

# Cold atoms

Lecture 5.

14<sup>th</sup> November, 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
...		
Lecture 5	ODLRO; BEC and symmetry breaking, coherent states	Nov 14
...		

# *Recapitulation*

# 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

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

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

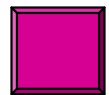
Momentum

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

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

Particle density

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



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

# Operators

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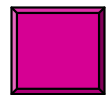
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# Hamiltonian

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

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

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

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

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

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

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

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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 of a homogeneous gas

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

# Hamiltonian of a homogeneous gas

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- conserves the particle number

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

- conserves the total momentum

$$[\mathcal{H}, \mathcal{P}_{x,y,z}] = 0$$

## Summary: two symmetries compared

Gauge invariance of the 1 <sup>st</sup> 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 <math>\psi^\dagger</math> as <math>\psi</math>.</p>	<p>selection rules</p> $\langle a_k a_{k'}   \mathcal{L}   a_{k''}^\dagger \rangle = 0$ <p>unless the total momentum transfer <math>-k - k' + k''</math> 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

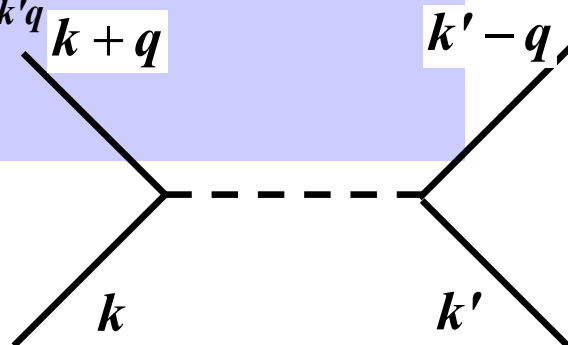
In the momentum representation

For the Fermi pseudopotential

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

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

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



Momentum conservation

$$(k + q) + (k' - q) - k - k' = 0$$

Particle number conservation

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

$$E55555F$$

## 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*)



# Basic idea

## Bogolyubov method

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

no interaction	weak interaction
$g = 0$	$g \neq 0$
$N = N_{\text{BE}} = \langle a_0^\dagger a_0 \rangle ? \quad 1$	$N = N_{\text{BE}} + \sum_{k \neq 0} \langle a_k^\dagger a_k \rangle \approx N_{\text{BE}} ? \quad 1$

The condensate dominates,  
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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

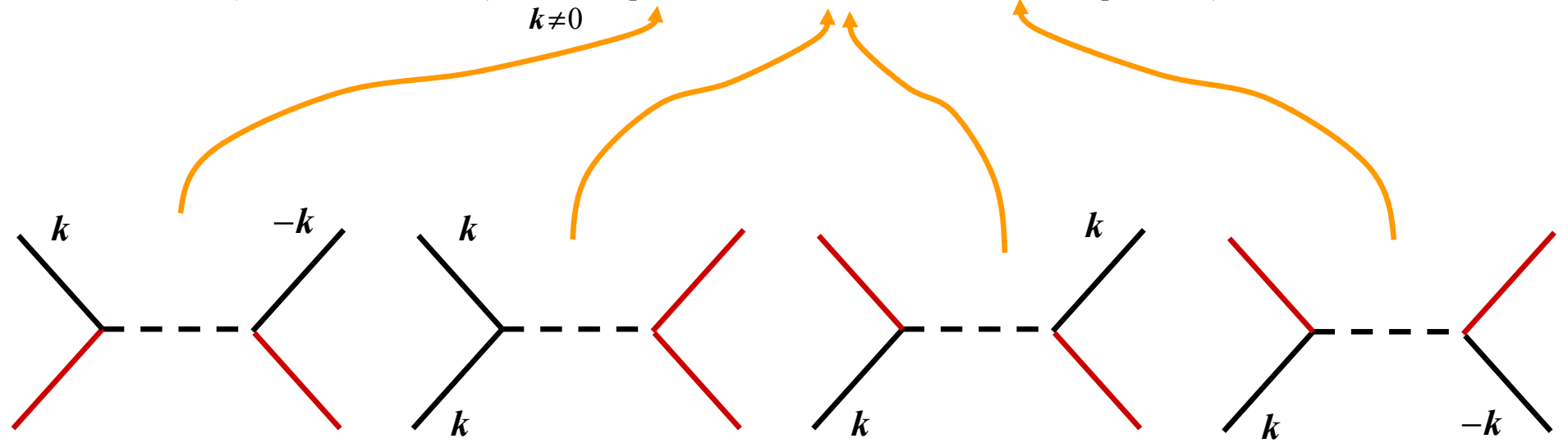
$$H = \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_k^\dagger a_k + \frac{1}{2} V^{-1} \sum_{kk'q} U a_{k+q}^\dagger a_{k'-q}^\dagger a_{k'} a_k$$

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

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

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

$N_0 = N - \sum_{k \neq 0} a_k^\dagger a_k$



— 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

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

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

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



# 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  $E$

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

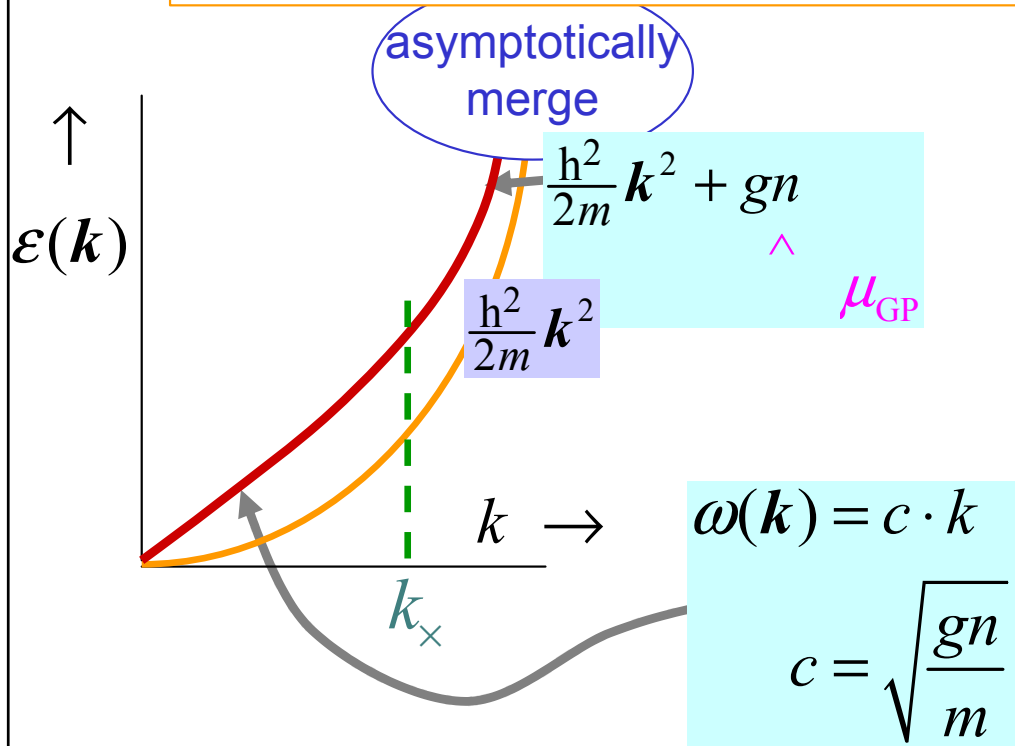
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ind. quasi-particles ground state energy  $E$

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



## 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  $^4\text{He}$
- 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 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

# Off-Diagonal Long Range Order

Analysis of BEC on the one-particle level  
ODLRO as a measure of coherence in the  
system

# Coherence in BEC: OPDM for non-interacting bosons

## *Off-Diagonal Long Range Order*

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

# Coherence in BEC: OPDM for non-interacting bosons

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

**Definition of OPDM** for **non**-interacting particles: Take an additive observable, like local density, or current density. Its average value for the whole assembly of atoms in a given equilibrium state  $|\{n_\alpha\}\rangle$ :

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

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$$= \text{Tr } \rho X \quad \rho = \sum_{\alpha} | \alpha \rangle \langle n_{\alpha} \rangle \langle \alpha |$$



# OPDM for homogeneous systems

In coordinate representation

$$\begin{aligned}\rho(\mathbf{r}, \mathbf{r}') &= \langle \mathbf{r} | \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle n_{\mathbf{k}} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle \langle n_{\mathbf{k}} \rangle \langle \mathbf{k} | \mathbf{r}' \rangle \\ &= \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle\end{aligned}$$

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

**CONDENSATE** lowest orbital with  $\mathbf{k}_0$



# OPDM for homogeneous systems: ODLRO

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

$$\rho(\mathbf{r} - \mathbf{r}') = \frac{1}{V} e^{i\mathbf{k}_0(\mathbf{r}-\mathbf{r}')} \langle n_0 \rangle + \frac{1}{V} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

coherent across the sample
*FT* of a smooth function has a finite range

$$\equiv \rho_{\text{BE}}(\mathbf{r} - \mathbf{r}') + \rho_{\text{G}}(\mathbf{r} - \mathbf{r}')$$

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$$\begin{aligned} \rho(\mathbf{0}) &= \rho_{\text{BE}}(\mathbf{0}) + \rho_{\text{G}}(\mathbf{0}) \\ &= n_{\text{BE}} + n_{\text{G}} \end{aligned}$$

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DISTANT OFF-DIAGONAL ELEMENT  $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$

$$\begin{aligned} \rho_{\text{BE}}(\mathbf{r} - \mathbf{r}') &\xrightarrow{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} n_{\text{BE}} \\ \rho_{\text{G}}(\mathbf{r} - \mathbf{r}') &\xrightarrow{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} 0 \\ \rho(\mathbf{r} - \mathbf{r}') &\xrightarrow{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} n_{\text{BE}} \end{aligned}$$

Off-Diagonal Long Range Order  
ODLRO

# From OPDM towards the macroscopic wave function

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

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coherent across the sample
FT of a smooth function has a finite range

$$= \Psi(\mathbf{r}) \Psi^*(\mathbf{r}') + \frac{1}{V} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

dyadic

## MACROSCOPIC WAVE FUNCTION

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

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

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## MACROSCOPIC WAVE FUNCTION

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

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

# ODLRO for interacting bosons

Basic expressions for the OPDM for a homogeneous system

$$\begin{aligned}\langle \mathbf{r} | \rho | \mathbf{r}' \rangle &= \langle \psi^\dagger(\mathbf{r}') \psi(\mathbf{r}) \rangle = V^{-1} \langle \sum e^{-i\mathbf{k}'\mathbf{r}'} a_{\mathbf{k}'}^\dagger \cdot \sum a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \rangle && \text{by definition} \\ &= V^{-1} \sum_{\mathbf{k}, \mathbf{k}'} e^{i\mathbf{k}\mathbf{r}} e^{-i\mathbf{k}'\mathbf{r}'} \langle a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} \rangle = V^{-1} \sum_{\mathbf{k}, \mathbf{k}'} e^{i\mathbf{k}\mathbf{r}} e^{-i\mathbf{k}'\mathbf{r}'} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \delta_{\mathbf{k}\mathbf{k}'} && \text{transl. invariance}\end{aligned}$$



Off-diagonal long range order

# ODLRO for interacting bosons

One particle density matrix

Basic expressions for the OPDM for a homogeneous system


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just like for  
non-  
interacting  
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General expression for the one particle density matrix with condensate

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

$$\mathbf{k}_0 \rightarrow 0, \langle n_0 \rangle = N_0$$

$$= V^{-1} e^{i\mathbf{k}_0(\mathbf{r}-\mathbf{r}')} \langle n_0 \rangle + V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

coherent across the sample

FT of a smooth function has a finite range

just like for non-interacting bosons

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coherent across the sample

$$\sum_{\mathbf{k} \neq \mathbf{k}_0}$$

FT of a smooth function has a finite range

$$= \psi(\mathbf{r}) \psi^*(\mathbf{r}') + V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

dyadic

$$\psi(\mathbf{r}) = \sqrt{\frac{N_0}{V}} \cdot e^{i\varphi} \cdot e^{i\mathbf{k}_0\mathbf{r}}$$

$\varphi$  an arbitrary phase

# ODLRO in the Bogolyubov theory

Basic expressions for the OPDM for a homogeneous system

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$$= V^{-1} e^{ik_0(\mathbf{r}-\mathbf{r}')} \langle n_0 \rangle + V^{-1} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

coherent across the sample

$$V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

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dyadic

$$\psi(\mathbf{r}) = \sqrt{\frac{N_0}{V}} \cdot e^{i\phi}$$

$\phi$  an arbitrary phase

just like for non-interacting bosons

**Interpretation in the Bogolyubov theory – at zero temperature**

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

**Rich microscopic content hinging on the Bogolyubov assumption**

# ODLRO in the Bogolyubov theory

Basic expressions for the OPDM for a homogeneous system

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

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General expression for the one particle density matrix with condensate

$$\rho(\mathbf{r}, \mathbf{r}') = V^{-1} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle \quad \boxed{k_0 \rightarrow 0, \langle n_0 \rangle = N_0}$$

$$= V^{-1} e^{i\mathbf{k}_0(\mathbf{r}-\mathbf{r}')} \langle n_0 \rangle + V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle$$

coherent across the sample

FT of a smooth function has a finite range

$$\Psi(\mathbf{r}) = \sqrt{\frac{N_0}{V}} \cdot e^{i\phi}$$

$\phi \in \mathbb{K}$  an arbitrary phase

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

just like for non-interacting bosons

**Interpretation in the Bogolyubov theory – at zero temperature**

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

**Rich microscopic content hinging on the Bogolyubov assumption**

# ODLRO in the Bogolyubov theory

Basic expressions for the OPDM for a homogeneous system

$$\begin{aligned} \langle \mathbf{r} | \rho | \mathbf{r}' \rangle &= \langle \psi^\dagger(\mathbf{r}') \psi(\mathbf{r}) \rangle = V^{-1} \langle \sum e^{-i\mathbf{k}'\mathbf{r}'} a_{\mathbf{k}'}^\dagger \cdot \sum a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \rangle && \text{by definition} \\ &= V^{-1} \sum_{\mathbf{k}, \mathbf{k}'} e^{i\mathbf{k}\mathbf{r}} e^{-i\mathbf{k}'\mathbf{r}'} \langle a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} \rangle = V^{-1} \sum_{\mathbf{k}, \mathbf{k}'} e^{i\mathbf{k}\mathbf{r}} e^{-i\mathbf{k}'\mathbf{r}'} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \delta_{\mathbf{k}\mathbf{k}'} && \text{transl. invariance} \end{aligned}$$

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$$k_0 \rightarrow 0, \langle n_0 \rangle = N_0$$

$$\begin{aligned} &= V^{-1} e^{ik_0(\mathbf{r}-\mathbf{r}')} \langle n_0 \rangle + V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle \\ &= \underbrace{\Psi(\mathbf{r}) \Psi^*(\mathbf{r}')}_{\text{dyadic}} + V^{-1} \sum_{\mathbf{k} \neq \mathbf{k}_0} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{k}} \rangle \end{aligned}$$

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

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

I.

explicit construction of the classical part of  
the field operators

## Quotation from Landau-Lifshitz IX [гл. III]

$\hat{\Psi}$ -операторов, которая меняет на 1 число частиц в конденсате, имеем, таким образом, по определению,

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

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

$$\begin{aligned} \lim_{N \rightarrow \infty} \langle m, N | \hat{E} | m, N+1 \rangle &= E, \\ \lim_{N \rightarrow \infty} \langle m, N+1 | \hat{E}^+ | m, N \rangle &= E^*; \end{aligned} \quad (26,3)$$

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

Если представить  $\hat{\Psi}$ -операторы в виде

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

то оставшая («надконденсатная») их часть переводит состояние  $|m, N\rangle$  в ортогональные ему состояния, т. е. матричные элементы<sup>1)</sup>

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

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

... that part of the  $\Psi$  operators, which changes the condensate particle number by 1, we have, then, by definition

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

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  $E$  is a complex number. These statements are strictly valid in the limit  $N \rightarrow \infty$ . The definition of the quantity  $E$  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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$$\hat{\Xi}|m, N+1\rangle = \Xi|m, N\rangle, \quad \hat{\Xi}^+|m, N\rangle = \Xi^*|m, N+1\rangle,$$

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  $\Xi$  is a complex number. These statements are strictly valid in the limit  $N \rightarrow \infty$ . The definition of the quantity  $\Xi$  has thus to be written in the form

$$\begin{aligned} \lim_{N \rightarrow \infty} \langle m, N | \hat{\Xi} | m, N+1 \rangle &= \Xi, \\ \lim_{N \rightarrow \infty} \langle m, N+1 | \hat{\Xi}^+ | m, N \rangle &= \Xi^*; \end{aligned} \quad (26,3)$$

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

If the  $\Psi$  operators are represented in the form

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

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

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

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

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

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Qui capere potest, capiat

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

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

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

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

$$\langle a_0 \rangle = \Lambda$$

**The ground state**

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

The above eigenvalue equation is known and defines the "ground" state  $\equiv$  Bogolyubov condensate state to be a **coherent state with the parameter  $\Lambda$**

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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

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

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

$$|\Lambda\rangle = e^{-|\Lambda|^2/2} \cdot e^{\Lambda a_0^\dagger} |\text{vac}\rangle$$

$$\langle \Lambda | a_0 | \Lambda \rangle = \Lambda$$

$$\langle \Lambda | a_0^\dagger a_0 | \Lambda \rangle = |\Lambda|^2$$

$$\langle \Lambda | a_0^\dagger a_0 a_0^\dagger a_0 | \Lambda \rangle = |\Lambda|^4 + |\Lambda|^2$$

$$\Delta n_0 = |\Lambda|$$

### Condensate

$$= |\Psi\rangle$$

$$= \sqrt{N_0} e^{i\phi}$$

$$\langle n_0 \rangle = N_0$$

$$\langle n_0^2 \rangle = N_0^2 + N_0$$

$$\Delta n_0 = \sqrt{N_0} = N_0$$

## New vacuum and the shifted field operators

Does all that make sense? Try to work in the full Fock space  $\mathbf{F}$  rather in its fixed  $N$  sub-space  $\mathbf{H}_N$  This implies using the "grand Hamiltonian"

$$H - \mu N$$

# L1: Thermodynamics: which environment to choose?

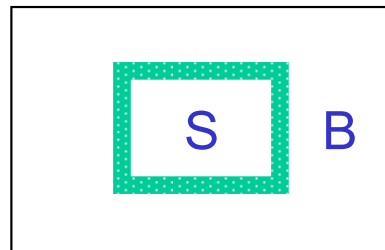
THE ENVIRONMENT IN THE THEORY SHOULD CORRESPOND TO THE EXPERIMENTAL CONDITIONS

... a truism difficult to satisfy

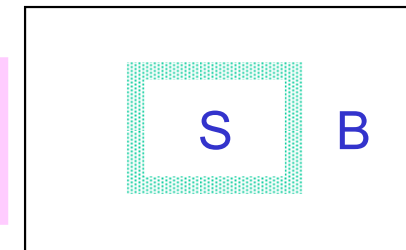
- 1 For large systems, this is not so sensitive for two reasons
  - System serves as a thermal bath or particle reservoir all by itself
  - Relative fluctuations (distinguishing mark) are negligible

- 2

	<u>Adiabatic system</u>	<u>Real system</u>	<u>Isothermal system</u>
SB heat exchange	– the slowest	medium fast process	the fastest



- temperature lag
- interface layer



- 3 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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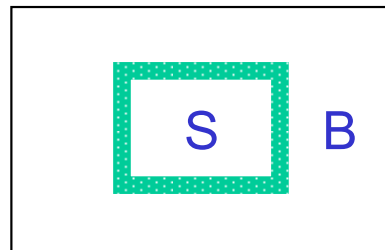
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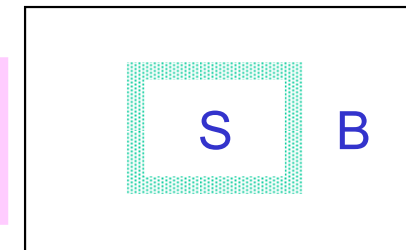
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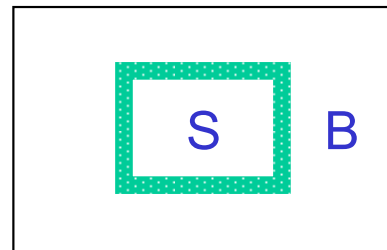
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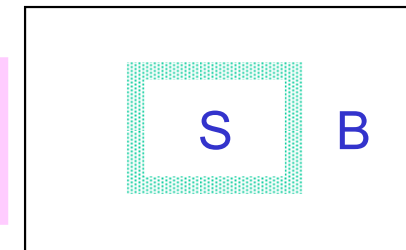
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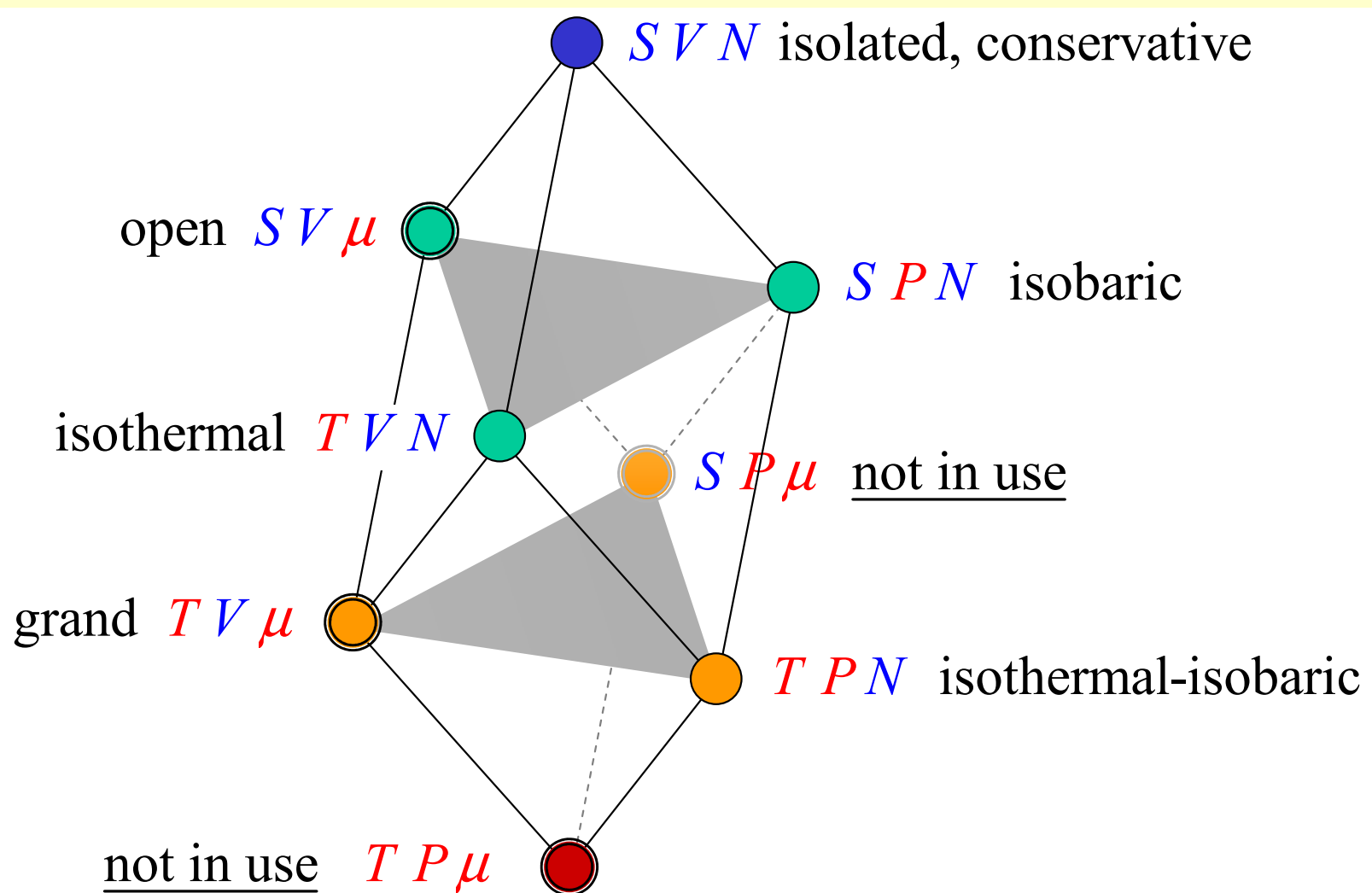
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**L1:** Homogeneous one component phase:  
 boundary conditions (environment) and state variables

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

b b b

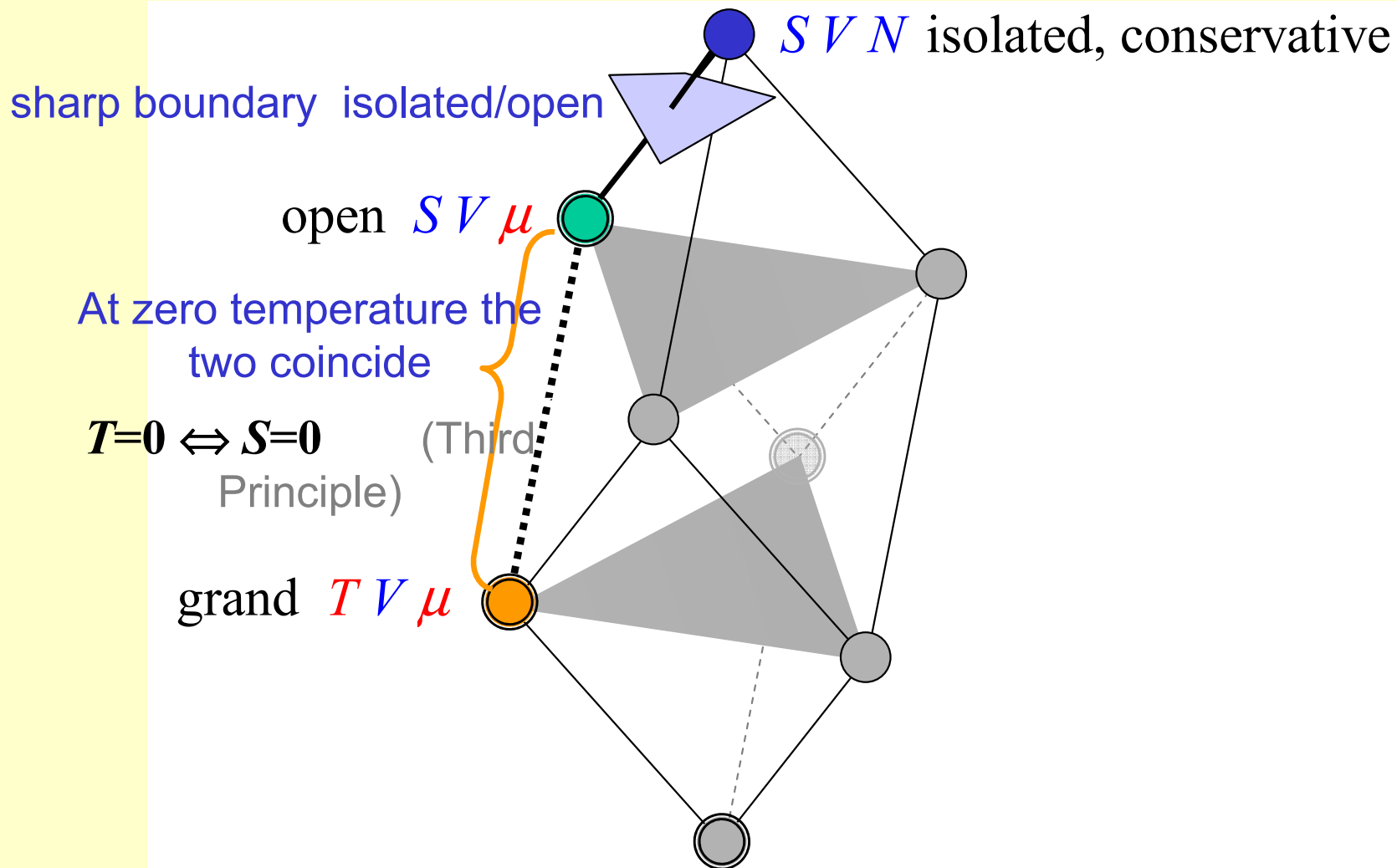
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## New vacuum and the shifted field operators

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Let us define the shifted field operator

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

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

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

$$\begin{aligned} (H - \mu N) |\Psi\rangle &= \sum \left( \frac{\hbar^2}{2m} \mathbf{k}^2 - \mu \right) a_k^\dagger a_k |\Psi\rangle \\ &= -\mu a_0^\dagger a_0 |\Psi\rangle = 0 \quad \text{for } \mu = 0 \end{aligned}$$

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$|\Psi\rangle$  ... a true eigenstate with  $\mathcal{E} = 0$ ,  $\mu$  the same as for the particle number conserving state  $|B\rangle = |N_0, 0, 0, \mathbf{K}, 0, \mathbf{K}\rangle = (N_0!)^{-1/2} (a_0^\dagger)^{N_0} |\text{vac}\rangle$

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

$$[b_0, b_0^\dagger] = 1, \quad b_0 |\Psi\rangle = 0 \quad \dots \text{new vacuum} \quad |\Psi\rangle = e^{-|\Lambda|^2/2} \cdot e^{\Lambda a_0^\dagger} |\text{vac}\rangle$$

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

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

$$\begin{aligned} (H - \mu N) |\Psi\rangle &= \sum \left( \frac{\hbar^2}{2m} \mathbf{k}^2 - \mu \right) a_k^\dagger a_k |\Psi\rangle \\ &= -\mu a_0^\dagger a_0 |\Psi\rangle = 0 \quad \text{for } \mu = 0 \end{aligned}$$

$|\Psi\rangle$  ... a true eigenstate with  $\mathcal{E} = 0$ ,  $\mu$  the same as for the particle number conserving state  $|B\rangle = |N_0, 0, 0, \mathbf{K}, 0, \mathbf{K}\rangle = (N_0!)^{-1/2} (a_0^\dagger)^{N_0} |\text{vac}\rangle$

**Two different, but macroscopically equivalent possibilities.**



## General case: the approximate vacuum

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

✓ Trial function ... a coherent state

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

✓ We should minimize the average grand energy

$$\begin{aligned} \langle \Psi | H - \mu N | \Psi \rangle &= \int d^3 r \Psi^*(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) - \mu \right) \Psi(\mathbf{r}) \\ &+ \frac{1}{2} \iint d^3 r d^3 r' \Psi^*(\mathbf{r}) \Psi(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') \Psi^*(\mathbf{r}') \Psi(\mathbf{r}') \end{aligned}$$

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

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

with the normalization condition

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

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

## More about the approximate vacuum

Approximate vacuum ... a coherent state

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

What is the OPDM?

$$\langle\Psi|\psi(\mathbf{r})|\Psi\rangle = \langle\Psi|\Psi(\mathbf{r})|\Psi\rangle = \Psi(\mathbf{r}), \quad \langle\Psi|\psi^\dagger(\mathbf{r})|\Psi\rangle = \langle\Psi|\Psi^*(\mathbf{r})|\Psi\rangle = \Psi^*(\mathbf{r})$$

$$\langle\mathbf{r}|\rho|\mathbf{r}'\rangle = \langle\psi^\dagger(\mathbf{r}')\psi(\mathbf{r})\rangle = \langle\Psi|\psi^\dagger(\mathbf{r}')\psi(\mathbf{r})|\Psi\rangle = \Psi(\mathbf{r})\Psi^*(\mathbf{r}')$$

Full ODLRO with the normalization condition  $\int d^3 r |\Psi(\mathbf{r})|^2 = N$

Explicit form of the coherent state

$$|\Psi\rangle = \exp\left\{-\frac{1}{2}\int d^3 r |\Psi(\mathbf{r})|^2\right\} \exp\left\{\int d^3 r \Psi(\mathbf{r})\psi^\dagger(\mathbf{r})\right\} |\text{vac}\rangle$$

$$\langle\Psi|\Psi\rangle = 1$$

**NOTE:** this is **not** a unitary transformation

## General case: the Bogolyubov transformation

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

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

$$[\eta(\mathbf{r}), \eta^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), \quad \eta(\mathbf{r})|\Psi\rangle = 0$$

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

$$H = \int d^3\mathbf{r} \eta^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) - \mu \right) \eta(\mathbf{r}) \\ + \frac{g}{2} \int d^3\mathbf{r} n_{\text{BE}}(\mathbf{r}) \left\{ \eta^\dagger(\mathbf{r}) \eta^\dagger(\mathbf{r}) + 4\eta^\dagger(\mathbf{r}) \eta(\mathbf{r}) + \eta(\mathbf{r}) \eta(\mathbf{r}) \right\}$$

Now eliminate the anomalous terms by the Bogolyubov transformation.

It is required that, in terms of the new field operators,

$$H = \sum_{\alpha} \varepsilon_{\alpha} b_{\alpha}^{\dagger} b_{\alpha} + E_0 \\ [b_{\alpha}, b_{\alpha'}^{\dagger}] = \delta_{\alpha\alpha'}, \quad [b_{\alpha}, b_{\alpha'}] = 0, \quad [b_{\alpha}^{\dagger}, b_{\alpha'}^{\dagger}] = 0$$

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$$[b_{\alpha}, b_{\alpha'}^{\dagger}] = \delta_{\alpha\alpha'}, \quad [b_{\alpha}, b_{\alpha'}] = 0, \quad [b_{\alpha}^{\dagger}, b_{\alpha'}^{\dagger}] = 0$$

This is achieved by the Bogolyubov transformation

$$\eta(\mathbf{r}) = \sum_{\alpha} u_{\alpha}(\mathbf{r}) b_{\alpha} + v_{\alpha}(\mathbf{r}) b_{\alpha}^{\dagger}$$
$$\eta^{\dagger}(\mathbf{r}) = \sum_{\alpha} v_{\alpha}^*(\mathbf{r}) b_{\alpha} + u_{\alpha}^*(\mathbf{r}) b_{\alpha}^{\dagger}$$

with  $\int d^3 \mathbf{r} \{ |u_{\alpha}|^2 - |v_{\alpha}|^2 \} = 1$

For  $u(\mathbf{r})$  and  $v(\mathbf{r})$  ... coupled Schrödinger-like Bogolyubov-de Gennes eqs.

$$\left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + 2g |\Psi(\mathbf{r})|^2 - \mu \right) u(\mathbf{r}) + g [\Psi(\mathbf{r})]^2 v^*(\mathbf{r}) = +\varepsilon \cdot u(\mathbf{r})$$

$$\left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + 2g |\Psi(\mathbf{r})|^2 - \mu \right) v(\mathbf{r}) + g [\Psi^*(\mathbf{r})]^2 u(\mathbf{r}) = -\varepsilon \cdot v(\mathbf{r})$$

## Detail: the mean-field for a homogeneous system

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

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

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### Homogeneous system:

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

$$\begin{aligned} \langle \Psi | H - \mu N | \Psi \rangle &= \int d^3\mathbf{r} \Psi^*(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) - \mu \right) \Psi(\mathbf{r}) \\ &\quad + \frac{1}{2} \iint d^3\mathbf{r} d^3\mathbf{r}' \Psi^*(\mathbf{r}) \Psi(\mathbf{r}) g \delta(\mathbf{r} - \mathbf{r}') \Psi^*(\mathbf{r}') \Psi(\mathbf{r}) \\ &= V \times \underbrace{\left( -\mu |\Psi|^2 + \frac{1}{2} g |\Psi|^4 \right)}_{\in(\Psi)} \end{aligned}$$

energy per unit volume

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

average particle density

## Detail: the mean-field for a homogeneous system

The GP equation reduces from differential to an algebraic one:

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

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

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

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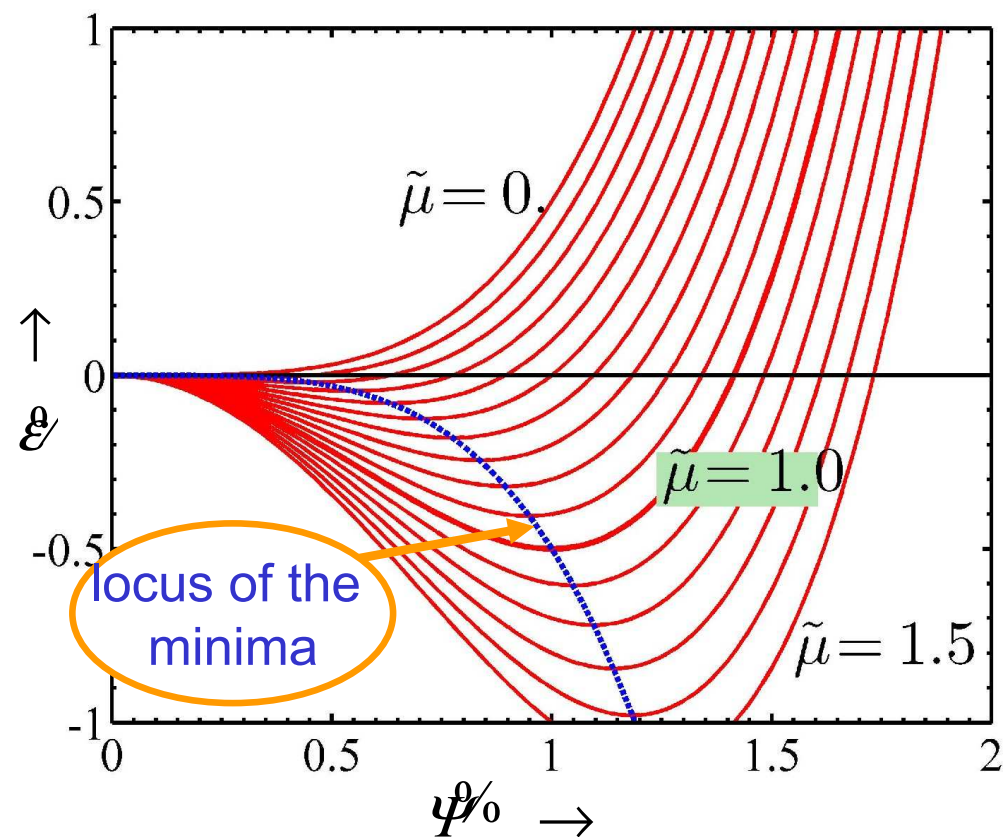
$$\Rightarrow n = |\Psi|_{\min}^2 = \frac{\mu}{g} \checkmark$$

## Plot in relative units

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

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

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



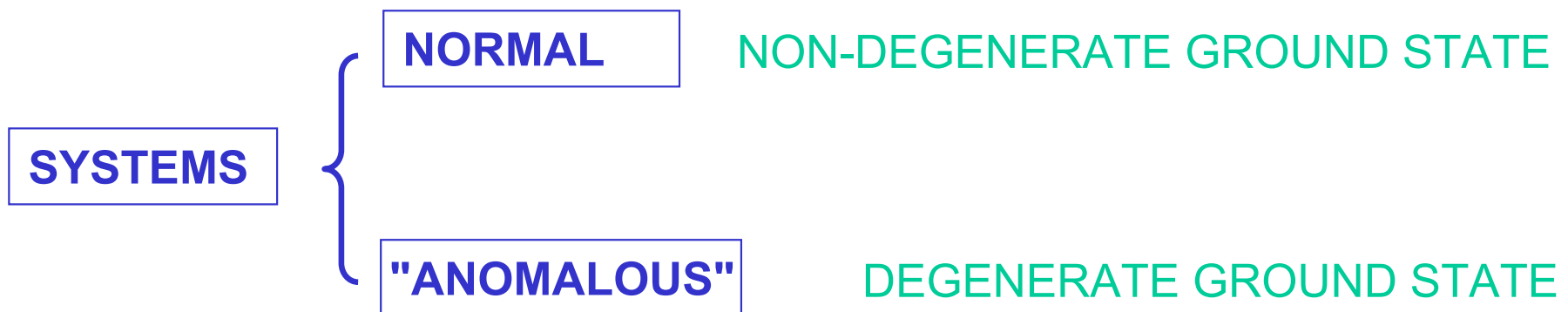


III.  
broken symmetry and quasi-averages

# Zero temperature limit of the grand canonical ensemble

$$\begin{aligned}\mathcal{P} &= Z^{-1} e^{-\beta(\mathcal{H}-\mu N)} \\ &= Z^{-1} \sum |\alpha N\rangle e^{-\beta(E_{\alpha N}-\mu N)} \langle \alpha N| \\ &\rightarrow Z^{-1} \sum |0N^0\rangle e^{-\beta(E_{0N^0}-\mu N^0)} \langle 0N^0| \propto \sum |0N^0\rangle \langle 0N^0|\end{aligned}$$

Picks up the correct ground state energy,  
all ground states are taken with equal statistical weight



# Degenerate ground state



Characterized by a classical order parameter ... **macroscopic quantity**

Typical cause: a symmetry degeneracy

Everything depends on the system characteristic parameters

Ginsburg – Landau phenomenological model

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

$$a > 0$$

stable equilibrium

non-degenerate

$$a < 0$$

metastable equilibrium

degenerate

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Characterized by a classical order parameter ... **macroscopic quantity**

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Ginsburg – Landau phenomenological model

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

spontaneous symmetry breaking

$$a > 0$$

stable equilibrium

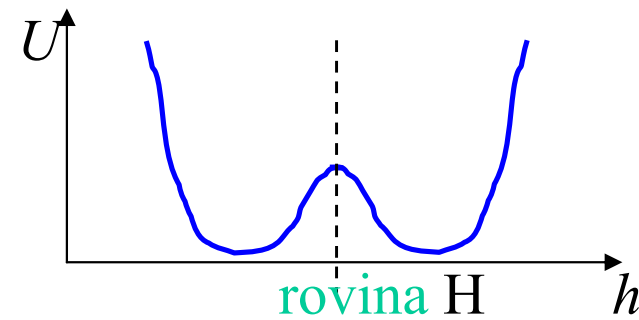
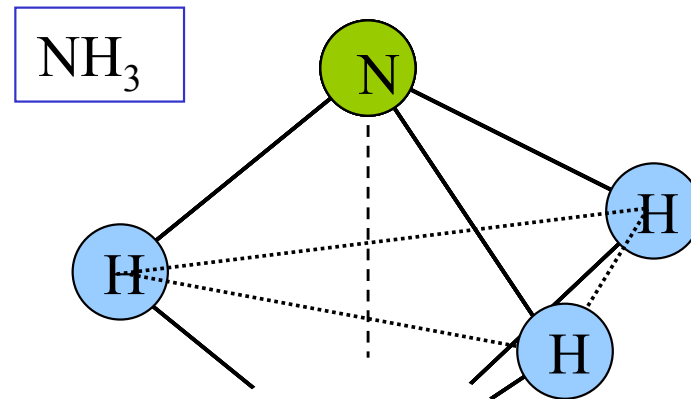
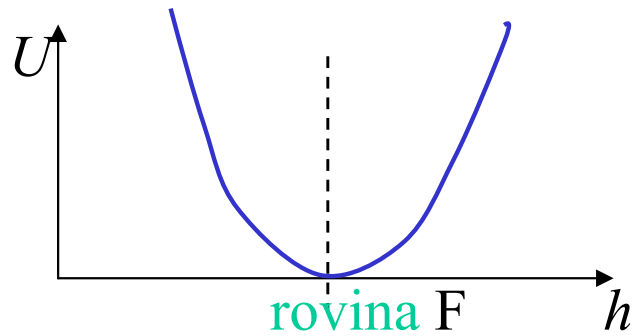
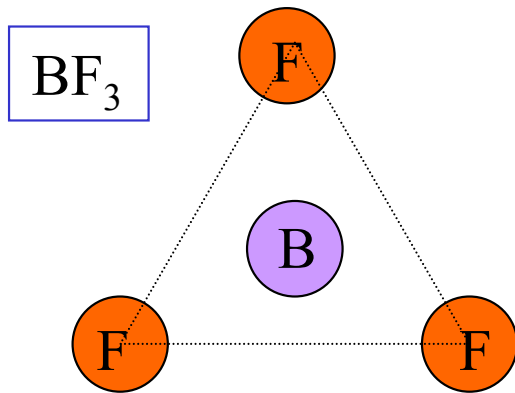
non-degenerate

$$a < 0$$

metastable equilibrium

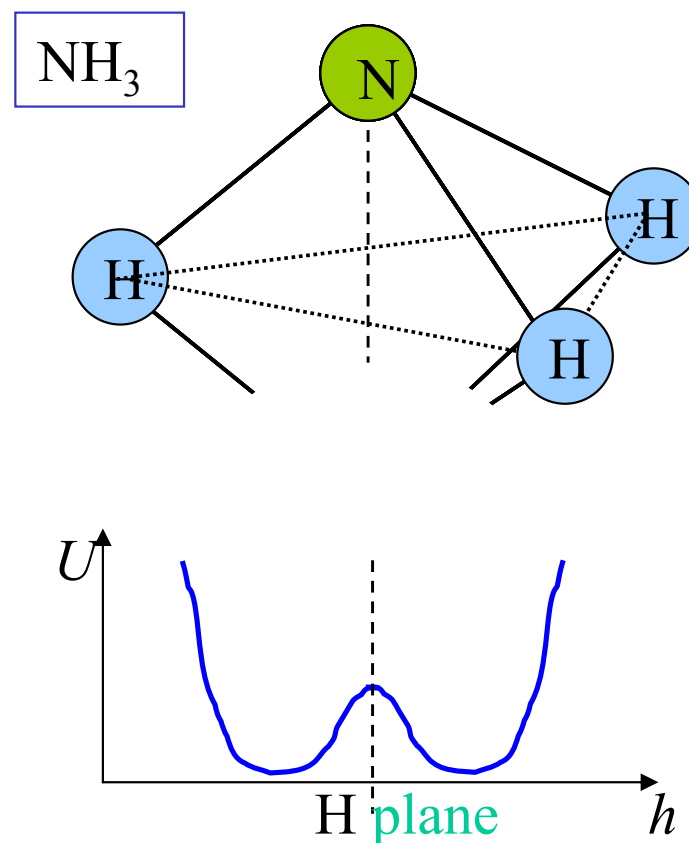
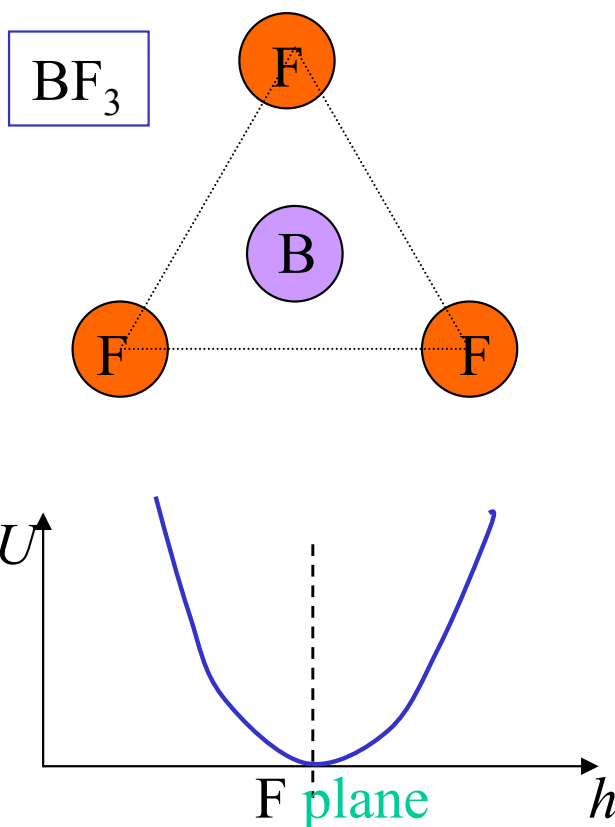
degenerate

# Rovnovážná struktura molekul $AB_3$



$U$  adiabatická potenciální energie

# Equilibrium structure of the $AB_3$ molecules

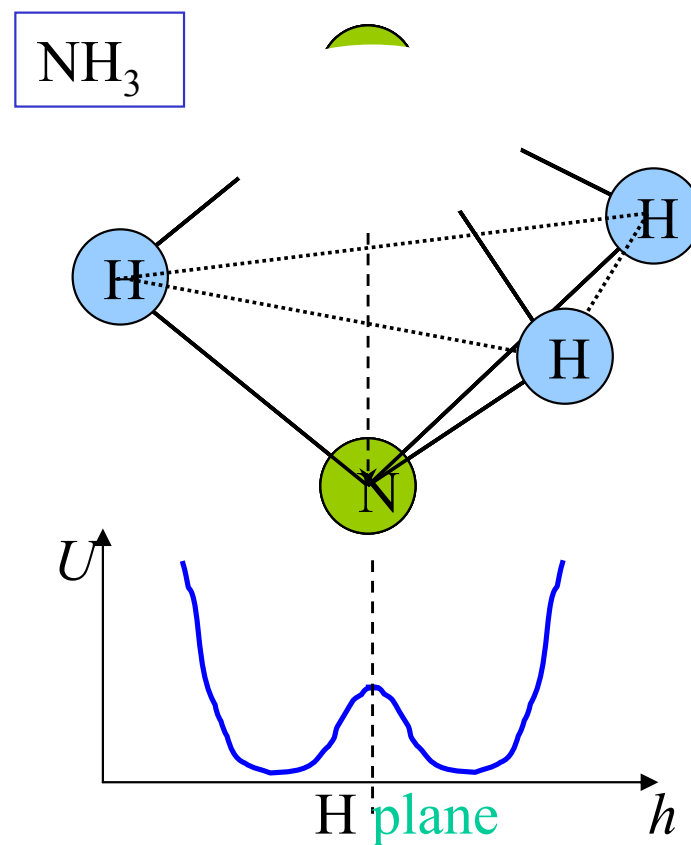
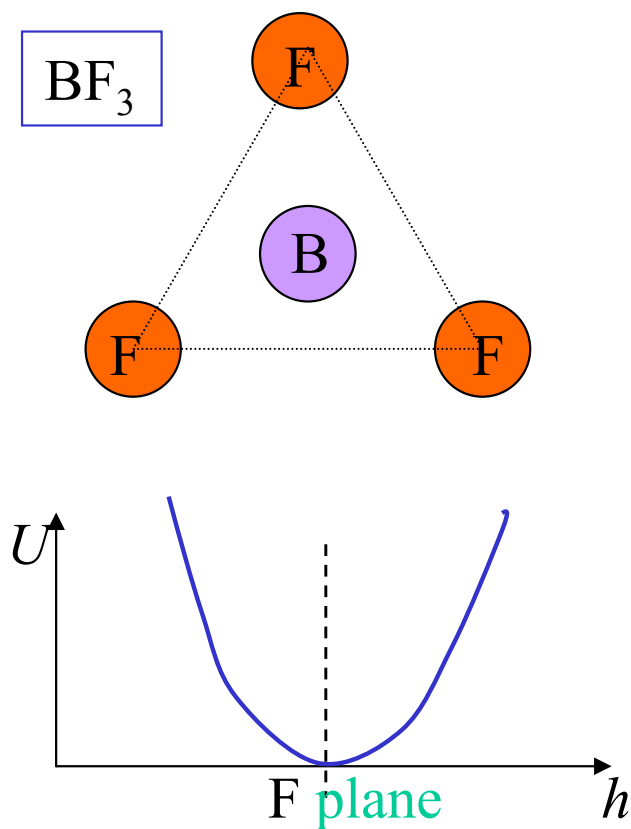


$U$  adiabatic potential energy

**stable equilibrium**  
**non-degenerate**  
**ground state**

**metastable equilibrium**  
**degenerate**  
**ground state**

# Equilibrium structure of the $AB_3$ molecules



$U$  adiabatic potential energy

**stable equilibrium**  
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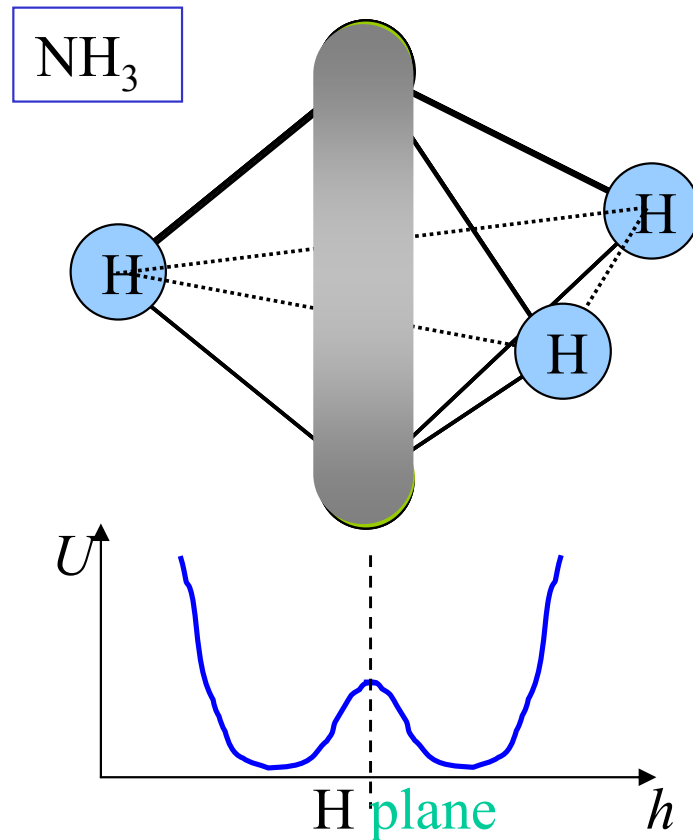
# Equilibrium structure of the $AB_3$ molecules

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

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

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

**degeneracy**

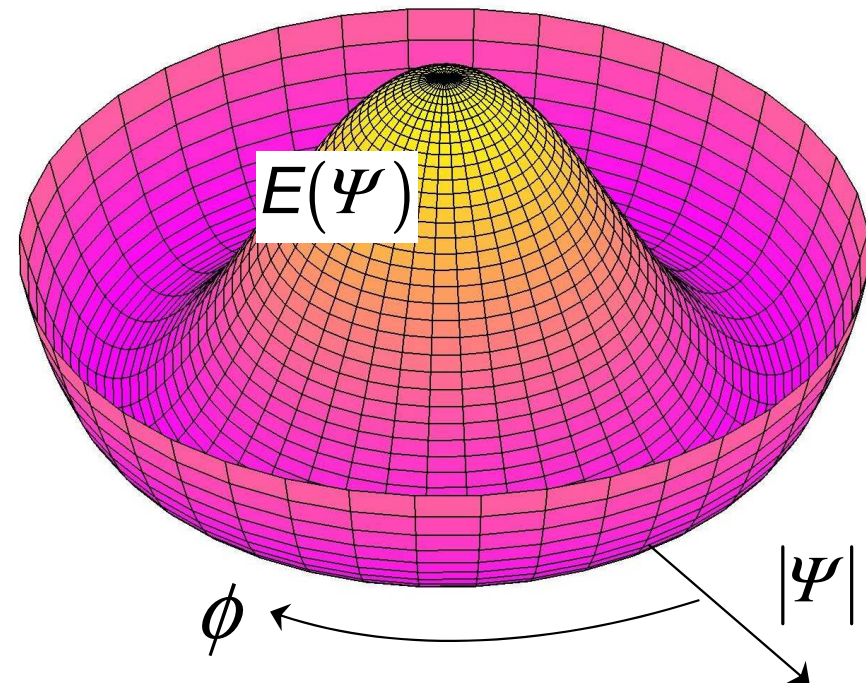
genuinely different  
for different  $\phi$

## Selection rule

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

$$\langle a_0 \rangle = \int d\phi \langle a_0 \rangle_\phi = 0$$

average over all degenerate states



"Mexican hat"

# Symmetry breaking – removal of the degeneracy

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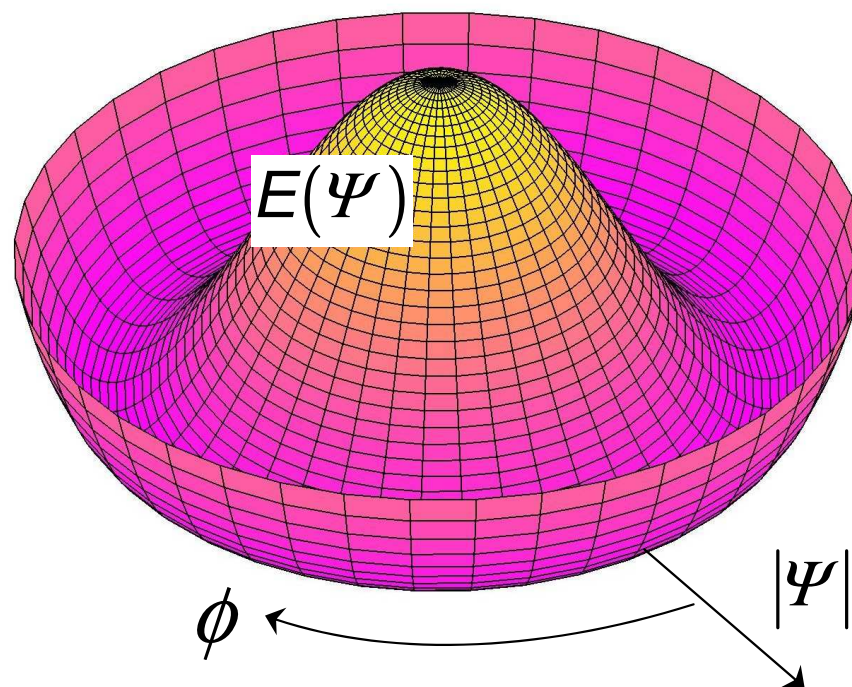
genuinely different  
for different  $\phi$

Symmetry broken by a small  
perturbation picking up one  $\phi$

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

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

particle number NOT conserved



"Mexican hat"

# Symmetry breaking – removal of the degeneracy

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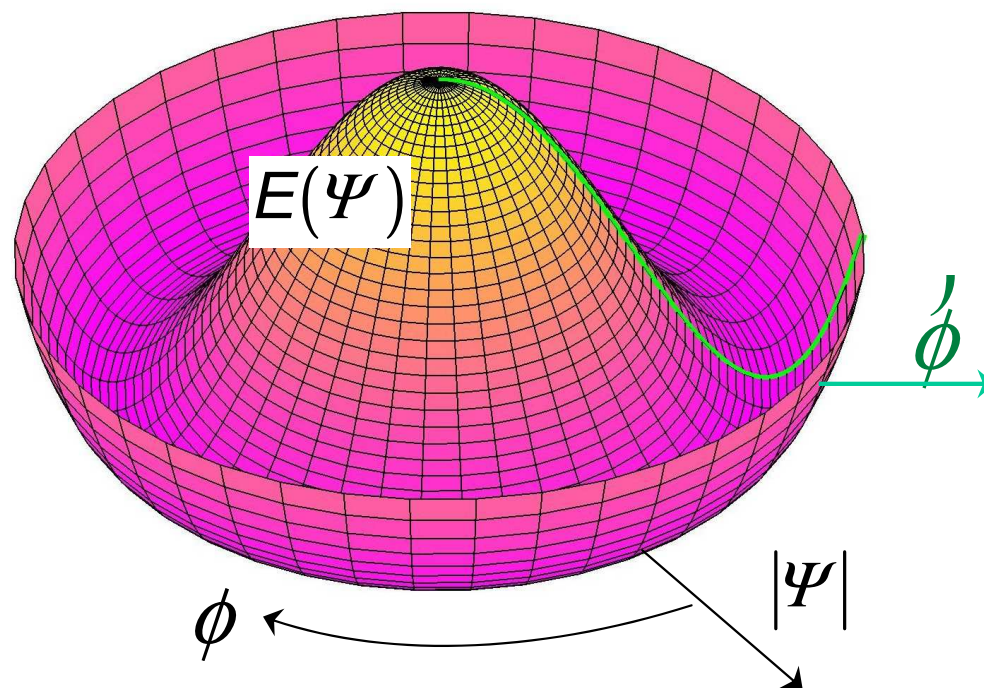
$$\mathcal{H} - \mu \mathcal{N} \rightarrow$$

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

particle number NOT conserved

For  $\lambda \rightarrow 0$

one particular phase selected



"Mexican hat"

100

## How the symmetry breaking works – ideal BE gas

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

$$\begin{aligned}\mathcal{H} - \mu\mathcal{N} - \lambda\left(a_0^\dagger e^{i\phi} + a_0 e^{-i\phi}\right) \\ &= -\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger e^{i\phi} + a_0 e^{-i\phi}\right) + \sum_{k \neq 0} \frac{\hbar^2}{2m} (\mathbf{k}^2 - \mu) a_k^\dagger a_k \\ &\rightarrow -\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger e^{i\phi} + a_0 e^{-i\phi}\right)\end{aligned}$$

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

Transformation:

$$\begin{aligned}-\mu a_0^\dagger a_0 - \lambda\left(a_0^\dagger e^{i\phi} + a_0 e^{-i\phi}\right) &= -\mu\left(a_0^\dagger a_0 + \frac{\lambda}{\mu} e^{i\phi} a_0^\dagger + \frac{\lambda}{\mu} e^{-i\phi} a_0\right) \\ &\equiv -\mu\left(a_0^\dagger a_0 - \Lambda a_0^\dagger - \Lambda^* a_0\right) = -\mu\left((a_0^\dagger - \Lambda^*)(a_0 - \Lambda) - \Lambda^* \Lambda\right) \\ &\equiv -\mu\left(b_0^\dagger b_0 - \Lambda^* \Lambda\right)\end{aligned}$$

# How the symmetry breaking works – ideal BE gas

Now we determine the many-body ground state

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

The lowest energy corresponds to

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

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

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

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

Infinitesimal symmetry breaking field  $\lambda \rightarrow 0$

$\lambda \rightarrow 0$  with  $N_0$  fixed:

$$\mu \rightarrow 0 - 0$$

$$\mathcal{E} \rightarrow 0$$

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

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

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

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

**Infinitesimal symmetry breaking field**  $\lambda \rightarrow 0$

$\lambda \rightarrow 0$  with  $N_0$  fixed:

$$\mu \rightarrow 0 - 0$$

$$\mathcal{E} \rightarrow 0$$

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

- 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  $\lambda \rightarrow 0$ , only then the thermodynamic limit  $N_0 \rightarrow \infty$

The end