Chaire Européenne du College de France (2004/2005)

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Lecture 3
28 Feb 05

Equation for the order parameter

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

This lecture:
- Gross-Pitaevskii theory
- Role of interactions and healing length.
- Thomas-Fermi and hydrodynamic limit
- Time dependent GP equation vs Bogoliubov equations.

Equation for order parameter can be derived starting form equation for field operator

$$< i\hbar \frac{\partial}{\partial t}\hat{\Psi}(r,t) > = < [-\frac{\hbar^2}{2m}\nabla^2 + V_{ext} + \int dr' \hat{\Psi}^+(r',t) V(r-r') \hat{\Psi}(r',t)] \hat{\Psi}(r,t) >$$

Replacing $\hat{\Psi}(r,t)$ with classical field $\Psi(r,t) = < \hat{\Psi}(r,t) >$ in interaction term requires proper procedure if V contains short range components

Simple procedure is applicable (in 3D) if

i) **range** of force and s-wave **scattering length a** are much **smaller** than **distance d** between particles

ii) **temperature** is sufficiently **low**

iii) only **macroscopic variations** of Ψ are considered (variation along distances much larger than a)

↓

Only low energy two-body scattering properties are relevant for describing the many-body problem.

IN PARTICULAR

- **scattering length a** is the only relevant interaction parameter.
- Equation for order parameter is properly derived by replacing V with **effective potential** $V_{eff} = g\delta(r-r')$ where $g = 4\pi\hbar^2 a/m$ is relevant coupling constant of problem.

Equation for order parameter becomes (Gross-Pitaevskii):

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = [-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r,t) + gn(r,t)]\Psi(r,t)$$

$$n(r,t) = |\Psi(r,t)|^2$$

density

- diluteness: $na^3 << 1$ (quantum fluctuations negligible)
- low temperature $T << T_C$ (thermal fluctuations negligble)

assumptions equivalent to treating field operator like a classical field:

$$\hat{\Psi}(r,t) = \Psi(r,t) + \cancel{\delta\hat{\Psi}}(r,t)$$

(density coincides with condensate density)

For non dilute gases and/or finite T one has

$$n(r,t) \neq n_0(r,t) = |\Psi(r,t)|^2$$

(density does not coincide with total density, see Lecture 4)

- **Gross-Pitaevskii** (GP) equation for order parameter plays role **analogous** to **Maxwell** equations in classical electrodynamics.
- **Condensate** wave function represents **classical limit of de Broglie wave** (corpuscolar nature of matter no longer important)

Important difference with respect to Maxwell equations:
GP contains Planck constant explicitly.
Follows from **different dispersion law** of photons and atoms:

from particles to waves: $p \to \hbar k, E \to \hbar\omega$

	particle (energy)		wave (frequency)
photons	$E = cp$	→	$\omega = ck$
atoms	$E = p^2 / 2m$	→	$\omega = \hbar k^2 / 2m$

GP eq. is non linear (analogy with **non linear optics)**
GP equation often called **non linear "Schroedinger equation"**
Equation for order parameter is **not equation for wave function**
(also equation for field operator is non linear)

Gross-Pitaevskii equation admits several types of solutions:

- **Stationary** solutions (e.g. ground state)

- Time dependent solutions
    - small amplitude oscillations (**elementary excitations**)
    - **large amplitude** solutions (e.g. expansion)

Sationary solutions of GP equation:

$$\Psi(r,t) = \Psi(r)e^{-i\mu t}$$

$$[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r) + gn(r)]\Psi(r) = \mu\Psi(r)$$

Gross-Pitaevskii equation at equilibrium

GP equation also derivable from variational approach

$$\frac{\delta(E-\mu N)}{\delta\Psi^*} = 0$$

$$E - \mu N = \int dr \left(\frac{\hbar^2}{2m}|\nabla\Psi|^2 + V_{ext}(r)|\Psi|^2 + \frac{1}{2}g|\Psi|^4 - \mu|\Psi|^2 \right)$$

Examples of solutions:
- **BEC in box** (this lecture)
- **BEC in harmonic trap** (this lecture)
- **Quantized vortices** (lecture 7)
- **BEC in periodic potentials** (lecture 9)

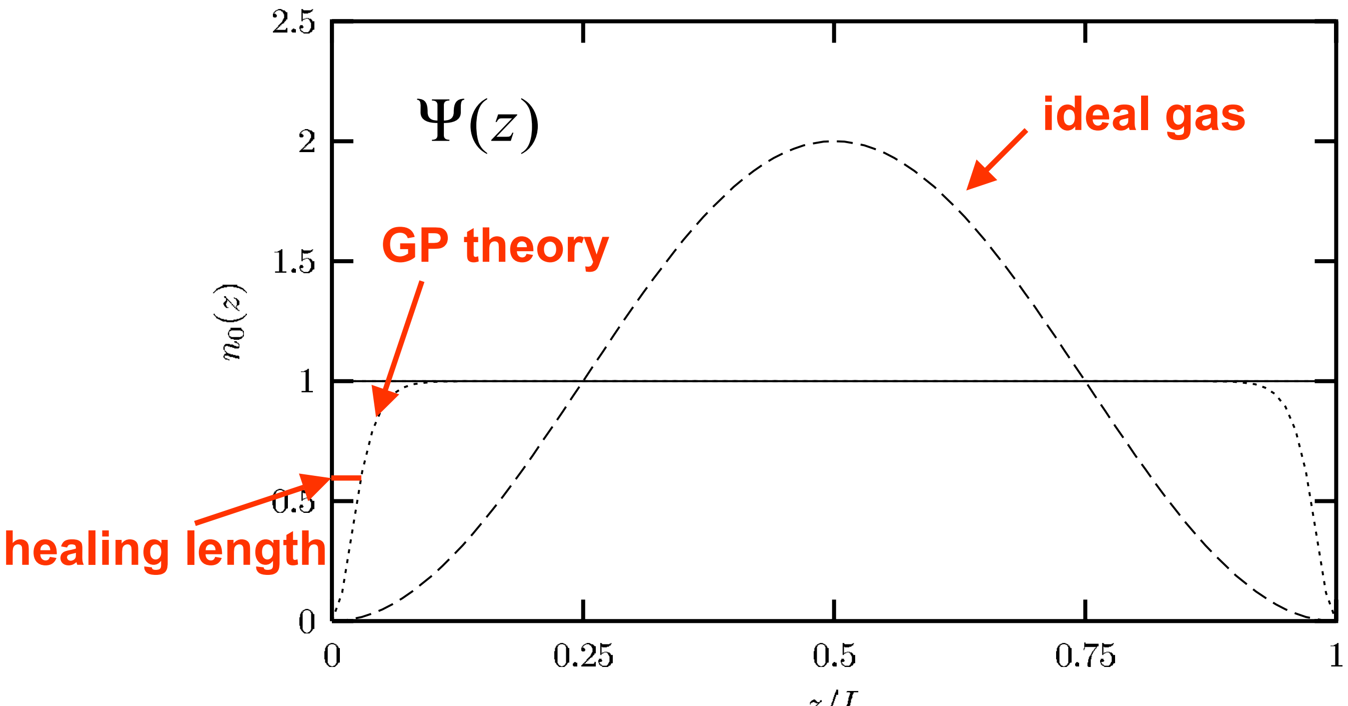
Example 1. BEC in a box (hard wall boundary conditions)

Non interacting ground state

$$\Psi = \sqrt{2\bar{n}}\,\sin(\pi z / L)$$

L: size of box

Wave function vanishes at the border



BEC in box. Role of interactions.

Gross-Pitaevskii equation can be rewritten in dimensionless form

$$\Psi \to \frac{1}{\sqrt{\bar{n}}}\Psi, z \to \bar{z} = \frac{z}{\varsigma}$$

where

$$\varsigma = \sqrt{\frac{\hbar^2}{2mg\bar{n}}} = \sqrt{\frac{1}{8\pi a\bar{n}}}$$

healing length (a>0)

Gross-Pitaevskii eq.:

$$-\frac{d^2}{d\bar{z}^2}\overline{\Psi}(\bar{z}) + \overline{\Psi}^3(\bar{z}) = \overline{\Psi}(\bar{z})$$

If $L >> \varsigma$ one can use boundary conditions: $\overline{\Psi}(0) = 0, \overline{\Psi}(\infty) = 1$

Solution:

$$\psi(z) = \sqrt{\bar{n}}\tanh\frac{z}{\sqrt{2}\varsigma}$$

Healing length ς : crucial parameter characterizing the interaction

If $L >> \varsigma$ the system can be considered **uniform** (except near the boundary

Interactions deeply modifying predictions of ideal gas

Example 2. BEC in harmonic trap

$$V_{ext} = \frac{1}{2} m \omega_{ho}^2 r^2$$

Non interacting ground state

$$n(r) \propto \exp(-r^2 / a_{ho}^2)$$

Gaussian with width $a_{ho} = \sqrt{\frac{\hbar}{m\omega_{ho}}}$

depends on $\hbar$

Role of interactions

Using a_{ho} and $\hbar\omega_{ho}$ as units of lengths and energy, and $\tilde{\Psi} = N^{-1/2} a_{ho}^{-3/2} \Psi$

normalized to

GP equation becomes

$$[-\tilde{\nabla}^2 + \tilde{r}^2 + 8\pi(Na/a_{ho})\tilde{\Psi}^2(\tilde{r})]\tilde{\Psi}(\tilde{r}) = 2\tilde{\mu}\tilde{\Psi}(\tilde{r})$$

Thomas-Fermi parameter

If $Na / a_{ho} << 1$ **Non interacting** ground state

If $Na / a_{ho} >> 1$ **Thomas-Fermi** limit (a>0)

In Thomas Fermi limit kinetic energy can be ignored and density profile takes the form (for n>0)

$$n(r) = \frac{1}{g}(\mu - V_{ext}(r))$$

Does **not** depend on $\hbar$ (see lecture 2)

Thomas-Fermi radius R is fixed by condition of vanishing density

$\mu = \frac{1}{2} m\omega_{ho}^2 R^2$ with μ fixed by normalization. One finds

$$\mu = \frac{1}{2}\hbar\omega_{ho}(15N\frac{a}{a_{ho}})^{2/5}$$

$$R = a_{ho}(15N\frac{a}{a_{ho}})^{1/5}$$

Thomas-Fermi condition $Na / a_{ho} >> 1$ implies $\mu >> \hbar\omega_{ho}, R >> a_{ho}$

and healing length $\varsigma << R$

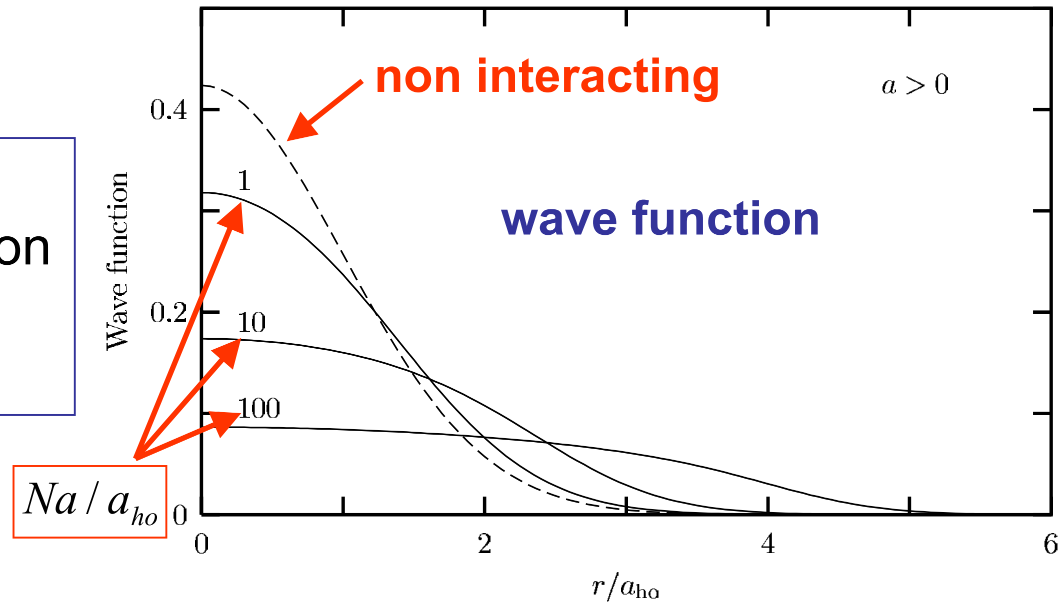
In fact $\mu = gn(0)$ and

$$\frac{\varsigma}{R} = \sqrt{\frac{\hbar^2}{2mgn(0)}}\frac{1}{R} = \frac{a_{ho}^2}{R^2} << 1$$

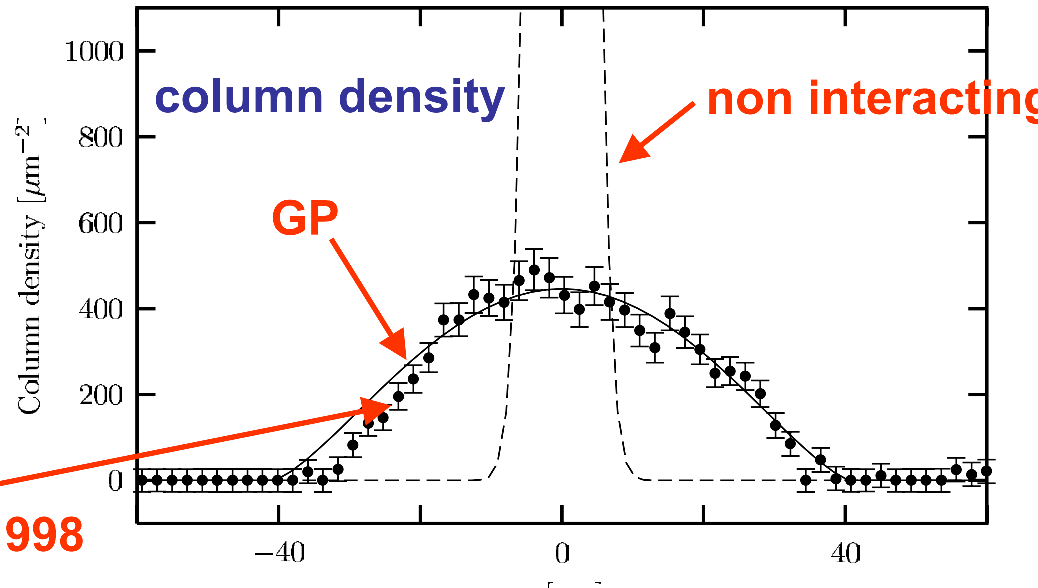
Some conclusions concerning equilibrium configurations

a >0

Thomas-Fermi parameter Na / a_{ho} drives the transition **from non interacting** to **Thomas-Fermi** limit



Huge effects due to **interaction** at equilibrium; **good agreement** with **experiments**



exp: Hau et al, 1998

Thomas-Fermi regime is compatible with diluteness condition

Gas parameter in the center of the trap

$$na^3 = \frac{\mu}{g} a^3 = 0.1 (N^{1/6} \frac{a}{a_{ho}})^{12/5}$$

Thomas-Fermi

$$Na / a_{ho} >> 1$$

Diluteness

$$N^{1/6} a / a_{ho} << 1$$

example: $a / a_{ho} = 10^{-3}, N = 10^6$

$$Na / a_{ho} = 10^3$$

$$N^{1/6} a / a_{ho} = 10^{-2}$$

Gross-Pitaevskii theory is not perturbative even if gas is dilute (role of BEC)!

a < 0

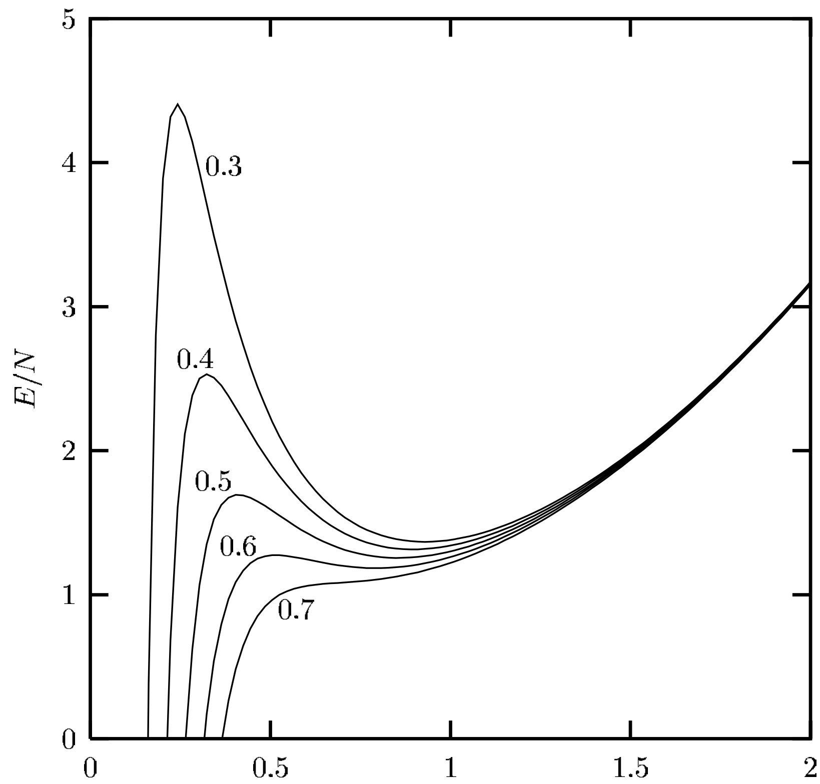
For **attractive** effective force TF limit is not available.
For **large N** system is **unstable** (**negative compressibility**).
Kinetic energy term term crucial to ensure metastable solution at finite N

Numerical solution of GP equation reveals existence of local minimum if $N\frac{|a|}{a_{ho}} < 0.58$ Ruprecht et al., 1995

Physical insight provided by variational approach based on Gaussian function

$$\psi(r) = \frac{N^{1/2}}{w^{3/2} a_{ho}^{3/2} \pi^{3/2}} e^{-r^2/2w^2 a_{ho}^2}$$

width of gaussian: variational parameter



First experiments on collapse in ^{85}Rb (JILA, 2001)

Time dependent Gross-Pitaevskii equation

$$i\hbar \frac{\partial}{\partial t}\Psi(r,t) = [-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r,t) + gn(r,t)]\Psi(r,t)$$

Equation can be rewritten in terms of the modulus and phase of the order parameter: $\Psi = \sqrt{n}e^{iS}$

Gross-Pitaevskii equation becomes equation for the density and for the velocity field $v_S = \hbar / m\nabla S$

$$\frac{\partial}{\partial t}n + \nabla(v_S n) = 0$$

quantum pressure

$$m\frac{\partial}{\partial t}v_S + \nabla(\frac{1}{2}mv_S^2 + V_{ext} + gn - \frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}) = 0$$

Origin of quantum pressure term.

Kinetic energy calculated in terms

of velocity field $v_S = \frac{\hbar}{m} \nabla S$ and density:

quantum pressure

$$E_{kin} = \frac{\hbar^2}{2m} \int dr |\nabla \Psi|^2 = \frac{m}{2} \int dr v_S^2 n + \frac{\hbar^2}{2m} \int dr \left(\nabla \sqrt{n} \right)^2$$

Hydrodynamic equations are recovered **if quantum pressure is negligible**
i.e, if during the oscillation the density varies over distances λ such that
$\hbar^2 / m\lambda^2 << gn$

In conclusion HD requires wavelengths larger than healing length $\lambda >> \varsigma$

(Thomas-Fermi approximation at equilibrium requires $R >> \varsigma$)

IN HYDRODYNAMIC LIMIT **PLANCK CONSTANT DISAPPEARS** FROM GP EQUATIONS

From Gross-Pitaevskii to Bogoliubov equations

Elementary excitations of the condensate can be studied in all regimes (not only in HD) by solving **linearized GP** equation with ansatz:

$$\Psi(t) = e^{-i\mu t}\left(\Psi_0 + u_j e^{-i\omega_j t} + v_j^* e^{i\omega_j t}\right)$$

After linearization:

$$\hbar\omega_j u_j = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext} - \mu + 2gn_0\right)u_j + g(\Psi_0)^2 v_j$$

$$-\hbar\omega_j v_j = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext} - \mu + 2gn_0\right)v_j + g(\Psi_0^*)^2 u_j$$

Bogoliubov equations

Bogoliubov equations have been derived in the framework of a theory for a **classical field** (time dependent Gross-Pitaevski theory)

Same equations can be also derived diagonalizing **quantum** Hamiltonian using **Bogoliubov transformations** (see lecture 4)

Some properties of Bogoliubov equations

i) $$(\omega_i - \omega_i^*)\int dr(|u_i|^2 - |v_i|^2) = 0$$

$\Rightarrow \omega_i$ is real, unless $\int dr|u_i|^2 = \int dr|v_i|^2$

(occurrence of complex solutions $\Longrightarrow$ **dynamic instability**, see lectures 6,9)

ii) $$\int dr(u_i u_j^* - v_i v_j^*) = 0$$ (orthoganility) if $\omega_i \neq \omega_j$

iii) For each solution u_i, v_i, ω_i
there exist another solution with $v_i^*, u_i^*, -\omega_i$
(the two solutions describe the **same physical** oscillation)

iv) If $\Psi(t) = e^{-i\mu t}(\Psi_0 + u_j e^{-i\omega_j t} + v_j^* e^{i\omega_j t})$ with u_i, v_i, ω_i solution of Bogoliubov eqs., energy change with respect to equilibrium is given by:

$$\delta E = \int dr(|u_i|^2 - |v_i|^2)\hbar\omega_i$$

Condition of **energetic stability** $\delta E > 0$ $\Rightarrow$ $$\omega_i \int dr(|u_i|^2 - |v_i|^2) > 0$$

Solution of Bogoliubov equations in uniform matter

In uniform matter one finds solutions of the form $u, v \propto e^{iqz}$

and dispersion law

$$\omega^2 = \hbar^2 \left(\frac{q^2}{2m}\right)^2 + q^2 c^2$$

Bogoliubov dispersion law

Wave length of the oscillation: $\lambda = 2\pi / q$

Healing length: $\varsigma = \hbar / \sqrt{2mgn} = \hbar / \sqrt{2}mc$

If $\lambda >> \varsigma$ **quantum pressure** is **negligible** and $\omega = cq$ (phonon)

If $\lambda << \varsigma$ **quantum pressure dominates** and $\omega = \hbar q^2 / 2m$ (free particle

Density response function in uniform matter

By adding density dependent perturbation of the form

$$\delta V_{ext} = -\lambda \exp(\eta t) \exp i(qz - \omega t)$$

$\eta \to 0^+$

the linearized solutions of time dependent GP eqs. can be written as

$$\Psi(t) = e^{-i\mu t} e^{\eta t} (\Psi_0 + u e^{i(qz-\omega t)} + v e^{-i(qz-\omega t)})$$

with u, v fixed by

$$\hbar(\omega + i\eta)u = \left(\frac{\hbar^2}{2m} q^2 + gn\right) u + gnv - \lambda \Psi_0$$

$$-\hbar(\omega + i\eta)v = \left(\frac{\hbar^2}{2m} q^2 + gn\right) v + gnu - \lambda \Psi_0$$

$$n = \Psi_0^2, \mu = gn$$

Response function is defined by relationship

$$\int e^{-iqz} \delta n(r,t) dr = \lambda e^{\eta t} e^{i(qz-\omega t)} \chi(q,\omega)$$

In our case we find

$$\chi(q,\omega) = N(u+v)/\lambda$$

Simple algebraic result for density response function:

$$\chi(q,\omega) = N\frac{q^2/m}{(\omega+i\eta)^2-\omega_B^2}$$

$$\omega_B^2 = \hbar^2\left(\frac{q^2}{2m}\right)^2 + q^2c^2$$

Poles of response function coincide with **Bogoliubov dispersion law**

Static response given by compressibility sum rule $\chi(q) = N/mc^2$

at large frequency exact **f-sum rule** result $\chi(q,\omega)_{\omega\to\infty} = Nq^2/m\omega^2$

imaginary part ⇨ **dynamic structure factor**: $\chi''(q,\omega) = \pi(S(q,\omega)-S(q,-\omega))$

from which one extracts result $S(q) = \hbar q^2/2m\omega_B(q)$

for **static structure factor** $NS(q) = \hbar\int d\omega S(q,\omega)$

(S(q) directly related to density fluctuations, see Lecture 4)

Some applications of time dependent Gross-Pitaevskii equations to trapped BEC's

Surface excitations ($n_r = 0, l \neq 0$) **and Landau's critical angular velocity (beyond the HD approximation, see lecture 2)**

Expansion and interference fringes generated by two separated condensates

Surface excitations ($n_r = 0, l \neq 0$) and Landau's critical angular velocity (beyond the HD approximation, see lecture 2)

$$\Omega_C = \min_l \frac{\varepsilon(l)}{l}$$

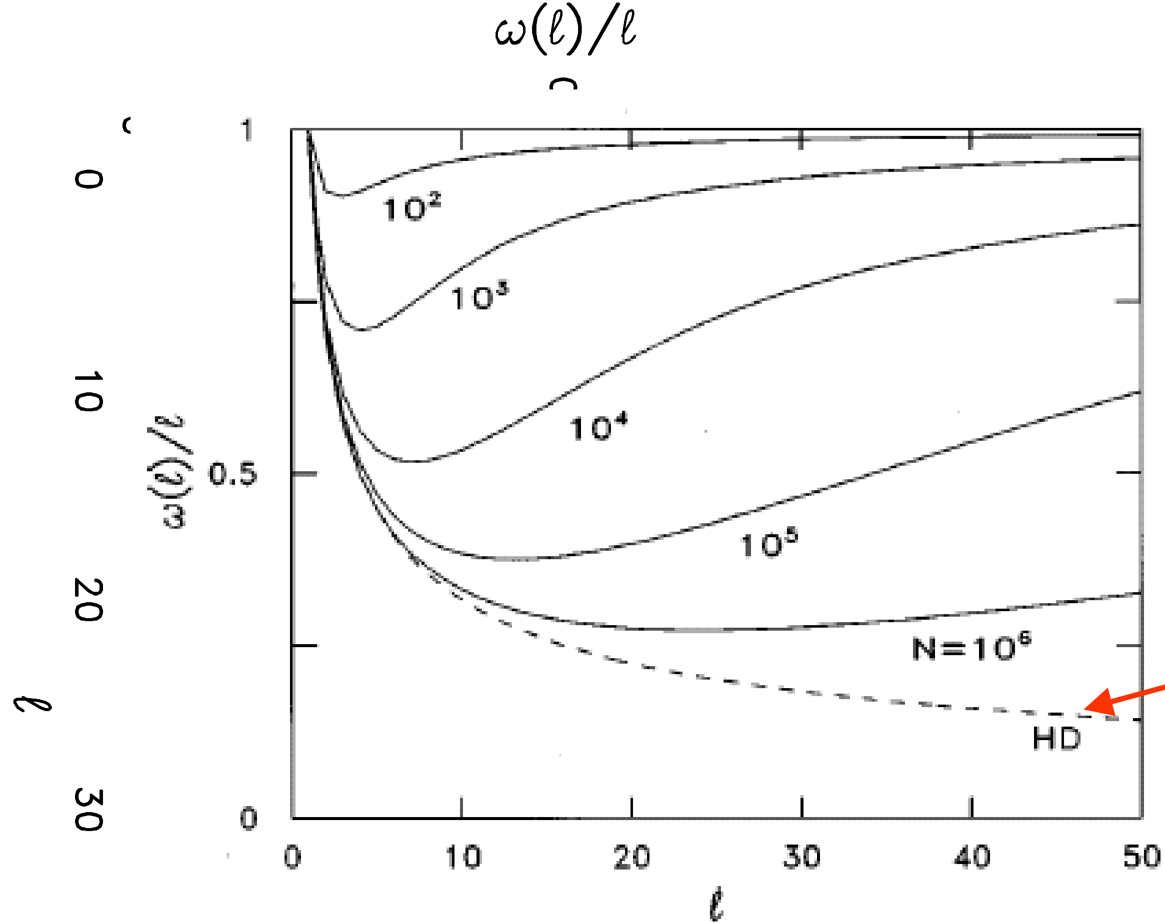
If $\Omega > \Omega_{cr}$ surface modes are unstable

In HD theory $\varepsilon(l) = \hbar\omega_{ho}\sqrt{l}$ and $\Omega_{cr} = 0$

Numerical solution of linearized GP eqs shows that, for fixed N, HD theory is accurate only for small values of of l and that

$$\Rightarrow \Omega_C = \min_l \frac{\varepsilon(l)}{l} \neq 0$$

Crucial role of quantum pressure ignored in hydrodynamic approximation



$$\frac{\omega_{HD}(l)}{l} = \frac{\omega_{ho}}{\sqrt{l}}$$

Angular velocity divided by angular momentum for surface excitations as a function of angular momentum for several values of N.
HD prediction recovered for **small** values of **angular momentum**.
For each value of N theory predicts critical value of angular velocity (Dalfovo et al. 1997).

$$\Omega_C = \min_l \frac{\varepsilon(l)}{l} \neq 0$$

Expansion and interference fringes generated by two separated condensates

Behaviour of velocity field of **single expanding condensate** is **correctly determined** by **hydrodynamic** equations. At large times: $\vec{v} = \vec{r}/t$

Recalling general expression $\vec{v} = (\hbar/m)\vec{\nabla}S$ for superfluid velocity field one can calculate time evolution of the phase of order parameter:

$$S(r,t) \to \frac{1}{2}\frac{mr^2}{\hbar t}$$

$$\Psi = \sqrt{n}e^{iS}$$

If two condensates are initially separated by distance d (along z-axis) after release of the trap they expand and eventually overlap.
For large times the relative phase of the two condensates is given by

$$S(x,y,z+d/2) - S(x,y,z-d/2) + \Phi \to (md/\hbar t)z + \Phi$$

Where Φ is relative phase of two condensates before expansion
Density profile can be calculated taking **linear superposition** of two waves

$$\Psi(r,t) = \Psi_a(r,t) + e^{i\Phi}\Psi_b(r,t)$$

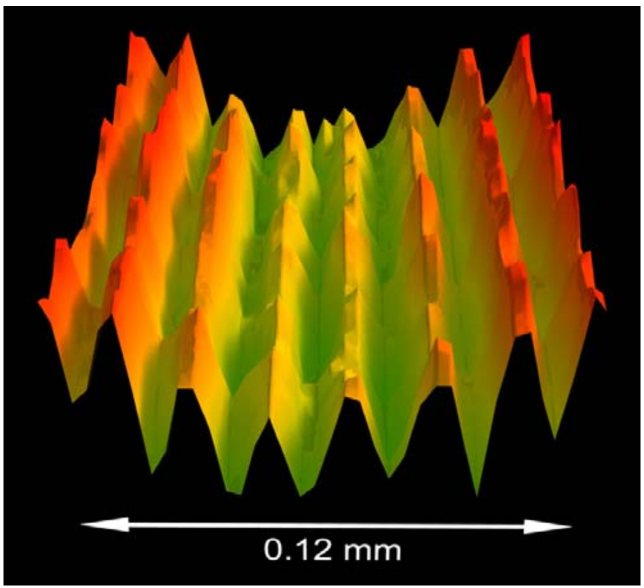
Linear superposition of wave functions **absent** in **hydrodynamic** theory

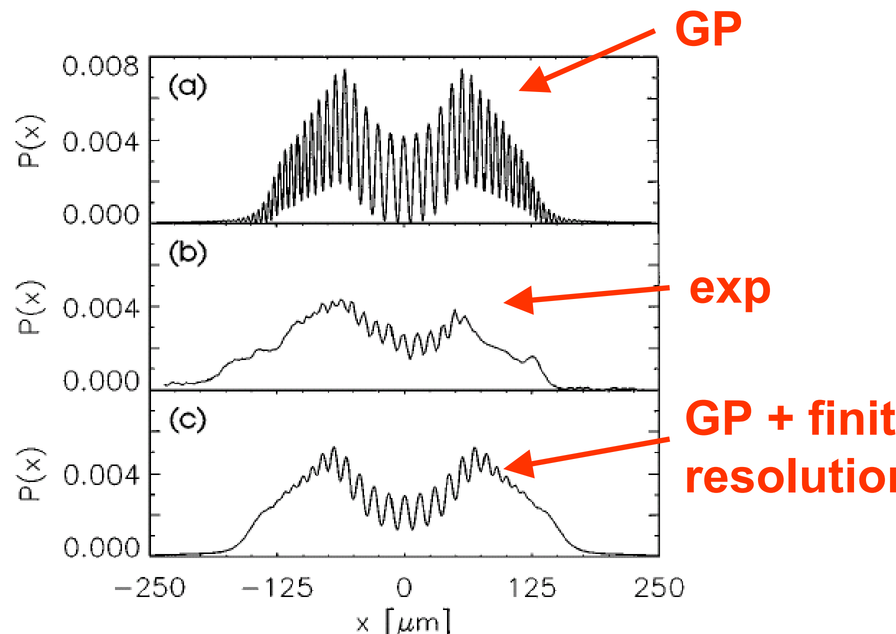
Spatial modulation of the relative phase results in spatial modulation of measured density:

$$n(r,t) = n_a(r,t) + n_b(r,t) + 2\sqrt{n_a(r,t)n_b(r,t)}\cos\left(\frac{md}{ht}z + \Phi\right)$$

Theory predicts interference fringes separated by spacing (spacing depends explicitly on Planck constant) $\lambda = \frac{ht}{md}$

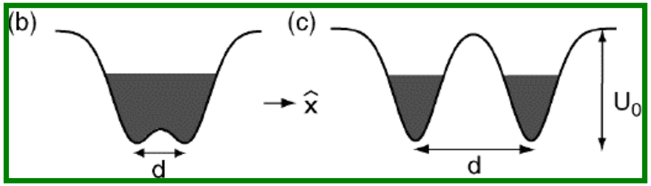
Full numerical solution of Gross-Pitaevskii equations (Rhorl et al. 1997) yields good agreement with experimental data.

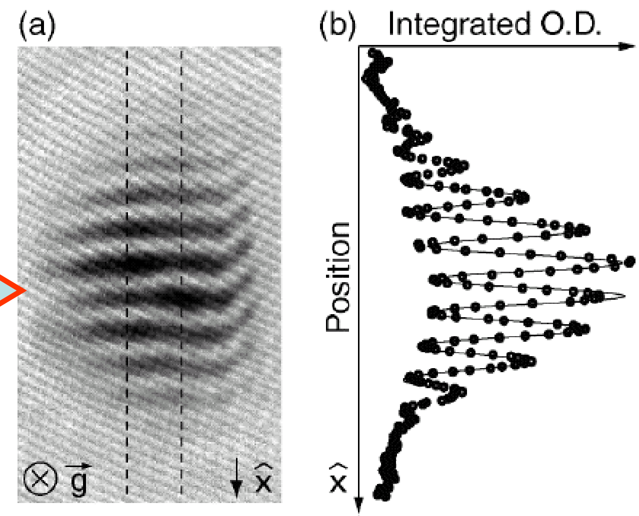




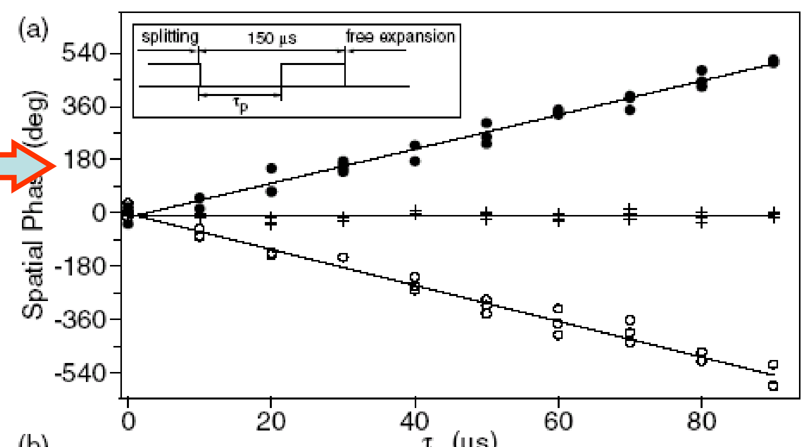
Recent experiments at MIT (Shin et al. 2004) and Heidelberg (Albiez et al. 2004) have measured time evolution of relative phase in double well

MIT 2004





Relative phase is determined measuring **interference fringes** after expansion:

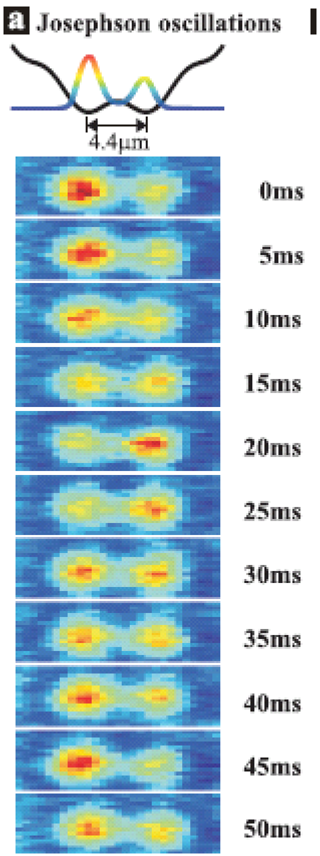


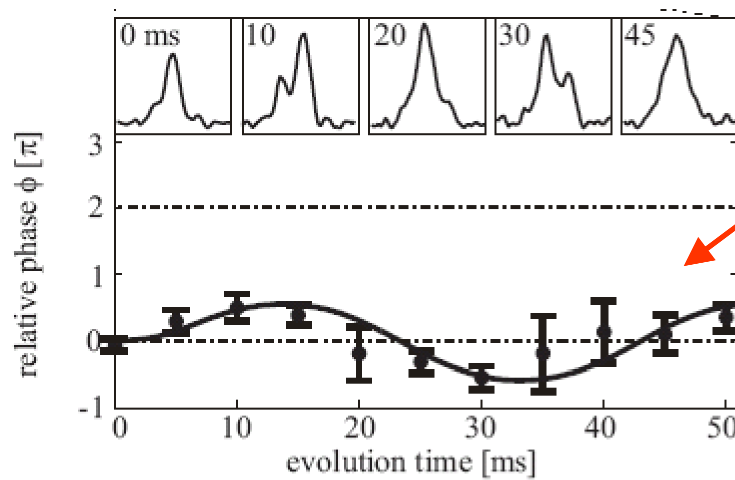
Relative phase evolves due to to applied ac Stark phase shift

Heidelberg 2004

Relative phase evolves in time because of Josephson oscillation between the two wells

opulation mbalance measured n situ





relativ phase

relative phase is measured by looking at **interference fringes** after expansion:

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

Next Lecture. **Fluctuations of the order parameter**.
Quantum fluctuations and BEC depletion.
Thermal depletion.
Shift of critical temperature due to interactions