 \right) \Psi(\mathbf{r}) = \mu \Psi(\mathbf{r})$$

Gross-Pitaevskii equation.

The lowest level coincides with the chemical potential

For a static condensate, the order parameter has ZERO PHASE.

Then

$$\Psi(\mathbf{r}) = \sqrt{N} \cdot \varphi_0(\mathbf{r}) = \sqrt{n(\mathbf{r})}$$

$$N [n] = N = \int d^3 \mathbf{r} |\Psi(\mathbf{r})|^2 = \int d^3 \mathbf{r} \cdot n(\mathbf{r}) = N$$

Gross-Pitaevskii equation – homogeneous gas

The GP equation simplifies

$$\left(-\frac{\hbar^2}{2m} \Delta + g |\Psi(\mathbf{r})|^2 \right) \Psi(\mathbf{r}) = \mu \Psi(\mathbf{r})$$

For periodic boundary conditions in a box with $V = L_x \cdot L_y \cdot L_z$

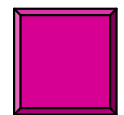
$$\varphi_0(\mathbf{r}) = \frac{1}{\sqrt{V}}$$

$$\Psi(\mathbf{r}) = \sqrt{N} \cdot \varphi_0(\mathbf{r}) = \sqrt{\frac{N}{V}} = \sqrt{n}$$

$$g |\Psi(\mathbf{r})|^2 \Psi(\mathbf{r}) = \mu \Psi(\mathbf{r}) \quad \dots \text{GP equation}$$

$$\underline{\mu = g |\Psi(\mathbf{r})|^2 = gn}$$

$$\underline{\frac{E}{N} = \frac{1}{N} \int d^3 \mathbf{r} \left\{ \frac{\hbar^2}{2m} (\nabla \sqrt{n})^2 + \cancel{V(\mathbf{r})n} + \frac{1}{2} g n^2 \right\} = \frac{1}{2} g n}$$



Field theoretic reformulation (second quantization)

Purpose:

- ⌘ go beyond the GPE \equiv mean field approximation
- ⌘ treat also the excitations

Field operator for spin-less bosons

Definition by commutation relations

$$\left[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}') \right] = \delta(\mathbf{r} - \mathbf{r}'), \quad \left[\psi(\mathbf{r}), \psi(\mathbf{r}') \right] = 0, \quad \left[\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}') \right] = 0$$

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

$$\{ |\kappa\rangle \} \quad \langle \kappa | \beta \rangle = \delta_{\kappa\beta} \quad |\psi\rangle = \sum |\kappa\rangle \langle \kappa | \psi \rangle, \quad \psi \dots \text{single particle state}$$

$$\langle \mathbf{r} | \kappa \rangle = \varphi_\kappa(\mathbf{r}) \quad \langle \mathbf{r} | \psi \rangle = \sum \langle \mathbf{r} | \kappa \rangle \langle \kappa | \psi \rangle$$

decomposition of the field operator

$$\psi(\mathbf{r}) = \sum \varphi_\kappa(\mathbf{r}) a_\kappa, \quad a_\kappa = \langle \kappa | \psi \rangle = \int d^3 \varphi_\kappa^*(\mathbf{r}) \psi(\mathbf{r})$$

$$\psi^\dagger(\mathbf{r}) = \sum \varphi_\kappa^*(\mathbf{r}) a_\kappa^\dagger$$

commutation relations

$$\left[a_\kappa, a_\lambda^\dagger \right] = \delta_{\kappa\lambda}, \quad \left[a_\kappa, a_\lambda \right] = 0, \quad \left[a_\kappa^\dagger, a_\lambda^\dagger \right] = 0$$

Action of the field operators in the Fock space

basis of single-particle states

$$\{|\kappa\rangle\} \quad \langle\kappa|\beta\rangle = \delta_{\kappa\beta} \quad |\psi\rangle = \sum |\kappa\rangle \langle\kappa|\psi\rangle, \quad \psi \dots \text{single particle state}$$

$$\langle\mathbf{r}|\kappa\rangle = \varphi_{\kappa}(\mathbf{r}) \quad \langle\mathbf{r}|\psi\rangle = \sum \langle\mathbf{r}|\kappa\rangle \langle\kappa|\psi\rangle$$

FOCK SPACE **F** space of many particle states

basis states ... symmetrized products of single-particle states **for bosons**

specified by the set of **occupation numbers** **0, 1, 2, 3, ...**

$$\{ \kappa_1, \kappa_2, \kappa_3, \mathbf{K}, \kappa_p, \mathbf{K} \}$$

$$\Psi_{\{\kappa\}} = |n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K}\rangle \quad n\text{-particle state} \quad n = \sum n_p$$

$$a_p^\dagger |n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K}\rangle = \sqrt{n_p + 1} |n_1, n_2, n_3, \mathbf{K}, n_p + 1, \mathbf{K}\rangle$$

$$a_p |n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K}\rangle = \sqrt{n_p} |n_1, n_2, n_3, \mathbf{K}, n_p - 1, \mathbf{K}\rangle$$

$$a_p^\dagger a_p |n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K}\rangle = n_p |n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K}\rangle$$

Action of the field operators in the Fock space

Average values of the field operators in the Fock states

Off-diagonal elements only!!! The diagonal elements vanish:

$$\begin{aligned} \langle n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} | a_p | n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} \rangle &= \\ \langle n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} | \sqrt{n_p} | n_1, n_2, n_3, \mathbf{K}, n_p - 1, \mathbf{K} \rangle &= 0 \end{aligned}$$

Creating a Fock state from the vacuum:

$$| n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} \rangle = \prod_p \frac{1}{\sqrt{n_p!}} (a_p^\dagger)^{n_p} | \text{vac} \rangle$$

Action of the field operators in the Fock space

Average values of the field operators in the Fock states

Off-diagonal elements only!!! The diagonal elements vanish:

$$\begin{aligned} \langle n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} | a_p | n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} \rangle &= \\ \langle n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} | \sqrt{n_p} | n_1, n_2, n_3, \mathbf{K}, n_p - 1, \mathbf{K} \rangle &= 0 \end{aligned}$$

Creating a Fock state from the vacuum:

$$| n_1, n_2, n_3, \mathbf{K}, n_p, \mathbf{K} \rangle = \prod_p \frac{1}{\sqrt{n_p!}} (a_p^\dagger)^{n_p} | \text{vac} \rangle$$

In particular, the condensate

$$| N_0, 0, 0, \mathbf{K}, 0, \mathbf{K} \rangle = \frac{1}{\sqrt{N_0!}} (a_0^\dagger)^{N_0} | \text{vac} \rangle$$

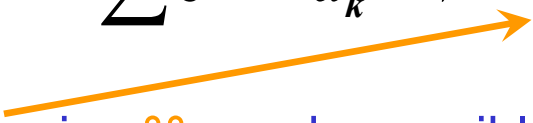
Field operator for spin-less bosons – cont'd

Important special case – an extended homogeneous system

Translational invariance suggests to use the

Plane wave representation (BK normalization)

$$\psi(\mathbf{r}) = V^{-1/2} \sum e^{i\mathbf{k}\mathbf{r}} a_{\mathbf{k}}, \quad a_{\mathbf{k}} = V^{-1/2} \int d^3 r e^{-i\mathbf{k}\mathbf{r}} \psi(\mathbf{r})$$

$$\psi^\dagger(\mathbf{r}) = V^{-1/2} \sum e^{-i\mathbf{k}\mathbf{r}} a_{\mathbf{k}}^\dagger = V^{-1/2} \sum e^{i\mathbf{k}\mathbf{r}} a_{-\mathbf{k}}^\dagger$$


The other form is \otimes made possible by the inversion symmetry (*parity*)

\otimes important, because the combination

$$u \cdot a_{\mathbf{k}} + v \cdot a_{-\mathbf{k}}^\dagger$$

corresponds to the momentum transfer by \mathbf{k}

Commutation rules do not involve a δ -function, because the BK momentum is discrete, albeit quasi-continuous:

$$\left[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger \right] = \delta_{\mathbf{k}\mathbf{k}'}, \quad \left[a_{\mathbf{k}}, a_{\mathbf{k}'} \right] = 0, \quad \left[a_{\mathbf{k}}^\dagger, a_{\mathbf{k}'}^\dagger \right] = 0$$

Operators

Additive observable

$$X = \sum X_j \quad \rightarrow \quad X = \iint d^3r d^3r' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | X | \mathbf{r}' \rangle \psi(\mathbf{r}')$$

General definition of the one particle density matrix – OPDM

$$\begin{aligned} \langle X \rangle &= \left\langle \iint d^3r d^3r' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | X | \mathbf{r}' \rangle \psi(\mathbf{r}') \right\rangle = \iint d^3r d^3r' \langle \mathbf{r} | X | \mathbf{r}' \rangle \underbrace{\langle \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}') \rangle}_{\langle \mathbf{r}' | \rho | \mathbf{r} \rangle} \\ &\equiv \iint d^3r d^3r' \langle \mathbf{r} | X | \mathbf{r}' \rangle \langle \mathbf{r}' | \rho | \mathbf{r} \rangle = \text{Tr } X \rho \end{aligned}$$

Particle number

$$N = \sum 1_{\text{OP},j} \quad \rightarrow \quad N = \int d^3r \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})$$

$$N = \sum a_k^\dagger a_k$$

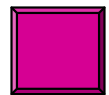
Momentum

$$\mathbf{P} = \sum \mathbf{p}_j \quad \rightarrow \quad \mathbf{P} = \int d^3r \psi^\dagger(\mathbf{r}) (-i\hbar \nabla) \psi(\mathbf{r})$$

$$\mathbf{P} = \sum \hbar \mathbf{k} \cdot a_k^\dagger a_k$$

Particle density

$$n_{\text{OP}}(\mathbf{r}) = \sum \delta(\mathbf{r} - \mathbf{r}_j) \quad \rightarrow \quad n_{\text{OP}}(\mathbf{r}) = \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})$$



$$n_{\text{OP}}(\mathbf{r}) = \frac{1}{V} \sum_q e^{i\mathbf{q}\mathbf{r}} \sum_k a_{\mathbf{k}-\mathbf{q}/2}^\dagger a_{\mathbf{k}+\mathbf{q}/2} \equiv \frac{1}{V} \sum_q e^{i\mathbf{q}\mathbf{r}} n_q$$

Hamiltonian

$$H = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) \quad \text{single-particle additive}$$

$$+ \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b) \quad \text{two-particle binary}$$

$$\rightarrow \int d^3\mathbf{r} \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \psi(\mathbf{r})$$

$$+ \frac{1}{2} \iint d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r})$$

Hamiltonian

$$H = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) \quad \text{single-particle additive}$$

acts in the N -particle sub-space $\mathbf{H}_N \subset \mathbf{F}$

$$+ \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b) \quad \text{two-particle binary}$$

$$\rightarrow \int d^3\mathbf{r} \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \psi(\mathbf{r})$$

acts in the whole Fock space \mathbf{F}

$$+ \frac{1}{2} \iint d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r})$$

Hamiltonian

$$H = \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) \quad \text{single-particle additive}$$

$$+ \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b) \quad \text{two-particle binary}$$

$$\rightarrow \int d^3\mathbf{r} \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \psi(\mathbf{r})$$

$$+ \frac{1}{2} \iint d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r})$$

acts in the N -particle sub-space $\mathbf{H}_N \subset \mathbf{F}$

acts in the whole Fock space \mathbf{F}

but \mathbf{K}

Particle number conservation

$$[H, N] = 0$$

Equilibrium density operators and the ground state (*ergodic property*)

$$\rho = \rho(H), \quad [N, \rho] = 0$$

On symmetries and conservation laws

Hamiltonian is conserving the particle number

Particle number conservation

$$[H, N] = 0$$

Equilibrium density operators and the ground state (*ergodic property*)

$$\rho = \rho(H), \quad [N, \rho] = 0$$

Typical selection rule

$$\langle \psi(\mathbf{r}) \rangle = \text{Tr} \psi(\mathbf{r}) \rho = 0$$

is a consequence:

$$\text{(similarly } \langle \psi \psi \rangle = 0, \langle \psi \psi \psi^\dagger \rangle = 0, \dots \text{)}$$

Proof:

$$0 = \text{Tr}(\psi[N, \rho]) = \text{Tr}(\rho[\psi, N]) = \text{Tr}(\rho\psi) \quad \text{Tr } A[B, C] = \text{Tr } C[A, B]$$

$$[\psi(x), \int dx' \psi^\dagger(x') \psi(x')] = \int dx' (\psi^\dagger(x') [\psi(x), \psi(x')] + [\psi(x), \psi^\dagger(x')] \psi(x')) = \psi(x)$$

QED

Deeper insight: gauge invariance of the 1st kind 

Gauge invariance of the 1st kind

Particle number conservation

$$[H, N] = 0$$

Equilibrium density operators and the ground state (*ergodic property*)

$$\rho = \rho(H), \quad [N, \rho] = 0$$

Gauge invariance of the 1st kind

$$[H, N] = 0 \iff e^{iN\varphi} H e^{-iN\varphi} = H \quad \text{unitary transform}$$

The equilibrium states have then the same invariance property:

$$[N, \rho] = 0 \iff e^{-iN\varphi} \rho e^{iN\varphi} = \rho$$

Selection rule rederived:

$$\text{Tr} \psi \rho = \text{Tr} \psi e^{-i\varphi N} \rho e^{i\varphi N} = \text{Tr} e^{i\varphi N} \psi e^{-i\varphi N} \rho = e^{i\varphi} \text{Tr} \psi \rho$$

$$(1 - e^{i\varphi}) \text{Tr} \psi \rho = 0 \implies \text{Tr} \psi(\mathbf{r}) \rho = \langle \psi(\mathbf{r}) \rangle = 0$$

Hamiltonian of a homogeneous gas

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq b} \sum_b U(\mathbf{r}_a - \mathbf{r}_b), \quad \boxed{V = \text{const.}}$$
$$= \int d^3\mathbf{r} \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V \right) \psi(\mathbf{r}) + \frac{1}{2} \iint d^3\mathbf{r} d^3\mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r})$$

To study the **symmetry properties** of the Hamiltonian

Proceed in three steps ...

in the direction reverse to that for the gauge invariance

Hamiltonian of the homogeneous gas

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq b} \sum_b U(\mathbf{r}_a - \mathbf{r}_b), \quad \boxed{V = \text{const.}}$$
$$= \int d^3 \mathbf{r} \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V \right) \psi(\mathbf{r}) + \frac{1}{2} \iint d^3 \mathbf{r} d^3 \mathbf{r}' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r})$$

- Translationally invariant system ... how to formalize (*and to learn more about the*

gauge invariance)

$$\boxed{T^\dagger(\mathbf{a}) \mathcal{H} T(\mathbf{a}) = \mathcal{H}, \quad \mathbf{a} \in R_3 \quad \dots \text{translation vector}}$$

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- Constructing the unitary operator $T(\mathbf{a})$

Translation in the one-particle orbital space

$$\underline{|T(\mathbf{a})\varphi(\mathbf{r}) = \varphi(\mathbf{r} - \mathbf{a})} = \sum \frac{1}{n!} (-\nabla \mathbf{a})^n \varphi(\mathbf{r}) = \sum \frac{1}{n!} \left(\frac{-i \mathbf{p} \mathbf{a}}{\hbar} \right)^n \varphi(\mathbf{r}) = \underline{e^{-i \mathbf{p} \mathbf{a} / \hbar} | \varphi(\mathbf{r})}$$

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- Constructing the unitary operator $T(\mathbf{a})$

$$\begin{aligned} \underline{T(\mathbf{a}) \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{K} \mathbf{r}_p, \mathbf{K} \mathbf{r}_N)} &= \Psi(\mathbf{r}_1 - \mathbf{a}, \mathbf{r}_2 - \mathbf{a}, \mathbf{r}_3 - \mathbf{a}, \mathbf{K} \mathbf{r}_p - \mathbf{a}, \mathbf{K} \mathbf{r}_N - \mathbf{a}) \\ &= \prod e^{-i \mathbf{p}_1 \mathbf{a} / \hbar} \Psi(\mathbf{r}_1, \mathbf{K} \mathbf{r}_N) = e^{-i \sum \mathbf{p}_1 \mathbf{a} / \hbar} \Psi(\mathbf{r}_1, \mathbf{K} \mathbf{r}_N) = \underline{e^{-i \mathcal{P} \mathbf{a} / \hbar}} \Psi(\mathbf{r}_1, \mathbf{K} \mathbf{r}_N) \end{aligned}$$

Hamiltonian of the homogeneous gas

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... compare $O(\varphi) = e^{-i \mathcal{N} \varphi}$

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... compare $O(\varphi) = e^{-i\mathcal{N}\varphi}$

- Infinitesimal translation

$$[\mathcal{H}, \mathcal{N}] = 0$$

$$\mathcal{H} = T^\dagger(\mathbf{a}) \mathcal{H} T(\mathbf{a}) = e^{+i\mathcal{P}\mathbf{a} / \hbar} \mathcal{H} e^{-i\mathcal{P}\mathbf{a} / \hbar} \approx \mathcal{H} + i/\hbar \mathcal{P}\mathbf{a} \mathcal{H} - i/\hbar \mathcal{H} \mathcal{P}\mathbf{a} + O(a^2)$$

$$\Rightarrow [\mathcal{H}, \mathcal{P}]\mathbf{a} = 0 \quad \Leftrightarrow \quad \boxed{[\mathcal{H}, \mathcal{P}_{x,y,z}] = 0} \quad \dots \text{momentum conservation}$$

Summary: two symmetries compared

Gauge invariance of the 1 st kind	Translational invariance
universal for atomic systems	specific for homogeneous systems
$O^\dagger(\varphi)\mathcal{H}O(\varphi) = \mathcal{H}, \quad \varphi \in \langle 0, 2\pi \rangle$ $O(\varphi) = e^{-i\mathcal{N}\varphi}$	$\mathcal{T}^\dagger(\mathbf{a})\mathcal{H}\mathcal{T}(\mathbf{a}) = \mathcal{H}, \quad \mathbf{a} \in R_3$ $\mathcal{T}(\mathbf{a}) = e^{-i\mathcal{P}\mathbf{a}/\hbar}$
global phase shift of the wave function	global shift in the configuration space
$[\mathcal{H}, \mathcal{N}] = 0$ <p>particle number conservation</p>	$[\mathcal{H}, \mathcal{P}_{x,y,z}] = 0$ <p>total momentum conservation</p>
$[\mathcal{N}, \mathcal{P}] = 0 \Leftrightarrow e^{-i\mathcal{N}\varphi} \mathcal{P} e^{i\mathcal{N}\varphi} = \mathcal{P}$ <p>for equilibrium states</p>	$[\mathcal{P}, \mathcal{P}] = 0 \Leftrightarrow e^{-\frac{i}{\hbar}\mathcal{P}\mathbf{a}} \mathcal{P} e^{\frac{i}{\hbar}\mathcal{P}\mathbf{a}} = \mathcal{P}$ <p>for equilibrium states</p>
<p>selection rules</p> $\langle \psi \mathcal{L} \psi^\dagger \rangle = 0$ <p>unless there are as many ψ^\dagger as ψ.</p>	<p>selection rules</p> $\langle a_k \mathcal{L} a_{k''}^\dagger \rangle = 0$ <p>unless the total momentum transfer $-\mathbf{k} - \mathbf{k}' + \mathbf{k}''$ is zero</p>

Hamiltonian of the homogeneous gas

In the momentum representation

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} V^{-1} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{k}}$$

$$U_{\mathbf{k}} = \int d^3 \mathbf{r} e^{-i\mathbf{k}\mathbf{r}} U(\mathbf{r})$$

Momentum conservation

$$(\mathbf{k} + \mathbf{q}) + (\mathbf{k}' - \mathbf{q}) - \mathbf{k} - \mathbf{k}' = 0$$

Particle number conservation

$$a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{k}}$$

Hamiltonian of the homogeneous gas

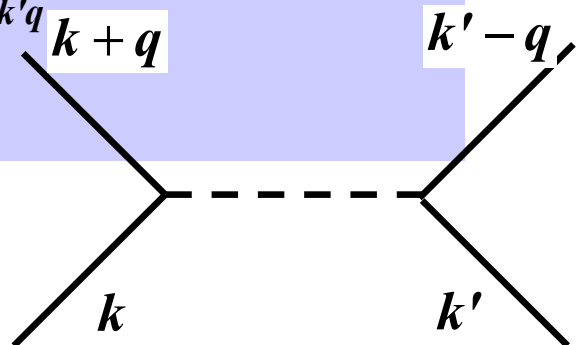
In the momentum representation

For the Fermi pseudopotential

$$U_q = U_0 \equiv U (= g)$$

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} V^{-1} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} U_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}}$$

$$U_{\mathbf{k}} = \int d^3 \mathbf{r} e^{-i\mathbf{k}\mathbf{r}} U(\mathbf{r})$$



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Particle number conservation

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Bogolyubov method

Originally, intended and conceived for extended (rather *infinite*) homogeneous system.

Reflects the 'Paradoxien der Unendlichen'

Basic idea

Bogolyubov method

is devised for boson quantum fluids with weak interactions – at $T=0$ now

no interaction

$$g = 0$$

$$N = N_{\text{BE}} = \langle a_0^\dagger a_0 \rangle ? \quad 1$$

weak interaction

$$g \neq 0$$

$$N = N_{\text{BE}} + \sum_{k \neq 0} \langle a_k^\dagger a_k \rangle \approx N_{\text{BE}} ? \quad 1$$

The condensate dominates,
but some particles are kicked out
by the interaction (*not thermally*)

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no interaction	weak interaction
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The condensate dominates,
but some particles are kicked out
by the interaction (*not thermally*)

Strange idea introduced by Bogolyubov

$$N_0 = \langle a_0^\dagger a_0 \rangle ? \quad 1 \Rightarrow \langle a_0^\dagger a_0 \rangle ? \quad a_0^\dagger a_0 - a_0 a_0^\dagger = 1 \Rightarrow \text{like } c\text{-numbers}$$

$$a_0 \approx \sqrt{N_0}, \quad a_0^\dagger \approx \sqrt{N_0}$$

$$N = N_0 + \sum_{k \neq 0} a_k^\dagger a_k \quad \dots \text{mixture of } c\text{-numbers and } q\text{-numbers}$$

Approximate Hamiltonian

Keep at most two particles out of the condensate, use $a_0 \approx \sqrt{N_0}$, $a_0^\dagger \approx \sqrt{N_0}$

$$H = \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_k^\dagger a_k + \frac{1}{2} V^{-1} \sum_{kk'q} U_q a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

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$$\rightarrow \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_k^\dagger a_k + \frac{UN_0}{2V} \sum_{k \neq 0} \left\{ a_k^\dagger a_{-k}^\dagger + 4a_k^\dagger a_k + a_k a_{-k} \right\} + \frac{UN_0^2}{2V}$$

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3rd & 4th order
neglected

2nd order
pair excitations

0th order
condensate

1st order

is zero

violates k-conservation

Approximate Hamiltonian

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2nd order

pair excitations

$$a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}} a_{\frac{k}{2}}$$

$$a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}} a_{\frac{k}{2}}$$

$$a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}}^\dagger a_{\frac{k}{2}} a_{\frac{k}{2}}$$

$$a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

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$a_{\underbrace{k+q}_0}^\dagger a_{\underbrace{k'-q}_0}^\dagger a_{k'} a_k$
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The idea: replace the unknown condensate occupation by the known particle number neglecting again higher than pair excitations

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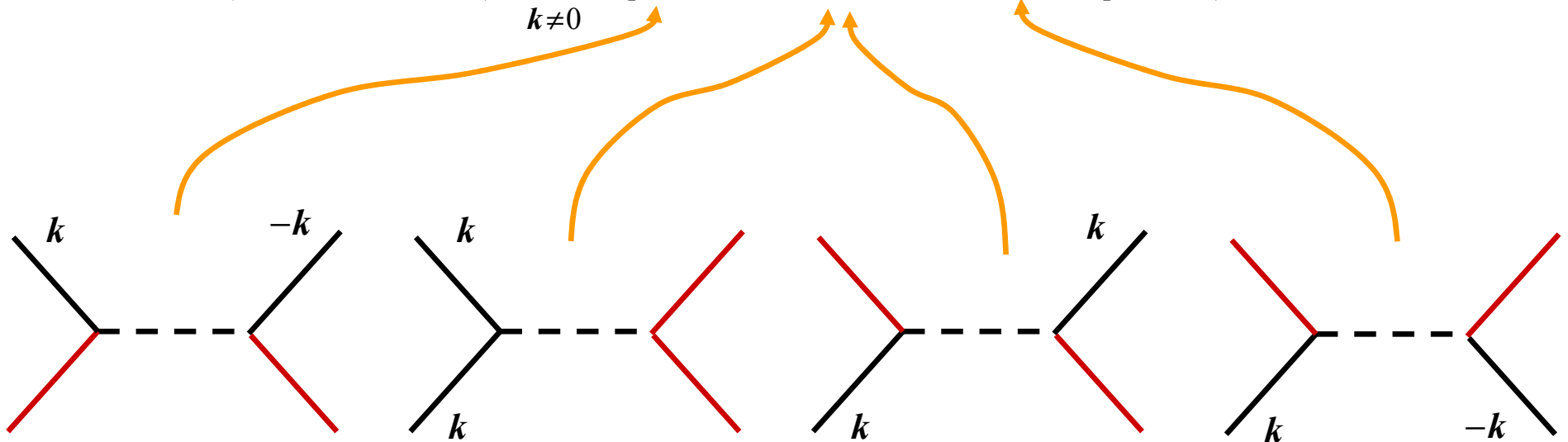
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— condensate particle

Bogolyubov transformation

Last rearrangement

$$H = \frac{1}{2} \sum_{\mathbf{k}} \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + gn \right) \{ a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} \} + \frac{gn}{2} \sum_{\mathbf{k}} \{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}} \} + \frac{gN^2}{2V}$$

mean field anomalous

Conservation properties: momentum ... YES, particle number ... NO

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NEW FIELD OPERATORS notice momentum conservation!!

$$b_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} + v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger$$
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requirements

① New operators should satisfy the boson commutation rules

$$\left[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger \right] = \delta_{\mathbf{k}\mathbf{k}'}, \quad \left[b_{\mathbf{k}}, b_{\mathbf{k}'} \right] = 0, \quad \left[b_{\mathbf{k}}^\dagger, b_{\mathbf{k}'}^\dagger \right] = 0$$

Bogolyubov transformation

Last rearrangement

$$H = \frac{1}{2} \sum_{\mathbf{k}} \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + gn \right) \left\{ a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} \right\} + \frac{gn}{2} \sum_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}} \right\} + \frac{gN^2}{2V}$$

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$$\left[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger \right] = \delta_{\mathbf{k}\mathbf{k}'}, \quad \left[b_{\mathbf{k}}, b_{\mathbf{k}'} \right] = 0, \quad \left[b_{\mathbf{k}}^\dagger, b_{\mathbf{k}'}^\dagger \right] = 0$$

$$\text{iff } u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$$

Bogolyubov transformation

Last rearrangement

$$H = \frac{1}{2} \sum_{\mathbf{k}} \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + gn \right) \left\{ a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} \right\} + \frac{gn}{2} \sum_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}} \right\} + \frac{gN^2}{2V}$$

mean field
anomalous

Conservation properties: momentum ... YES, particle number ... NO

NEW FIELD OPERATORS notice momentum conservation!!

$$\begin{array}{l|l} b_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} + v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger & a_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \\ b_{-\mathbf{k}}^\dagger = v_{\mathbf{k}} a_{\mathbf{k}} + u_{\mathbf{k}} a_{-\mathbf{k}}^\dagger & a_{-\mathbf{k}}^\dagger = -v_{\mathbf{k}} b_{\mathbf{k}} + u_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \end{array}$$

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Bogolyubov transformation

- ② In terms of the new operators, the anomalous terms in the Hamiltonian have to vanish

$$\begin{aligned} H &= \frac{1}{2} \sum \left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn \right) \left\{ a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}} \right\} + \frac{gn}{2} \sum_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}} \right\} + \frac{gN^2}{2V} \\ &= \sum \left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn \right) \left\{ u_{\mathbf{k}}^2 b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + v_{\mathbf{k}}^2 b_{\mathbf{k}} b_{\mathbf{k}}^\dagger + u_{\mathbf{k}} v_{\mathbf{k}} (b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{\mathbf{k}} b_{-\mathbf{k}}) \right\} \\ &\quad + \frac{gn}{2} \sum_{\mathbf{k}} 2u_{\mathbf{k}} v_{\mathbf{k}} \left\{ (b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{\mathbf{k}} b_{\mathbf{k}}^\dagger) + (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) (b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{\mathbf{k}} b_{-\mathbf{k}}) \right\} \\ &\quad + \frac{gN^2}{2V} \end{aligned}$$

$$\Rightarrow \left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn \right) u_{\mathbf{k}} v_{\mathbf{k}} + \frac{gn}{2} (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) = 0$$
$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$$

$$u_{\mathbf{k}}^2 = \left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn + \varepsilon(\mathbf{k}) \right) / 2\varepsilon(\mathbf{k}) \quad v_{\mathbf{k}}^2 = \left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn - \varepsilon(\mathbf{k}) \right) / 2\varepsilon(\mathbf{k})$$

$$\varepsilon(\mathbf{k}) = \sqrt{\left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn \right)^2 - (gn)^2}$$

Bogolyubov transformation – result

Without quoting the transformation matrix

$$H = \frac{1}{2} \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \{ b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}} \} + \frac{gN^2}{12V} + \text{higher order constant}$$

independent quasiparticles ground state energy E

$$\varepsilon(\mathbf{k}) = \sqrt{\left(\frac{\hbar^2}{2m} \mathbf{k}^2 + gn\right)^2 - (gn)^2} = \sqrt{\frac{\hbar^2}{2m} \mathbf{k}^2} \sqrt{\frac{\hbar^2}{2m} \mathbf{k}^2 + 2gn}$$

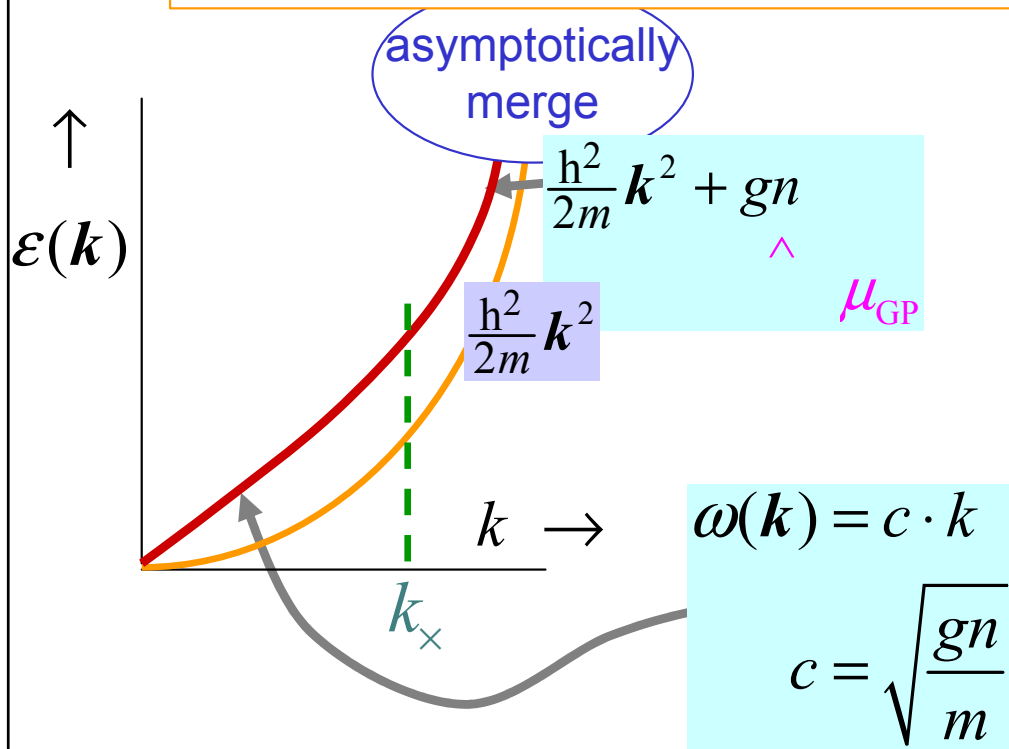
Bogolyubov transformation – result

Without quoting the transformation matrix

$$H = \frac{1}{2} \sum \epsilon(k) b_k^\dagger b_k + \frac{gN^2}{2V} + \text{higher order constant}$$

ind. quasi-particles ground state energy E

$$\epsilon(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m} + gn\right)^2 - (gn)^2} = \sqrt{\frac{\hbar^2 k^2}{2m}} \sqrt{\frac{\hbar^2 k^2}{2m} + 2gn}$$



high energy region

quasi-particles are nearly just particles

sound region

quasi-particles are collective excitations

cross-over

$$k_x = \sqrt{\frac{4mgn}{\hbar^2}}$$

defines scale for k

More about the sound part of the dispersion law

- Entirely dependent on the interactions, both the magnitude of the velocity and the linear frequency range determined by g

$$\omega(\mathbf{k}) = c \cdot k$$

- Can be shown to really be a sound:

$$\text{a) } c = \sqrt{\frac{\kappa}{\rho}} = \sqrt{\frac{V \partial_{VV} E}{m \cdot n}}, \quad E = \frac{gN^2}{2V} + L$$

$$c = \sqrt{\frac{gn}{m}}$$

$$\text{b) } b_k^\dagger = u_k a_k^\dagger + v_k a_{-k} \xrightarrow{k \rightarrow 0} u_k (a_k^\dagger + a_{-k})$$

$$n_k = \sum_q a_{q-k/2}^\dagger a_{q+k/2} \approx (a_k^\dagger + a_{-k})$$

- Even a weakly interacting gas exhibits superfluidity; the ideal gas does not.
- The phonons are actually Goldstone modes corresponding to a broken symmetry
- The dispersion law has no **roton** region, contrary to the reality in ^4He
- The dispersion law bends upwards \Rightarrow quasi-particles are unstable, can decay

Particles and quasi-particles

At zero temperature, there are no quasi-particles, just the condensate.

Things are different with the true particles. Not all particles are in the condensate, but they are not thermally agitated in an incoherent way, they are a part of the fully coherent ground state

$$\langle a_k^\dagger a_k \rangle = \langle (-v_k b_k + u_k b_{-k}^\dagger)(u_k b_{-k} - v_k b_k^\dagger) \rangle = v_k^2 \neq 0$$

The total fraction of particles outside of the condensate is

$$\frac{N - N_0}{N} \approx \frac{8}{3\sqrt{\pi}} \frac{a_s^{3/2} n^{1/2}}{\sqrt{a_s^3 n}}$$

square root of the
gas parameter
is
the expansion
variable

What is the Bogolyubov approximation about

The results for various quantities are

$$\begin{aligned} N_0 &\approx N \times \left(1 - \frac{8}{3\sqrt{\pi}} a_s^{3/2} n^{1/2} \right) \\ E &\approx \frac{gn}{2} N \times \left(1 + \frac{128}{15\sqrt{\pi}} a_s^{3/2} n^{1/2} \right) \\ \mu &\approx gn \times \left(1 + \frac{32}{3\sqrt{\pi}} a_s^{3/2} n^{1/2} \right) \end{aligned}$$

square root of the gas parameter
 $\sqrt{a_s^3 n}$
is the expansion variable

general
pattern

$$[\text{BG}] \approx [\text{GP}] \times \left(1 + \frac{L}{L \sqrt{\pi}} a_s^{3/2} n^{1/2} \right)$$

The Bogolyubov theory is the lowest order correction to the mean field (Gross-Pitaevskii) approximation

It provides thus the criterion for the validity of the mean field results

It is the simplest genuine field theory for quantum liquids with a condensate

Trying to understand the Bogolyubov
method

Notes to the contents of the Bogolyubov theory

- The first consistent microscopic theory of the ground state and elementary excitations (quasi-particles) for a quantum liquid (1947)
- The quantum condensate turns into the classical order parameter in the thermodynamic limit $\mathcal{N} \rightarrow \infty, \mathcal{V} \rightarrow \infty, \mathcal{N} / \mathcal{V} = n = \text{const.}$
- The Bogolyubov transformation became one of the standard technical means for treatment of "anomalous terms" in many body Hamiltonians (...de Gennes)

- Central point of the theory is the assumption

$$a_0 \approx \sqrt{N_0}, \quad a_0^\dagger \approx \sqrt{N_0}$$

- Its introduction and justification intuitive, surprisingly lacks mathematical rigor. Two related problems:

lowering operator \longleftarrow ? \longrightarrow gauge symmetry, s. rule

$$a_0 |G, N\rangle \in \mathbf{H}_{N-1} \quad \langle G, N | a_0 | G, N\rangle = \sqrt{N_0} \quad \langle a_0 \rangle = 0$$

- Additional assumptions: something of a crutch/bar to study of finite systems
 - homogeneous system
 - infinite system

Infinity as a problem: philosophical, mathematical, physical

What next ???

- Off-diagonal long range order and the Bogolyubov ground state
- Coherent state as the GP vacuum
- Spontaneous symmetry breaking

The end