Chaire Européenne du Collège de France (2004/2005)

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Lecture 1
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Bose-Einstein condensation and long range order

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BEC INFM

Bose-Einstein condensation and superfluidity

Key concepts in low temperature physics . Recent major progress in atomic quantum gases (main object of the present course)

Non trivial intercorrelated effects:

- **Role of interactions** (are interactions friends or enemies of BEC and superfluidity? Tunability of interaction)
- **Non uniform** nature of the confinement (harmonic, periodic); BEC in both momentum and **coordinate** space;
- **Dimensionality**; (1D and 2D configurations now achievable)

- **BEC** (can be defined at **equilibrium**)
- **Superfluidity** (mainly related to **transport** phenomena)

Natural link between BEC and superfluidity provided by order parameter

$$\Psi = |\Psi| e^{iS}$$

sqrt of condensate density

$$v_S = \frac{\hbar}{m} \nabla S$$

Superfluid velocity (irrotationality)

Plan of the course

Lecture 1. **BEC and long range order**
- Long range order, eigenvalues of density matrix
- order parameter and concept of classical field
- BEC in ideal gas (3D harmonic trapping)
- interactions and BEC fragmentation (uniform gas, double potential)

Lecture 2. **Superfluidity and hydrodynamics.**
Landau criterion (galilean vs rotational). Hydrodynamic theory of superfluids. Collective oscillations and expansion.

Lecture 3. **Equation for the order parameter**.
Gross-Pitaevskii theory. Healing length.
Time dependent theory. Bogoliubov equations.

Lecture 4. **Fluctuations of the order parameter**.
Quantum fluctuations and BEC depletion.
Thermal depletion. Shift of critical temperature.

Lecture 5. **BEC in low dimensions**.
Theorems on long range order. Algebraic decay in low D. Mean field and beyond mean field. Collective oscillations in 1D gas.

Lecture 6. **Moment of inertia and superfluidity.**
Irrotational vs rotatational flow. Moment of inertia. Scissors. Expansion of rotating BEC.

Lecture 7. **Quantized vortices.**
Quantization of circulation. Nucleation of vortices. Measurement of angular momentum. Vortex lattice. Collective oscillations.

Lecture 8. **Ultracold Fermi gases.**
Ideal Fermi gas in harmonic trap. Role of interactions. BCS-BEC crossover. Unitarity and universality. Effects of superfluidity.

Lecture 9. **BEC in periodic potentials.**
Momentum distribution and interference. Bloch oscillations. Josephson oscillations. Superfluid vs insulator phase.

Some references:

- F. Dalfovo et al. Rev. Mod Phys. **71**, 463 (1999)
- "Bose-Einstein Condensation in Atomic Gases", Enrico Fermi Summer School, M. Inguscio et al. (1999) (collection of experimental and theoretical papers)
- A. Leggett, Rev. Mod. Phys. **73**, 307 (2001)
- E. Cornell, W. Ketterle and C. Weiman, Nobel Lectures Rev. Mod. Phys. **74** (2002)
- C. Pethick and H. Smith, "Bose-Einstein Condensation in Dilute Bose Gases", Cambridge University Press (2002)
- L. Pitaevskii and S. Stringari "Bose-Einstein Condensation", Oxford University Press (2003)

systematically employed in this course

1-body density matrix and long-range order

$$n^{(1)}(r,r') = \left\langle \hat{\Psi}^{+}(r)\hat{\Psi}(r') \right\rangle$$

(Bose field operators)

Relevant observables related to 1-body density:

- **Density**: $n(r) = n^{(1)}(r,r)$

- **Momentum distribution**:

$$n(p) = (2\pi\hbar)^{-3}\int dRdsn^{(1)}(R+s/2),R-s/2)e^{-ips/\hbar}$$

In uniform systems

$$n^{(1)}(r,r') = n^{(1)}(s) = \frac{1}{V}\int dpn(p)e^{ips/\hbar}$$

If n(p) is smooth function → $n^{(1)}(s)_{s\to\infty} = 0$

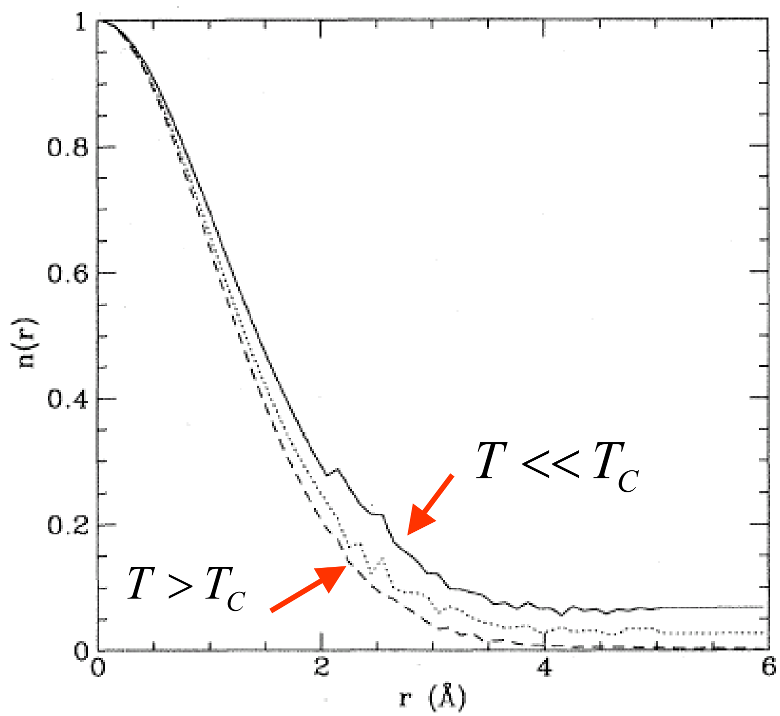
If $n(p) = N_0\delta(p) + \tilde{n}(p)$ → $n^{(1)}(s)_{s\to\infty} = n_0 = \dfrac{N_0}{V}$

Smooth function

Off-diagonal long range order
(Landau, Lifschitz, Penrose, Onsager)

Example of calculation of density matrix in highly correlated many-body system: liquid He4

(Ceperley, Pollock 1987)



Long range order and eigenvalues of density matrix

$$\int dr' n^{(1)}(r,r')\varphi_i(r') = n_i \varphi_i(r)$$

$$n^{(1)}(r,r') = \sum_i n_i \varphi_i^*(r)\varphi_i(r')$$

BEC occurs when $n_o \equiv N_0 >> 1$. It is then convenient to rewrite density matrix by separating contribution arising from condensate:

$$n^{(1)}(r,r') = N_0 \varphi_0^*(r)\varphi_i(r') + \sum_{i\neq 0} n_i \varphi_i^*(r)\varphi_i(r')$$

For large N the sum can be replaced by integral which tends to zero at large distances.
Viceversa contribution from condensate remains finite up to distances $|r-r'|$ fixed by size of φ_0

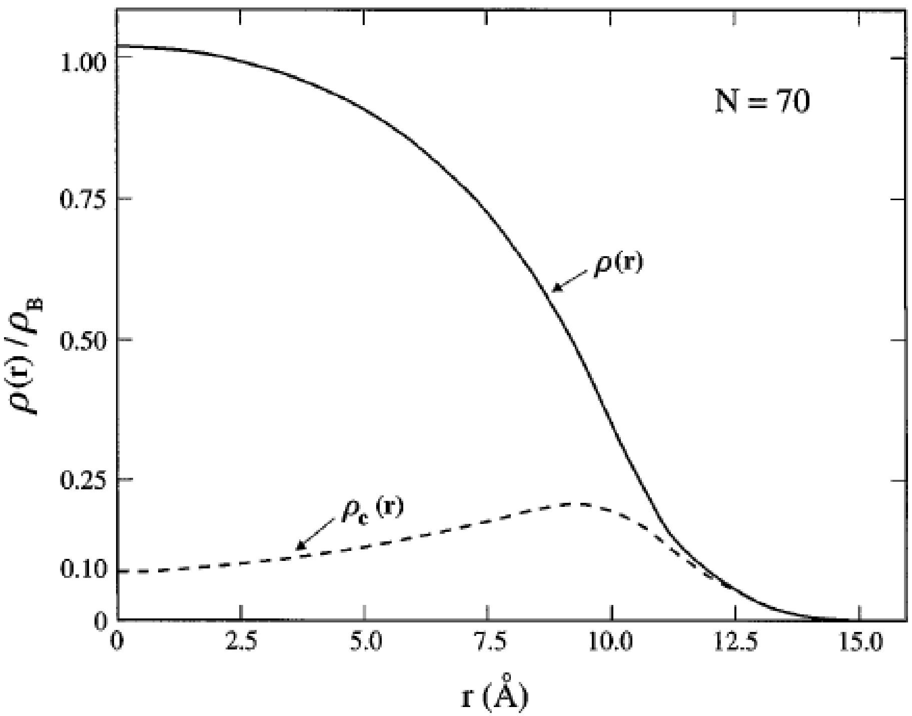
BEC and long range order: consequence of macroscopic occupation of a single-partice state.
Procedure holds also in **non uniform** and **finite** size systems.

Diagonalization of 1-body density matrix in a "small" droplet of liquid He4 at T=0

(Lewart, Pandharipande and Pieper, Phys. Rev. B (1988))

TABLE III. Number of particles having a given angular momentum for the 70-atom ^{4}He drop. The number of particles in the condensate is shown separately.

l	N_l	
Condensate	25.33	26.46
0	1.13	
1	3.74	
2	5.06	
3	5.51	
4	5.55	
5	4.92	
6	4.20	
7	3.63	
8	2.98	
9	1.97	
10	1.32	
Total	65.34	



In bulk condensate fraction is 0.1. In the droplet the fraction is larger because of **surface effects**.
Condensate density is close to 0.1 in the center of the droplet.
It increases and reaches 1 at the surface.

ORDER PARAMETER

Diagonalization of 1-body density matrix permits to identify single-particle wave functions φ_i . In terms of such functions one can write field operator in the form:

$$\hat{\Psi}(r) = \varphi_0(r)\hat{a}_0 + \sum_{i\neq 0} \varphi_i(r)\hat{a}_i$$

If $N_0 >> 1$ one can use Bolgoliubov approximation

$$\hat{a}_0, \hat{a}_0^+ \to \sqrt{N_0}$$

(non commutativity $[\hat{a}_0, \hat{a}_0^+] = 1$ inessential for most physical properties within 1/N approximation).

From field operator to classical field

Bogoliubov approximation is equivalent to treating the macroscopic component of the field operator as a classical field (true also in liquid helium):

$$\hat{\Psi}(r) = \Psi_0(r) + \delta\hat{\Psi}(r)$$

thermal and quantum fluctuations

with

$$\Psi_0(r) = \sqrt{N_0}\,\varphi_0(r)$$

$$\delta\hat{\Psi}(r) = \sum_{i\neq 0} \varphi_i(r)\hat{a}_i$$

Usually fluctuations $\delta\hat{\Psi}(r)$ are small in dilute gases at T=0 ⇒ **field operator** is **classical object** (analogy with classical limit of QED, see Lecture 3).

In helium quantum fluctuations are instead always crucial

$$\Psi_0(r) = |\Psi_0(r)| e^{iS(r)}$$

Order parameter

- Complex function
- Defined up to a constant phase factor
- Fixing the phase $S \Rightarrow$ breaking of gauge symmetry
- Corresponds to average $\Psi_o(r) = <\hat{\Psi}(r)>$ where average means

$$<\hat{\Psi}(r)> = <N|\hat{\Psi}(r)|N+1>$$

- For stationary configurations $|N(t)> = e^{-iE(N)t/\hbar}|N>$ time evolution is hence fixed by chemical potential $\mu = \frac{\partial E}{\partial N}$

$$\Psi_0(r,t) = e^{-i\mu t/\hbar}\Psi_0(r)$$

Chemical potential: fundamental parameter in Bose-Einstein condensates. Fixes time evolution of the phase

Behaviour of BEC in non interacting gas (grand canonical ensemble):

$$H_0\varphi_i = \varepsilon_i\varphi_i$$

$$n_i = \frac{1}{\exp[(\varepsilon_i - \mu)/k_B T] - 1}$$

value of μ is fixed by normalization condition $\sum_i n_i = N$

BEC starts when chemical potential takes minimum value, so close to ε_0 ($\varepsilon_0 - \mu << k_B T$) that occupation number $n_0 \equiv N_0$ of i=0 state becomes large and comparable to N:

$$N_0 \approx \frac{k_B T}{\varepsilon_0 - \mu} >> 1$$

If $\varepsilon_i - \mu >> \varepsilon_0 - \mu$ for i>0 one can replace μ with ε_0 and occupation number of i-state **does not depend** any more on **N**

Mechanism of BEC:

$$N = N_0 + \sum_{i\neq 0} \frac{1}{\exp[(\varepsilon_i - \varepsilon_0)/k_B T] - 1}$$

number of atoms out of the condensate depends only on T (not on N)

Condition fixes value of critical temperature

3D gas in harmonic potential

$$V_{ext} = \frac{1}{2} m\left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right]$$

$$\varepsilon(n_x, n_y, n_z) = (n_x + \frac{1}{2})\hbar\omega_x + (n_y + \frac{1}{2})\hbar\omega_y + (n_z + \frac{1}{2})\hbar\omega_z$$

BEC starts at $\mu = \varepsilon(0,0,0)$

$$N_T = \sum_{n_x, n_y, n_z \neq 0} \frac{1}{\exp\left[\beta\hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z)\right] - 1}$$

If $k_B T >> \hbar\omega_i$ one can transform sum into integral (semiclassical approximation)
Integration yields:
(N_T increases with T, independent of N)

$$\omega_{ho} = (\omega_x \omega_y \omega_z)^{1/3}$$

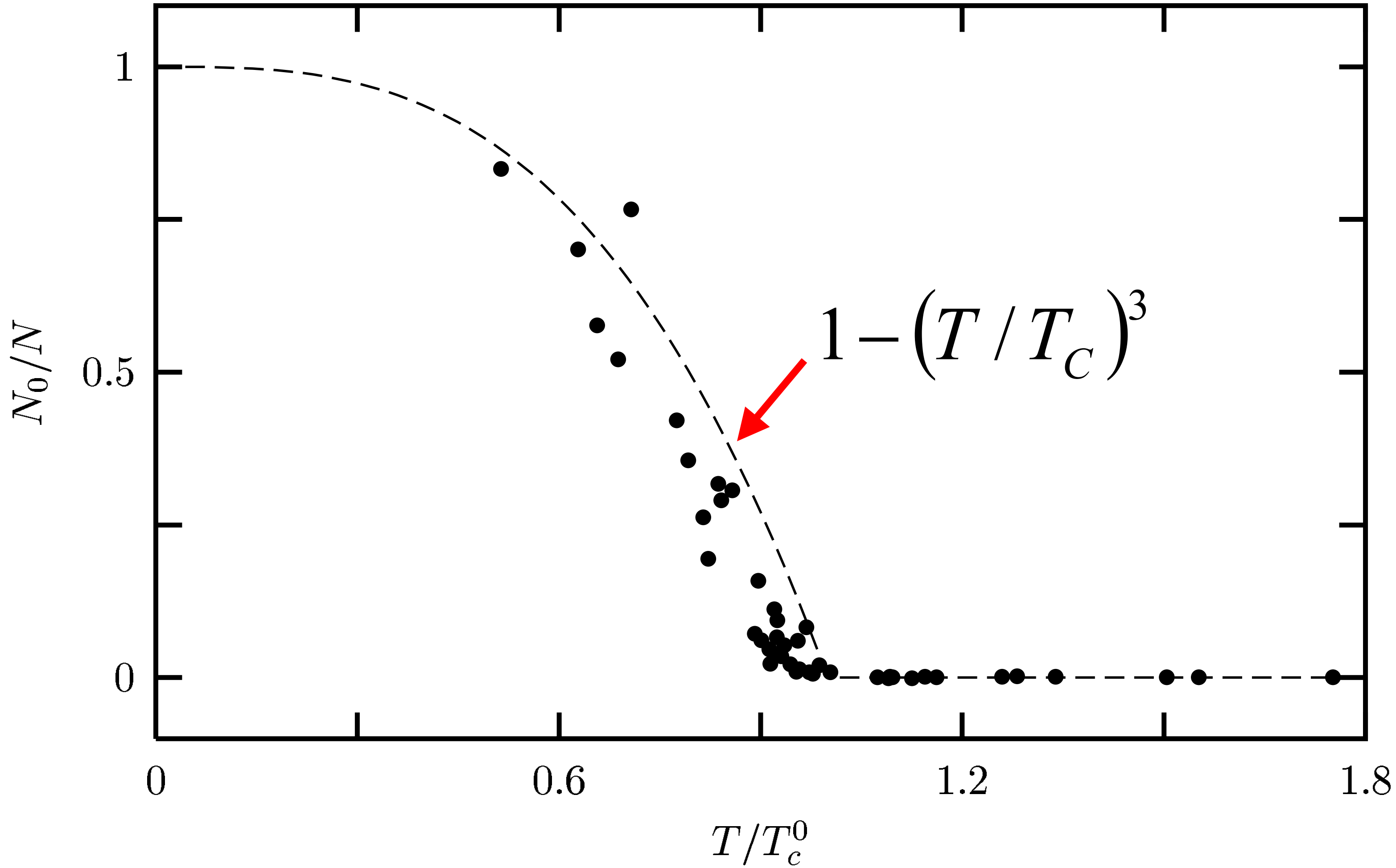
$$N_T = \left(\frac{k_B T}{\hbar\omega_{ho}}\right)^3 g_3(1)$$

Condition $N_T = N$ then yields

$$k_B T_c = 0.94\hbar\omega_{ho} N^{1/3}$$

and

$$N_0(T) = N\left(1 - \frac{T^3}{T_c^3}\right)$$



CONDENSATE FRACTION (Jila 96)
EXPERIMENTAL EVIDENCE
FOR PHASE TRANSITION

ROLE OF INTERACTIONS ON BEC: SOME QUESTIONS

- Do interactions modify shape of order parameter?
- Do interactions **reinforce or weaken** BEC?
- Do they enhance or decrease **critical temperature**?
- Can BEC be **fragmented**? (more than one s.p. state with macroscopic occupancy?)

No general answer

Effects depend on dimensionality, sign of interaction, nature of trapping (harmonic, double well,periodic..)

BEC fragmentation and role of interactions

- Robustness of BEC ensured by (repulsive) two-body interactions in uniform configurations **(mean field effect)**
- If trapping is not uniform (ex.: double well), interactions can work in opposite direction **(quantum fluctuations)**

BEC fragmentation and Nozieres' argument

Compare energy of two different configurations for a gas confined in **uniform** box:

$$|bec\rangle = \frac{1}{\sqrt{N!}}(a_0^+)^N |vac\rangle$$

atoms occupy same sp state (BEC state)

$$|frg\rangle = \frac{1}{\sqrt{N_0!N_1!}}(a_0^+)^{N_0}(a_1^+)^{N_1}|vac\rangle$$

atoms occupy two orthogonal sp states (fragmented BEC)

$$N = N_0 + N_1$$

$$H = H_0 + H_{\text{int}}$$

momenta of sp states

Since $p_0 = 0, p_1 \approx V^{-1/3}$, H_0 (kinetic energy) gives negligible contribution

$$H_{\text{int}} = \frac{g}{2}\int dr \hat{\Psi}^+(r)\hat{\Psi}^+(r)\hat{\Psi}(r)\hat{\Psi}(r)$$

Express field operator in terms of 0- and 1- sp states

$$\hat{\Psi}(r) = \varphi_0(r)\hat{a}_0 + \varphi_1(r)\hat{a}_1$$

$$\hat{\Psi}^+(r)\hat{\Psi}^+(r)\hat{\Psi}(r)\hat{\Psi}(r) =$$
$$[(\varphi_0^*)^2(\hat{a}_0^+)^2 + (\varphi_1^*)^2(\hat{a}_1^+)^2 + 2\varphi_0^*\varphi_1^*\hat{a}_0^+\hat{a}_1^+]\times$$
$$[(\varphi_0)^2(\hat{a}_0)^2 + (\varphi_1)^2(\hat{a}_1)^2 + 2\varphi_0\varphi_1\hat{a}_0\hat{a}_1]$$

$(N_0, N_1 >> 1)$

$$E\ (frg) = \frac{1}{2}g[N_0^2\int|\varphi_0|^4 + N_1^2\int|\varphi_1|^4 + 4N_0N_1\int|\varphi_0|^2|\varphi_1|^2]$$

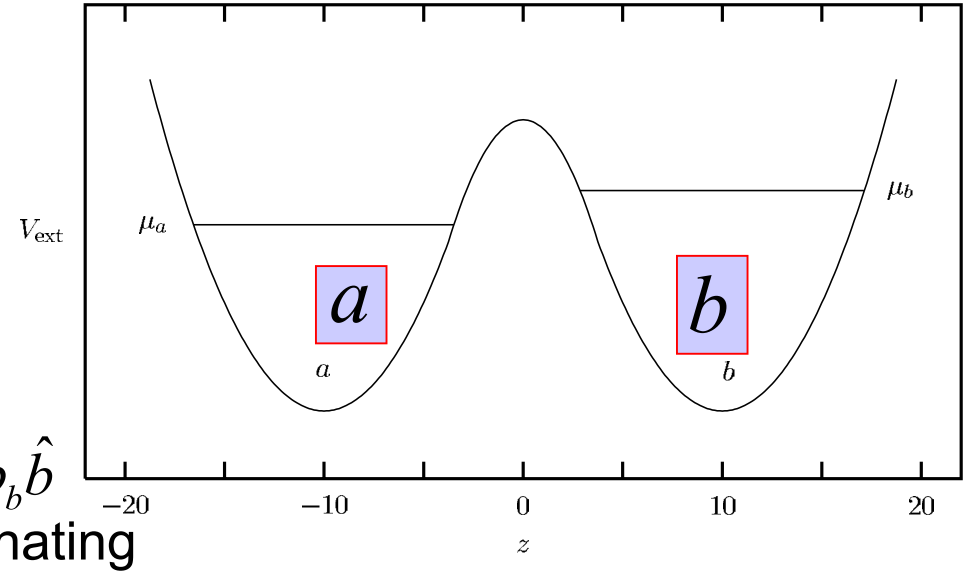
$$E(bec) = \frac{1}{2}g(N_0 + N_1)^2\int|\varphi_0|^4$$

Since $|\varphi_0|^2 = |\varphi_1|^2$ (**full overlap between s.p. wave functions**)

$$\Delta E = E(frg) - E(bec) = gN_0N_1\int|\varphi_0|^4 > 0$$

fragmentation is inhibited by repulsive interactions (mean field effect)

If condensates are separated interactions favour fragmentation Example:
BEC in double well potential



By writing field operator as $\hat{\Psi} = \varphi_a \hat{a} + \varphi_b \hat{b}$ and neglecting higher order terms originating from overlap between wave functions a and b the many-body Hamiltonian

$$H = \int dr \hat{\Psi}^+(r)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r)\right)\hat{\Psi}(r) + \frac{g}{2}\int dr \hat{\Psi}^+(r)\hat{\Psi}^+(r)\hat{\Psi}(r)\hat{\Psi}(r)$$

takes Boson Hubbard form

$$H = \frac{E_C}{4}(\hat{a}^+\hat{a}^+\hat{a}\ \hat{a} + \hat{b}^+\hat{b}^+\hat{b}\ \hat{b}) - \frac{\delta_J}{2}(\hat{a}^+\hat{b} + \hat{b}^+\hat{a})$$

tunneling

with $E_C = 2g\int \varphi_a^4$ and $\delta_J = -2\int dr \varphi_a(r)(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r))\varphi_b(r)$

In the absence of interaction ($E_C = 0$) the eigenstates of H are:

$$|\varphi_0\rangle = (\hat{a}^+ + \hat{b}^+)|vac\rangle$$

$$|\varphi_1\rangle = (\hat{a}^+ - \hat{b}^+)|vac\rangle$$

$$\delta_J = \varepsilon_1 - \varepsilon_0$$

We are now ready to compare interaction energy between

$$\left|bec\right\rangle = \frac{1}{\sqrt{N!2^N}}(a^+ + b^+)^N \left|vac\right\rangle$$

(ground state in the absence of two-body interaction)

$$\left|frg_{01}\right\rangle = \frac{1}{\sqrt{N/2!\,N/2!\,2^N}}(\hat{a}^+ + \hat{b}^+)^{N/2}(\hat{a}^+ - \hat{b}^+)^{N/2}\left|vac\right\rangle$$

$$\left|frg_{ab}\right\rangle = \frac{1}{\sqrt{N/2!\,N/2!}}(a^+)^{N/2}(b^+)^{N/2}\left|vac\right\rangle$$

Nozieres' argument applies to configurations $\left|bec\right\rangle$ and $\left|frg_{01}\right\rangle$

since wave functions $\varphi_a \pm \varphi_b$ fully overlap in space:
interactions make $\left|bec\right\rangle$ robust against $\left|frg_{01}\right\rangle$

Different behaviour if one considers configurations $|bec\rangle$ and $|frg_{ab}\rangle$ (φ_a and φ_b do not overlap!)

Comparison between interaction energy in $|\quad\rangle$ and $|frg_{ab}\rangle$

$$E_{\text{int}}(bec) = \frac{E_C}{8} N(N-1)$$

$$E_{\text{int}}(frg_{ab}) = \frac{E_C}{4}[N_a(N_a-1) + N_b(N_b-1)] =$$

$$= \frac{E_C}{8} N(N-2) < E_{\text{int}}(bec)$$

!!

interactions favour BEC fragmentation ($E_C > 0$)

(role of quantum fluctuations, see Lecture 4)

In general competition between interaction and tunneling

Can we distinguish experimentally between $| \quad \rangle$ and $| \quad \rangle$?

Look at interference fringes in density after expansion (Lecture 3) or in 'in situ' momentum distribution

$$n(p) = < \hat{\Psi}^+(p)\hat{\Psi}(p) >$$
$$\hat{\Psi}(p) = \varphi_a(p)\hat{a} + \varphi_b(p)\hat{b}$$

Assume, for simplicity:

φ_a and φ_b do not overlap in coordinate space; they **fully** overlap in **momentum** space

$$\varphi_a(z) = \varphi_b(z+d)$$
$$\varphi_a(p) = e^{-ipd/\hbar}\varphi_b(p)$$
$$n_a(p) = n_b(p)$$

With BEC

$$|bec\rangle = \frac{1}{\sqrt{N!2^N}}(a^+ + b^+)^N |vac\rangle$$

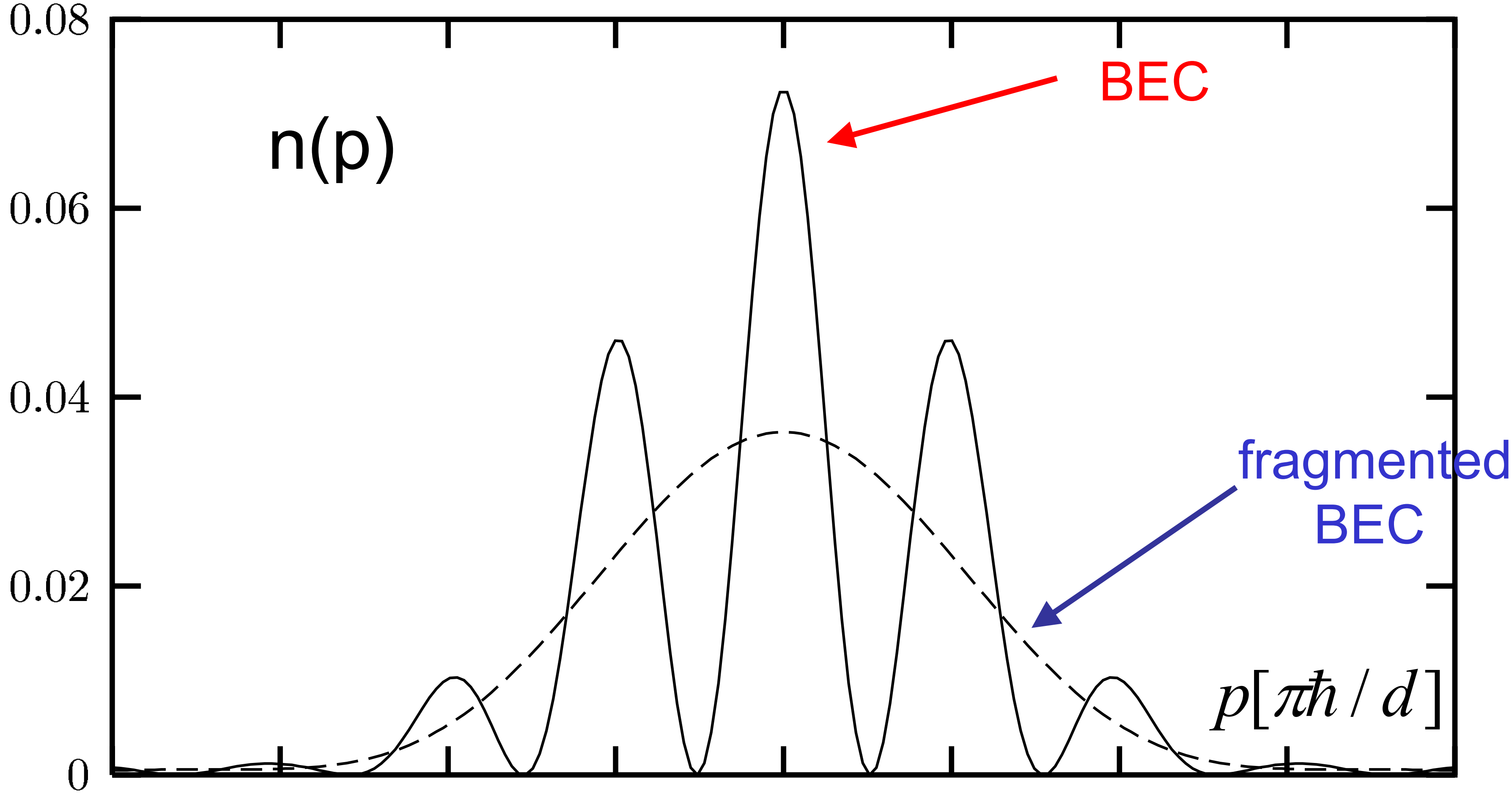
$$n(z) = n_a(z) + n_b(z)$$
$$n(p) = 2(1+\cos(pd/\hbar))n_a(p)$$

With BEC fragmentation

$$|frg_{ab}\rangle = \frac{1}{\sqrt{N/2!N/2!}}(a^+)^{N/2}(b^+)^{N/2}|vac\rangle$$

$$n(z) = n_a(z) + n_b(z)$$
$$n(p) = 2n_a(p)$$

Momentum distribution in double well potential



1-body density

$$n^{(1)}(z) = \frac{1}{V}\int dp\, n(p) e^{-ipz/\hbar}$$

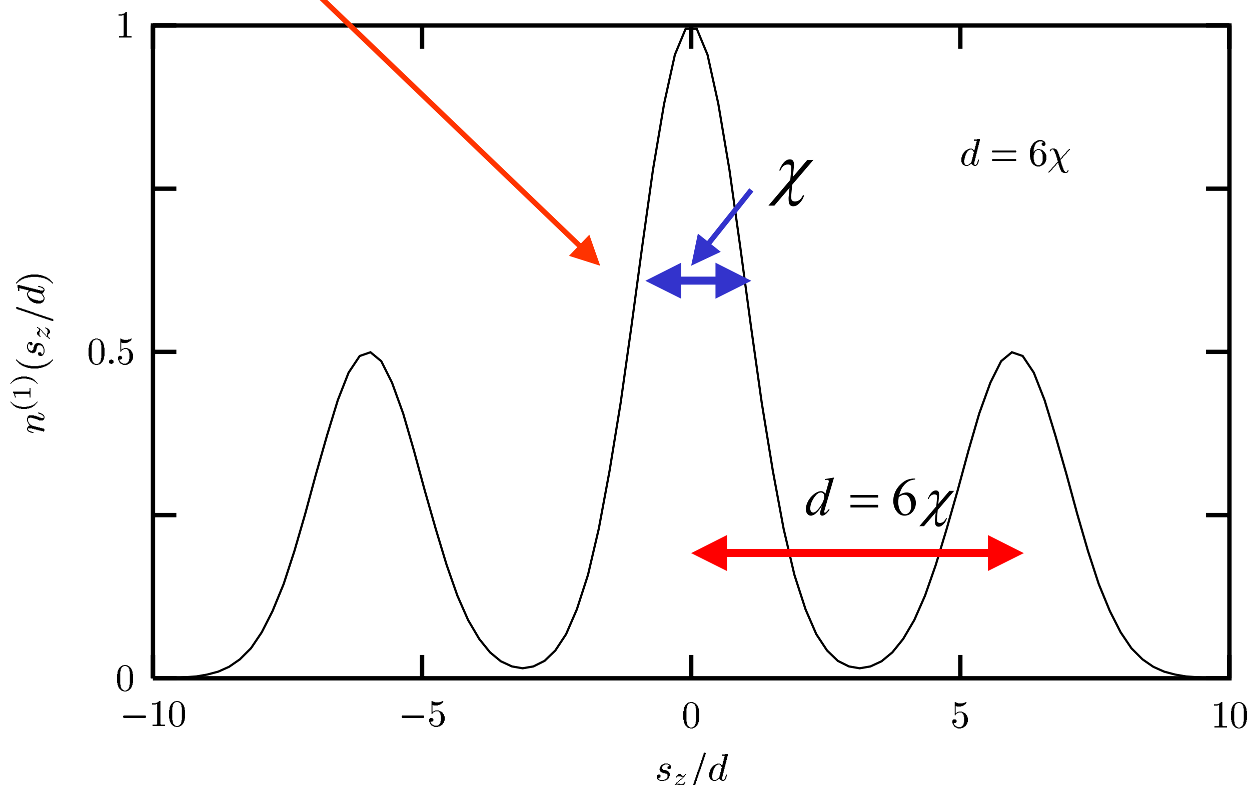
With BEC fragmentation

$$n^{(1)}(z) = N e^{-z^2/2\chi^2}$$

With BEC

$$n^{(1)}(z) = N[e^{-z^2/2\chi^2} + (e^{-(z+d)^2/2\chi^2} + e^{-(z-d)^2/2\chi^2})/2]$$

width of each condensate



long range order

Measurement of the phase

Results for momentum distribution described in last slides correspond to **averaging** procedure. Result of single measurement (**via for example inelastic photon scattering**) can be different:

- If the state is **coherent** (BEC) each measurement will reproduce same positions of peaks of n(p) (the **phase is reproducible**).
- If condensates are in **fragmented BEC** state the measurement process will "**create**" the relative phase S_r and the measured momentum distribution will exhibit interference fringes according to the law

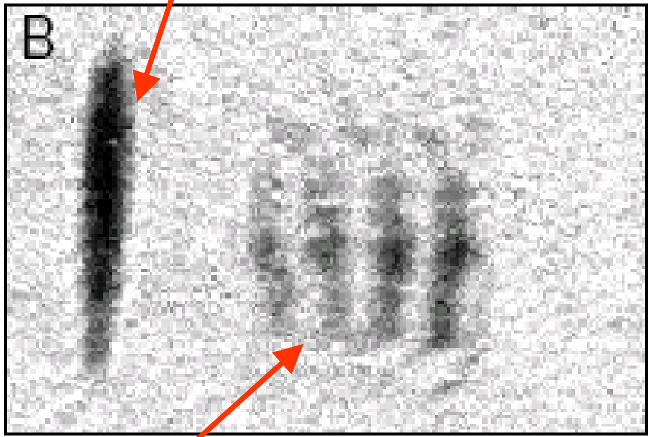
$$n(p) = 2[1 + \cos(pd/\hbar + S_r)]n_a(p)$$

In this case the value of the **phase is random** and the **averaging** procedure **washes out** interference effects in n(p).

- Measurements of the phase are more easily obtained by imaging **density distribution** after **release** of the traps. The two **condensates overlap** in coordinate space giving rise to interference **fringes** (Lecture 3).
- Measurement of **momentum distribution** has the advantage of determining the **phase in situ** (non destructive measurement).

unresolved condensates

In situ measurement of the **phase** in momentum distribution (double well configuration) Saba et al., MIT 2005



oscillations in the stream of outcoupled atoms $\propto n(p)$

This lecture

Lecture 1. **BEC and long range order.**
Long range order and order parameter.
BEC fragmentation and role of interactions.

Next lecture

Lecture 2. **Superfluidity and hydrodynamics.**
Landau criterion (galilean vs rotational). Hydrodynamic theory of superfluids. Collective oscillations and expansion.