

Lecture 2: Weak Interactions and BEC

Previous lecture:

- Ideal gas model gives a fair intuition for occurrence of BEC but is *unphysical* (infinite compressibility, shape of condensate....)
- Order parameter and its equation of motion
- Slow (low energy) scattering of atoms and interaction parameter
- Gross-Pitaevskii equation. Amplitude and phase of the order parameter
- Super current and superfluid velocity. Irrotational hydrodynamics.
- Solution of GPE in uniform and non-uniform case. Thomas-Fermi Approximation

Order parameter

Density matrix

$$\rho^{(1)}(\mathbf{x}, \mathbf{y}) = \langle \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{y}) \rangle = \sum_{\alpha} n_{\alpha} \psi_{\alpha}^*(\mathbf{x}) \psi_{\alpha}(\mathbf{y})$$

Field operator

$$\hat{\Psi}(\mathbf{x}) = \sum_{\alpha} \psi_{\alpha}(\mathbf{x}) \hat{a}_{\alpha}$$

Creation and annihilation operators

$$[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}] = \delta_{\alpha, \beta} \quad [\hat{a}_{\alpha}, \hat{a}_{\beta}] = 0$$

$$\langle \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha} \rangle = n_{\alpha}$$

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Neglecting quantum fluctuations

$$\alpha = 0 \quad N_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle \gg 1$$

Neglect commutator $[\hat{a}_0, \hat{a}_0^\dagger] = 1$

$$\hat{a}_0^\dagger = \hat{a}_0 = \sqrt{N_0} \quad \text{- a (large) number}$$

Classical field and quantum fluctuations:

$$\hat{\Psi}(\mathbf{x}) = \Psi_0(\mathbf{x}) + \delta\hat{\Psi}(\mathbf{x}) = \sqrt{N_0}\psi_0(\mathbf{x}) + \sum_{\alpha \neq 0} \psi_\alpha(\mathbf{x})\hat{a}_\alpha$$

Equation of motion

$$\hat{H} = \int d\mathbf{x} \left[\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \cdot \nabla \hat{\Psi} + U(\mathbf{x}, t) |\hat{\Psi}(\mathbf{x})|^2 \right] + \\ + \frac{1}{2} \int d\mathbf{x} d\mathbf{y} |\hat{\Psi}(\mathbf{x})|^2 V(\mathbf{x} - \mathbf{y}) |\hat{\Psi}(\mathbf{y})|^2$$

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{x}, t) = [\hat{\Psi}, \hat{H}] =$$

$$= \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{x}, t) + \int d\mathbf{y} V(\mathbf{x} - \mathbf{y}) |\hat{\Psi}(\mathbf{y})|^2 \right] \hat{\Psi}(\mathbf{x}, t)$$

Interaction term

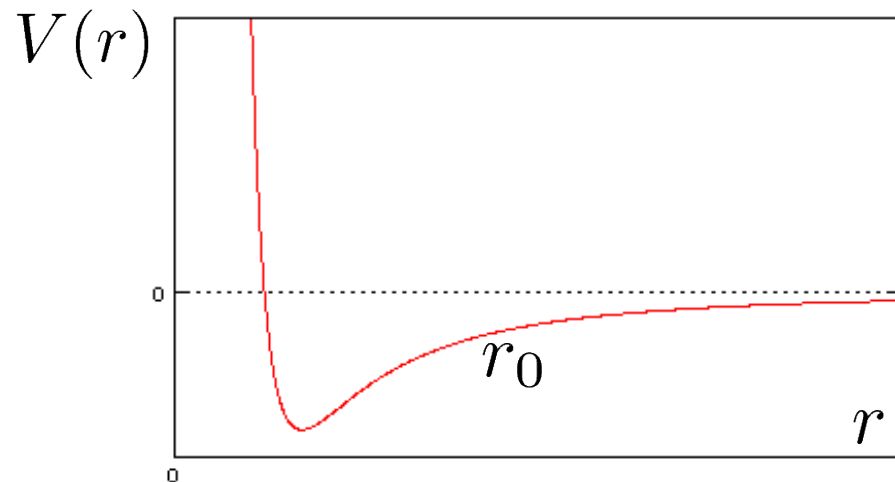
Replacing the field operator by its 'classical' part $\hat{\Psi}(\mathbf{x}, t) \rightarrow \Psi_0(\mathbf{x}, t)$
and assuming slow changes of $\Psi_0(\mathbf{x}, t)$ we put

$$\hat{\Psi}(\mathbf{x}, t) \int d\mathbf{y} V(\mathbf{x} - \mathbf{y}) |\hat{\Psi}(\mathbf{y})|^2 \rightarrow g |\Psi_0(\mathbf{x}, t)|^2 \Psi_0(\mathbf{x}, t)$$

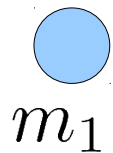
Questions:

1. What is 'slow changes'?
2. What is the value of coupling?

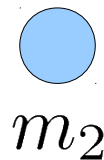
$$g \sim \int d\mathbf{x} V(\mathbf{x})$$



Scattering theory



$V(r)$



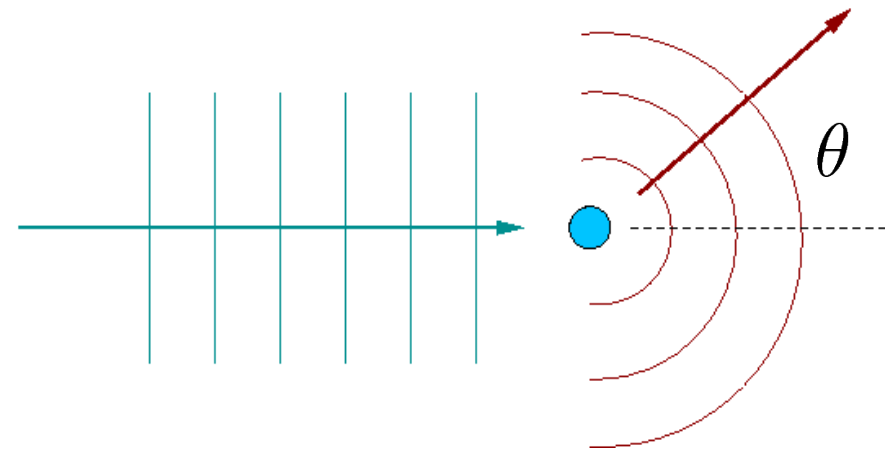
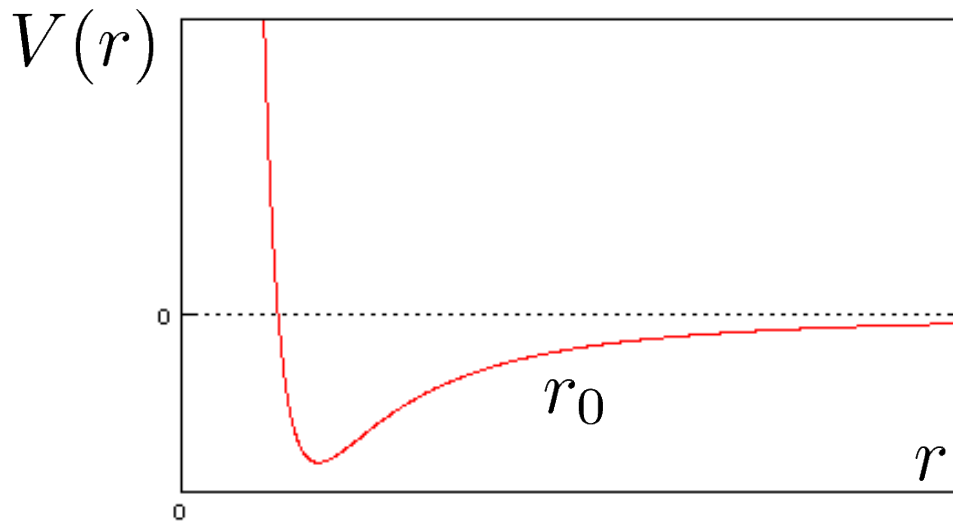
Schrödinger equation for effective particle with reduced mass

$$m^* = m_1 m_2 / (m_1 + m_2)$$

and relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

$$\left(-\frac{\hbar^2}{2m^*} \nabla^2 + V(r) \right) \psi(\mathbf{r}) = \frac{\hbar^2 k^2}{2m^*} \psi(\mathbf{r})$$

Asymptotic solution



Beyond the range r_0 of the interatomic potential the solution of the Schrödinger equation simplifies

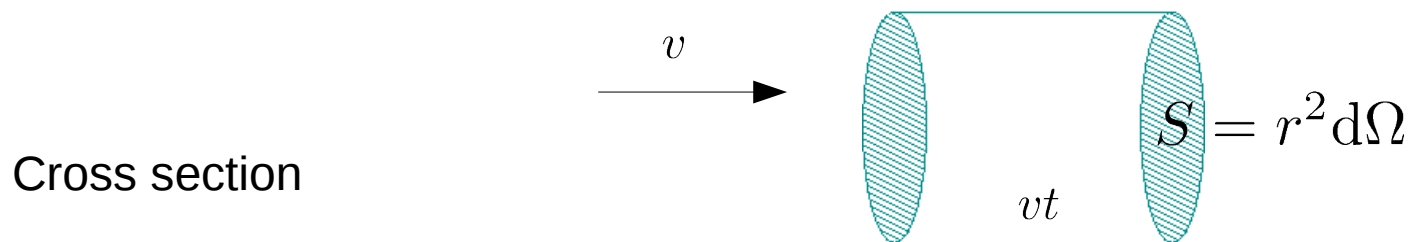
$$\psi(\mathbf{r}) = e^{ikz} + f(\theta) \frac{e^{ikr}}{r}$$

↙
↖ scattering amplitude

Incoming current density

$$j = \frac{\hbar}{m} \text{Im} \psi^* \nabla \psi = \frac{\hbar k}{m} = v$$

Scattering Amplitude



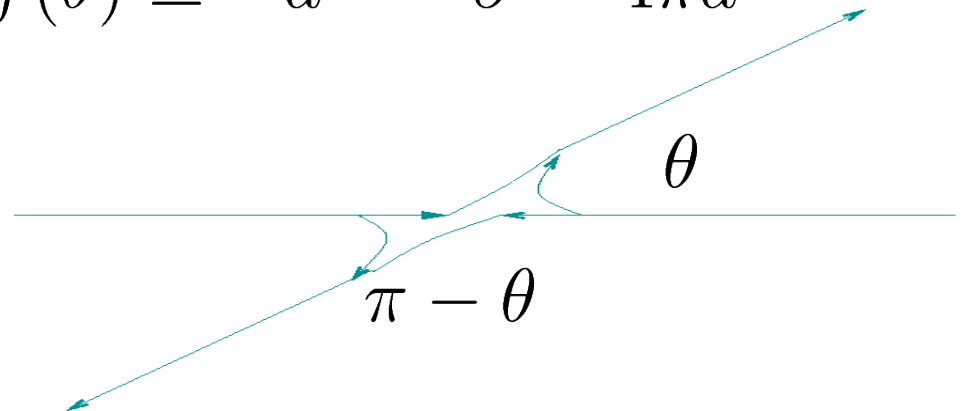
$$d\sigma = \frac{|\psi(\mathbf{r})|^2 dV}{vt} = |f(\theta)|^2 d\Omega = |f(\theta)|^2 \sin\theta d\theta d\phi$$

s-scattering, independent of angle

$$f(\theta) \simeq -a \quad \sigma = 4\pi a^2$$

identical particles (bosons/fermions)

$$d\sigma = |f(\theta) \pm f(\pi - \theta)|^2 d\Omega$$



Partial waves

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} P_l(\cos \theta) \frac{\chi_{kl}(r)}{kr} \quad P_l(x) \text{ - Legendre polynomials}$$

Radial equation

$$-\frac{d^2 \chi_{kl}}{dr^2} + \frac{l(l+1)}{r^2} \chi_{kl} + \frac{2m^*}{\hbar^2} V(r) \chi_{kl} = k^2 \chi_{kl}$$

Large distances $r \gg r_0$ $\chi_{kl} = A_l \sin \left(kr - \frac{\pi l}{2} + \delta_l \right)$

Comparison

$$\begin{aligned} f(\theta) \frac{e^{ikr}}{r} &= \psi(\mathbf{r}) - e^{ikr \cos \theta} = \\ &= \sum_{l=0}^{\infty} P_l(\cos \theta) \frac{A_l i^{-l} e^{-i\delta_l}}{2ikr} \left(e^{ikr+2i\delta_l} - e^{-ikr+i\pi l} \right) \\ &\quad - \sum_{l=0}^{\infty} P_l(\cos \theta) \frac{2l+1}{2ikr} \left(e^{ikr} - e^{-ikr+i\pi l} \right) \end{aligned}$$

Only outgoing wave $A_l = (2l+1)i^l e^{i\delta_l}$

Scattering amplitude

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) (e^{2i\delta_l} - 1)$$

$$\sigma = 2\pi \int_0^{\pi} |f(\theta)|^2 \sin \theta d\theta = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

bosons: $l = 0, 2, 4, \dots$

fermions: $l = 1, 3, 5, \dots$

phase shifts $\delta_l = \delta_l(k)$

must be calculated from the solution of the Schrödinger equations.

The situation becomes simpler if the energy of scattered particles is small....

Slow collisions

For $kr_0 \ll 1$ there exists a parametrically large region

$$r_0 \ll r \ll 1/k$$

where right hand side $\sim k^2$ is not important and $V(r) \sim 0$:

Analysis of the solutions for each l gives

$$f_l = \frac{1}{2ik} (e^{2i\delta_l} - 1) \sim k^{2l}$$

And one neglects all $l > 0$

S-wave amplitude

$$\frac{d^2 \chi_{k0}}{dr^2} = 0 \qquad \chi_{k0} = c_0(1 - r/a)$$

On the other hand one can already use the asymptotic form of wavefunction

$$\chi_{k0} = e^{i\delta_0} \sin(kr + \delta_0) = e^{i\delta_0} (\sin \delta_0 + k \cos \delta_0 r)$$

$$c_0 = e^{i\delta_0} \sin \delta_0 \qquad \tan \delta_0 \simeq \delta_0 = -ak \simeq f_0 k$$

Born approximation

To calculate a one has to solve Schrödinger equation for $r < r_0$

For small interaction potential $V(\mathbf{r})$ perturbation theory gives

$$f_0 = -a = -\frac{m^*}{2\pi\hbar^2} \int d\mathbf{r} V(\mathbf{r})$$

Details of the potential are not important for small energy scattering as long as they yield the same value of the scattering length.

Let us define an effective potential $V_{\text{eff}} = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r})$

giving the same value of scattering length as $V(\mathbf{r})$ non-perturbatively

Dilute atomic gas

Below BEC transition

$$k \sim k_T = 1/\Lambda_T \ll n^{1/3}$$

And collisions are always slow: $kr_0 \ll 1$

Interatomic interactions can be safely characterised by the corresponding scattering length a

Weak interactions (diluteness) condition is the condition on *gas parameter*

$$n|a|^3 \ll 1$$

Gross – Pitaevskii Equation

Replacing the field operator by its 'classical' part $\hat{\Psi}(\mathbf{x}, t) \rightarrow \Psi_0(\mathbf{x}, t)$

and assuming slow changes of $\Psi_0(\mathbf{x}, t)$ over the lengths $\sim a$
we obtain GPE:

$$i\hbar \frac{\partial}{\partial t} \Psi_0(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{x}, t) + g |\Psi_0(\mathbf{x})|^2 \right] \Psi_0(\mathbf{x}, t)$$

with coupling constant $g = \int d\mathbf{y} V_{\text{eff}}(\mathbf{y}) = \frac{4\pi\hbar^2 a}{m}$

$V(\mathbf{x}), V_{\text{eff}}(\mathbf{x}) = g\delta(\mathbf{x})$ have the same scattering length

Condensate density and phase

The order parameter $\Psi_0(\mathbf{x}, t)$ has meaning of *macroscopic wavefunction*

$$\int d\mathbf{x} |\Psi_0(\mathbf{x})|^2 = N_0$$

Condensate density $n_0(\mathbf{x}) = |\Psi_0(\mathbf{x})|^2$

Moreover the macroscopic wavefunction has a **PHASE**

$$\Psi_0(\mathbf{x}, t) = \sqrt{n_0(\mathbf{x}, t)} e^{iS(\mathbf{x}, t)}$$

Phase and current

Multiplying Gross Pitaevskii Equation

$$i\hbar \frac{\partial}{\partial t} \Psi_0(\mathbf{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{x}, t) + g|\Psi_0(\mathbf{y})|^2 \right] \Psi_0(\mathbf{x}, t)$$

by its complex conjugate and integrating by parts one gets *continuity equation*

$$\frac{\partial}{\partial t} n_0(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) = 0$$

for density and *supercurrent*

$$\mathbf{j}(\mathbf{x}, t) = \frac{\hbar}{2im} (\Psi_0^* \nabla \Psi_0 - \Psi_0 \nabla \Psi_0^*) = n_0 \frac{\hbar}{m} \nabla S$$


Hydrodynamic form of GPE

Substituting 'polar' representation of order parameter

$$\Psi_0(\mathbf{x}, t) = \sqrt{n_0(\mathbf{x}, t)} e^{iS(\mathbf{x}, t)}$$

into GPE and separating real and imaginary parts

$$\frac{\partial}{\partial t} n(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) = 0$$
$$\hbar \frac{\partial}{\partial t} S + \left(\frac{m \mathbf{v}_s^2}{2} + U + gn - \frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} \right) = 0$$

quantum pressure 

Superfluid velocity

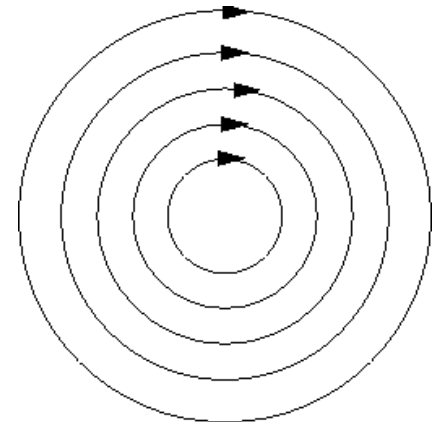
$$\mathbf{v}_s(\mathbf{x}, t) = \frac{\hbar}{m} \nabla S(\mathbf{x}, t)$$

is irrotational, i.e. $\nabla \times \mathbf{v}_s = \frac{\hbar}{m} \nabla \times \nabla S = 0$

for example consider uniform rotation $\mathbf{v}(\mathbf{r}) = \boldsymbol{\Omega} \times \mathbf{r}$

cannot be described by velocity field $\mathbf{v}_s(\mathbf{x}, t)$

- rotation can only enter in form of singular points of phase
where $n_0(\mathbf{x}) = 0$

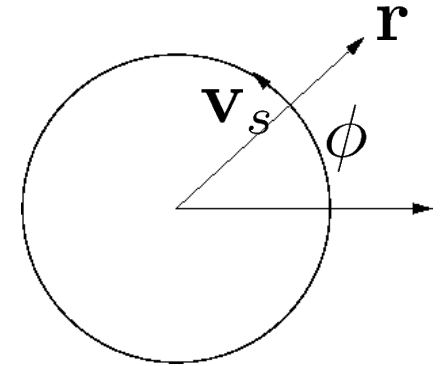


Vortex

Cylindrical coordinates

$$\Psi_s(r, \phi) = |\Psi_s(r)| e^{is\phi}$$

$$L_z = \hbar s N$$



$$\mathbf{v}_s = \frac{\hbar}{m} \frac{1}{r} \frac{\partial S}{\partial \phi} \hat{\phi} = \frac{\hbar}{m} \frac{s}{r} \hat{\phi}$$

$$\oint \mathbf{v}_s \cdot d\mathbf{l} = 2\pi s \frac{\hbar}{m}$$

$$\nabla \times \mathbf{v}_s = 2\pi s \frac{\hbar}{m} \delta(\mathbf{r}) \hat{z}$$

$$n(r) = |\Psi_s(r)|^2 \sim r^{2s}$$

Vortices

Superfluid velocity behaves differently from rigid rotation

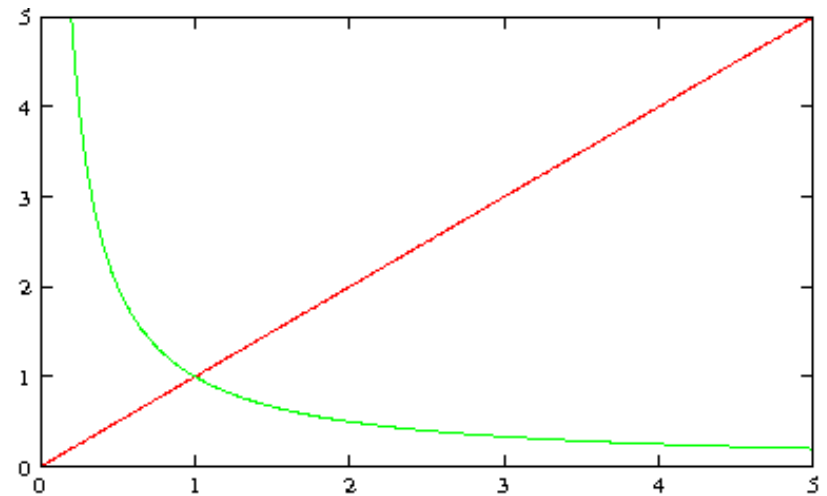
Vortex configuration costs more energy

$$\Delta E = E_{s=1} - E_{s=0}$$

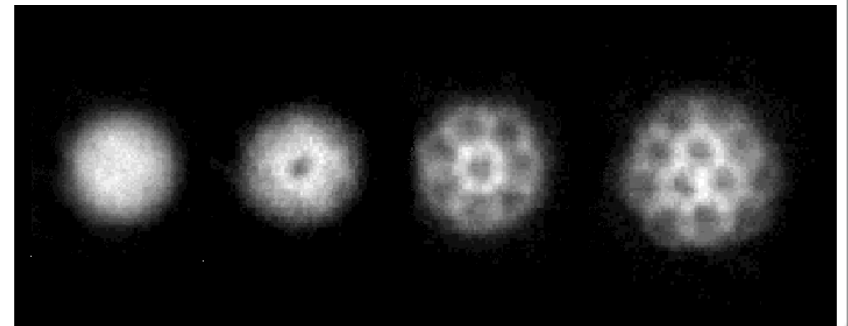
But can be favoured in the rotating frame

$$E_{\text{rot}} = E_0 - \Omega L_z$$

above critical rotation Ω_c



J. Dalibard, 2001



Time dependence and chemical potential

Density matrix at large distances

$$\langle \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{y}) \rangle \quad \rightarrow \quad \langle \hat{\Psi}^\dagger(\mathbf{x}) \rangle \langle \hat{\Psi}(\mathbf{y}) \rangle = \Psi_0^\dagger \Psi_0$$

$$\Psi_0 = \langle \hat{\Psi} \rangle = \langle N | \hat{\Psi} | N + 1 \rangle$$

$$\Psi_0(t) = e^{-i\mu t/\hbar} \langle N | \hat{\Psi} | N + 1 \rangle$$

Chemical potential $\mu = E_{N+1} - E_N$

Uniform case

Non Linear Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_0(\mathbf{x}) - \mu\Psi_0(\mathbf{x}) + g|\Psi_0(\mathbf{x})|^2\Psi_0(\mathbf{x}) = 0$$

is solved with uniform solution $\Psi_0 = \sqrt{n}$

Mean field $\mu = \frac{\partial E_0}{\partial N} = gn$ $P = -\partial E_0/\partial V = gn^2/2$

* $E_0 = \frac{1}{2}Ngn$ Compressibility and sound velocity $\frac{1}{mc^2} = \frac{\partial n}{\partial P} = \frac{1}{gn}$

Condensate in a box

Close to the boundary

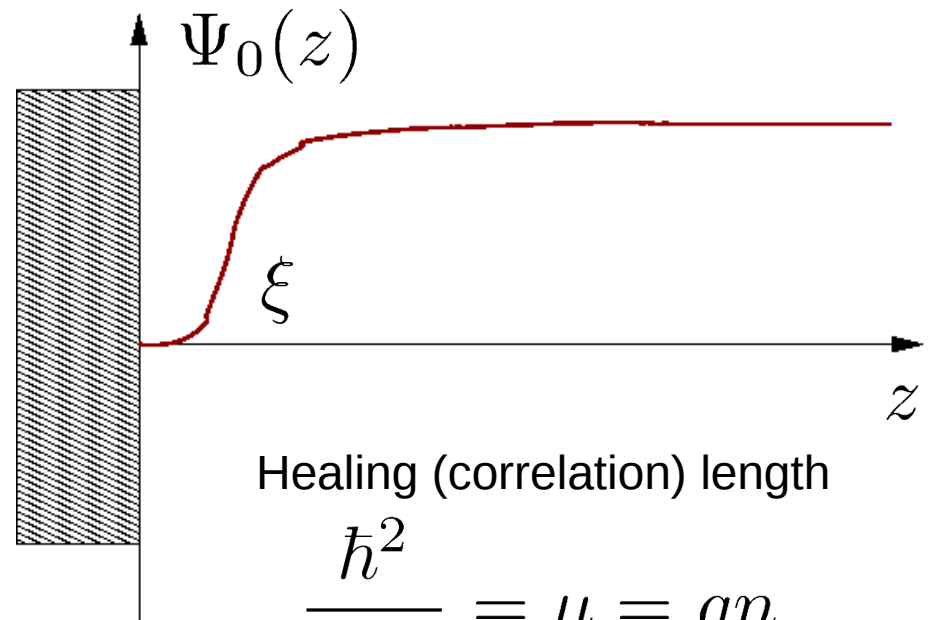
$$\Psi_0(\mathbf{x}) = \sqrt{n} f(z/\xi)$$

$$-\frac{1}{2} \frac{d^2}{dz^2} f + f^3 - f = 0$$

$$f(0) = 0, \quad f(\infty) = 1$$

$$f(z) = \tanh(z)$$

*



Healing (correlation) length

$$\frac{\hbar^2}{m\xi^2} = \mu = gn$$

$$\xi = \frac{\hbar}{\sqrt{mgn}}$$

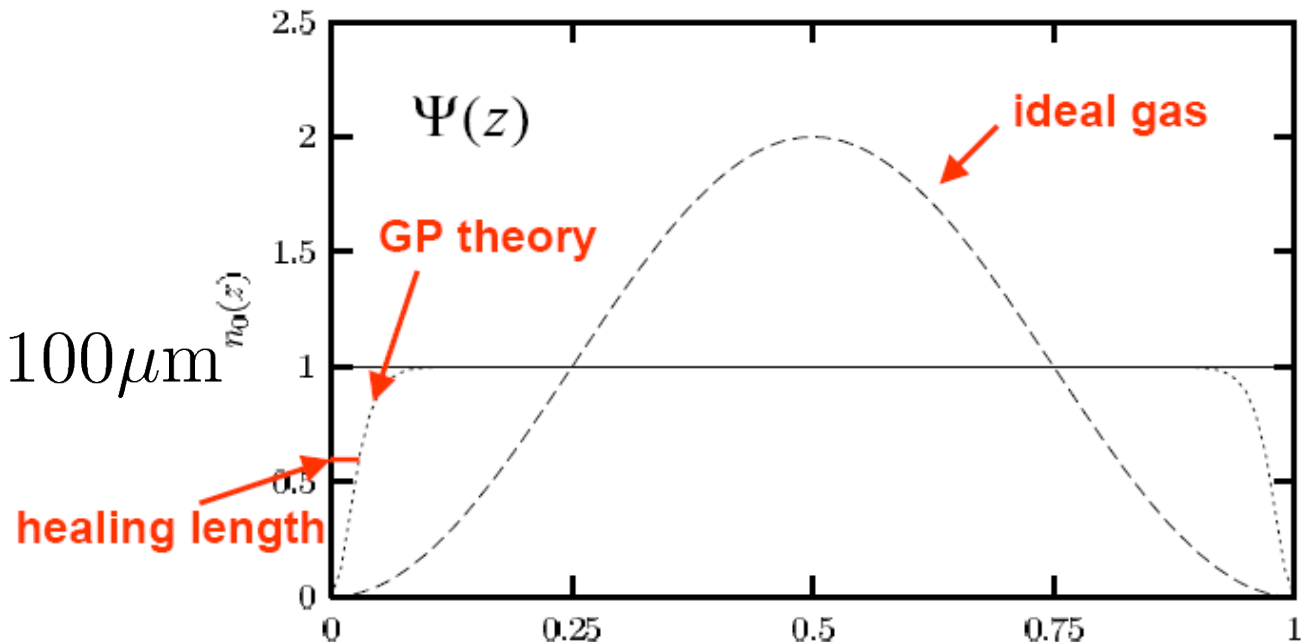
Nonlinearity is important

$$\Psi_0 = \sqrt{n} \tanh(z/\xi)$$

Compare with ground state of free particle in a box: $\Psi_0(z) \sim \sin \pi z/L$

Typical values

$$\xi \sim 1\mu\text{m} \ll L \sim 100\mu\text{m}$$



Harmonic trap

$$V(\mathbf{x}) = \frac{1}{2}m\omega_{\text{ho}}^2 x^2$$

typical length

$$a_{\text{ho}} = \sqrt{\frac{\hbar}{m\omega_{\text{ho}}}}$$

Non interacting particles

$$n(\mathbf{x}) = |\Psi(\mathbf{x})|^2 \sim \exp\left(-\frac{x^2}{a_{\text{ho}}^2}\right)$$

Thomas-Fermi approximation: assume the condensate changes on much larger lengthscales

~~$$-\frac{\hbar^2}{2m}\nabla^2\Psi_0(\mathbf{x}) - (\mu - U(\mathbf{x}))\Psi_0(\mathbf{x}) + g|\Psi_0(\mathbf{x})|^2\Psi_0(\mathbf{x}) = 0$$~~

Local Density Approximation

$$\Psi_0(\mathbf{x}) = \sqrt{n_{\text{TF}}(\mathbf{x})}$$

$$\mu - U(\mathbf{x}) = gn_{\text{TF}}(\mathbf{x}) > 0$$

$$n(0) = \mu/g$$

Inverted parabola

$$n_{\text{TF}}(\mathbf{x}) = n(0) \left(1 - \frac{x^2}{R_{\text{TF}}^2} \right)$$

$$\frac{m\omega_{\text{ho}}^2 R_{\text{TF}}^2}{2} = \mu$$

Thomas Fermi Radius $R_{\text{TF}} = \sqrt{\frac{2\mu}{m\omega_{\text{ho}}^2}} \gg \xi(0) = \hbar/\sqrt{mgn(0)}$

Thomas – Fermi parameter

$$* \quad N = \int d\mathbf{x} n_{\text{TF}}(\mathbf{x}) \quad \mu = \frac{\hbar\omega_{\text{ho}}}{2} \left(\frac{15Na}{a_{\text{ho}}} \right)^{2/5}$$

if $N \frac{a}{a_{\text{ho}}} \gg 1$

$$R_{\text{TF}} = a_{\text{ho}} \left(\frac{15Na}{a_{\text{ho}}} \right)^{1/5}$$

$$\mu \gg \omega_{\text{ho}} \quad \text{and} \quad R_{\text{TF}} \gg a_{\text{ho}}$$

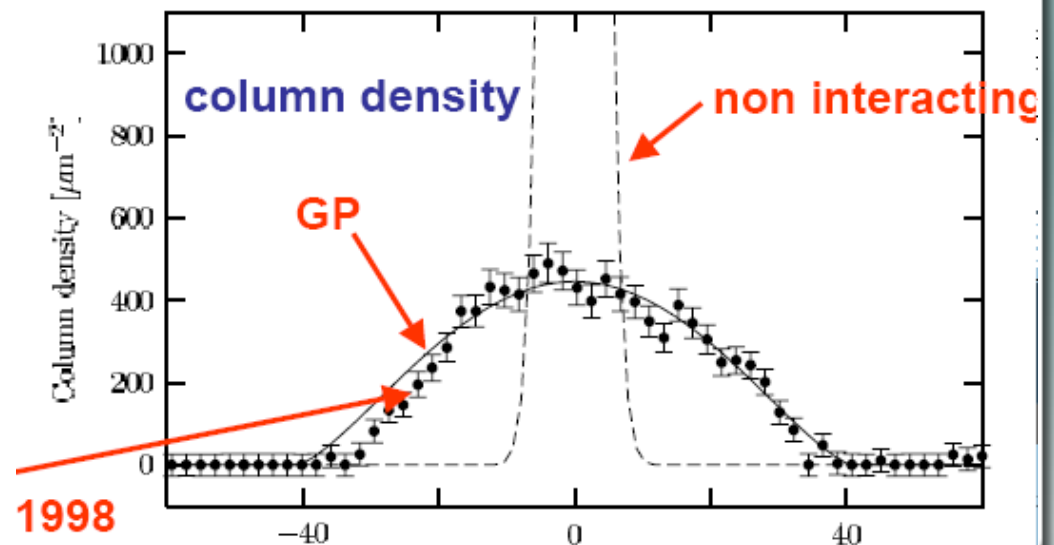
$$\frac{\xi(0)}{R_{\text{TF}}} = \frac{a_{\text{ho}}^2}{R_{\text{TF}}^2} \ll 1$$

Local density approximation is valid

Thomas-Fermi density profile

Quantum pressure $-\frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n} \sim \frac{\hbar^2}{mR_{\text{TF}}^2} \ll \frac{\hbar^2}{m\xi^2} = \mu$

$$n_{\text{TF}}(\mathbf{x}) = n(0) \left(1 - \frac{x^2}{R_{\text{TF}}^2}\right)$$



Conclusions of Lecture 2

- Order parameter has amplitude and phase and its dynamics is governed by Gross – Pitaevskii Equation
- Interactions enter through the scattering length of the potential
- Phase plays important role and leads to unusual irrotational hydrodynamics. In particular rigid rotation is forbidden
- The typical scale on which order parameter change its value is governed by healing length
- If the external trap is sufficiently slow function of coordinates one neglects quantum pressure term in GPE and uses Thomas-Fermi approximation. Usually it works fine for large number of particles