

Cold atoms

Lecture 6.

29th November, 2006

Preliminary plan/reality in the fall term

Lecture 1	Something about everything (see next slide)	Sep 22
...	The textbook version of BEC in extended systems	
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	
...		

The class before last:
Interacting atoms

L4: Scattering length, pseudopotential

Beyond the potential radius, say 3σ , the scattered wave propagates in free space

For small energies, the scattering is purely isotropic, the s-wave scattering. The outside wave is

$$\psi \propto \frac{\sin(kr + \delta_0)}{r}$$

For very small energies the radial part becomes just

$$r - a_s, \quad a_s \dots \text{the scattering length}$$

This may be extrapolated also into the interaction sphere (we are not interested in the short range details)

Equivalent potential ("pseudopotential")

$$U(r) = g \cdot \delta(r)$$
$$g = \frac{4\pi a_s \hbar^2}{m}$$

The class before last:
Mean-field treatment of interacting atoms

L4: Many-body Hamiltonian and the Hartree approximation

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

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

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

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

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

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

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

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

self-consistent
system

L4: Gross-Pitaevskii equation at zero temperature

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

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

Putting

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

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

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

This is the celebrated **Gross-Pitaevskii equation**.

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

Then

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

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

The lowest level coincides with the chemical potential

Gross-Pitaevskii equation – homogeneous gas

The GP equation simplifies

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

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

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

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

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

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

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

Previous class:
Field theoretic reformulation
(second quantization)

L5: Field operator for spin-less bosons

Definition by commutation relations

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

basis of single-particle states (κ complete set of quantum numbers)
decomposition of the field operator

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

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

commutation relations

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

Plane wave representation (BK normalization)

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

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

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

L5: 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 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

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

Hamiltonian

$$\begin{aligned} H &= \sum_a \frac{1}{2m} p_a^2 + V(\mathbf{r}_a) + \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b) \\ &= \int d^3r \psi^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \psi(\mathbf{r}) + \frac{1}{2} \iint d^3r d^3r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \end{aligned}$$

Previous class:
Bogolyubov method

L5: Basic idea

Bogolyubov method

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

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

The condensate dominates.

Strange idea

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

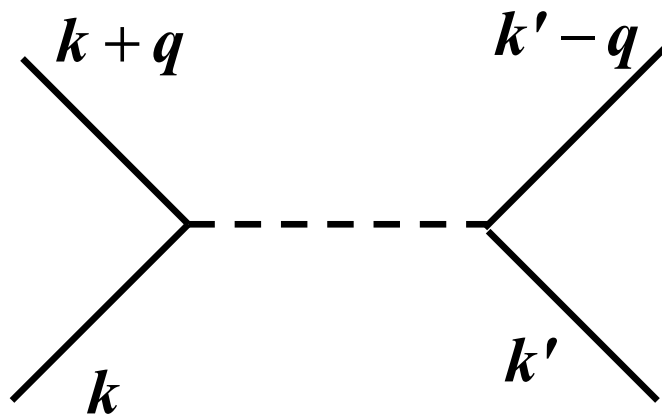
$$a_0 \approx \sqrt{N_0}, \quad a_0^\dagger \approx \sqrt{N_0}$$

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

L5: Hamiltonian of the homogeneous gas

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

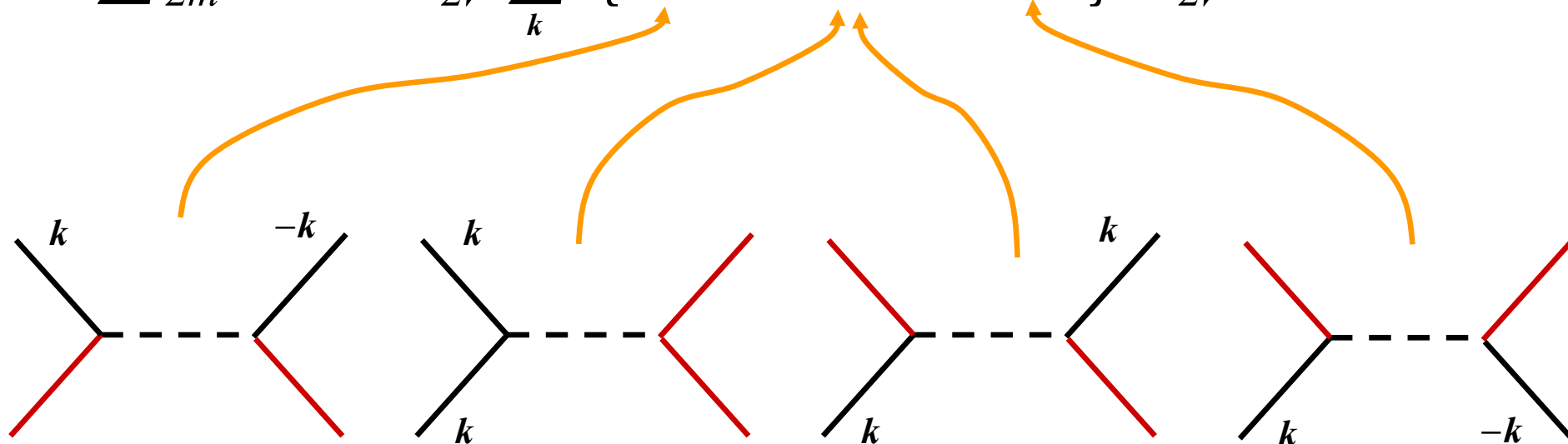
$$U_{\mathbf{k}} = \int d^3 \mathbf{r} e^{-i\mathbf{k}\mathbf{r}} U(\mathbf{r})$$



L5: Approximate Hamiltonian

Keep at most two particles out of the condensate

$$\begin{aligned}
 H &= \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} V^{-1} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} U_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}} \\
 &= \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{UN_0}{2V} \sum_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + 4a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{\mathbf{k}} a_{-\mathbf{k}} \right\} + \frac{UN_0^2}{2V} \\
 &= \sum \frac{\hbar^2}{2m} \mathbf{k}^2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{UN}{2V} \sum_{\mathbf{k}} \left\{ a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + 2a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{\mathbf{k}} a_{-\mathbf{k}} \right\} + \frac{UN^2}{2V}
 \end{aligned}$$



— condensate particle

L5: Bogolyubov transformation

Last rearrangement

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

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

NEW FIELD OPERATORS notice momentum conservation!!

$$\begin{array}{l|l} b_k = u_k a_k + v_k a_{-k}^\dagger & a_k = u_k b_k - v_k b_{-k}^\dagger \\ b_{-k}^\dagger = v_k a_k + u_k a_{-k}^\dagger & a_{-k}^\dagger = -v_k b_k + u_k b_{-k}^\dagger \end{array}$$

requirements

- 1 New operators should satisfy the boson commutation rules

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

$$\text{iff } u_k^2 - v_k^2 = 1$$

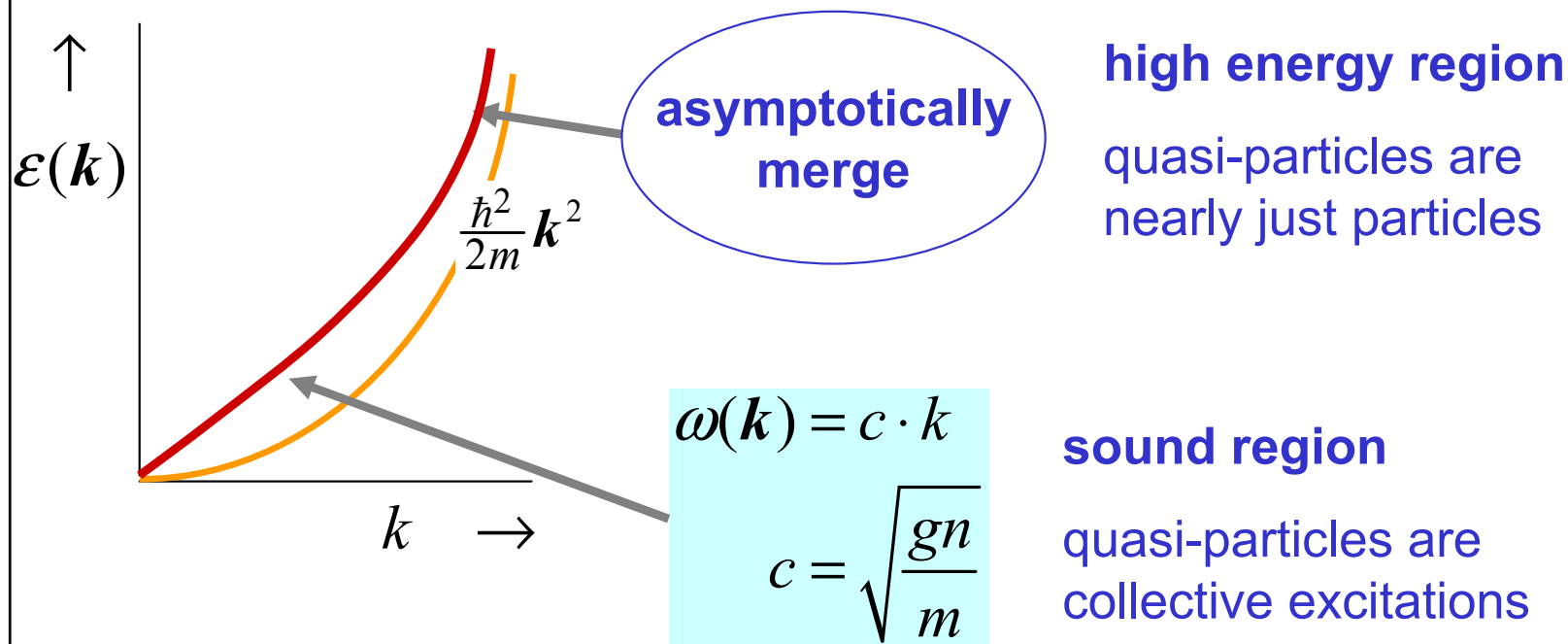
- 2 When introduced into the Hamiltonian, the anomalous terms have to vanish

L5: Bogolyubov transformation – result

Without quoting the transformation matrix

$$H = \frac{1}{2} \sum \underbrace{\varepsilon(\mathbf{k}) \{a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}}\}}_{\text{independent quasiparticles}} + \frac{UN^2}{2V} + \text{higher order constant}$$

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



L5: 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:

$$c = \sqrt{\frac{\kappa}{\rho}} = \sqrt{\frac{V \partial_{VV} E}{m \cdot n}}, \quad E = \frac{UN^2}{2V} + \dots$$

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

- 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
- 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 amount of the particles outside of the condensate is

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

the gas parameter
is
the expansion variable

Trying to understand the Bogolyubov
method

L5: Action of the field operators in the Fock space

basis of single-particle states

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

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

FOCK SPACE 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, ...**

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

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

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

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

Average values of the field operators in the Fock states

$$a_p^\dagger \left| n_1, n_2, n_3, \dots, n_p, \dots \right\rangle = \sqrt{n_p + 1} \left| n_1, n_2, n_3, \dots, n_p + 1, \dots \right\rangle$$

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

$$\left\langle n_1, n_2, n_3, \dots, n_p, \dots \left| a_p \right| n_1, n_2, n_3, \dots, n_p, \dots \right\rangle =$$

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

Off-diagonal elements only!!!

L5: Hamiltonian conserves the particle number

Particle number conservation

$$[H, N] = 0$$

Equilibrium density operators and the ground state

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

Typical selection rule

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

is a consequence of the gauge invariance of the 1st kind:

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

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This is at odds with the Bogolyubov idea

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

which leads to

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

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which leads to

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

Perhaps the ground state does not conserve the particle number??

First try:
Coherent ground state

Reformulation of the Bogolyubov requirements

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

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

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

The ground state

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

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

For a coherent state, there is no problem with the particle number conservation. It has a rather uncertain particle number, but a well defined phase:

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

explicit form

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

Bogolyubov condition

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

$$\langle n_0 \rangle = N$$

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

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

$$\Delta N_0 = |\Lambda|$$

$$\Delta n_0 = \sqrt{N} = \langle n_0 \rangle / \sqrt{N} \square \langle n_0 \rangle$$

New vacuum and the shifted field operators

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

$$H - \mu N$$

Let us define the shifted field operator

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

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

What next? Example: BE system without interactions – ideal Bose gas

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

Here, $|\Psi\rangle$ is a true eigenstate, μ coincides with the previous result for the particle number conserving state. **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

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

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

General case: the Bogolyubov transformation

Define

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

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

$$\boxed{\varphi(\mathbf{r}) = u(\mathbf{r})\eta(\mathbf{r}) + v(\mathbf{r})\eta^\dagger(\mathbf{r}) \quad \varphi^\dagger(\mathbf{r}) = v^*(\mathbf{r})\eta(\mathbf{r}) + u^*(\mathbf{r})\eta^\dagger(\mathbf{r})}$$

$$[\varphi(\mathbf{r}), \varphi^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}') \quad \text{iff} \quad |u(\mathbf{r})|^2 - |v(\mathbf{r})|^2 = 1$$

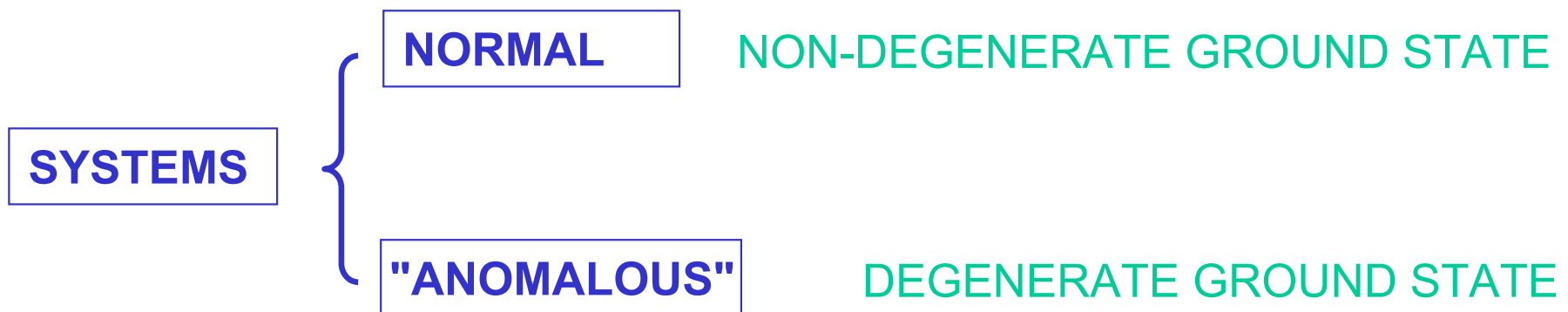
$$\eta(\mathbf{r}) = u^*(\mathbf{r})\varphi(\mathbf{r}) - v(\mathbf{r})\varphi^\dagger(\mathbf{r}) \quad \eta^\dagger(\mathbf{r}) = -v^*(\mathbf{r})\varphi(\mathbf{r}) + u(\mathbf{r})\varphi^\dagger(\mathbf{r})$$

Second try:
Quasi-averages and broken symmetry

Zero temperature limit of the grand canonical ensemble

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

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

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

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

spontaneous symmetry breaking

$$a > 0$$

stable equilibrium

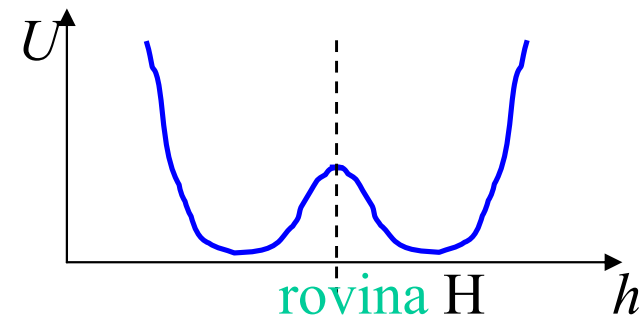
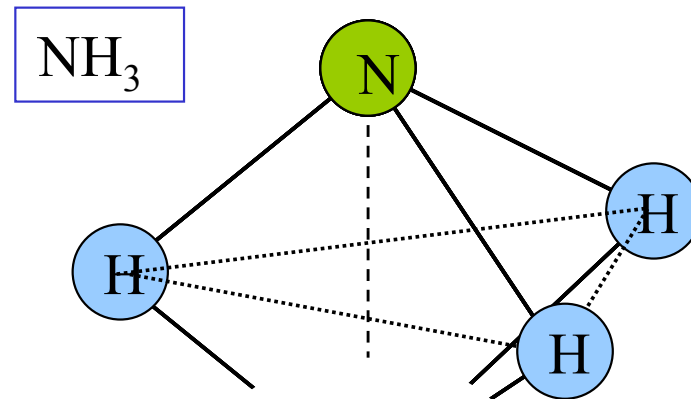
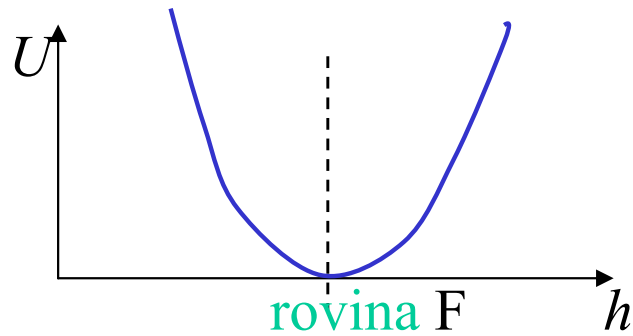
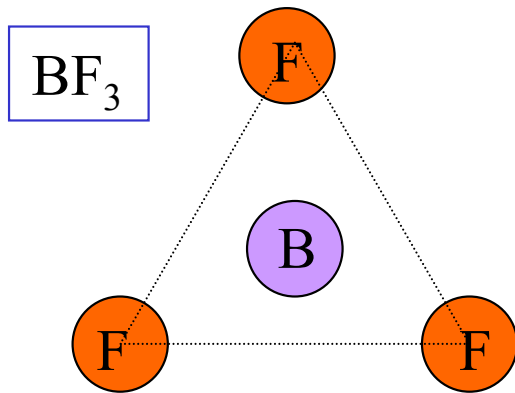
non-degenerate

$$a < 0$$

metastable equilibrium

degenerate

Rovnovážná struktura molekul AB_3



U adiabatická potenciální energie

The end

ADDITIONAL NOTES

On the way to the mean-field Hamiltonian

ADDITIONAL NOTES

On the way to the mean-field Hamiltonian

① First, the following exact transformations are performed

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

$$\hat{V} = \sum_a V(\mathbf{r}_a) = \int d^3 \mathbf{r} V(\mathbf{r}) \sum_a \delta(\mathbf{r} - \mathbf{r}_a) \equiv \int d^3 \mathbf{r} V(\mathbf{r}) \cdot \hat{n}(\mathbf{r})$$

particle density operator

$$\hat{U} = \frac{1}{2} \sum_{a \neq b} \sum U(\mathbf{r}_a - \mathbf{r}_b) = \frac{1}{2} \int d^3 \mathbf{r} d^3 \mathbf{r}' U(\mathbf{r} - \mathbf{r}') \sum_{a \neq b} \sum \delta(\mathbf{r} - \mathbf{r}_a) \delta(\mathbf{r}' - \mathbf{r}_b)$$

$$= \frac{1}{2} \int d^3 \mathbf{r} d^3 \mathbf{r}' U(\mathbf{r} - \mathbf{r}') \sum_a \delta(\mathbf{r} - \mathbf{r}_a) \left\{ \sum_b \delta(\mathbf{r}' - \mathbf{r}_b) - \delta(\mathbf{r} - \mathbf{r}') \right\}$$

$\hat{n}(\mathbf{r})$
 $\hat{n}(\mathbf{r}')$
TRICK!!
eliminates **SI**
(self-interaction)

$$\hat{H} = \hat{W} + \int d^3 \mathbf{r} V(\mathbf{r}) \cdot \hat{n}(\mathbf{r}) + \frac{1}{2} \int d^3 \mathbf{r} d^3 \mathbf{r}' U(\mathbf{r} - \mathbf{r}') \hat{n}(\mathbf{r}) \{ \hat{n}(\mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}') \}$$

ADDITIONAL NOTES

On the way to the mean-field Hamiltonian

② Second, a specific many-body state is chosen, which defines the mean field:

$$\Psi \rightarrow n(\mathbf{r}) = \langle \hat{n}(\mathbf{r}) \rangle \equiv \langle \Psi | \hat{n}(\mathbf{r}) | \Psi \rangle$$

Then, the operator of the (quantum) density fluctuation is defined:

$$\hat{n}(\mathbf{r}) = n(\mathbf{r}) + \Delta \hat{n}(\mathbf{r})$$

$$\hat{n}(\mathbf{r}) \hat{n}(\mathbf{r}') = \hat{n}(\mathbf{r}) n(\mathbf{r}') + n(\mathbf{r}) \hat{n}(\mathbf{r}') + \Delta \hat{n}(\mathbf{r}) \Delta \hat{n}(\mathbf{r}') - n(\mathbf{r}) n(\mathbf{r}')$$

The Hamiltonian, still exactly, becomes

$$\begin{aligned} \hat{H} = & \hat{W} + \int d^3 r \left\{ V(\mathbf{r}) + \int d^3 r' U(\mathbf{r} - \mathbf{r}') n(\mathbf{r}') \right\} \cdot \hat{n}(\mathbf{r}) \\ & - \frac{1}{2} \int d^3 r d^3 r' U(\mathbf{r} - \mathbf{r}') n(\mathbf{r}) n(\mathbf{r}') \\ & + \frac{1}{2} \int d^3 r d^3 r' U(\mathbf{r} - \mathbf{r}') \left\{ \Delta \hat{n}(\mathbf{r}) \Delta \hat{n}(\mathbf{r}') - \hat{n}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \right\} \end{aligned}$$

ADDITIONAL NOTES

On the way to the mean-field Hamiltonian

③ In the last step, the third line containing exchange, correlation and the self-interaction correction is neglected. The mean-field Hamiltonian of the main lecture results: ←

$$V_H(\mathbf{r})$$

substitute back
 $\hat{n}(\mathbf{r}) = \sum_a \delta(\mathbf{r} - \mathbf{r}_a)$
and integrate

$$+\frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' U(\mathbf{r} - \mathbf{r}') \{ \cancel{\Delta \hat{n}(\mathbf{r}) \Delta \hat{n}(\mathbf{r}')} - \hat{n}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \}$$

REMARKS

- Second line ... an additive constant compensation for double-counting of the Hartree interaction energy
- In the original (variational) Hartree approximation, the self-interaction is not left out, leading to non-orthogonal Hartree orbitals

BACK

Variational approach
to the condensate ground state

ADDITIONAL NOTES

Variational estimate of the condensate properties

① VARIATIONAL PRINCIPLE OF QUANTUM MECHANICS

The ground state and energy are uniquely defined by

$$E = \langle \Psi | \hat{H} | \Psi \rangle \leq \langle \Psi' | \hat{H} | \Psi' \rangle \quad \text{for all } |\Psi'\rangle \in \mathcal{H}_N^S, \langle \Psi' | \Psi' \rangle = 1$$

In words, $|\Psi'\rangle$ is a normalized symmetrical wave function of N particles. The minimum condition in the variational form is

$$\delta \langle \Psi | \hat{H} | \Psi \rangle = 0 \quad \text{equivalent with the SR} \quad \hat{H} | \Psi \rangle = E | \Psi \rangle$$

② HARTREE VARIATIONAL ANSATZ FOR THE CONDENSATE WAVE F.

For our many-particle Hamiltonian,

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

the true ground state is approximated by the condensate for non-interacting particles (Hartree Ansatz, here identical with the symmetrized Hartree-Fock)

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_p, \dots, \mathbf{r}_N) = \varphi_0(\mathbf{r}_1) \varphi_0(\mathbf{r}_2) \cdots \varphi_0(\mathbf{r}_p) \cdots \varphi_0(\mathbf{r}_N)$$

ADDITIONAL NOTES

Variational estimate of the condensate properties

Here, φ_0 is a normalized real spinless orbital. It is a functional variable to be found from the variational condition

$$\delta \mathcal{E}[\varphi_0] = \delta \langle \Psi[\varphi_0] | \hat{H} | \Psi[\varphi_0] \rangle = 0 \quad \text{with} \quad \langle \Psi[\varphi_0] | \Psi[\varphi_0] \rangle = 1 \Leftrightarrow \langle \varphi_0 | \varphi_0 \rangle = 1$$

Explicit calculation yields

$$\mathcal{E}[\varphi_0] = \frac{\hbar^2}{2m} N \int d^3 \mathbf{r} (\nabla \varphi_0(\mathbf{r}))^2 + N \int d^3 \mathbf{r} V(\mathbf{r}) (\varphi_0(\mathbf{r}))^2 + \frac{1}{2} N(N-1) g \int d^3 \mathbf{r} (\varphi_0(\mathbf{r}))^4$$

Variation of energy with the use of a Lagrange multiplier:

$$\delta \left\{ N^{-1} \mathcal{E}[\varphi_0] - \mu \langle \varphi_0 | \varphi_0 \rangle \right\}$$

$$\varphi_0 = \varphi_0(\mathbf{r}), \quad \delta \varphi_0 = \delta \varphi_0(\mathbf{r})$$

$$= \frac{2\hbar^2}{2m} \int d^3 \mathbf{r} \delta \varphi_0 \cdot (-\Delta \varphi_0) + 2 \int d^3 \mathbf{r} \delta \varphi_0 \cdot (V(\mathbf{r}) - \mu) \varphi_0 + \frac{4}{2} (N-1) g \int d^3 \mathbf{r} \delta \varphi_0 \cdot \varphi_0^3$$

This results into the GP equation derived here in the variational way:

$$\left(\frac{1}{2m} p^2 + V(\mathbf{r}) + (N - 1) g |\varphi_0(\mathbf{r})|^2 \right) \varphi_0(\mathbf{r}) = \mu \varphi_0(\mathbf{r})$$

eliminates self-interaction

BACK

ADDITIONAL NOTES

Variational estimate of the condensate properties

② ANNEX Interpretation of the Lagrange multiplier μ

The idea is to identify it with the chemical potential. First, we modify the notation to express the particle number dependence

$$\mathcal{E}_N[\varphi] = N \left\{ \langle \varphi | \frac{1}{2m} p^2 | \varphi \rangle + \langle \varphi | V | \varphi \rangle + \frac{1}{2} (N-1) g \int d^3 r \varphi^4 \right\}$$

$$E_N = \mathcal{E}_N[\varphi_{0N}], \quad \left(\frac{1}{2m} p^2 + V(\mathbf{r}) + (N-1) g |\varphi_{0N}(\mathbf{r})|^2 \right) \varphi_0(\mathbf{r}) = \mu_N \varphi_{0N}(\mathbf{r})$$

The first result is that μ is not the average energy per particle:

$$E_N / N = \mathcal{E}_N[\varphi_{0N}] / N = \langle \varphi_{0N} | \frac{1}{2m} p^2 | \varphi_{0N} \rangle + \langle \varphi_{0N} | V | \varphi_{0N} \rangle + \frac{1}{2} (N-1) g \int d^3 r \varphi_{0N}^4$$

from the GPE

$$\mu_N = \langle \varphi_{0N} | \frac{1}{2m} p^2 | \varphi_{0N} \rangle + \langle \varphi_{0N} | V | \varphi_{0N} \rangle + (N-1) g \int d^3 r \varphi_{0N}^4$$

ADDITIONAL NOTES

Variational estimate of the condensate properties

Compare now systems with N and $N-1$ particles:

$$E_N = \mathcal{E}_N[\varphi_{0N}] = \mathcal{E}_{N-1}[\varphi_{0N}] + \mu_N \geq \mathcal{E}_{N-1}[\varphi_{0,N-1}] + \mu_N = E_{N-1} + \mu_N$$



In the "thermodynamic" asymptotics of large N , the inequality tends to equality. This only makes sense, and can be proved, for $g > 0$.

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Reminescent of the Derivation:

theorem in the HF theory of atoms.

$$\begin{aligned} \mathcal{E}_N[\varphi] &= N \langle \varphi | \frac{1}{2m} p^2 | \varphi \rangle + N \langle \varphi | V | \varphi \rangle + \frac{1}{2} N(N-1) g \int d^3 r \varphi^4 \\ \mathcal{E}_{N-1}[\varphi] &= (N-1) \langle \varphi | \frac{1}{2m} p^2 | \varphi \rangle + (N-1) \langle \varphi | V | \varphi \rangle + \frac{1}{2} (N-1)(N-2) g \int d^3 r \varphi^4 \\ \mathcal{E}_N - \mathcal{E}_{N-1} &= \underbrace{\langle \varphi | \frac{1}{2m} p^2 | \varphi \rangle + \langle \varphi | V | \varphi \rangle + \frac{1}{2} (N(N-1) - (N-1)(N-2)) g \int d^3 r \varphi^4}_{\mu_N \text{ for } \varphi \mapsto \varphi_{0N}} \end{aligned}$$

ADDITIONAL NOTES

Variational estimate of the condensate properties

③ SCALING ANSATZ FOR A SPHERICAL PARABOLIC TRAP

The potential energy has the form

$$V(\mathbf{r}) = \frac{1}{2} m \omega_0^2 \cdot r^2 = \frac{1}{2} m \omega_0^2 (x^2 + y^2 + z^2)$$

Without interactions, the GPE reduces to the SE for isotropic oscillator

$$\left(\frac{1}{2m} p^2 + \frac{1}{2} m \omega_0^2 \cdot r^2 \right) \varphi_0(\mathbf{r}) = \frac{3}{2} \hbar \omega_0 \varphi_0(\mathbf{r})$$

The solution (for the ground state orbital) is

$$\varphi_{00}(\mathbf{r}) = A_0^3 e^{-\frac{1}{2} \frac{r^2}{a_0^2}}, \quad a_0 = \sqrt{\frac{\hbar}{m \omega_0}}, \quad \hbar \omega_0 = \frac{\hbar^2}{m a_0^2}, \quad A_0 = (a_0^2 \pi)^{-1/4}$$

We (have used and) will need two integrals:

$$I_1(\sigma) = \int_{-\infty}^{+\infty} du e^{-\frac{u^2}{\sigma^2}} = \sigma \sqrt{\pi}, \quad I_2(\sigma) = \int_{-\infty}^{+\infty} du e^{-\frac{u^2}{\sigma^2}} u^2 = \frac{1}{2} \sigma^3 \sqrt{\pi}$$

ADDITIONAL NOTES

Variational estimate of the condensate properties

SCALING ANSATZ

The condensate orbital will be taken in the form

$$\varphi_0(\mathbf{r}) = A^3 e^{-\frac{1}{2} \frac{r^2}{b^2}}, \quad A = (b^2 \pi)^{-1/4}$$

It is just like the ground state orbital for the isotropic oscillator, but with a rescaled size. This is reminiscent of the well-known scaling for the ground state of the helium atom.

Next, the total energy is calculated for this orbital

$$\begin{aligned} \mathcal{E}[\varphi_0] &= \frac{\hbar^2}{2m} N \int d^3 \mathbf{r} (\nabla \varphi_0(\mathbf{r}))^2 + N \int d^3 \mathbf{r} V(\mathbf{r}) (\varphi_0(\mathbf{r}))^2 + \frac{1}{2} N(N-1) g \int d^3 \mathbf{r} (\varphi_0(\mathbf{r}))^4 \\ &= \frac{1}{2} \hbar \omega_0 N A^6 \left\{ \frac{a_0^2}{b^4} \int d^3 \mathbf{r} e^{-\frac{r^2}{b^2}} r^2 + \frac{1}{a_0^2} \int d^3 \mathbf{r} e^{-\frac{r^2}{b^2}} r^2 + (N-1) A^6 \frac{m a_0^2}{\hbar^2} g \int d^3 \mathbf{r} e^{-\frac{2r^2}{b^2}} \right\} \end{aligned}$$

ADDITIONAL NOTES

Variational estimate of the condensate properties

For an explicit evaluation, we (have used and) will use the identities:

$$\frac{\hbar^2}{m} = \hbar\omega_0 a_0^2, \quad m\omega_0^2 = \frac{\hbar\omega_0}{a_0^2}, \quad A^2 = \frac{1}{I_1(b)} = \frac{1}{b\sqrt{\pi}}, \quad g = \frac{4\pi\hbar^2 a_s}{m}$$

$$\mathcal{E}[\varphi_0] =$$

The integrals, by the Fubini theorem, are a product of three:

$$= \hbar\omega_0 N \left\{ \frac{3I_2(b) (I_1(b))^2}{2b\sqrt{\pi} (I_1(b))^2} \left\{ \frac{a_0^2}{b^4} + \frac{1}{a_0^2} \right\} + (N-1) \frac{1}{2b^3\pi^{3/2}} \frac{ma_0^2}{\hbar^2} \frac{4\pi\hbar^2 a_s}{m} \frac{(I_1(b/\sqrt{2}))^3}{(I_1(b))^3} \right\}$$

Finally,

$$\mathcal{E}[\varphi_0] = \hbar\omega_0 N \left\{ \frac{3}{4} \left\{ \frac{a_0^2}{b^2} + \frac{b^2}{a_0^2} \right\} + \frac{(N-1) a_s}{\sqrt{2\pi} a_0} \cdot \frac{a_0^3}{b^3} \right\} \equiv \hbar\omega_0 N \cdot \tilde{E}(\tilde{\sigma})$$

dimension-less
energy per particle

$$\tilde{E}(\tilde{\sigma}) = \frac{3}{4} \left\{ \frac{1}{\tilde{\sigma}^2} + \tilde{\sigma}^2 \right\} + \eta \cdot \frac{1}{\tilde{\sigma}^3}$$

$$\tilde{\sigma} = \frac{b}{a_0}$$

dimension-less
orbital size

This expression is plotted in the figures in the main lecture.

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ADDITIONAL NOTES

