Cold atoms

Lecture 7.

21st February, 2007

Preliminary plan/reality in the fall term

Lecture 1 …	Something about everything (see next slide) The textbook version of BEC in extended systems	Sep 22
Lecture 2 …	thermodynamics, grand canonical ensemble, extended gas: ODLRO, nature of the BE phase transition	Oct 4
Lecture 3 …	atomic clouds in the traps – independent bosons, what is BEC?, "thermodynamic limit", properties of OPDM	Oct 18
Lecture 4 …	atomic clouds in the traps – interactions, GP equation at zero temperature, variational prop., chem. potential	Nov 1
Lecture 5 …	Infinite systems: Bogolyubov theory	Nov 15
Lecture 6 …	BEC and symmetry breaking, coherent states	Nov 29
Lecture 7 …	Time dependent GP theory. Finite systems: BEC theory preserving the particle number	

Recapitulation

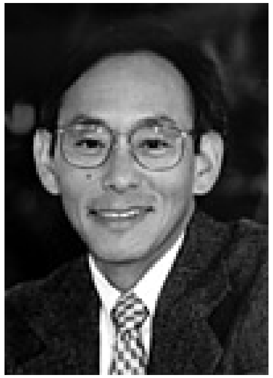
Offering many new details and
alternative angles of view

BEC in atomic clouds

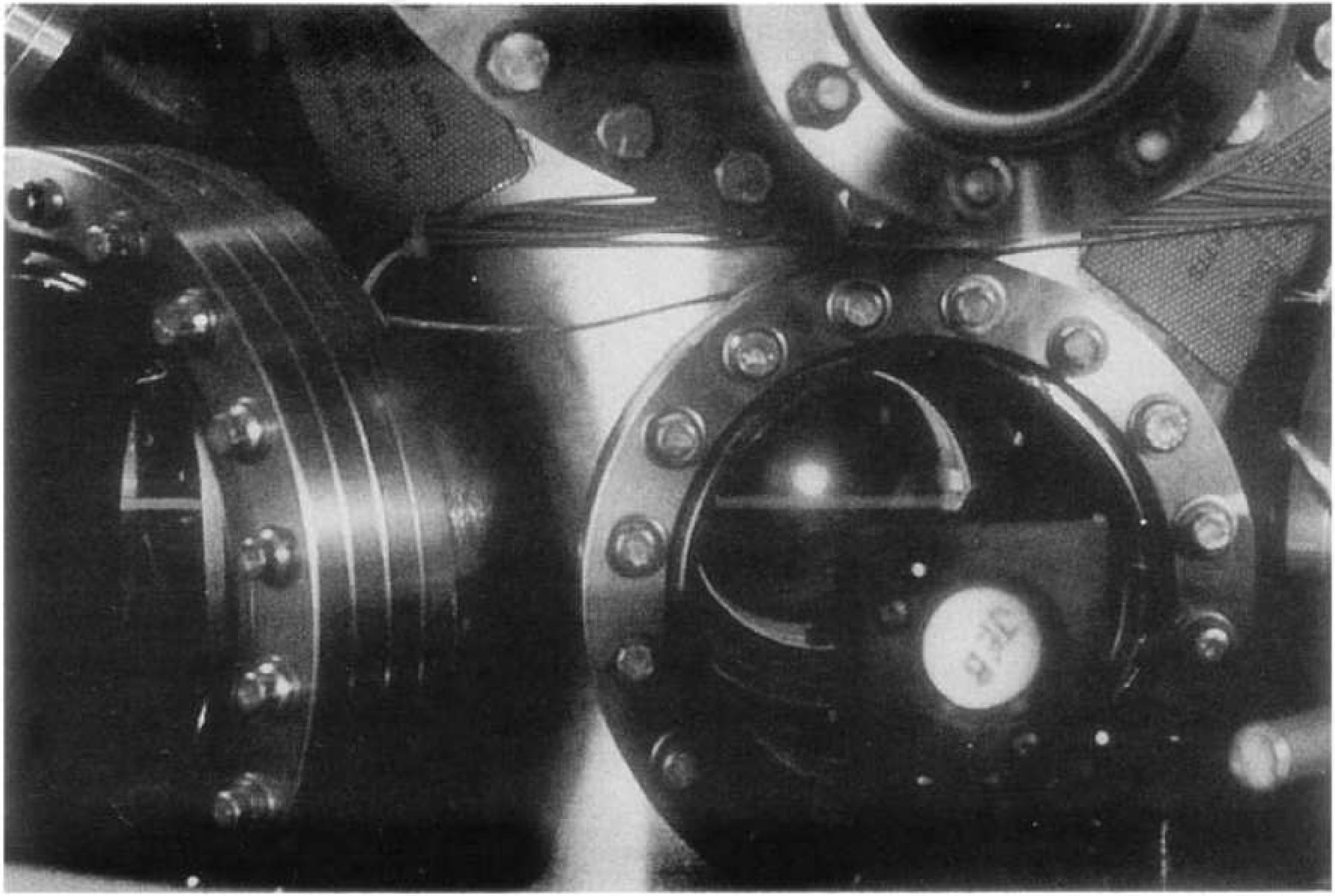
Nobelists I. Laser cooling and trapping of atoms

The Nobel Prize in Physics 1997

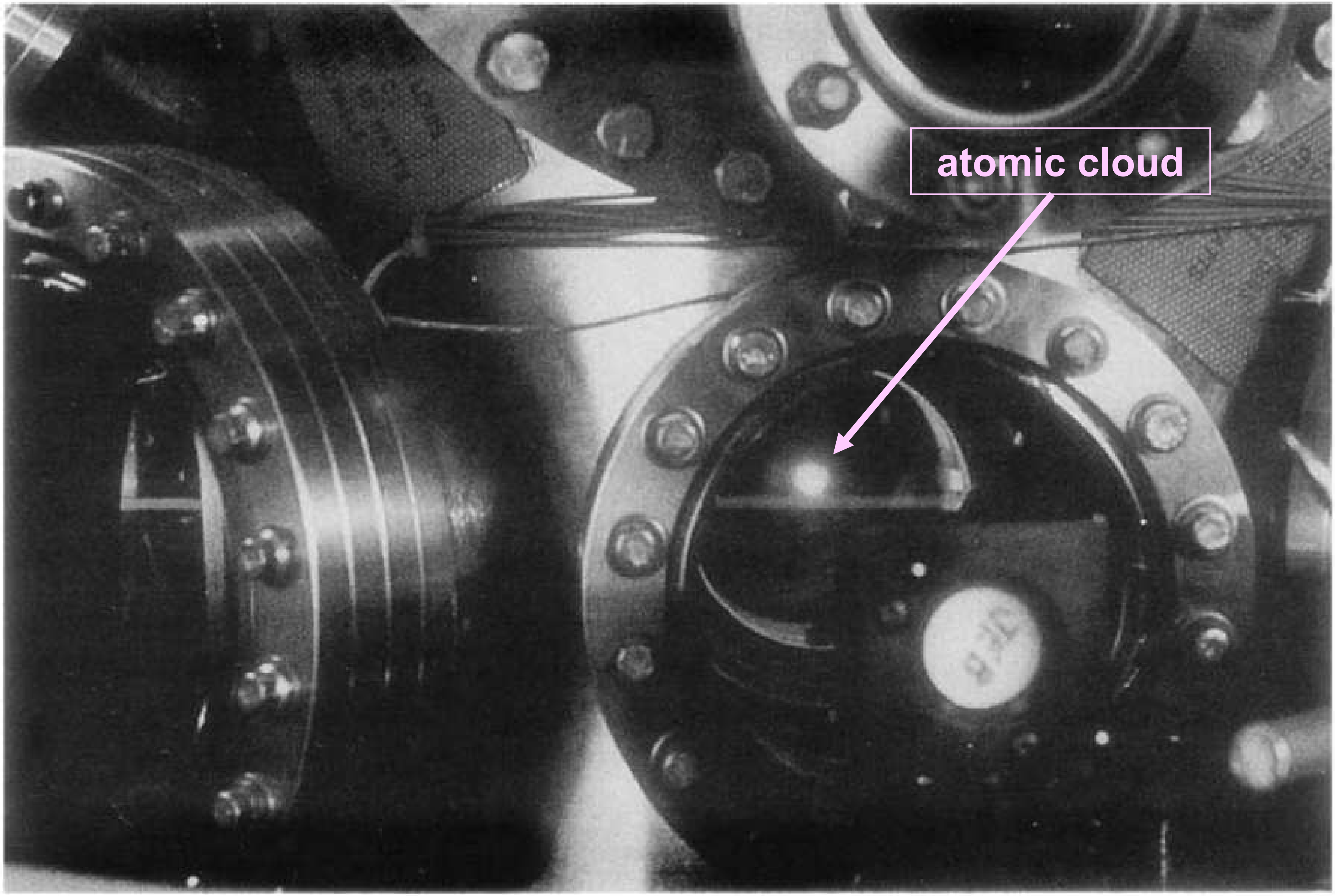
"for development of methods to cool and trap atoms with laser light"

		
Steven Chu	**Claude Cohen-Tannoudji**	**William D. Phillips**
1/3 of the prize	1/3 of the prize	1/3 of the prize
USA	France	USA
Stanford University Stanford, CA, USA	Collège de France; École Normale Supérieure Paris, France	National Institute of Standards and Technology Gaithersburg, MD, USA
b. 1948	b. 1933 (in Constantine, Algeria)	b. 1948

Doppler cooling in the Chu lab



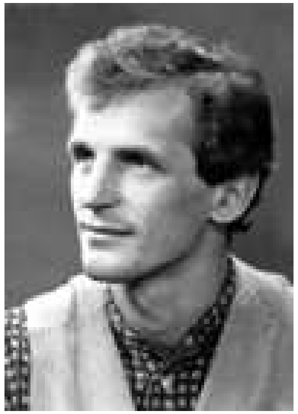
Doppler cooling in the Chu lab

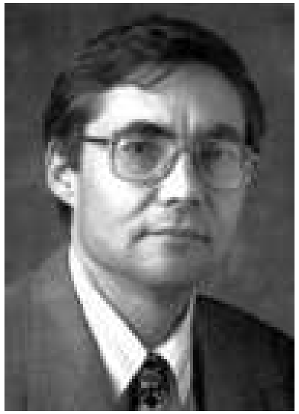


Nobelists II. BEC in atomic clouds

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"

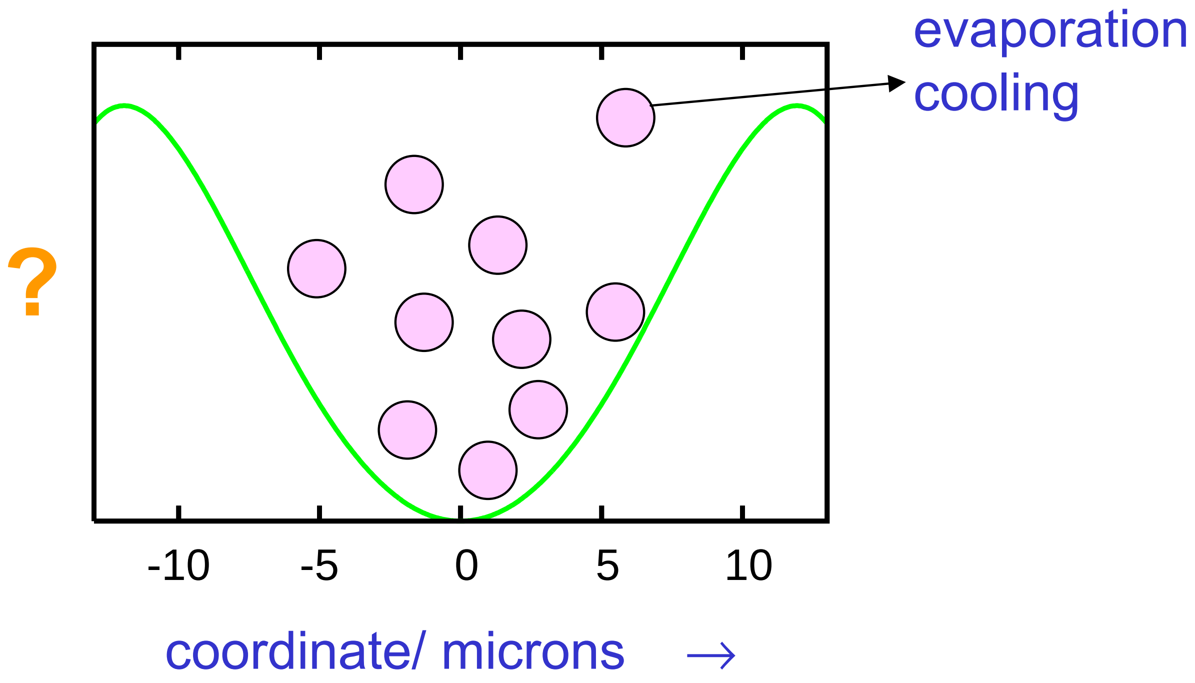




Eric A. Cornell	Wolfgang Ketterle	Carl E. Wieman
1/3 of the prize	1/3 of the prize	1/3 of the prize
USA	Federal Republic of Germany	USA
University of Colorado, JILA Boulder, CO, USA	Massachusetts Institute of Technology (MIT) Cambridge, MA, USA	University of Colorado, JILA Boulder, CO, USA
b. 1961	b. 1957	b. 1951

Trap potential

Typical profile

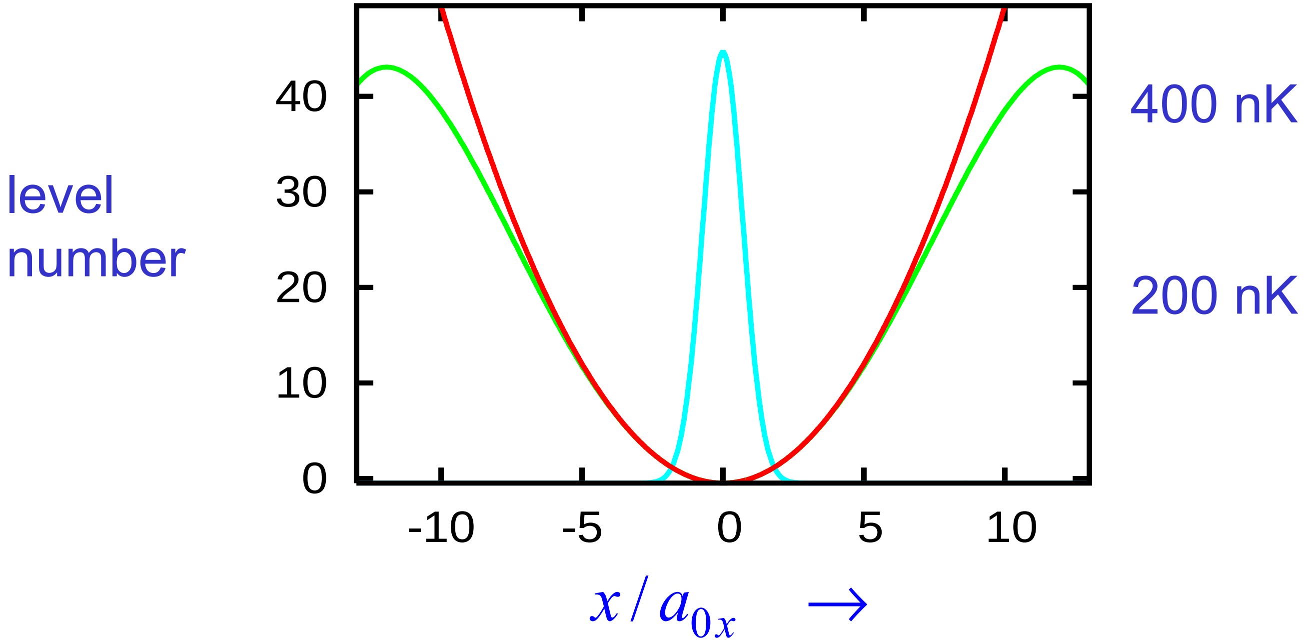


This is just one direction

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



$$^{87}\mathrm{Rb}$$
$$a_0 = 1\,\mu\mathrm{m}$$
$$\hbar\omega = 10\ \mathrm{nK}$$
$$N \sim 10^6\ \mathrm{at.}$$

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

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

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

characteristic energy

characteristic length

BEC observed by TOF in the velocity distribution

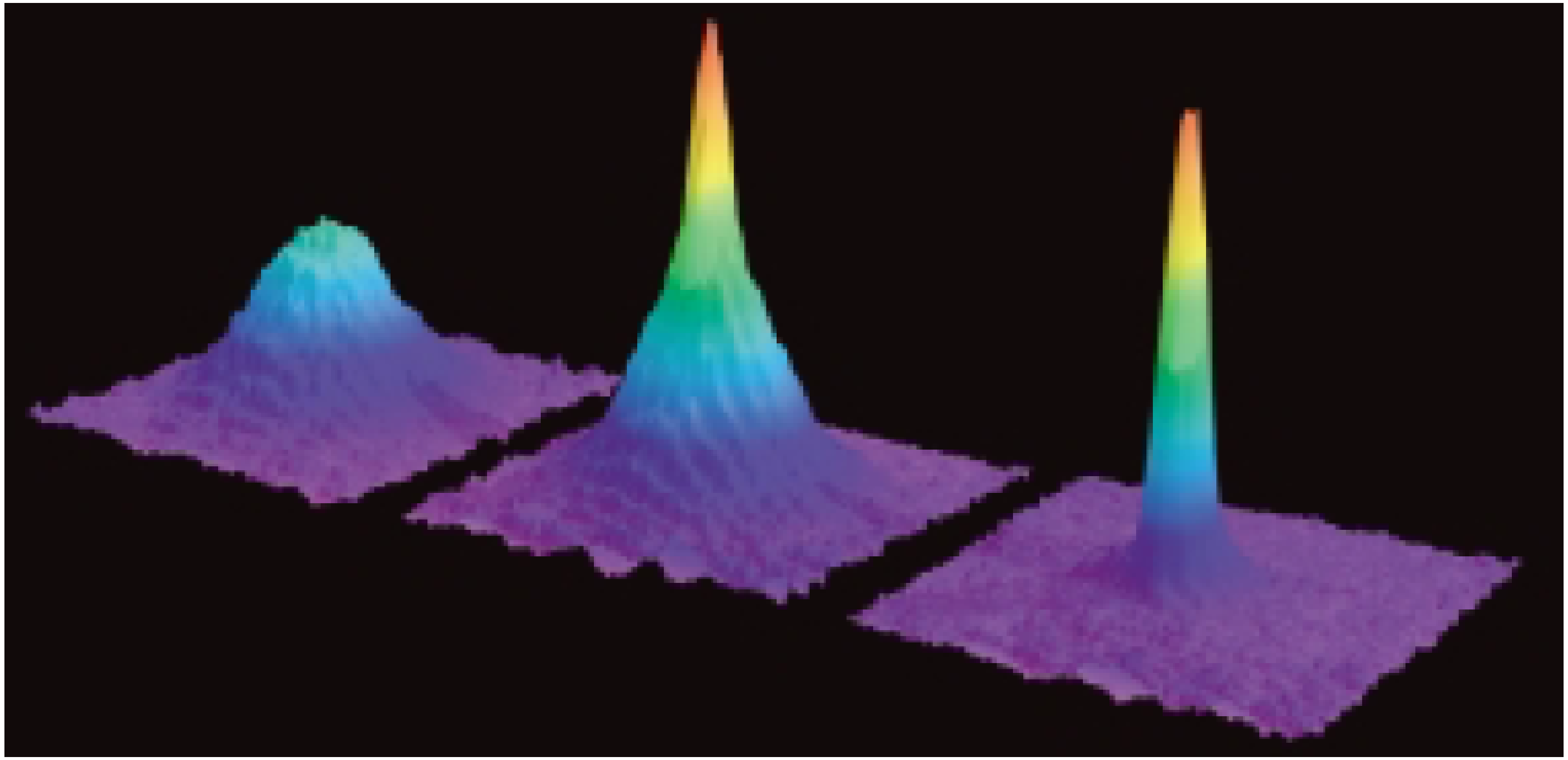
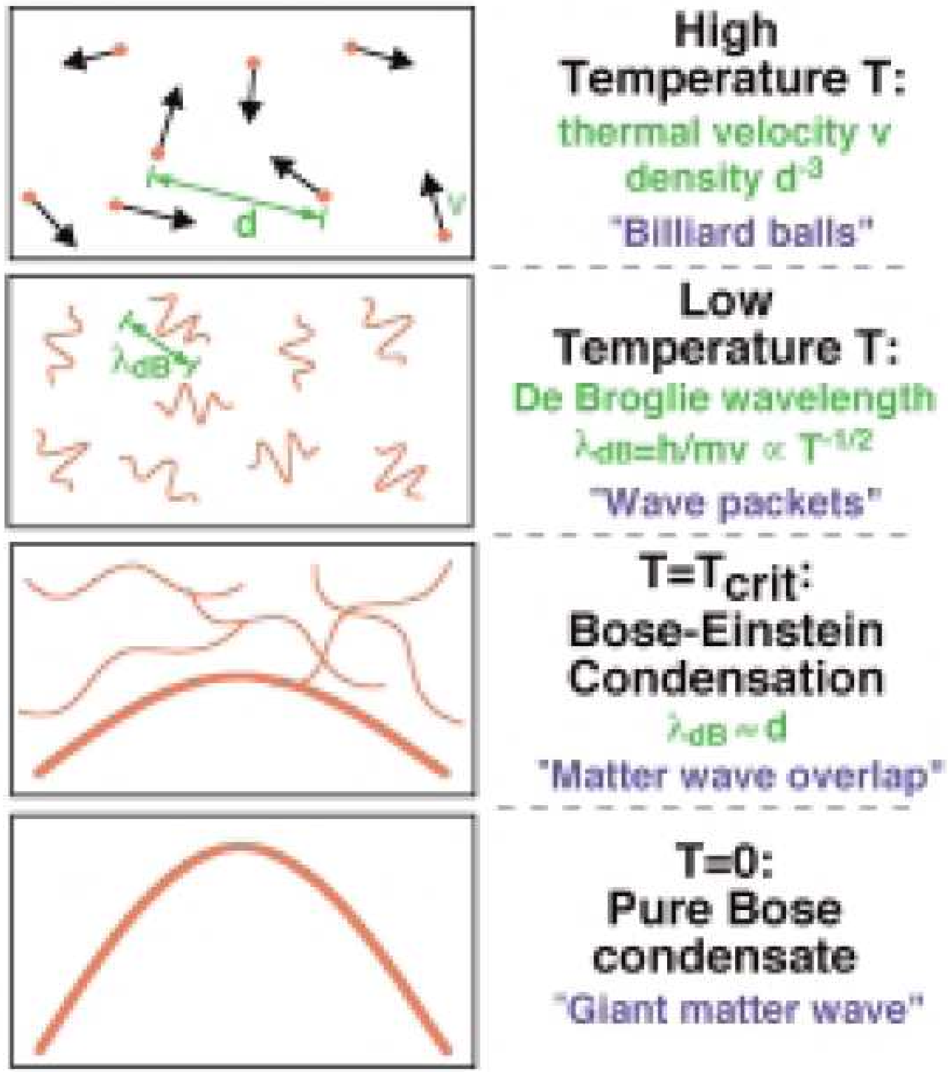


Figure 7. Observation of Bose-Einstein condensation by absorption imaging. Shown is absorption vs. two spatial dimensions. The Bose-Einstein condensate is characterized by its slow expansion observed after 6 ms time-of-flight. The left picture shows an expanding cloud cooled to just above the transition 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 μK.

Ketterle explains BEC to the King of Sweden



Simple estimate of T_C (following the Ketterle slide)

The quantum breakdown sets on when

the wave clouds of the atoms start overlapping

mean interatomic distance → $$\left(\frac{V}{N}\right)^{\frac{1}{3}} \approx \frac{h}{\sqrt{mk_B T_c}}$$ ← thermal de Broglie wavelength

Critical temperature

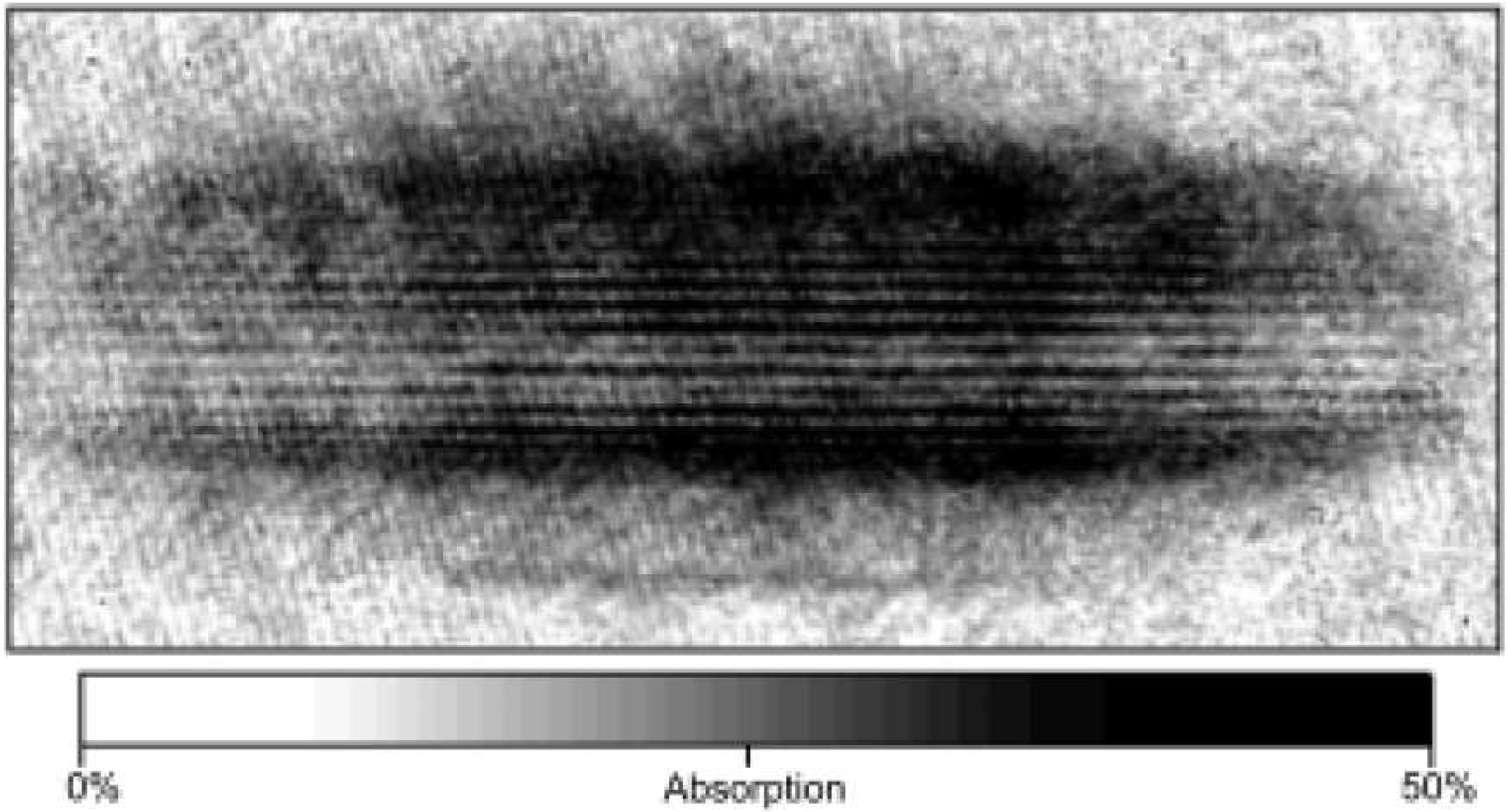
ESTIMATE

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

TRUE EXPRESSION

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

Interference of atoms



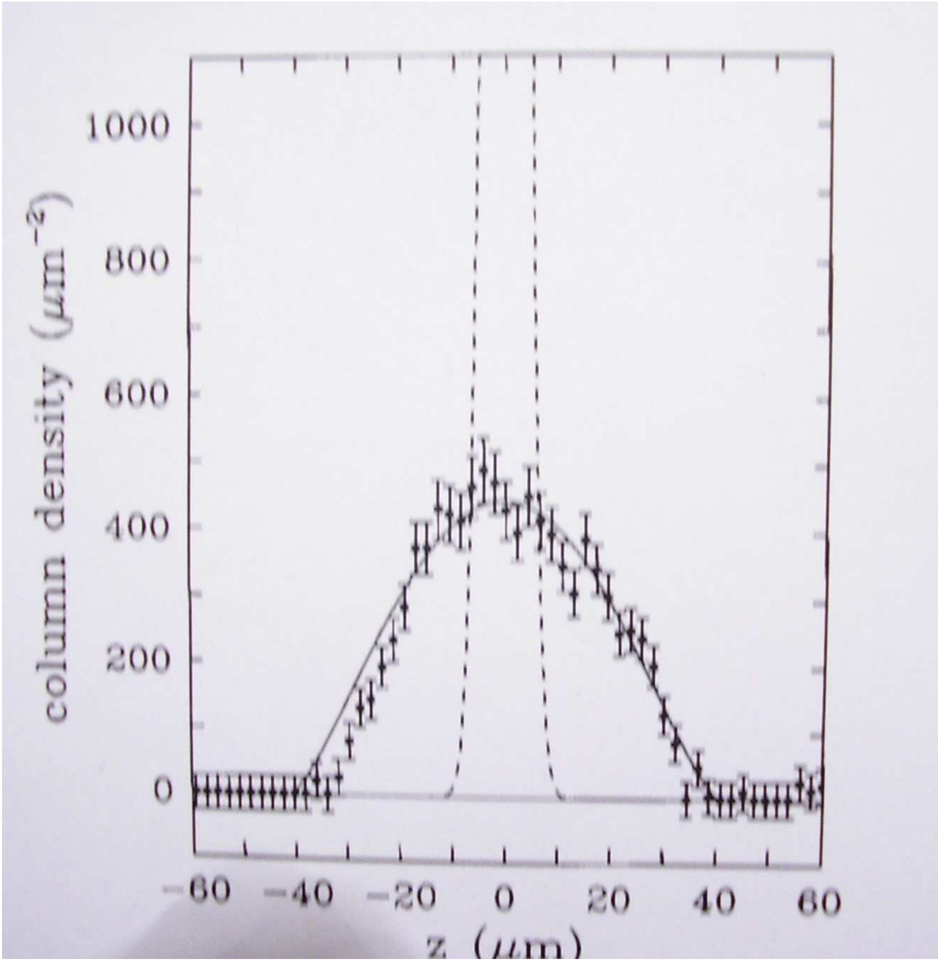
Two coherent condensates are interpenetrating and interfering.
Vertical stripe width …. 15 μm
Horizontal extension of the cloud …. 1,5mm

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

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

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

replaced by an effective potential, Fermi pseudopotential

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

$$g = \frac{4\pi a_s \hbar^2}{m}, \qquad a_s \quad \ldots \quad \text{the scattering length}$$

Experimental data

	C_6 (a.u.)	β_6 (a.u.)	a_0 (a.u.)
$^7Li_2$	1388 [a]	65	−27.3 [b]
$^{23}Na_2$	1472 [c]	89	77.3 [d]
$^{39}K_2$	3897 [e]	129	−33 [f]
$^{85}Rb_2$	4700 [g]	164	−369 [g]
$^{87}Rb_2$	4700 [g]	165	106 [g]
$^{133}Cs_2$	6890 [h]	197	2400 [h]

Mean-field treatment of interacting atoms

Many-body Hamiltonian and the Hartree approximation

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

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

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

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

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

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

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

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

Putting

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

we obtain a closed equation for the order parameter:

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

The lowest level coincides with the chemical potential

This is the celebrated Gross-Pitaevskii equation.

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

Then

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

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

Gross-Pitaevskii equation – homogeneous gas

The GP equation simplifies

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

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

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

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

$$g\left|\Psi(\boldsymbol{r})\right|^2\Psi(\boldsymbol{r}) = \mu\Psi(\boldsymbol{r}) \quad \text{... GP equation}$$

$$\boxed{\mu = g\left|\Psi(\boldsymbol{r})\right|^2 = gn}$$

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

Field theoretic reformulation (second quantization)

Purpose: go beyond the GP approximation, treat also the excitations

Field operator for spin-less bosons

Definition by commutation relations

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

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

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

$$\langle\boldsymbol{r}|\kappa\rangle=\varphi_{\kappa}(\boldsymbol{r}) \qquad \langle\boldsymbol{r}|\psi\rangle=\sum\langle\boldsymbol{r}|\kappa\rangle\langle\kappa|\psi\rangle$$

decomposition of the field operator

$$\psi(\boldsymbol{r}) = \sum\varphi_{\kappa}(\boldsymbol{r})\ a_{\kappa}, \quad a_{\kappa}=\text{"}\langle\kappa|\psi\rangle\text{"}=\int \mathrm{d}^3\,\varphi^*_{\kappa}(\boldsymbol{r})\psi(\boldsymbol{r})$$

$$\psi^{\dagger}(\boldsymbol{r}) = \sum\varphi^*_{\kappa}(\boldsymbol{r})\ a^{\dagger}_{\kappa}$$

commutation relations

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

Action of the field operators in the Fock space

basis of single-particle states

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

$$\langle\boldsymbol{r}|\kappa\rangle = \varphi_\kappa(\boldsymbol{r}) \qquad \langle\boldsymbol{r}|\psi\rangle = \sum\langle\boldsymbol{r}|\kappa\rangle\langle\kappa|\psi\rangle$$

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, …**

$$\{\kappa_1, \kappa_2, \kappa_3, \ldots, \kappa_p, \ldots\}$$

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

$$\boxed{\begin{aligned} a_p^\dagger|n_1, n_2, n_3, \ldots, n_p, \ldots\rangle &= \sqrt{n_p+1}\,|n_1, n_2, n_3, \ldots, n_p+1, \ldots\rangle \\ a_p|n_1, n_2, n_3, \ldots, n_p, \ldots\rangle &= \sqrt{n_p}\,|n_1, n_2, n_3, \ldots, n_p-1, \ldots\rangle \end{aligned}}$$

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:

$$\left\langle n_1, n_2, n_3, \ldots, n_p, \ldots \right| a_p \left| n_1, n_2, n_3, \ldots, n_p, \ldots \right\rangle =$$
$$\left\langle n_1, n_2, n_3, \ldots, n_p, \ldots \right| \sqrt{n_p} \left| n_1, n_2, n_3, \ldots, n_p - 1, \ldots \right\rangle = 0$$

Creating a Fock state from the vacuum:

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

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)

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

$$\psi^\dagger(\boldsymbol{r}) = V^{-1/2}\sum \mathrm{e}^{-\mathrm{i}\boldsymbol{kr}}\ a^\dagger_{\boldsymbol{k}} = V^{-1/2}\sum \mathrm{e}^{\mathrm{i}\boldsymbol{kr}}\ a^\dagger_{\boldsymbol{-k}}$$

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

⌘ important, because the combination

$$u\cdot a_{\boldsymbol{k}} + v\cdot a^\dagger_{\boldsymbol{-k}}$$

corresponds to the momentum transfer by $\boldsymbol{k}$

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

$$\left[a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}\right] = \delta_{\boldsymbol{kk}'}, \quad \left[a_{\boldsymbol{k}}, a_{\boldsymbol{k}'}\right] = 0, \quad \left[a^\dagger_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}\right] = 0$$

Operators

Additive observable

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

General definition of the one particle density matrix – OPDM

$$\langle X\rangle = \left\langle \iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\,\psi^\dagger(\boldsymbol{r})\langle \boldsymbol{r}|X|\boldsymbol{r}'\rangle\psi(\boldsymbol{r}')\right\rangle = \iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\,\langle \boldsymbol{r}|X|\boldsymbol{r}'\rangle \underbrace{\langle \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')\rangle}_{\langle \boldsymbol{r}'|\rho|\boldsymbol{r}\rangle}$$

$$\equiv \iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\,\langle \boldsymbol{r}|X|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\rho|\boldsymbol{r}\rangle = \mathrm{Tr}\,X\rho$$

Particle number

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

$$N = \sum a_\kappa^\dagger a_\kappa$$

Momentum

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

$$\boldsymbol{P} = \sum \hbar\boldsymbol{k}\cdot a_\kappa^\dagger a_\kappa$$

Hamiltonian

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

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

$$\rightarrow \int \mathrm{d}^3\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) \right) \psi(\boldsymbol{r})$$

$$+\tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

Hamiltonian

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

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

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

$$\to \int \mathrm{d}^3\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) \right) \psi(\boldsymbol{r})$$

acts in the whole Fock space $\mathbf{F}$

$$+\tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

Hamiltonian

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

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

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acts in the whole Fock space $\mathbf{F}$

$$+\tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

but …

Particle number conservation

$$[H, N] = 0$$

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

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

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*)

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

Typical selection rule

$$\boxed{\langle \psi(\boldsymbol{r}) \rangle = \mathrm{Tr}\, \psi(\boldsymbol{r}) P = 0}$$

is a consequence: (similarly $\langle \psi\psi \rangle = 0, \langle \psi\psi\psi^\dagger \rangle = 0, \dots$)

Proof:

$$0 = \mathrm{Tr}\big(\psi[\mathcal{N}, \mathcal{P}]\big) = \mathrm{Tr}\big(\mathcal{P}[\psi, \mathcal{N}]\big) = \mathrm{Tr}\big(\mathcal{P}\psi\big) \qquad \mathrm{Tr}\, A[B,C] = \mathrm{Tr}\, C[A,B]$$

$$[\psi(x), \textstyle\int \mathrm{d}\, x' \psi^\dagger(x')\psi(x')] = \int \mathrm{d}\, x' (\psi^\dagger(x')[\psi(x), \psi(x')] + [\psi(x), \psi^\dagger(x')]\psi(x')) = \psi(x)$$

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

$$[H, N] = 0 \quad \Leftrightarrow \quad \mathrm{e}^{\mathrm{i}N\varphi} H \, \mathrm{e}^{-\mathrm{i}N\varphi} = H \quad \text{unitary transform}$$

The equilibrium states have then the same invariance property:

$$[N, \rho] = 0 \quad \Leftrightarrow \quad \mathrm{e}^{-\mathrm{i}N\varphi} \rho \, \mathrm{e}^{\mathrm{i}N\varphi} = \rho$$

Selection rule rederived:

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

$$(1 - \mathrm{e}^{\mathrm{i}\varphi})\, \mathrm{Tr}\, \psi\rho = 0 \quad \Rightarrow \mathrm{Tr}\, \psi(\boldsymbol{r})\rho = \langle \psi(\boldsymbol{r}) \rangle = 0$$

Hamiltonian of a homogeneous gas

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq} \sum_b U(\boldsymbol{r}_a - \boldsymbol{r}_b), \qquad \boxed{V = \text{const.}}$$

$$= \int \mathrm{d}^3\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V \right) \psi(\boldsymbol{r}) + \tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

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

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq b} \sum U(\boldsymbol{r}_a - \boldsymbol{r}_b), \qquad \boxed{V = \text{const.}}$$

$$= \int \mathrm{d}^3\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \Big(-\tfrac{\hbar^2}{2m}\Delta + V\Big) \psi(\boldsymbol{r}) + \tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

- Translationally invariant system … how to formalize (*and to learn more about the gauge invariance*)

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

Hamiltonian of the homogeneous gas

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq b}\sum U(\boldsymbol{r}_a - \boldsymbol{r}_b), \qquad \boxed{V = \text{const.}}$$

$$= \int \mathrm{d}^3 \boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V \right) \psi(\boldsymbol{r}) + \tfrac{1}{2} \iint \mathrm{d}^3 \boldsymbol{r}\, \mathrm{d}^3 \boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r} - \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

- Translationally invariant system … how to formalize (*and to learn more about the gauge invariance*)

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

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

Translation in the one-particle orbital space

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

Hamiltonian of the homogeneous gas

$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a \neq} \sum_b U(\boldsymbol{r}_a - \boldsymbol{r}_b), \qquad \boxed{V = \text{const.}}$$

$$= \int \mathrm{d}^3\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V \right) \psi(\boldsymbol{r}) + \tfrac{1}{2} \iint \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') U(\boldsymbol{r}-\boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

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$$\mathcal{T}(\boldsymbol{a}) \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots \boldsymbol{r}_p, \ldots \boldsymbol{r}_N) = \Psi(\boldsymbol{r}_1 - \boldsymbol{a}, \boldsymbol{r}_2 - \boldsymbol{a}, \boldsymbol{r}_3 - \boldsymbol{a}, \ldots \boldsymbol{r}_p - \boldsymbol{a}, \ldots \boldsymbol{r}_N - \boldsymbol{a})$$

$$= \prod \mathrm{e}^{-\mathrm{i}\, \boldsymbol{p}_\ell \boldsymbol{a}/\hbar}\, \Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N) = \mathrm{e}^{-\mathrm{i} \sum \boldsymbol{p}_\ell \boldsymbol{a}/\hbar}\, \Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N) = \mathrm{e}^{-\mathrm{i} \mathcal{P} \boldsymbol{a}/\hbar}\, \Psi(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N)$$

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$$=\prod \mathrm{e}^{-\mathrm{i}\,\boldsymbol{p}_\ell\boldsymbol{a}/\hbar}\,\Psi(\boldsymbol{r}_1,\dots\boldsymbol{r}_N)=\mathrm{e}^{-\mathrm{i}\sum\boldsymbol{p}_\ell\boldsymbol{a}/\hbar}\,\Psi(\boldsymbol{r}_1,\dots\boldsymbol{r}_N)=\mathrm{e}^{-\mathrm{i}\mathcal{P}\boldsymbol{a}/\hbar}\,\Psi(\boldsymbol{r}_1,\dots\boldsymbol{r}_N)$$

$$\boxed{\mathcal{T}(\boldsymbol{a})=\mathrm{e}^{-\mathrm{i}\mathcal{P}\boldsymbol{a}/\hbar}} \qquad \text{... compare} \quad O(\varphi)=\mathrm{e}^{-\mathrm{i}\mathcal{N}\varphi}$$

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$$H = \sum_a \frac{1}{2m} p_a^2 + V + \frac{1}{2} \sum_{a} \neq \sum_{b} U(\boldsymbol{r}_a - \boldsymbol{r}_b), \qquad \boxed{V = \text{const.}}$$

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$$\boxed{\mathcal{T}(\boldsymbol{a}) = \mathrm{e}^{-\mathrm{i} \mathcal{P} \boldsymbol{a}/\hbar}} \qquad \text{... compare} \quad O(\varphi) = \mathrm{e}^{-\mathrm{i} \mathcal{N} \varphi}$$

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

- Infinitesimal translation

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

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

Summary: two symmetries compared

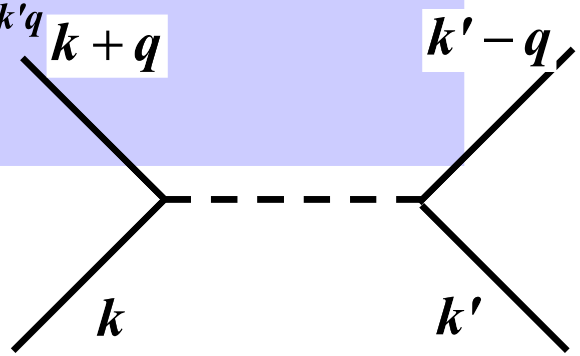
Gauge invariance of the 1st kind	Translational invariance
universal for atomic systems	specific for homogeneous systems
$O^\dagger(\varphi)\mathcal{H}O(\varphi)=\mathcal{H},\quad \varphi\in\langle 0,2\pi\rangle$ $O(\varphi)=\mathrm{e}^{-\mathrm{i}\mathcal{N}\varphi}$	$\mathcal{T}^\dagger(\boldsymbol{a})\mathcal{H}\mathcal{T}(\boldsymbol{a})=\mathcal{H},\quad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

Hamiltonian of the homogeneous gas

In the momentum representation

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

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



Momentum conservation

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

Particle number conservation

$$a^\dagger a^\dagger a \ a$$

Hamiltonian of the homogeneous gas

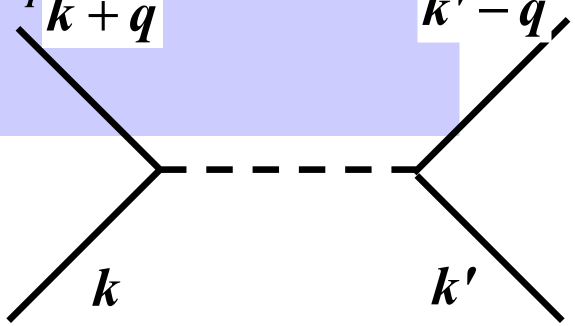
In the momentum representation

For the Fermi pseudopotential

$$U_{\boldsymbol{q}} = U_0 \equiv U \ (= g)$$

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

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



Momentum conservation

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

Particle number conservation

$$a^\dagger a^\dagger a \ a$$

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	weak interaction
$g = 0$	$g \neq 0$
$N = N_{\mathrm{BE}} = \left\langle a_0^\dagger a_0 \right\rangle \gg 1$	$N = N_{\mathrm{BE}} + \sum_{\boldsymbol{k} \neq 0} \left\langle a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \right\rangle \approx N_{\mathrm{BE}} \gg 1$

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

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The condensate dominates,
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Strange idea introduced by Bogolyubov

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

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

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

Approximate Hamiltonian

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

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

Approximate Hamiltonian

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$$H = \sum \frac{\hbar^2}{2m} \boldsymbol{k}^2 a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{1}{2} V^{-1} \sum_{\boldsymbol{kk'q}} U \; a_{\boldsymbol{k+q}}^\dagger, a_{\boldsymbol{k'-q}}^\dagger a_{\boldsymbol{k'}} a_{\boldsymbol{k}}$$

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

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

3rd & 4th order
neglected

2nd order
pair excitations

0th order
condensate

1st order
is zero
violates k-conservation

Approximate Hamiltonian

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

$$H = \sum \frac{\hbar^2}{2m}\boldsymbol{k}^2 a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \tfrac{1}{2}V^{-1}\sum_{\boldsymbol{kk'q}} U \; a_{\boldsymbol{k}+\boldsymbol{q}}^\dagger a_{\boldsymbol{k}'-\boldsymbol{q}}^\dagger a_{\boldsymbol{k}'} a_{\boldsymbol{k}}$$

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use $N_0 = N - \sum_{\boldsymbol{k}\neq 0} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}$

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

The idea: replace the unknown condensate occupation by the known particle number neglecting again higher than pair excitations

Approximate Hamiltonian

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$$= \sum \frac{\hbar^2}{2m}\boldsymbol{k}^2 a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{UN}{2V}\sum_{\boldsymbol{k}\neq 0}\left\{a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger + 2a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + a_{\boldsymbol{k}} a_{-\boldsymbol{k}}\right\} + \frac{UN^2}{2V}$$

The idea: replace the <u>unknown</u> condensate occupation by the <u>known</u> particle number neglecting again higher than pair excitations

Approximate Hamiltonian

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

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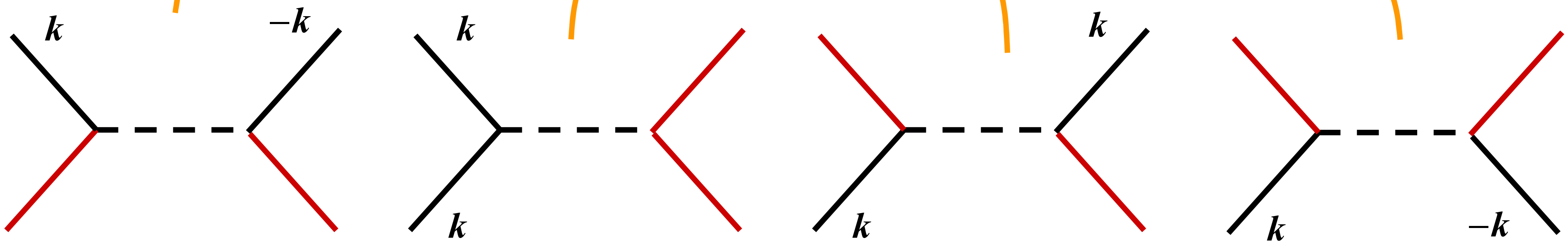


condensate particle

Bogolyubov transformation

Last rearrangement

$$H = \frac{1}{2}\sum \underbrace{\left(\frac{\hbar^2}{2m}\boldsymbol{k}^2 + gn\right)}_{\text{mean field}}\left\{a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} + a^\dagger_{-\boldsymbol{k}} a_{-\boldsymbol{k}}\right\} + \frac{gn}{2}\sum_{\boldsymbol{k}} \underbrace{\left\{a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}} + a_{\boldsymbol{k}} a_{-\boldsymbol{k}}\right\}}_{\text{anomalous}} + \frac{gN^2}{2V}$$

Conservation properties: momentum … YES, particle number … NO

Bogolyubov transformation

Last rearrangement

$$H=\frac{1}{2}\sum\underbrace{\left(\frac{\hbar^2}{2m}\boldsymbol{k}^2+gn\right)}_{\text{mean field}}\left\{a_{\boldsymbol{k}}^{\dagger}a_{\boldsymbol{k}}+a_{-\boldsymbol{k}}^{\dagger}a_{-\boldsymbol{k}}\right\}+\frac{gn}{2}\sum_{\boldsymbol{k}}\underbrace{\left\{a_{\boldsymbol{k}}^{\dagger}a_{-\boldsymbol{k}}^{\dagger}+a_{\boldsymbol{k}}a_{-\boldsymbol{k}}\right\}}_{\text{anomalous}}+\frac{gN^2}{2V}$$

Conservation properties: momentum … YES, particle number … NO

NEW FIELD OPERATORS notice momentum conservation!!

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

requirements

❶ New operators should satisfy the boson commutation rules

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

$$\textbf{iff}\quad u_{\boldsymbol{k}}^2-v_{\boldsymbol{k}}^2=1$$

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

Bogolyubov transformation – result

Without quoting the transformation matrix

$$H = \tfrac{1}{2}\sum \underbrace{\varepsilon(\boldsymbol{k})\left\{b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}} + b_{-\boldsymbol{k}}^{\dagger} b_{-\boldsymbol{k}}\right\}}_{\text{independent quasiparticles}} + \underbrace{\frac{gN^2}{2V} + \text{higher order constant}}_{\text{ground state energy } E}$$

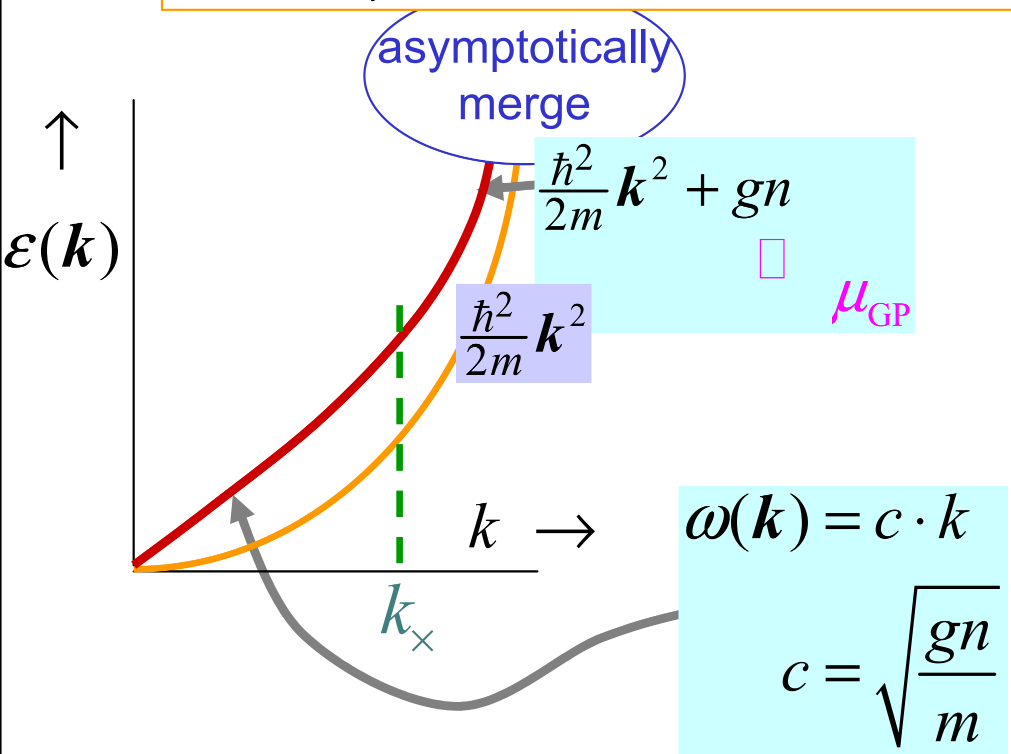
$$\varepsilon(\boldsymbol{k}) = \sqrt{\left(\frac{\hbar^2}{2m}\boldsymbol{k}^2 + gn\right)^2 - (gn)^2} = \sqrt{\frac{\hbar^2}{2m}\boldsymbol{k}^2}\sqrt{\frac{\hbar^2}{2m}\boldsymbol{k}^2 + 2gn}$$

Bogolyubov transformation – result

Without quoting the transformation matrix

$$H = \frac{1}{2}\sum \underbrace{\varepsilon(\boldsymbol{k})\, b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}}}_{\text{ind. quasi-particles}} + \underbrace{\frac{gN^2}{2V} + \text{higher order constant}}_{\text{ground state energy } E}$$

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



high energy region

quasi-particles are nearly just particles

sound region

quasi-particles are collective excitations

cross-over

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

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

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

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

- Can be shown to really be a sound:

$$c = \text{"}\sqrt{\frac{\kappa}{\rho}}\text{"} = \sqrt{\frac{V \partial_{VV} E}{m \cdot n}}\,, \qquad E = \frac{gN^2}{2V} + \cdots$$

- 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 ^{4}He
- 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 <u>all</u> 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

$$\left\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \right\rangle = \left\langle \left(-v_{\mathbf{k}} b_{\mathbf{k}} + u_{\mathbf{k}} b_{-\mathbf{k}}^{\dagger} \right) \left(u_{\mathbf{k}} b_{-\mathbf{k}} - v_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} \right) \right\rangle = v_{\mathbf{k}}^{2} \neq 0$$

The total fraction of particles outside of the condensate is

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

square root of the gas parameter is the expansion variable

What is the Bogolyubov approximation about

The results for various quantities are

$$N_0 \approx N\times\left(1 - \frac{8}{3\sqrt{\pi}} a_s^{3/2} n^{1/2}\right)$$

$$E \approx \frac{gn}{2} N\times\left(1 + \frac{128}{15\sqrt{\pi}} a_s^{3/2} n^{1/2}\right)$$

$$\mu \approx gn\times\left(1 + \frac{32}{3\sqrt{\pi}} a_s^{3/2} n^{1/2}\right)$$

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

general pattern

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

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 microsopic 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 $\mathcal{N} \to \infty, \quad \mathcal{V} \to \infty, \quad \mathcal{N} / \mathcal{V} = n = \text{ const.}$
- 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

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

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

$$\text{lowering operator} \quad \longleftarrow \quad ? \quad \longrightarrow \quad \text{gauge symmetry, s. rule}$$

$$a_0 \left| G, N \right\rangle \in \mathrm{H}_{N-1} \qquad \left\langle G, N \right| a_0 \left| G, N \right\rangle = \sqrt{N_0} \qquad \left\langle a_0 \right\rangle = 0$$

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

Infinity as a problem: philosophical, mathematical, physical

ODLRO in the Bogolyubov theory

Basic expressions for the OPDM for a homogeneous system

$$\langle \boldsymbol{r}' | \rho | \boldsymbol{r} \rangle = \left\langle \psi^\dagger(\boldsymbol{r}) \psi(\boldsymbol{r}') \right\rangle = V^{-1} \left\langle \sum \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{r}} a_{\boldsymbol{k}}^\dagger \cdot \sum \mathrm{e}^{\mathrm{i}\boldsymbol{k}'\boldsymbol{r}'} a_{\boldsymbol{k}'} \right\rangle \qquad \text{by definition}$$

$$= V^{-1} \sum_{\boldsymbol{k},\boldsymbol{k}'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}'\boldsymbol{r}'} \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{r}} \left\langle a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}'} \right\rangle = V^{-1} \sum_{\boldsymbol{k},\boldsymbol{k}'} \mathrm{e}^{\mathrm{i}\boldsymbol{k}'\boldsymbol{r}'} \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{r}} \left\langle a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \right\rangle \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad \text{transl. invariance}$$

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General expression for the one particle density matrix with condensate

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

$$\boxed{\boldsymbol{k}_0 \to 0,\ \langle n_0 \rangle = N_0}$$

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

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

$$\Psi(\boldsymbol{r}) = \sqrt{\frac{N_0}{V}} \cdot \mathrm{e}^{\mathrm{i}\varphi} \cdot \mathrm{e}^{\mathrm{i}\boldsymbol{k}_0\boldsymbol{r}}$$

$\varphi \ldots$ an arbitrary phase

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Interpretation in the Bogolyubov theory – at zero temperature

$$\rho(\boldsymbol{r},\boldsymbol{r}') = V^{-1/2}\langle a_0\rangle \cdot V^{-1/2}\langle a_0^\dagger\rangle + V^{-1}\sum_{\boldsymbol{k}\neq\boldsymbol{k}_0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')} v_{\boldsymbol{k}}^2$$

Rich microscopic content hinging on the Bogolyubov assumption

Three methods of reformulating the Bogolyubov theory

In the original BEC theory … no need for non-zero averages of linear field operators

Why so important? … microscopic view of the condensate phase
quasi-particles and superfluidity
basis for a perturbation treatment of Bose fluids

We shall explore three approaches having a common basic idea:

⌘ relax the particle number conservation ⌘ work in the thermodynamic limit

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I	explicit construction of the classical part of the field operators	*Pitaevski in* LL IX (1978)
II	the condensate represented by a coherent state	*Cummings & Johnston* (1966) *Langer, Fisher & Ambegaokar* (1967 – 1969)
III	spontaneous symmetry breakdown, particle number conservation violated	*Bogolyubov* (1960) *Hohenberg&Martin* (1965) *P W Anderson* (1983 – book)

I.
explicit construction of the classical part of the field operators

Quotation from Landau-Lifshitz IX

ψ-операторов, которая меняет на 1 число частиц в конденсате, имеем, таким образом, по определению,

$$\hat{\Xi}\,|m, N+1\rangle = \Xi\,|m, N\rangle, \quad \hat{\Xi}^+\,|m, N\rangle = \Xi^*\,|m, N+1\rangle,$$

где символы $|m, N\rangle$ и $|m, N+1\rangle$ обозначают два «одинаковых» состояния, отличающихся только числом частиц в системе, а Ξ — некоторое комплексное число. Эти утверждения справедливы строго в пределе $N \to \infty$. Поэтому определение величины Ξ следует записать в виде

$$\lim_{N\to\infty} \langle m, N|\hat{\Xi}|m, N+1\rangle = \Xi,$$
$$\lim_{N\to\infty} \langle m, N+1|\hat{\Xi}^+|m, N\rangle = \Xi^*; \qquad (26,3)$$

переход к пределу совершается при заданном конечном значении плотности жидкости N/V.

Если представить ψ-операторы в виде

$$\hat{\Psi} = \hat{\Xi} + \hat{\Psi}', \quad \hat{\Psi}^+ = \hat{\Xi}^+ + \hat{\Psi}'^+, \qquad (26,4)$$

то остальная («надконденсатная») их часть переводит состояние $|m, N\rangle$ в ортогональные ему состояния, т. е. матричные элементы [1])

$$\lim_{N\to\infty} \langle m, N|\hat{\Psi}'|m, N+1\rangle = 0, \quad \lim_{N\to\infty} \langle m, N+1|\hat{\Psi}'^+|m, N\rangle = 0. \qquad (26,5)$$

В пределе $N \to \infty$ разница между состояниями $|m, N\rangle$ и $|m, N+1\rangle$ исчезает вовсе, и в этом смысле величина Ξ становится средним значением оператора $\hat{\Psi}$ по этому состоянию. Подчеркнем, что характерным для системы с конденсатом является именно конечность этого предела.

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… that part of the Ψ operators, which changes the condensate particle number by 1, we have, then, by definition

$$\hat{\Xi}|m, N+1\rangle = \Xi|m, N\rangle, \quad \hat{\Xi}^+|m, N\rangle = \Xi^*|m, N+1\rangle,$$

the symbols $|m, N\rangle$ и $|m, N+1\rangle$ denoting two "identical" states, differing only by the number of the particles in the system, and Ξ is a complex number. These statements are strictly valid in the limit $N \longrightarrow \infty$. The definition of the quantity Ξ has thus to be written in the form

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the limiting transition is to be performed at a given fixed value of the liquid density N/V.

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If the Ψ operators are represented in the form

$$\hat{\Psi} = \hat{\Xi} + \hat{\Psi}', \quad \hat{\Psi}^{+} = \hat{\Xi}^{+} + \hat{\Psi}'^{+}, \qquad (26,4)$$

then their remaining ("supercondensate") parts transform the state $|m, N\rangle$ to states which are orthogonal to it, that is, the matrix elements are

$$\lim_{N\to\infty} \langle m, N|\hat{\Psi}'|m, N+1\rangle = 0, \quad \lim_{N\to\infty} \langle m, N+1|\hat{\Psi}'^{+}|m, N\rangle = 0. \qquad (26,5)$$

In the limit $N \longrightarrow \infty$, the difference between the states $|m, N\rangle$ and $|m, N+1\rangle$ vanishes entirely and in this sense the quantity Ξ becomes the mean value of the operator $\hat{\Psi}$ over this state.

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Qui capere potest, capiat

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Let anyone accept this who can

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Kdo můžeš pochopiti, pochop

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II.
the condensate represented by a coherent state

Reformulation of the Bogolyubov requirements

Bogolyubov himself and his faithful followers never speak of the many particle wave function. Looks like he wanted

$$a_0 \left|\Psi\right\rangle = \Lambda \left|\Psi\right\rangle, \quad \Lambda = \sqrt{N_0}\, \mathrm{e}^{\mathrm{i}\phi}\,, \quad \text{so that}$$

$$\left\langle a_0 \right\rangle = \Lambda$$

The ground state

This is in contradiction with the selection rule, $\left\langle a_0 \right\rangle = 0$

The above eigenvalue equation is known and defines the ground state to be a **coherent state with the parameter Λ**

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HISTORICAL REMARK

⌘ The coherent states (not their name) discovered by Schrödinger as the minimum uncertainty wave packets, obtained by shifting the ground state of a harmonic oscillator.

⌘ These states were introduced into the quantum theory of the coherence of light by Roy Glauber (NP 2005). Hence the name.

⌘ The uses of the coherent states in the many body theory and quantum field theory have been manifold.

About the coherent states

OUR BASIC DEFINITION

$$a_0 \left|\Psi\right\rangle = \Lambda \left|\Psi\right\rangle, \quad \Lambda = \sqrt{N_0}\,\mathrm{e}^{\mathrm{i}\phi}, \quad \left\langle a_0 \right\rangle = \Lambda$$

If a particle is removed from a coherent state, it remains unchanged (*cf*. the Pitaevskii requirement above). It has a rather uncertain particle number, but a reasonably well defined phase

General coherent state	Condensate
$\left\|\Lambda\right\rangle = \mathrm{e}^{-\left\|\Lambda\right\|^2/2} \cdot \mathrm{e}^{\Lambda a_0^\dagger} \left\|\mathrm{vac}\right\rangle$	$= \left\|\Psi\right\rangle$
$\left\langle \Lambda \right\| a_0 \left\| \Lambda \right\rangle = \Lambda$	$= \sqrt{N_0}\,\mathrm{e}^{\mathrm{i}\phi}$
$\left\langle \Lambda \right\| a_0^\dagger a_0 \left\| \Lambda \right\rangle = \left\|\Lambda\right\|^2$	$\left\langle n_0 \right\rangle = N_0$
$\left\langle \Lambda \right\| a_0^\dagger a_0 a_0^\dagger a_0 \left\| \Lambda \right\rangle = \left\|\Lambda\right\|^4 + \left\|\Lambda\right\|^2$	$\left\langle n_0^2 \right\rangle = N_0^2 + N_0$
$\Delta n_0 = \left\|\Lambda\right\|$	$\Delta n_0 = \sqrt{N_0} \ll N_0$

New vacuum and the shifted field operators

Does all that make sense? Try to work in the full Fock space F rather in its fixed N sub-space H_N This implies using the "grand Hamiltonian"

$$H - \mu N$$

L1: *Thermodynamics*: which environment to choose?

THE ENVIRONMENT IN THE THEORY SHOULD CORRESPOND
TO THE EXPERIMENTAL CONDITIONS

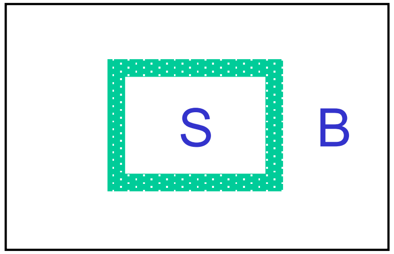
… a truism difficult to satisfy

❶ For large systems, this is not so sensitive for two reasons

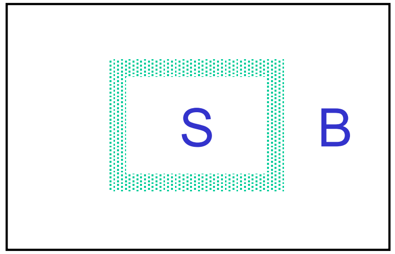
- System serves as a thermal bath or particle reservoir all by itself
- Relative fluctuations (distinguishing mark) are negligible

❷

	Adiabatic system	Real system	Isothermal system
SB heat exchange –	the slowest	medium fast process	the fastest



- temperature lag
- interface layer



❸ Atoms in a trap: ideal model … isolated. In fact: unceasing energy exchange (laser cooling). A small number of atoms may be kept (one to, say, 40). With 10^7, they form a bath already. Besides, they are cooled by evaporation and they form an open (albeit non-equilibrium) system.

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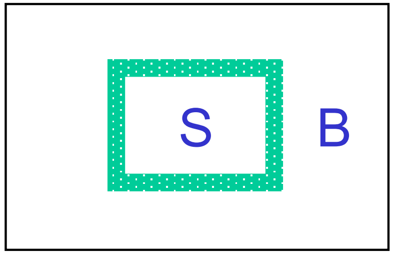

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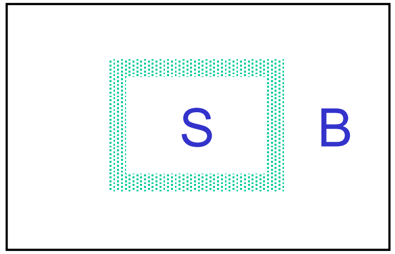

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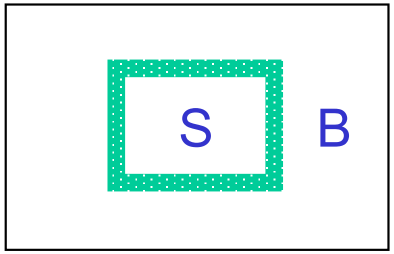

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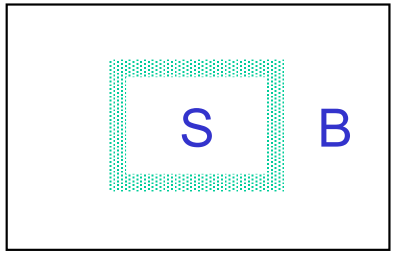

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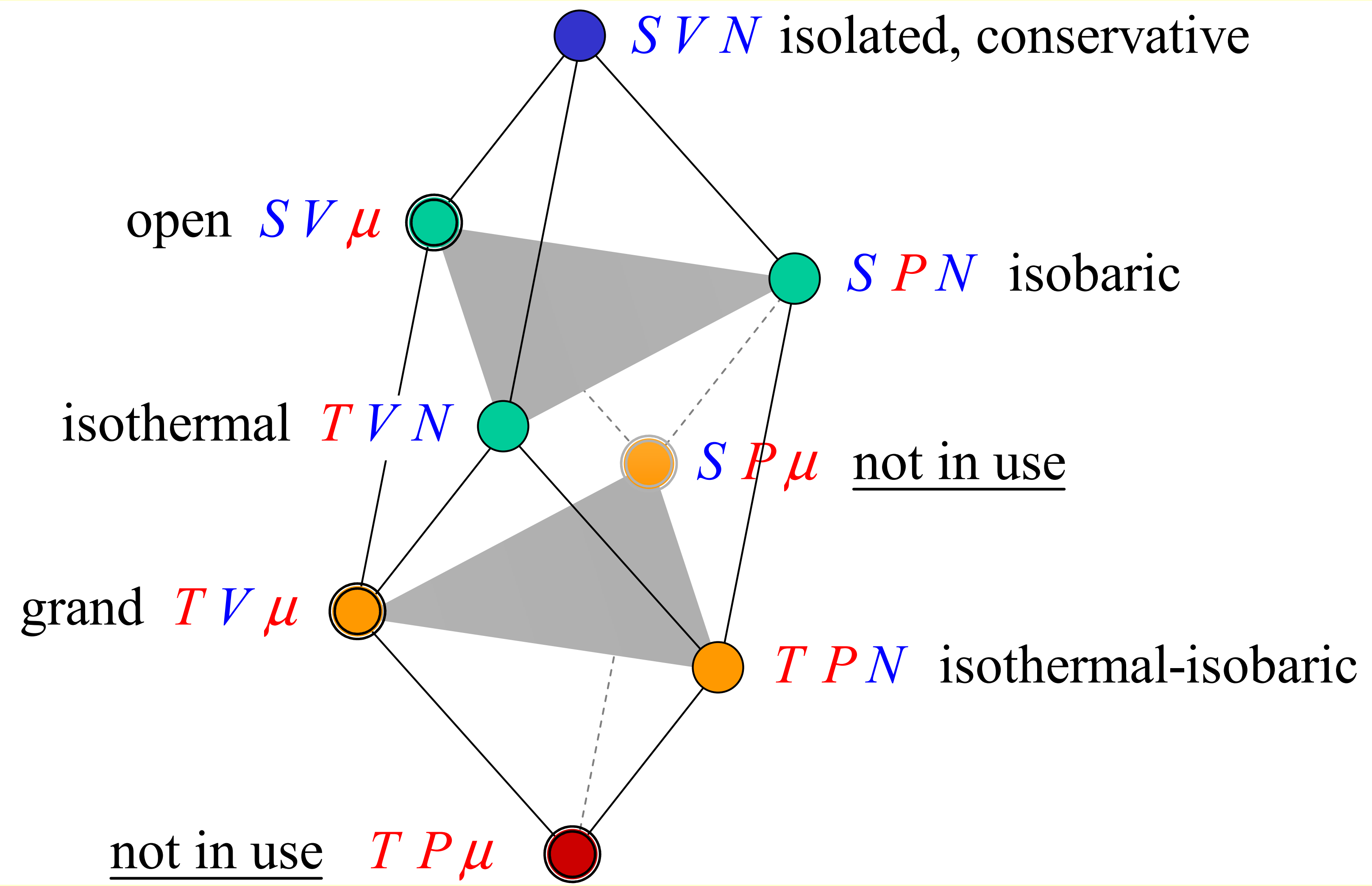
L1: Homogeneous one component phase: boundary conditions (environment) and state variables

$S\ V\ N$ additive variables, have densities $s = S/V \quad n = N/V$ "extensive"

$\updownarrow\ \updownarrow\ \updownarrow$

$T\ P\ \mu$ dual variables, intensities "intensive"

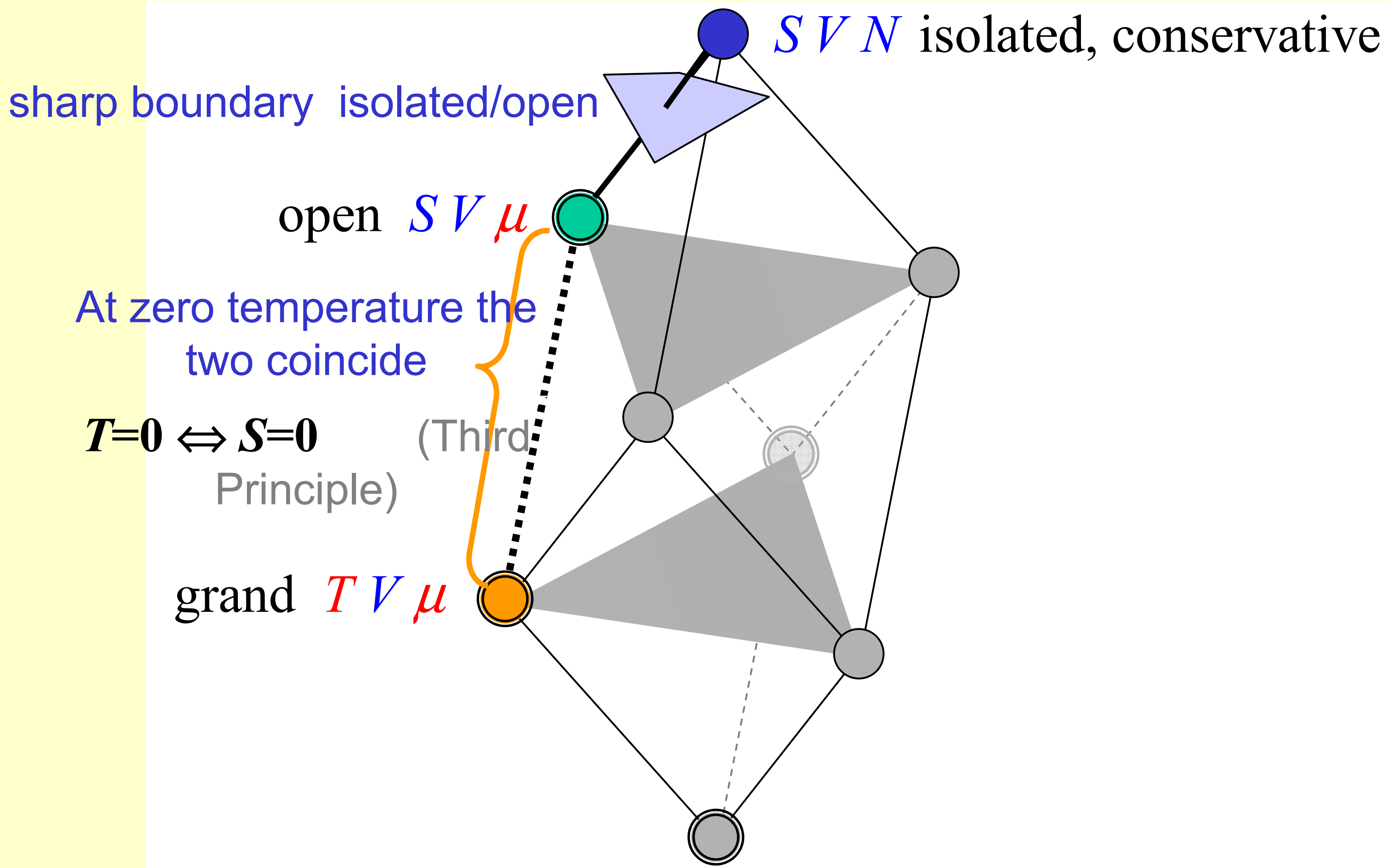


L1: Homogeneous one component phase:
boundary conditions (environment) and state variables

$S\ V\ N$ additive variables, have densities $s = S/V \quad n = N/V$ "extensive"

$\updownarrow \ \updownarrow \ \updownarrow$

$T\ P\ \mu$ dual variables, intensities "intensive"



New vacuum and the shifted field operators

Does all that make sense? Try to work in the full Fock space F rather in its fixed N sub-space H_N This implies using the "grand Hamiltonian"

$$H - \mu N$$

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$$H - \mu N$$

Let us define the shifted field operator

$$b_0 = a_0 - \Lambda, \quad b_0^\dagger = a_0^\dagger - \Lambda^*$$

$$\left[b_0, b_0^\dagger \right] = 1, \quad b_0 \left| \Psi \right\rangle = 0 \; \ldots \; \text{new vacuum}$$

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What next? … is this coherent state able to represent the condensate?

Test example: ideal Bose gas – limit of a BE system without interactions

$$(H - \mu N) \left| \Psi \right\rangle = \sum \left(\frac{\hbar^2}{2m} \boldsymbol{k}^2 - \mu \right) a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \left| \Psi \right\rangle$$

$$= -\mu a_0^\dagger a_0 \left| \Psi \right\rangle = 0 \quad \text{for} \quad \mu = 0$$

Here, $\left| \Psi \right\rangle$ is a true eigenstate, μ coincides with the previous result for the particle number conserving state $\left| B \right\rangle = \left| N_0, 0, 0, \ldots, 0, \ldots \right\rangle$

Two different, but macroscopically equivalent possibilities.

General case: the approximate vacuum

$$H = \int \mathrm{d}^3 \boldsymbol{r}\, \psi^\dagger(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{r})\right)\psi(\boldsymbol{r}) + \frac{1}{2}\iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r'}\,\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r'})U(\boldsymbol{r}-\boldsymbol{r'})\psi(\boldsymbol{r'})\psi(\boldsymbol{r})$$

$g\delta(\boldsymbol{r}-\boldsymbol{r}')$

- Non-zero interaction, repulsive forces make the lowest energies N dependent
- Inhomogeneous, possibly finite, system with a confinement potential
- There is no privileged symmetry related basis of one-particle orbitals

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$$g\delta(\boldsymbol{r}-\boldsymbol{r}')$$

- Trial function … a coherent state a marked generalization!!

$$\psi(\boldsymbol{r}) |\Psi\rangle = \Psi(\boldsymbol{r}) |\Psi\rangle$$

- We should minimize the average grand energy

$$\langle \Psi | H - \mu N | \Psi \rangle = \int \mathrm{d}^3 \boldsymbol{r}\, \Psi^*(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) - \mu \right) \Psi(\boldsymbol{r})$$
$$+ \tfrac{1}{2} \iint \mathrm{d}^3 \boldsymbol{r}\, \mathrm{d}^3 \boldsymbol{r}'\, \Psi^*(\boldsymbol{r}) \Psi(\boldsymbol{r}) U(\boldsymbol{r}-\boldsymbol{r}') \Psi^*(\boldsymbol{r}') \Psi(\boldsymbol{r}')$$

This is precisely the energy functional of the Hartree type we met already

and the Euler-Lagrange equation is the good old Gross-Pitaevski equation

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

with the normalization condition

$$N[n] = N = \int \mathrm{d}^3 \boldsymbol{r} \left| \Psi(\boldsymbol{r}) \right|^2$$

General case: the approximate vacuum

$$H=\int \mathrm{d}^3\boldsymbol{r}\,\psi^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta+V(\boldsymbol{r})\right)\psi(\boldsymbol{r})+\tfrac{1}{2}\iint \mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'\,\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')U(\boldsymbol{r}-\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r})$$

$$g\delta(\boldsymbol{r}-\boldsymbol{r}')$$

Trial function … a coherent state a marked generalization!!

$$\psi(\boldsymbol{r})|\Psi\rangle=\Psi(\boldsymbol{r})|\Psi\rangle$$

We should minimi

$$\langle\Psi|H -\quad \mu)\Psi(\boldsymbol{r})$$

$$-\boldsymbol{r}')\Psi^*(\boldsymbol{r}')\Psi(\boldsymbol{r}')$$

This is precisely … we met already

and the Euler-L … itaevski equation

$$\Psi(\boldsymbol{r})$$

with the normal

PROPERTIES OF THE COHERENT GROUND STATE

- Ground state in the mean field approximation
- All particles at zero temperature are in the condensate
- $|\Psi(\boldsymbol{r})|^2=n(\boldsymbol{r})$

General case: perturbative expansion

Define the shifted field operators and the condensate as the new vacuum

$$\eta(\boldsymbol{r}) = \psi(\boldsymbol{r}) - \Psi(\boldsymbol{r}), \quad \eta^\dagger(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r}) - \Psi^*(\boldsymbol{r})$$

$$\left[\eta(\boldsymbol{r}), \eta^\dagger(\boldsymbol{r}')\right] = \delta(\boldsymbol{r} - \boldsymbol{r}') \text{ etc.}, \quad \eta(\boldsymbol{r})\left|\boldsymbol{\Psi}\right\rangle = 0$$

Expansion parameter … concentration of the supra-condensate particles

deviation from the MF condensate = η-operators

If we keep only the terms not more than quadratic in the new operators, the resulting approximate Hamiltonian becomes

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If we keep only the terms not more than quadratic in the new operators, the resulting approximate Hamiltonian becomes

$$\begin{aligned} H - \mu N = &\int \mathrm{d}^3\boldsymbol{r}\, \Psi^*(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + \tfrac{1}{2} g n_{\mathrm{BE}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r}) \\ &+\int \mathrm{d}^3\boldsymbol{r}\, \eta^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + g n_{\mathrm{BE}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r}) + \text{h.c.} \\ &+\int \mathrm{d}^3\boldsymbol{r}\, \eta^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu\right)\eta(\boldsymbol{r}) \\ &+\tfrac{g}{2}\int \mathrm{d}^3\boldsymbol{r}\, n_{\mathrm{BE}}(\boldsymbol{r})\left\{\eta^\dagger(\boldsymbol{r})\eta^\dagger(\boldsymbol{r}) + 4\eta^\dagger(\boldsymbol{r})\eta(\boldsymbol{r}) + \eta(\boldsymbol{r})\eta(\boldsymbol{r})\right\} \end{aligned}$$

Here (*see in a moment*)

$$n_{\mathrm{BE}}(\boldsymbol{r}) = \left|\Psi(\boldsymbol{r})\right|^2$$

General case: perturbative expansion

$$H - \mu N = \int \mathrm{d}^3\boldsymbol{r}\, \Psi^*(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + \tfrac{1}{2} g n_{\mathrm{BE}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r})$$

$$+\int \mathrm{d}^3\boldsymbol{r}\, \eta^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + g n_{\mathrm{BE}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r}) + \mathrm{h.c.}$$

$$+\int \mathrm{d}^3\boldsymbol{r}\, \eta^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu\right)\eta(\boldsymbol{r})$$

$$+\tfrac{g}{2}\int \mathrm{d}^3\boldsymbol{r}\, n_{\mathrm{BE}}(\boldsymbol{r})\left\{\eta^\dagger(\boldsymbol{r})\eta^\dagger(\boldsymbol{r}) + 4\eta^\dagger(\boldsymbol{r})\eta(\boldsymbol{r}) + \eta(\boldsymbol{r})\eta(\boldsymbol{r})\right\}$$

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\end{aligned}
$$

1. The linear part must vanish to have minimum at $\eta = 0$. This is identical with the Gross-Pitaevskii equation and justifies the identification

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General case: perturbative expansion

$$
\begin{aligned}
H - \mu N = &\int \mathrm{d}^3\boldsymbol{r}\left(-\tfrac{1}{2}\right) g n_{\mathrm{BE}}^2(\boldsymbol{r}) \\
&\cancel{+\int \mathrm{d}^3\boldsymbol{r}\,\eta^\dagger(\boldsymbol{r})\left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + g n_{\mathrm{BE}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r})} + \mathrm{h.c.} \\
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&+\tfrac{g}{2}\int \mathrm{d}^3\boldsymbol{r}\, n_{\mathrm{BE}}(\boldsymbol{r})\left\{\eta^\dagger(\boldsymbol{r})\eta^\dagger(\boldsymbol{r}) + 4\eta^\dagger(\boldsymbol{r})\eta(\boldsymbol{r}) + \eta(\boldsymbol{r})\eta(\boldsymbol{r})\right\}
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2. The zero-th order part simplifies – substitute from the GPE
3. There remains to eliminate the anomalous terms from the quadratic part: **Bogolyubov transformation**

General case: the Bogolyubov transformation

A simple method: use EOM for the field operators

$$\mathrm{i}\partial_t \eta(\boldsymbol{r},t) = \left[\eta(\boldsymbol{r},t), H - \mu N\right]$$
$$= \left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + 2g n_{\mathrm{BE}}(\boldsymbol{r})\right)\eta(\boldsymbol{r},t) + g n_{\mathrm{BE}}(\boldsymbol{r})\eta^\dagger(\boldsymbol{r},t)$$
$$-\mathrm{i}\partial_t \eta^\dagger(\boldsymbol{r},t) = \left[\eta^\dagger(\boldsymbol{r},t), H - \mu N\right]$$
$$= \left(-\tfrac{\hbar^2}{2m}\Delta + V(\boldsymbol{r}) - \mu + 2g n_{\mathrm{BE}}(\boldsymbol{r})\right)\eta^\dagger(\boldsymbol{r},t) + g n_{\mathrm{BE}}(\boldsymbol{r})\eta(\boldsymbol{r},t)$$

These are linear eqs. To find their mode structure, make a linear ansatz

$$\eta(\boldsymbol{r},t) = \sum b_k u_k(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}E_k t} + b_k^\dagger v_k^*(\boldsymbol{r})\mathrm{e}^{+\mathrm{i}E_k t}$$
$$\eta^\dagger(\boldsymbol{r},t) = \sum b_k v_k(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}E_k t} + b_k^\dagger u_k^*(\boldsymbol{r})\mathrm{e}^{+\mathrm{i}E_k t}$$

Reminescent of the old *u* and *v* for infinite system.

Substitute into the EOM and separate individual frequencies.

Bogolyubov – de Gennes eqs. are obtained.

General case: the Bogolyubov transformation

Bogolyubov – de Gennes eqs.

$$E_k u_k = \left(-\frac{\hbar^2}{2m}\Delta + V - \mu + 2g n_{\mathrm{BE}}\right) u_k + g n_{\mathrm{BE}} v_k^*$$

$$-E_k v_k = \left(-\frac{\hbar^2}{2m}\Delta + V - \mu + 2g n_{\mathrm{BE}}\right) v_k + g n_{\mathrm{BE}} u_k^*$$

Strange coupled "Schrödinger" equations.

Strange orthogonality relations:

$$\int \mathrm{d}^3\boldsymbol{r} \left(u_k^* u_\ell - v_k^* v_\ell\right)(\boldsymbol{r}) = \delta_{k\ell}$$

It is our choice to normalize to unity

$$\int \mathrm{d}^3\boldsymbol{r} \left(u_k v_\ell - v_k u_\ell\right)(\boldsymbol{r}) = 0$$

The definition of the QP field operators can be inverted

$$\eta(\boldsymbol{r}) = \sum b_k u_k(\boldsymbol{r}) + b_k^\dagger v_k^*(\boldsymbol{r})$$

$$\eta^\dagger(\boldsymbol{r}) = \sum b_k v_k(\boldsymbol{r}) + b_k^\dagger u_k^*(\boldsymbol{r})$$

$$\boxed{\begin{aligned} b_k &= \int \mathrm{d}^3\boldsymbol{r} \left(+u_k^* \eta - v_k^* \eta^\dagger\right)(\boldsymbol{r}) \\ b_k^\dagger &= \int \mathrm{d}^3\boldsymbol{r} \left(-v_k \eta + u_k \eta^\dagger\right)(\boldsymbol{r}) \end{aligned}}$$

General case: the Bogolyubov transformation

These field operators satisfy the correct commutation rules

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

Finally,

$$H - \mu N = \int \mathrm{d}^3\boldsymbol{r} \left(-\tfrac{1}{2}\right) g n_{\mathrm{BE}}^2(\boldsymbol{r}) + \sum \left\{ E_k b_k^\dagger b_k - \int \mathrm{d}^3\boldsymbol{r} \left| v_k(\boldsymbol{r}) \right|^2 \right\}$$

a neat QP form of the grand Hamiltonian.

Detail: the mean-field for a homogeneous system

Before: minimize the energy functional with fixed particle number N, find the chemical potential μ afterwards

Now: minimize the grand energy functional with fixed chemical potential, find the average particle number in the process

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Now: minimize the grand energy functional with fixed chemical potential, find the average particle number in the process

Homogeneous system:

order parameter $\quad \Psi(\boldsymbol{r}) \equiv \Psi = \text{ const. } = \sqrt{N_0/V} \equiv \sqrt{n}$

$$\langle \Psi | H - \mu N | \Psi \rangle = \int \mathrm{d}^3 \boldsymbol{r}\, \Psi^*(\boldsymbol{r}) \left(-\tfrac{\hbar^2}{2m} \Delta + V(\boldsymbol{r}) - \mu \right) \Psi(\boldsymbol{r})$$

$$+ \tfrac{1}{2} \iint \mathrm{d}^3 \boldsymbol{r}\, \mathrm{d}^3 \boldsymbol{r}'\, \Psi^*(\boldsymbol{r}) \Psi(\boldsymbol{r}) g \delta(\boldsymbol{r} - \boldsymbol{r}') \Psi^*(\boldsymbol{r}') \Psi(\boldsymbol{r})$$

$$= V \times \Big(\underbrace{-\mu |\Psi|^2 + \tfrac{1}{2} g |\Psi|^4}_{\in(\Psi)} \Big)$$

energy per unit volume $\quad \in(\Psi)$

$$\langle \Psi | N | \Psi \rangle = \int \mathrm{d}^3 \boldsymbol{r}\, \Psi^*(\boldsymbol{r}) \Psi(\boldsymbol{r}) = V \times \underbrace{|\Psi|^2}_{n(\Psi)}$$

average particle density $\quad n(\Psi)$

Detail: the mean-field for a homogeneous system

The GP equation reduces from differential to an algebraic one:

$$\frac{\partial}{\partial x}\in(x)=0, \quad |\Psi|\equiv x$$

$$-2\mu x+\tfrac{1}{2}g\cdot 4x^3=0, \quad |\Psi|_{\max}=0, \quad \boxed{|\Psi|_{\min}=\sqrt{\frac{\mu}{g}},} \quad \in_{\min}=-\tfrac{1}{2}g|\Psi|_{\min}^4=-\frac{\mu^2}{2g}$$

$$\Rightarrow \quad \boxed{n=|\Psi|_{\min}^2=\frac{\mu}{g}}$$

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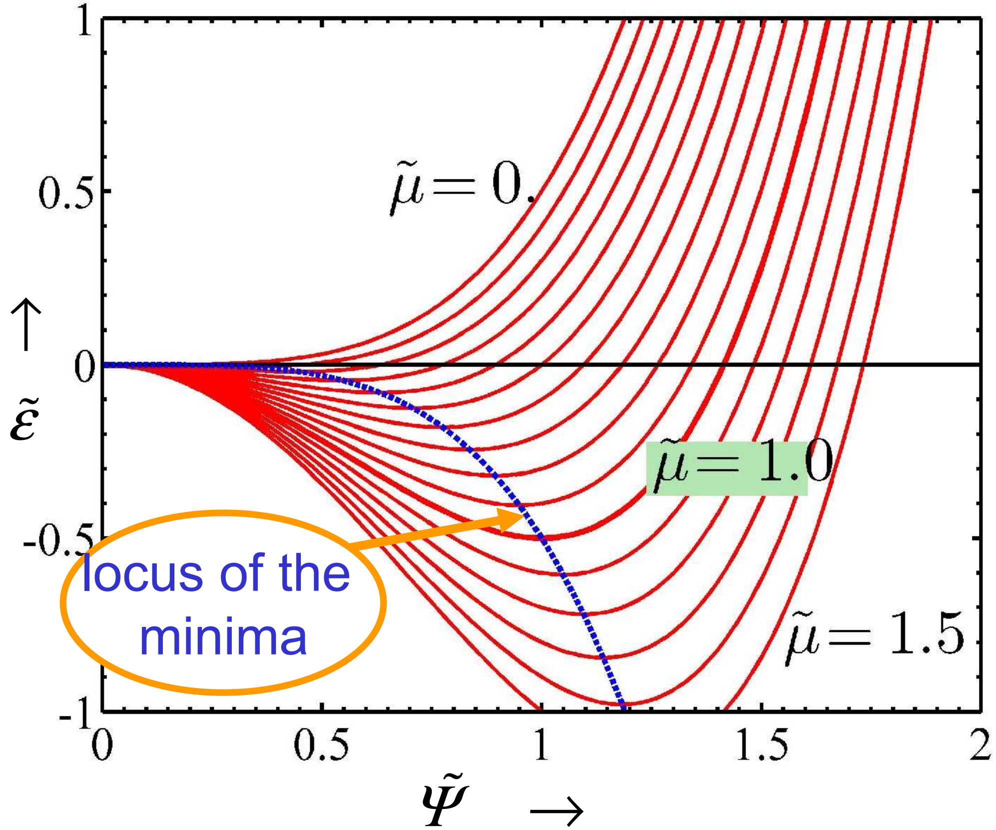
$$\Rightarrow \quad \boxed{n=|\Psi|_{\min}^2=\frac{\mu}{g}}$$

<u>Plot in relative units</u>

choose $\mu_{\text{ref}}; \quad |\Psi_{\text{ref}}|=\sqrt{\mu_{\text{ref}}/g}$

$\mu=\tilde{\mu}\cdot\mu_{\text{ref}} \qquad |\Psi|=\tilde{\Psi}\cdot|\Psi_{\text{ref}}|$

$\in=\tilde{\varepsilon}\cdot g|\Psi_{\text{ref}}|^4$



III.
broken symmetry and quasi-averages

Zero temperature limit of the grand canonical ensemble

$$\mathcal{P} = Z^{-1}\,\mathrm{e}^{-\beta(\mathcal{H}-\mu\mathcal{N})}$$
$$= Z^{-1}\sum\left|\alpha N\right\rangle \mathrm{e}^{-\beta(E_{\alpha N}-\mu N)}\left\langle \alpha N\right|$$
$$\to Z^{-1}\sum\left|0\tilde{N}\right\rangle \mathrm{e}^{-\beta(E_{0\tilde{N}}-\mu\tilde{N})}\left\langle 0\tilde{N}\right| \propto \sum\left|0\tilde{N}\right\rangle\left\langle 0\tilde{N}\right|$$

Picks up the correct ground state energy,

all ground states are taken with equal statistical weight

SYSTEMS

- **NORMAL** — NON-DEGENERATE GROUND STATE
- **"ANOMALOUS"** — DEGENERATE GROUND STATE

Degenerate ground state

SYSTEMS

- **NORMAL** — NON-DEGENERATE GROUND STATE
- **"ANOMALOUS"** — DEGENERATE GROUND STATE

Characterized by a <u>classical order parameter</u> … **macroscopic quantity**
Typical cause: a symmetry degeneracy
Everything depends on the system characteristic parameters
Ginsburg – Landau phenomenological model

$$\mathcal{E}(\Psi) = a\Psi^2 + b\Psi^4$$

$a > 0$
stable equilibrium
non-degenerate

$a < 0$
metastable equilibrium
degenerate

Degenerate ground state

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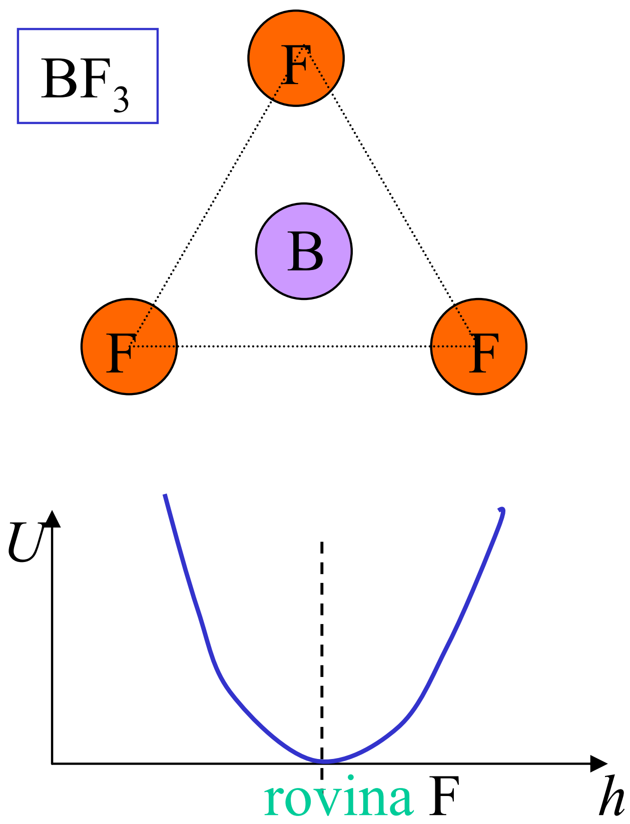
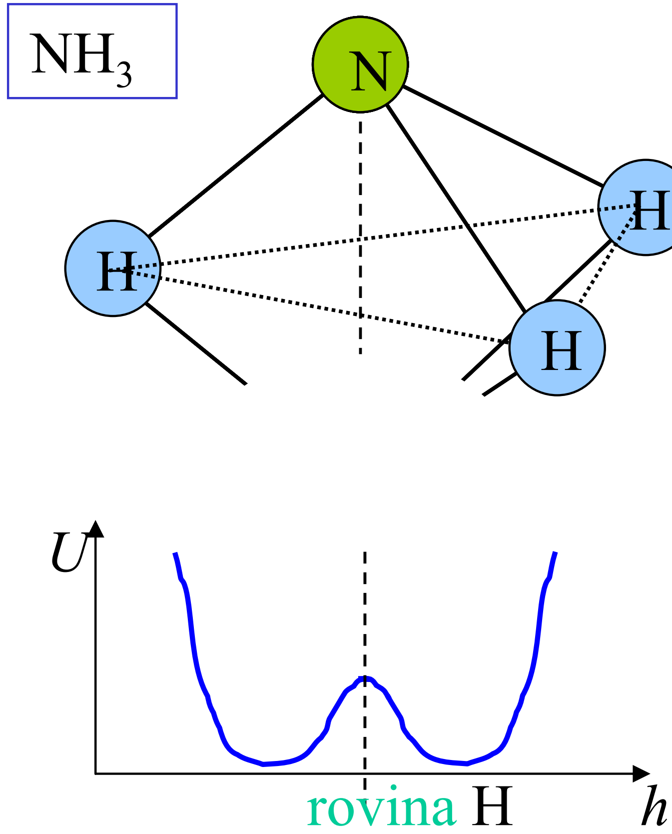
spontaneous symmetry breaking

$a > 0$	$a < 0$
stable equilibrium	metastable equilibrium
non-degenerate	degenerate

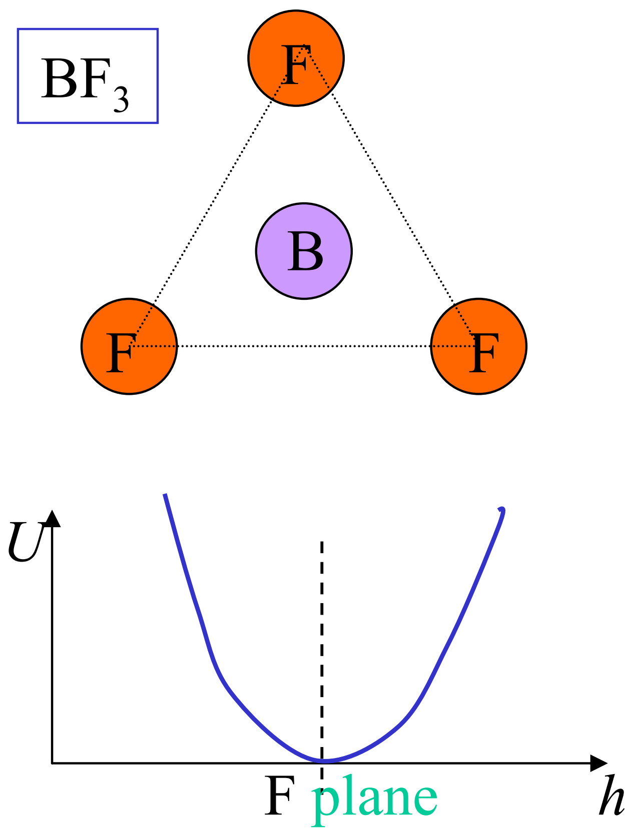
Rovnovážná struktura molekul AB_3

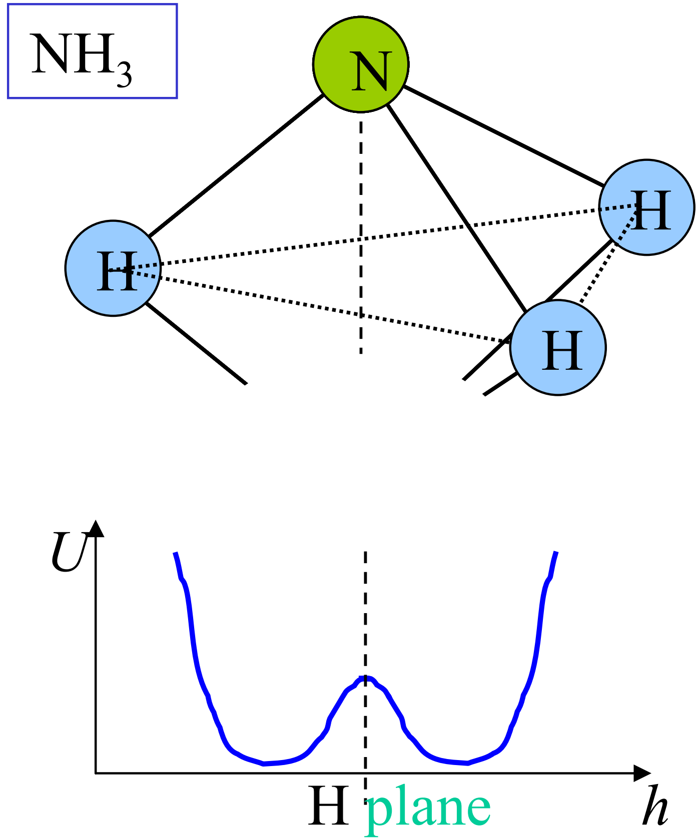




U adiabatická potenciální energie

Equilibrium structure of the AB_3 molekules



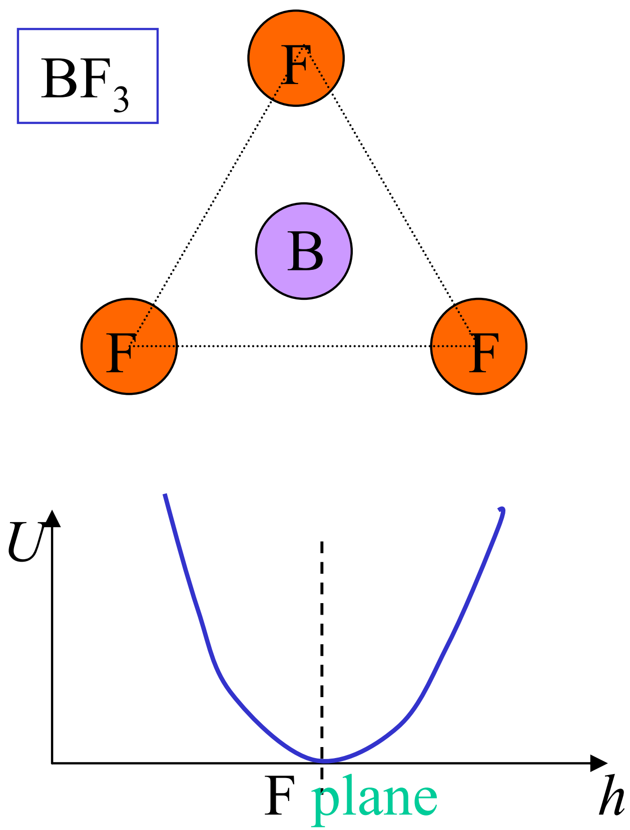


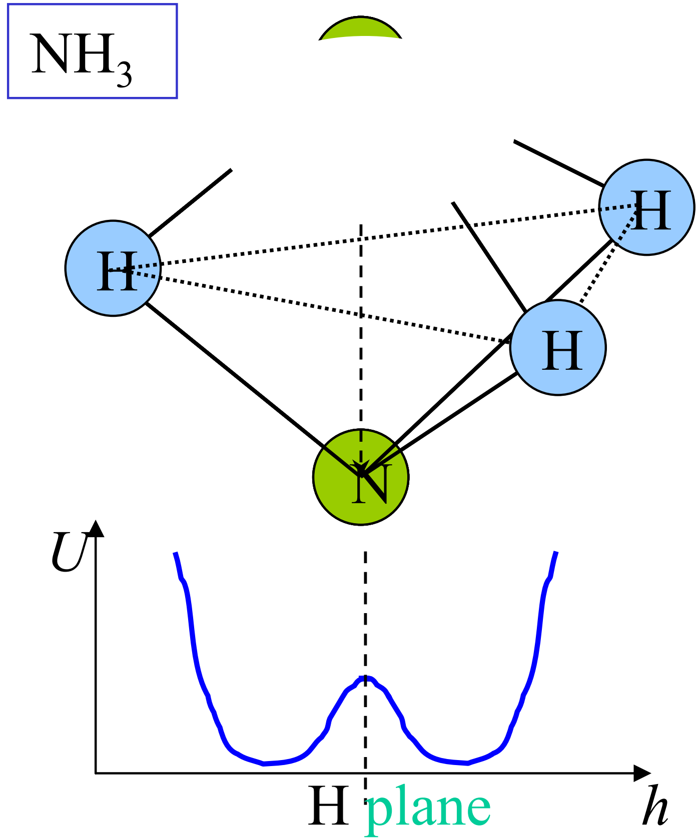
U adiabatic potential energy

stable equilibrium
non-degenerate
ground state

metastable equilibrium
degenerate
ground state

Equilibrium structure of the AB_3 molekules





U adiabatic potential energy

stable equilibrium
non-degenerate
ground state

metastable equilibrium
degenerate
ground state

Equilibrium structure of the AB_3 molekules

Ammonia molecule

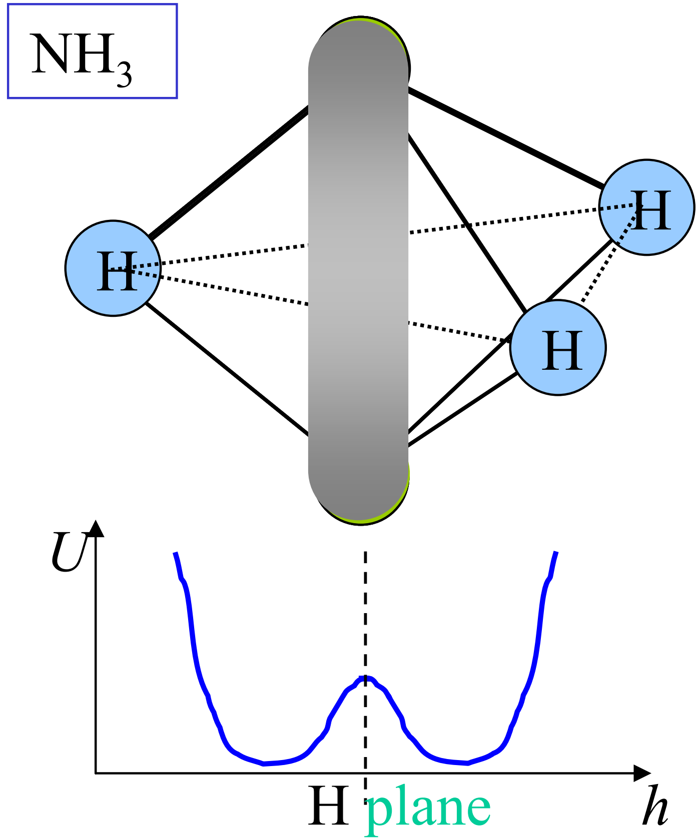
pyramidal molecule.

two minima of potential energy separated by a ***barrier***.

Different from a typical extended system:

⌘ **Small system:**
quantum *barrier & tunneling*

⌘ **Discrete symmetry broken:**
discrete set of equivalent equilibria states



Broken continouous symmetries in extended systems

Three popular cases

System	Isotropic ferromagnet	Atomic crystal lattice	Bosonic gas/liquid
Hamiltonian	Heisenberg spin Hamiltonian	Distinguishable atoms with int.	Bosons with short range interactions
Symmetry	3D rotational in spin space	Translational	Global gauge invariance
Order parameter	homogeneous magnetization	periodic particle density	macroscopic wave function
Symmetry breaking field	external magnetic field	"empty lattice" potential	particle source/drain
Goldstone modes	magnons	acoustic phonons	sound waves

For a nearly exhaustive list see the PWA book of 1983

Bose condensate - degeneracy of the ground state

The coherent ground state

mean field energy $$E(\Psi) = \left(-\mu|\Psi|^2 + \tfrac{1}{2} g |\Psi|^4\right)$$

order parameter $$\Psi = \sqrt{\langle N_0 \rangle} \cdot \mathrm{e}^{\mathrm{i}\phi} \quad \text{any from } (0, 2\pi)$$

mf ground state $$|\Psi\rangle = \mathrm{e}^{-\frac{1}{2}|\Psi|^2} \cdot \mathrm{e}^{\sqrt{N_0}\cdot \mathrm{e}^{\mathrm{i}\phi} a_0^\dagger} |\mathrm{vac}\rangle$$

degeneracy

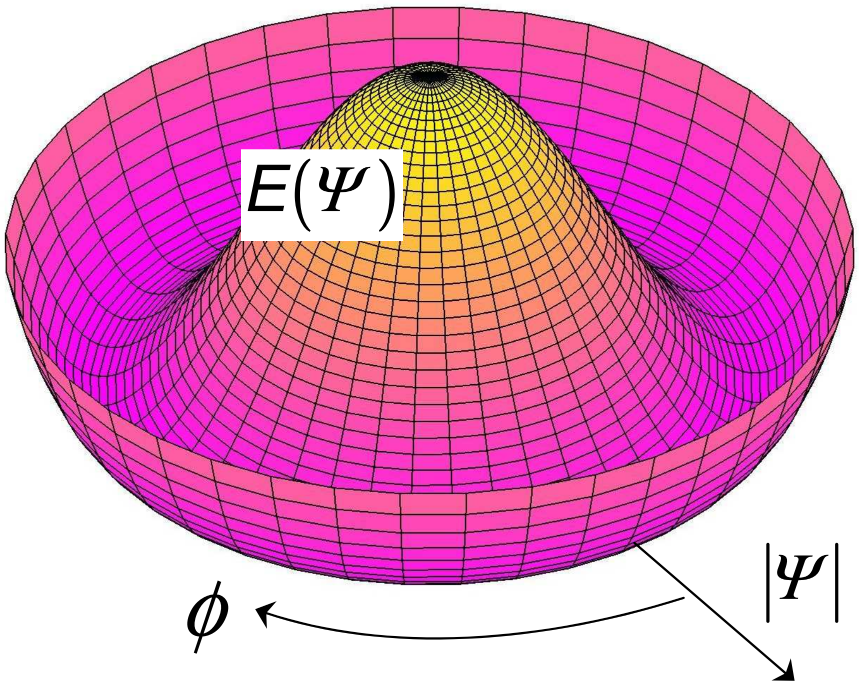
genuinely different for different ϕ

Selection rule

$$\langle a_0 \rangle_\phi = |\Psi| \mathrm{e}^{\mathrm{i}\phi} \neq 0$$

$$\langle a_0 \rangle = \int \mathrm{d}\phi \langle a_0 \rangle_\phi = 0$$

average over all degenerate states



"Mexican hat"

Symmetry breaking – removal of the degeneracy

The coherent ground state

mean field energy $E(\Psi) = \left(-\mu|\Psi|^2 + \frac{1}{2} g |\Psi|^4\right)$

order parameter $\Psi = \sqrt{\langle N_0 \rangle} \cdot \mathrm{e}^{\mathrm{i}\phi}$ any from $(0,2\pi)$

degeneracy

mf ground state $|\Psi\rangle = \mathrm{e}^{-\frac{1}{2}|\Psi|^2} \cdot \mathrm{e}^{\sqrt{N_0} \cdot \mathrm{e}^{\mathrm{i}\phi} a_0} |\mathrm{vac}\rangle$

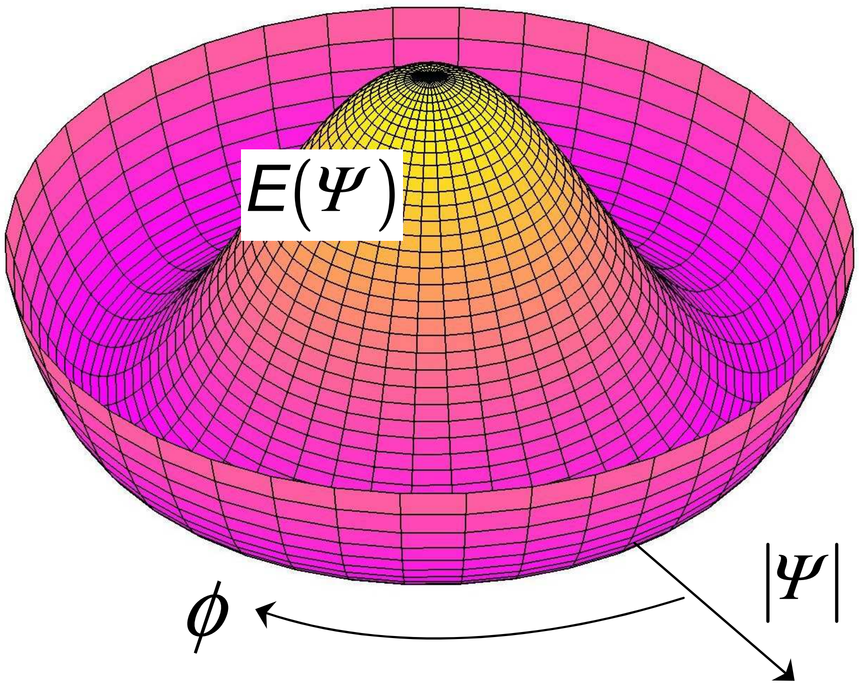
genuinely different for different ϕ

Symmetry broken by a small perturbation picking up one ϕ

$$\mathcal{H} - \mu\mathcal{N} \rightarrow$$

$$\mathcal{H} - \mu\mathcal{N} - \lambda\left(a_0^\dagger \mathrm{e}^{\mathrm{i}\phi} + a_0 \mathrm{e}^{-\mathrm{i}\phi}\right)$$

particle number NOT conserved



"Mexican hat"

Symmetry breaking – removal of the degeneracy

The coherent ground state

mean field energy $E(\Psi) = \left(-\mu|\Psi|^2 + \tfrac{1}{2} g |\Psi|^4\right)$

order parameter $\Psi = \sqrt{\langle N_0 \rangle} \cdot e^{i\phi}$ any from $(0, 2\pi)$

degeneracy

mf ground state $|\Psi\rangle = e^{-\frac{1}{2}|\Psi|^2} \cdot e^{\sqrt{N_0} \cdot e^{i\phi} a_0} |\text{vac}\rangle$

genuinely different for different ϕ

Symmetry broken by a small perturbation picking up one ϕ

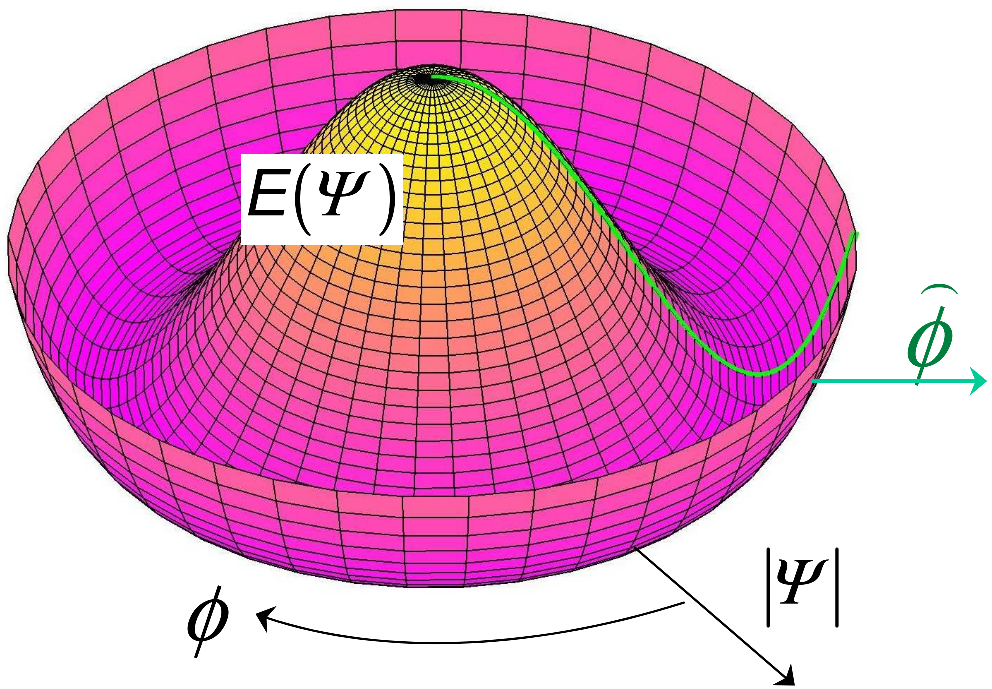
$$\mathcal{H} - \mu\mathcal{N} \rightarrow$$

$$\mathcal{H} - \mu\mathcal{N} - \lambda\left(a_0^\dagger e^{i\phi} + a_0 e^{-i\phi}\right)$$

particle number NOT conserved

For $\lambda \rightarrow 0$

one particular phase selected



"Mexican hat"

How the symmetry breaking works – ideal BE gas

Without interactions, the ground level is uncoupled from the excited levels:

$$\mathcal{H} - \mu\mathcal{N} - \lambda\left(a_0^\dagger\,\mathrm{e}^{\mathrm{i}\phi} + a_0\,\mathrm{e}^{-\mathrm{i}\phi}\right)$$

$$= -\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger\,\mathrm{e}^{\mathrm{i}\phi} + a_0\,\mathrm{e}^{-\mathrm{i}\phi}\right) + \sum_{\boldsymbol{k}\neq 0}\frac{\hbar^2}{2m}\left(\boldsymbol{k}^2 - \mu\right)a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}$$

$$\to -\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger\,\mathrm{e}^{\mathrm{i}\phi} + a_0\,\mathrm{e}^{-\mathrm{i}\phi}\right)$$

The control parameter is the chemical potential μ, but it will be adjusted to yield a fixed average particle number in the condensate.

Transformation:

$$-\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger\,\mathrm{e}^{\mathrm{i}\phi} + a_0\,\mathrm{e}^{-\mathrm{i}\phi}\right) = -\mu\left(a_0^\dagger a_0 + \frac{\lambda}{\mu}\mathrm{e}^{\mathrm{i}\widehat{\phi}}\,a_0^\dagger + \frac{\lambda}{\mu}\mathrm{e}^{-\mathrm{i}\widehat{\phi}}\,a_0\right)$$

$$\equiv -\mu\left(a_0^\dagger a_0 - \Lambda a_0^\dagger - \Lambda^* a_0\right) = -\mu\left(\left(a_0^\dagger - \Lambda^*\right)\left(a_0 - \Lambda\right) - \Lambda^*\Lambda\right)$$

$$\equiv -\mu\left(b_0^\dagger b_0 - \Lambda^*\Lambda\right)$$

How the symmetry breaking works – ideal BE gas

Now we determine the many-body ground state

$$-\mu\left(b_0^\dagger b_0 - \Lambda^* \Lambda\right)\left|\Psi\right\rangle = \mathcal{E}\left|\Psi\right\rangle, \qquad \boxed{b_0 = a_0 - \Lambda, \quad \Lambda = -\lambda\mu^{-1}\,\mathrm{e}^{\mathrm{i}\widehat{\phi}}, \quad \mu \le 0}$$

The lowest energy corresponds to

$$b_0\left|\Psi\right\rangle = 0, \quad \text{i.e.} \quad a_0\left|\Psi\right\rangle = \Lambda\left|\Psi\right\rangle \quad \text{... coherent state}$$

$$\Lambda^*\Lambda = \left\langle\Psi\right|a_0^\dagger a_0\left|\Psi\right\rangle = N_0, \quad \Lambda = \sqrt{N_0}\,\mathrm{e}^{\mathrm{i}\widehat{\phi}}$$

$$\mathcal{E} = \mu\Lambda^*\Lambda = \mu N_0 \qquad \mu = -\lambda/\sqrt{N_0}$$

The control parameter is the chemical potential μ, but it will be adjusted to yield a fixed average particle number in the condensate.

Infinitesimal symmetry breaking field $\lambda \to 0$

$\underline{\lambda \to 0 \ \text{ with } \ N_0 \ \text{ fixed:}}$

$$\mu \to 0 - 0$$

$$\mathcal{E} \to 0$$

$$\Lambda = \sqrt{N_0}\,\mathrm{e}^{\mathrm{i}\widehat{\phi}}, \quad \left|\Psi\right\rangle \ \text{ fixed}$$

How the symmetry breaking works – ideal BE gas

Now we determine the many-body ground state

$$-\mu\left(b_0^\dagger b_0 - \Lambda^* \Lambda\right)\left|\Psi\right\rangle = \mathcal{E}\left|\Psi\right\rangle, \qquad \boxed{b_0 = a_0 - \Lambda, \quad \Lambda = -\lambda\mu^{-1}\,\mathrm{e}^{\mathrm{i}\widehat{\phi}}, \quad \mu \le 0}$$

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$$\mu \to 0 - 0$$

$$\mathcal{E} \to 0$$

$$\Lambda = \sqrt{N_0}\,\mathrm{e}^{\mathrm{i}\widehat{\phi}}, \quad \left|\Psi\right\rangle \ \text{ fixed}$$

- The coherent state is the exact ground state for the ideal BE gas
- The order parameter picks up the phase from the perturbing field
- The order of limits: first $\lambda \to 0$, only then the thermodynamic limit $N_0 \to \infty$

The end