ECT* Workshop
January 2015

Basic concepts of cold atomic gases

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Lecture #2

Stationary GP

By inserting this

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

into the GP equation

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

one finds the stationary GP equation:

$$\boxed{\left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + g\left|\Psi_0(\mathbf{r})\right|^2\right]\Psi_0(\mathbf{r}) = \mu\Psi_0(\mathbf{r})}$$

It gives the **ground state** of the condensate and all possible **stationary** states (vortices, solitons, etc.)

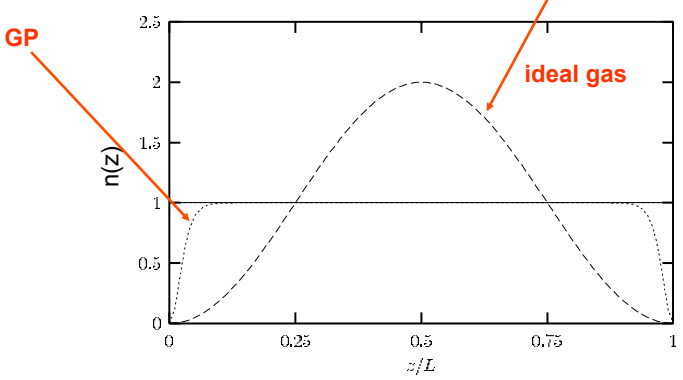
Stationary GP: BEC in a box

Example: 1D box of size *L* and hard walls.

Solution of Schrödinger equation for free particles: $\Psi_0 = \sqrt{2\bar{n}}\,\sin(\pi z / L)$

average density

GP equation with $a > 0$



Stationary GP: BEC in a box

In order to stress the role of interaction in GP, let us rescale the units:

$$\Psi_0 \to \frac{1}{\sqrt{\bar{n}}}\Psi_0 \quad , \quad z \to \frac{z}{\xi}$$

where $\xi = \sqrt{\frac{\hbar^2}{2mg\bar{n}}} = \sqrt{\frac{1}{8\pi a\bar{n}}}$ healing length

The GP equation becomes:

$$-\frac{d^2}{dz^2}\Psi_0(z) + \Psi_0^3(z) = \Psi_0(z)$$

If $L >> \xi$ one can use the boundary conditions: $\Psi_0(0) = 0, \Psi_0(\infty) = 1$

and the solution is:

$$\Psi_0(z) = \sqrt{\bar{n}}\,\tanh\frac{z}{\sqrt{2}\xi}$$

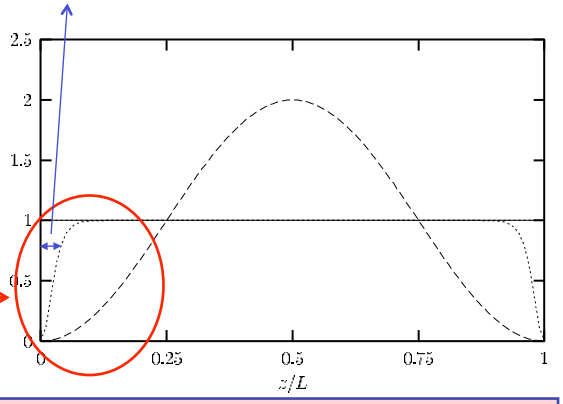
Stationary GP: BEC in a box

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

healing length

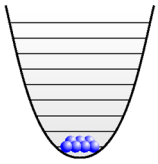
crucial parameter characterizing the interaction

$$\Psi_0(z) = \sqrt{\bar{n}}\tanh\frac{z}{\sqrt{2}\xi}$$



If $L >> \xi$ GP predictions differ significantly from those of an ideal gas !

Stationary GP: harmonic trap



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

Noninteracting ground state: $\Psi_0(r) \propto \exp(-r^2/a_{ho}^2)$

$$a_{ho} = \sqrt{\hbar / m\omega_{ho}}$$

depends on ħ

Role of interactions:

Using a_{ho} and $\hbar\omega_{ho}$ as units of lengths and energy, and $\tilde{\Psi} = N^{-1/2}a_{ho}^{-3/2}\Psi_0$

normalized to 1

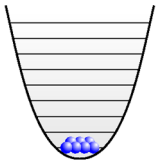
GP equation becomes

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

Thomas-Fermi parameter

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

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



Stationary GP: harmonic trap

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

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) + g|\Psi_0(\mathbf{r})|^2 \right] \Psi_0(\mathbf{r}) = \mu \Psi_0(\mathbf{r})$$

and thus

$$|\Psi_0(\mathbf{r})|^2 = n(\mathbf{r}) = \frac{1}{g}[\mu - V_{ext}(\mathbf{r})]$$

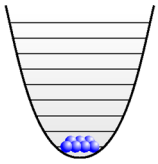
Thomas-Fermi density profile

In an isotropic harmonic potential the density is an inverted parabola with radius $R = a_{ho}(15Na / a_{ho})^{1/5}$

The chemical potential is fixed by the normalization to N: $\mu = gn(0) = (1/2)\hbar\omega_{ho}(15Na / a_{ho})^{2/5}$

The Thomas-Fermi $Na / a_{ho} >> 1$ limit implies:

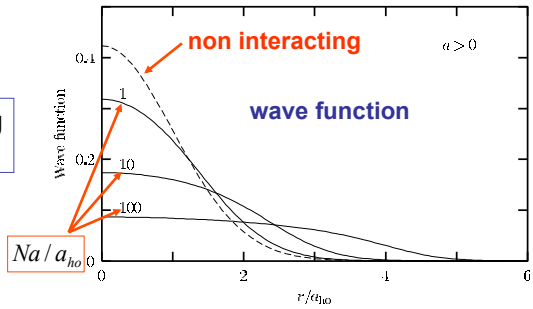
$$\mu >> \hbar\omega_{ho} \quad , \quad R >> a_{ho} \quad , \quad R >> \xi$$



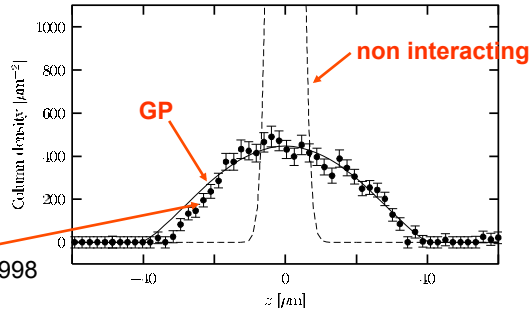
Stationary GP

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) + g|\Psi_0(\mathbf{r})|^2 \right] \Psi_0(\mathbf{r}) = \mu \Psi_0(\mathbf{r})$$

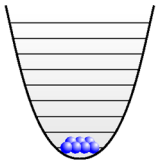
from noninteracting to Thomas-Fermi:



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



exp: Hau et al, 1998



Stationary GP: harmonic trap

Note: Thomas-Fermi regime is compatible with diluteness condition

Gas parameter in the center of the trap → $na^3 = \mu a^3 / g = 0.1(N^{1/6} a / a_{ho})^{12/5}$

Thomas-Fermi if $Na / a_{ho} >> 1$

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

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

$Na / a_{ho} = 10^3$ $\qquad$ $N^{1/6} a / a_{ho} = 10^{-2}$

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

Time-dependent Gross-Pitaevskii equation

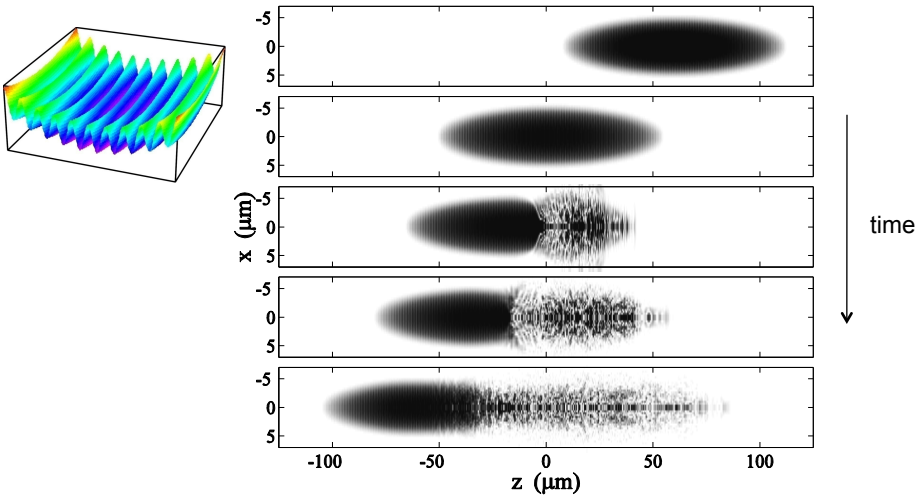
$$i\hbar \frac{\partial}{\partial t} \Psi_0(\mathbf{r},t) = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) + g \left| \Psi_0(\mathbf{r},t) \right|^2 \right] \Psi_0(\mathbf{r},t)$$

This equation can be

- ✓ Numerically solved (GP simulations)
- ✓ Linearized for small oscillations (Bogoliubov equations)
- ✓ Rewritten in terms of density and velocity (T=0 hydrodynamics)

Time-dependent Gross-Pitaevskii equation

Numerical integration.
Example: a BEC oscillating in a trap + optical lattice. Onset of instabilities.



Time-dependent Gross-Pitaevskii equation

Linearization for small oscillations

Ansatz: $\Psi_0(\mathbf{r},t) = e^{-i\mu t}[\,\Psi_0(\mathbf{r}) + u_j(\mathbf{r})e^{-i\omega_j t} + v_j^*(\mathbf{r})e^{i\omega_j t}\,]$

Zero-order in *u* and *v*: $\left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + g\left|\Psi_0(\mathbf{r})\right|^2\right]\Psi_0(\mathbf{r}) = \mu\Psi_0(\mathbf{r})$

First-order in *u* and *v*:

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

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

Bogoliubov equations !

u and *v* are Bogoliubov quasiparticle amplitudes.

ħω are quasiparticle energies.

n_0 is the ground state density: $n_0(\mathbf{r}) = \left|\Psi_0(\mathbf{r})\right|^2$

Time-dependent Gross-Pitaevskii equation

Linearization for small oscillations

Ansatz: $\Psi_0(\mathbf{r},t) = e^{-i\mu t}[\Psi_0(\mathbf{r}) + u_j(\mathbf{r})e^{-i\omega_j t} + v_j^*(\mathbf{r})e^{i\omega_j t}]$

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

Bogoliubov equations !

Note: the **same equations** can be also derived diagonalizing **quantum** Hamiltonian using **Bogoliubov transformations**.

interacting particles → noninteracting quasiparticles

Bogoliubov equations

Some properties of *u* and *v:*

$\int d\mathbf{r}(u_i u_j^* - v_i v_j^*) = \delta_{ij}$ orthogonality and normalization

$(\omega_i - \omega_i^*)\int d\mathbf{r}(|u_i|^2 - |v_i|^2) = 0 \Rightarrow \omega_i$ are real, unless $\int d\mathbf{r}|u_i|^2 = \int d\mathbf{r}|v_i|^2$

occurrence of complex solutions $\Longrightarrow$ **dynamic instability**

If $\Psi_0(\mathbf{r},t) = e^{-i\mu t}(\Psi_0 + u_j e^{-i\omega_j t} + v_j^* e^{i\omega_j t})$, with u_j, v_j, ω_j solution of Bogoliubov eqs., then the energy change with respect to equilibrium is:

$$\delta E = \hbar\omega_j \int d\mathbf{r}\left(|u_j|^2 - |v_j|^2\right)$$

Condition of **energetic stability** $\delta E > 0 \Longrightarrow \omega_j \int dr(|u_j|^2 - |v_j|^2) > 0$

Bogoliubov equations

Solutions of Bogoliubov equations in a uniform gas: $u, v \propto e^{i\mathbf{q}\cdot\mathbf{r}}$

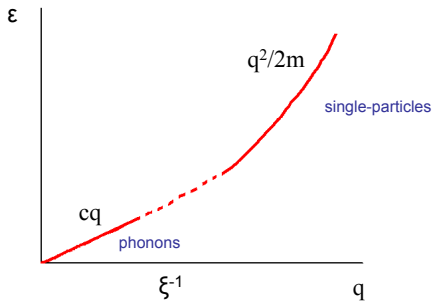
Bogoliubov dispersion law $\omega^2 = \hbar^2 \left(\frac{q^2}{2m} \right)^2 + q^2 c^2$ with $c = \sqrt{g n_0 / m}$

Wavelength of the oscillation:

$\lambda = 2\pi / q$

to be compared with the healing length

$\xi = \hbar / \sqrt{2 m g n_0} = \hbar / \sqrt{2} m c$



Bogoliubov equations

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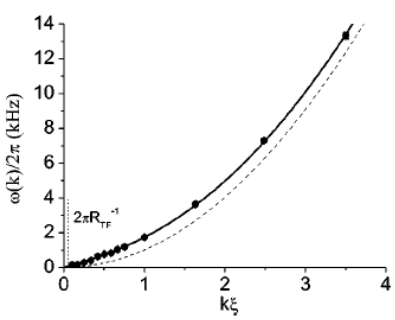
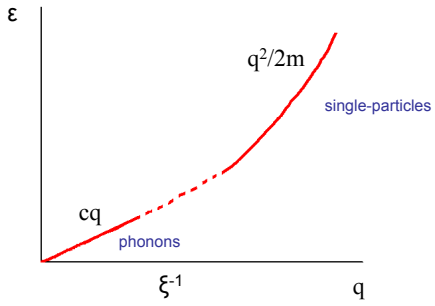
Experiments (Davidson et al.):



Rev. of Mod. Phys. **77**, 187 (2005)



Bogoliubov equations

Solutions of Bogoliubov equations in a uniform gas: $u, v \propto e^{i\mathbf{q}\cdot\mathbf{r}}$

Bogoliubov dispersion law

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

with $c = \sqrt{g n_0 / m}$

In nonuniform systems: numerical solutions

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

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

Time-dependent Gross-Pitaevskii equation

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

This equation can be

- ✓ Numerically solved (GP simulations)
- ✓ Linearized for small oscillations (Bogoliubov equations)
- ✓ Rewritten in terms of density and velocity (T=0 hydrodynamics)

Time-dependent Gross-Pitaevskii equation

Rewritten in terms of density and velocity

Write $\Psi_0 = \sqrt{n}\, e^{iS}$ with

$n = |\Psi_0|^2$ density

$\mathbf{v}_S = (\hbar / m)\nabla S$ velocity

and insert into

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

$$\frac{\partial}{\partial t} n + \nabla\cdot(\mathbf{v}_S n) = 0$$

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

Time-dependent Gross-Pitaevskii equation

Rewritten in terms of density and velocity

Write $\Psi_0 = \sqrt{n}\, e^{iS}$ with

$n = |\Psi_0|^2$ density

$\mathbf{v}_S = (\hbar / m)\nabla S$ velocity

$$\frac{\partial}{\partial t} n + \nabla\cdot(\mathbf{v}_S n) = 0$$

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quantum pressure

These look like hydrodynamic equations, except for quantum pressure

Time-dependent Gross-Pitaevskii equation

What is quantum pressure in terms of energy density:

$$n = |\Psi_0|^2$$
$$\mathbf{v}_S = (\hbar / m)\nabla S$$

GP kinetic energy:

$$E_{kin} = \frac{\hbar^2}{2m}\int d\mathbf{r}\,|\nabla\Psi_0|^2 = \frac{m}{2}\int d\mathbf{r}\, v_S^2 n + \frac{\hbar^2}{2m}\int d\mathbf{r}\left(\nabla\sqrt{n}\right)^2$$

energy of the condensate flow

quantum pressure

To be compared with mean-field energy density $\approx gn$

Time-dependent Gross-Pitaevskii equation

$$\frac{\partial}{\partial t}n + \nabla\cdot(\mathbf{v}_S n) = 0$$
$$m\frac{\partial}{\partial t}\mathbf{v}_S + \nabla\left(\frac{1}{2}mv_S^2 + V_{ext} + gn - \frac{\hbar^2}{2m\sqrt{n}}\nabla^2\sqrt{n}\right) = 0$$

Hydrodynamic equations are obtained when quantum pressure is negligible, i.e., if during the oscillation the density varies over distances λ such that

$\hbar^2 / m\lambda^2 << gn$ or $\boxed{\lambda >> \xi}$

Time-dependent Gross-Pitaevskii equation

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v}_S n) = 0$$

$$m \frac{\partial}{\partial t} \mathbf{v}_S + \nabla \left(\frac{1}{2} m v_S^2 + V_{ext} + gn - \cancel{\frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n}} \right) = 0$$

$\lambda >> \xi$

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v}_S n) = 0$$

$$m \frac{\partial}{\partial t} \mathbf{v}_S + \nabla \left(\frac{1}{2} m v_S^2 + V_{ext} + gn \right) = 0$$

Note: **Planck constant** has disappeared !

Hydrodynamic equations of a superfluid at T=0

v_s is the superfluid velocity.

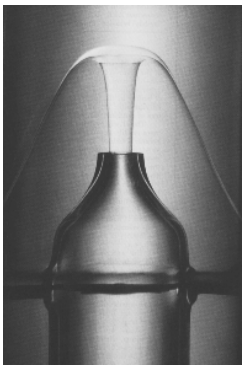
The velocity field is irrotational!

There is no viscosity in these equations!

Superfluidity

"[…] from a modern point of view, superfluidity is not a single phenomenon but a complex of phenomena"

[A.J. Leggett, Rev. Mod. Phys. 73, 307 (2001)]



Superfluidity

Landau criterion for superfluidity

Case #1: Fluid at rest in the presence of moving walls or impurities, at T=0.

The dynamics in the moving frame is governed by $H = H_0 - \mathbf{v}\cdot\mathbf{p}$

The fluid can absorb energy and momentum **only** through the creation of elementary excitations.

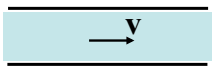
At T=0 excitations can be created only if $\varepsilon(p) - \mathbf{v}\cdot\mathbf{p} < 0$

If $\boxed{v_c = \min_p \frac{\varepsilon(p)}{p} \neq 0}$ the fluid remains at rest for $v \leq v_c$

Superfluidity

Landau criterion for superfluidity

Case #2: Fluid moving in the presence of walls or impurities at rest, at T=0.



Similar arguments as before

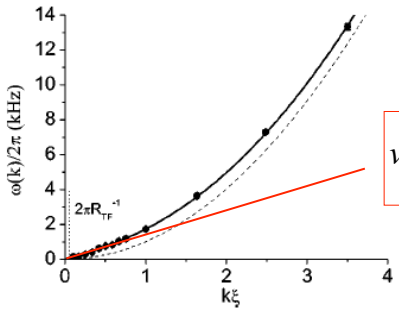
The fluid can absorb energy and momentum **only** through the creation of elementary excitations.

if $\boxed{v_c = \min_p \frac{\varepsilon(p)}{p} \neq 0}$ the current will not decay for $v \leq v_c$ (**persistent current**)

Superfluidity

Landau criterion for superfluidity

In a dilute (weakly interacting) BEC, the spectrum of Bogoliubov quasiparticles is



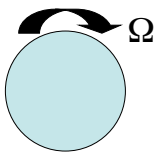
$$v_c = \min_p \frac{\varepsilon(p)}{p} = c$$

The system is superfluid: it flows without dissipation below a critical velocity!!

Superfluidity

Landau criterion for superfluidity

Case #3: fluid at rest in a rotating bucket



Dynamics in rotating frame governed by $H = H_0 - \Omega \hat{l}_z$

Fluid at rest if $\Omega < \Omega_C$ where $\Omega_C = \min_l \frac{\varepsilon(l)}{l}$

$\varepsilon(l) \equiv$ energy of elementary excitation

$l \equiv$ angular momentum of elementary excitation

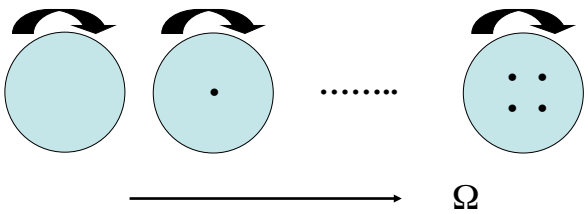
$\Omega_C \neq 0 \Longleftrightarrow$ Landau criterion for superfluidity

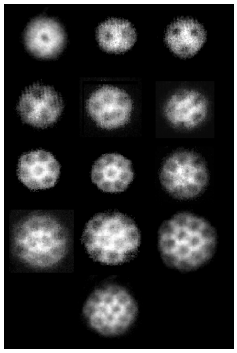
Superfluidity

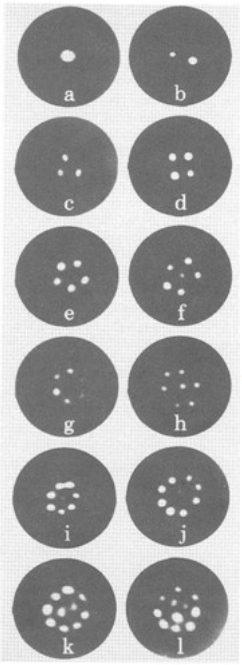
Landau criterion for superfluidity

Case #3: fluid at rest in a rotating bucket

The superfluid does not follow the rotation of the bucket for small Ω, but at higher Ω it can lower its energy by nucleating vortices!

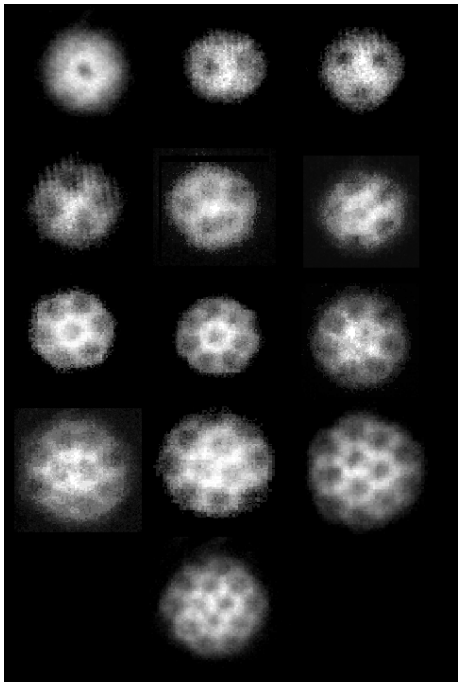






Quantized vortices in BEC (Dalibard et al., 2001)

Quantized vortices in superfluid helium (Packard et al. 1979)



Superfluidity and quantized vortices

A **BEC** behaves as an irrotational **superfluid**, as a consequence of

$$\Psi_0 = \sqrt{n}\, e^{iS}$$

with

$$n = |\Psi_0|^2$$
$$\mathbf{v}_S = \hbar / m \nabla S$$

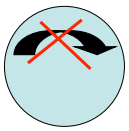
The velocity field is the gradient of a scalar

$$\nabla \times \mathbf{v}_S = 0$$

$$\oint d\ell \cdot \mathbf{v}_S = 0$$

For any closed path in a simply connected geometry

No rotation!



Superfluidity and quantized vortices

$$\oint d\ell \cdot \mathbf{v}_S = 0$$

For any closed path in a simply connected geometry

However, if the system is not simply connected (e.g., it has a hole), than one can choose a path such that

$$\oint d\ell \cdot \mathbf{v}_S = \frac{\hbar}{m} \underbrace{\oint d\ell \cdot \nabla S}_{\Delta S = 2k\pi,\quad k = 0, \pm 1, \pm 2, \ldots} = k \frac{h}{m}$$

quantized circulation!

This condition follows from the single-valuedness of the function

$$\Psi_0 = \sqrt{n}\, e^{iS}$$

Quantized vortex!

Superfluidity and quantized vortices

$$\oint d\ell \cdot \mathbf{v}_S = 0$$

For any closed path in a simply connected geometry

However, if the system is not simply connected (e.g., it has a hole), than one can choose a path such that

$$\oint d\ell \cdot \mathbf{v}_S = \frac{\hbar}{m} \underbrace{\oint d\ell \cdot \nabla S}_{\Delta S = 2k\pi, \quad k = 0, \pm 1, \pm 2, \ldots} = k \frac{h}{m}$$

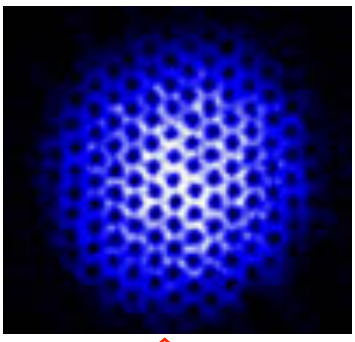
quantized circulation!

This condition follows from the single-valuedness of the function

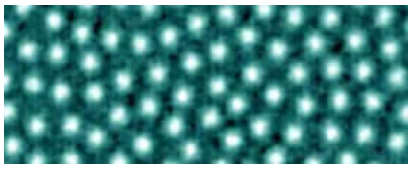
$$\Psi_0 = \sqrt{n}\, e^{iS}$$

or quantized circulation in a toroidal geometry

Superfluidity and quantized vortices



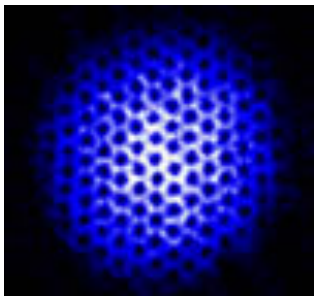
Vortex lattice in BEC (JILA, 2002)

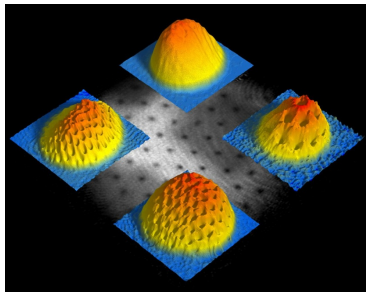


Abrikosov lattice in type II superconductors

Superfluidity and quantized vortices

Many experiments on quantized vorticity in BECs in the last 15 years!
A lot of interesting physics: vortex nucleation, vortex arrays, fast rotations and Lowest Landau Level regime, quantum turbulence, BKT transition in 2D, Tkachenko waves, Kelvin modes, persistent currents in toroidal traps, etc.

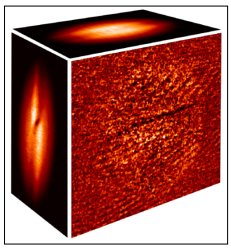


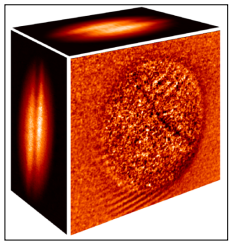


For a review, see A.Fetter, Rev. Mod. Phys. 81, 647 (2009)

Superfluidity and quantized vortices

Recent results in Trento: solitonic vortices in BEC of sodium.





BEC and superfluid hydrodynamics

From GP equation, neglecting quantum pressure:

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v}_S n) = 0$$

$$m \frac{\partial}{\partial t} \mathbf{v}_S + \nabla \left(\frac{1}{2} m v_S^2 + V_{ext} + gn \right) = 0$$

Hydrodynamic equations of a superfluid at T=0

Can be rewritten in the form

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v}_S n) = 0$$

$$m \frac{\partial}{\partial t} \mathbf{v}_S + \nabla \left(\frac{1}{2} m v_S^2 + V_{ext} + \mu(n) \right) = 0$$

In this form they are more general !

$\longrightarrow$ this Euler equation is equivalent to the equation for the phase:

$$\hbar \frac{\partial}{\partial t} S = -\left(\frac{1}{2} m v_S^2 + V_{ext} + \mu \right)$$

local chemical potential

BEC and superfluid hydrodynamics

Hydrodynamic eqs of superfluids at T=0

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v}_S n) = 0$$

$$m \frac{\partial}{\partial t} \mathbf{v}_S + \nabla \left(\frac{1}{2} m v_S^2 + V_{ext} + \mu(n) \right) = 0$$

These equations can be obtained, independently of GP, starting from the equation for the bosonic field operator in uniform systems, imposing Galilean invariance, and using a local density approximation for a slowly varying order parameter.

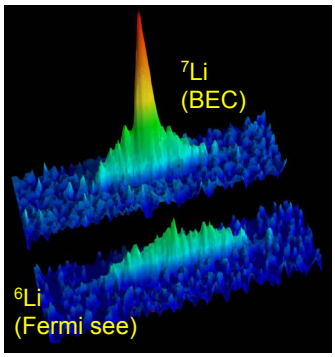
In this context, ***n*** is the **total** density and the superfluid velocity is $v_S = \frac{\hbar}{m} \nabla S$

- ✓ Equations are **classical** (do not depend on Planck constant).
- ✓ Velocity field is **irrotational** (role of the **phase**).
- ✓ Condensate density does not enter HD eqs.
- ✓ HD valid for **macroscopic** phenomena (length scales >> healing length)
- ✓ HD applicable to both **Bose** and **Fermi** superfluids.
- ✓ HD equations depend on **equation of state** *μ(n)* (sensitive to quantum correlations, statistics, dimensionality, ...).
- ✓ HD equations can be linearized for small oscillations.

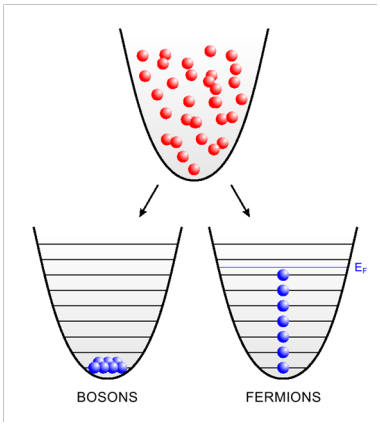
Fermions

Ultracold fermions

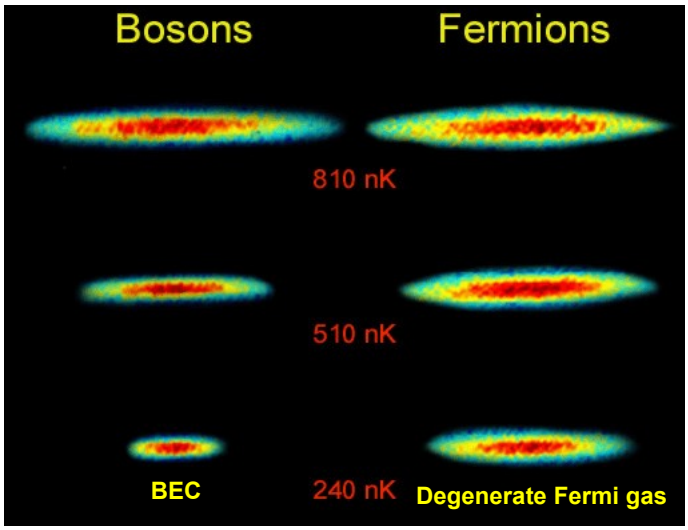
- Condensation is only possible for BOSONS.
- FERMIONS behave differently, due to Pauli.



(Salomon, ENS, 2001)



Observing quantum statistics



(Rice, 2001)

Ultracold fermions

Ideal fermions in a trap

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

if $N >> 1, \quad k_B T >> \hbar\omega_{ho}$ one can use semiclassical approximation

$$f(r,p) = \frac{1}{\exp[(p^2/2m + V_{ext}(r) - \mu)/k_B T] + 1}$$

distribution function

normalization can be written as:

$$N = \iint \frac{drdp}{(2\pi\hbar)^3} f(r,p) = \frac{1}{2(\hbar\omega_{ho})^3} \int d\varepsilon \frac{\varepsilon^2}{\exp[(\varepsilon - \mu)/k_B T] + 1}$$

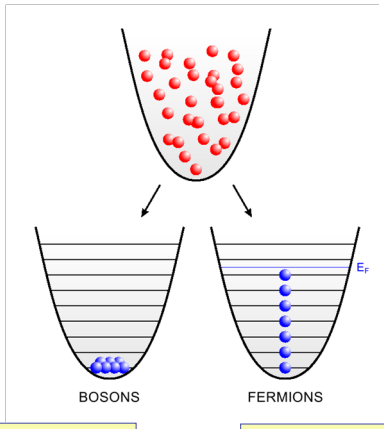
At T=0: $\mu \to E_F; \quad f(r,p) \to \Theta(p^2/2m + V_{ext} - E_F)$ step function

One gets $E_F = \hbar\omega_{ho}(6N)^{1/3}$

Same dependence as BEC critical temperature

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

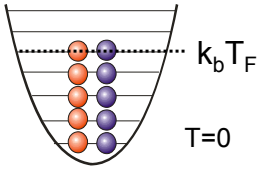
Ultracold fermions



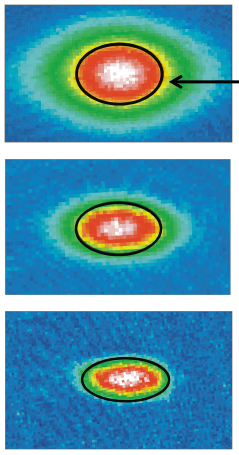
$k_B T << k_B T_c = 0.94\,\hbar\omega_{ho} N^{1/3}$

$k_B T << k_B T_F = E_F = 1.82\,\hbar\omega_{ho} N^{1/3}$

Ultracold fermions



Density profile



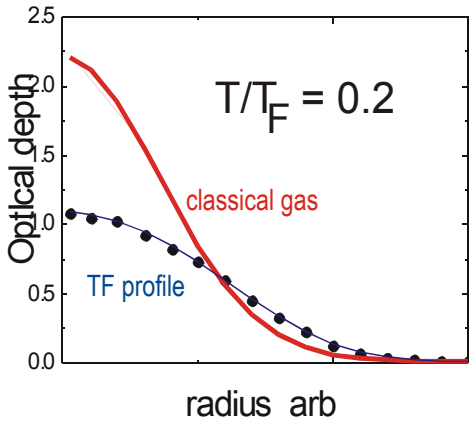
T/T_F=0.77

E_F

T/T_F=0.27

T/T_F=0.11

(Regal et al., JILA)



Ultracold fermions

Another consequence of Pauli exclusion principle:

Fermions of the **same atomic species** and in the **same spin state** do not interact in s-wave scattering **!!**

Just a (almost) free degenerate Fermi gas…

Ultracold fermions

Another consequence of Pauli exclusion principle:

Fermions of the **same atomic species** and in the **same spin state** do not interact in s-wave scattering **!!**

Just a (almost) free degenerate Fermi gas…

BUT what about a **mixture of two spin states** or two species **?**

- s-wave scattering is possible and dominates at low temperature
- s-wave scattering length can be tuned thanks to Feshbach resonances

Ultracold fermions

A dilute mixture of two spin states or two species, interacting via a contact interaction (low-energy s-wave scattering):

$$\hat{H}_{\text{int}} = g\int d\mathbf{r}\,\hat{\Psi}^{+}_{\uparrow}(\mathbf{r})\hat{\Psi}^{+}_{\downarrow}(\mathbf{r})\hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r})$$

with $g = 4\pi\hbar^2 a/m$

If **a < 0** atoms can form bound pairs (bosons) and undergo BCS superfluidity

Ultracold fermions

BCS theory $a<0$ $k_F|a|<<1$

Pairing between spin-up and -down atoms **in momentum space (Cooper pairs).**

Order parameter characterizing the long range order of **two-body** density matrix.

$$\Delta(\mathbf{r}) = \left\langle \hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r}) \right\rangle$$

Quasi-particle excitation spectrum has a **gap:**

$$\varepsilon(p) = \sqrt{\Delta^2_{gap} + [p^2/2m) - \mu]^2}$$

½ of the energy required to break a pair

BCS **critical temperature**:

$$T_c = 0.28\,T_F \exp\left[-\frac{\pi}{2k_F|a|}\right]$$

Note: this prefactor contains Gorkov and Melik-Barkhudarov corrections to BCS (renormalization of scattering length due to screening effects)

Note: this can be very small if $k_F|a|$ is small !

Same physics of weak coupling superconductors!

Ultracold fermions

A dilute mixture of two spin states or two species, interacting via a contact interaction (low-energy s-wave scattering):

$$\hat{H}_{\text{int}} = g\int d\mathbf{r}\,\hat{\Psi}^{+}_{\uparrow}(\mathbf{r})\hat{\Psi}^{+}_{\downarrow}(\mathbf{r})\hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r})$$

with $g = 4\pi\hbar^2 a/m$

If **a < 0** atoms can form bound pairs (bosons) and undergo BCS superfluidity

If **a > 0** atoms can form bound molecules (bosons) and undergo BEC.

Ultracold fermions

BEC of molecules $a > 0$ $k_F|a| << 1$

When the scattering length *a* is positive, the interaction can produce **bound molecules** (bosons) of size *a*.

If $k_F|a|$ is small, the size of molecules is much smaller than the average distance between them (gas of bosonic dimers).

By solving the two-body scattering problem one finds the molecular binding energy:

$$E = -\frac{\hbar^2}{ma^2}$$

At low T, molecules form a BEC. The critical temperature for a gas of bosons of mass *2m* (molecules) at density *n* is directly related to value of Fermi energy of fermions of mass *m* at the same density.

In a uniform gas: $T_{BEC} = 0.2T_F$ In a harmonic trap: $T_{BEC} = 0.5T_F$

Critical temperature for superfluidity is much **higher in BEC than in BCS** side where it is exponentially small.

Ultracold fermions

A dilute mixture of two spin states or two species, interacting via a contact interaction (low-energy s-wave scattering):

$$\hat{H}_{\text{int}} = g \int d\mathbf{r}\, \hat{\Psi}^{+}_{\uparrow}(\mathbf{r})\hat{\Psi}^{+}_{\downarrow}(\mathbf{r})\hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r})$$

with $g = 4\pi\hbar^2 a / m$

If **a < 0** atoms can form bound pairs (bosons) and undergo BCS superfluidity

If **a > 0** atoms can form bound molecules (bosons) and undergo BEC.

Ultracold fermions

A dilute mixture of two spin states or two species, interacting via a contact interaction (low-energy s-wave scattering):

$$\hat{H}_{\text{int}} = g \int d\mathbf{r}\, \hat{\Psi}^{+}_{\uparrow}(\mathbf{r})\hat{\Psi}^{+}_{\downarrow}(\mathbf{r})\hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r})$$

with $g = 4\pi\hbar^2 a / m$

If **a < 0** atoms can form bound pairs (bosons) and undergo BCS superfluidity

If **a > 0** atoms can form bound molecules (bosons) and undergo BEC.

In both cases one gets deep modifications of many-body wave function.
The ideal Fermi gas is no longer a proper starting point.

No perturbative theories

Ultracold fermions

A dilute mixture of two spin states or two species, interacting via a contact interaction (low-energy s-wave scattering):

$$\hat{H}_{\text{int}} = g\int d\mathbf{r}\,\hat{\Psi}^{+}_{\uparrow}(\mathbf{r})\hat{\Psi}^{+}_{\downarrow}(\mathbf{r})\hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r})$$

with $g = 4\pi\hbar^2 a/m$

If **a < 0** atoms can form bound pairs (bosons) and undergo BCS superfluidity

If **a > 0** atoms can form bound molecules (bosons) and undergo BEC.

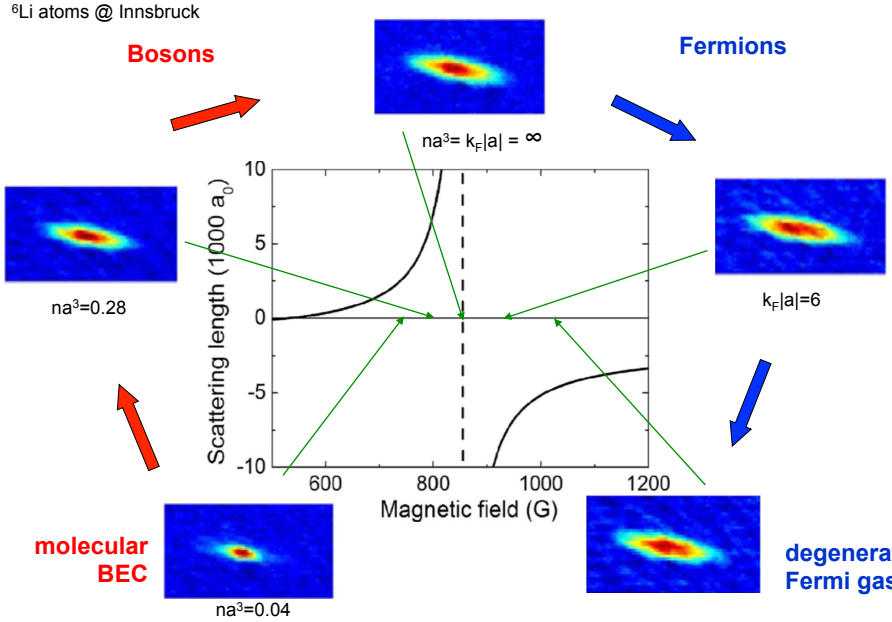
The scattering length can be tuned at will when the atomic species exhibits Feshbach resonances.

BCS-BEC crossover

scattering length

Ultracold fermions

BCS-BEC crossover
^{6}Li atoms @ Innsbruck

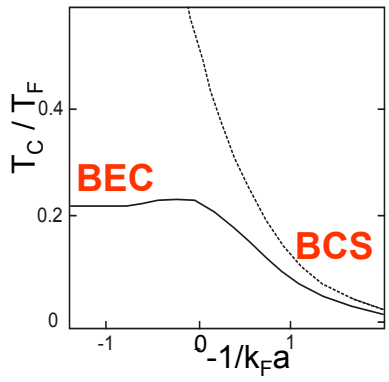


Theory of the BCS-BEC crossover

First theoretical approach developed by Leggett (1980).
Nozieres and Schmitt-Rink (1985) generalized the gap equation of BCS theory to include the whole resonance region.

Theory predicts (Randeria,1993):

- critical temperature and equation of state as a function of dimensionless the parameter $k_F a$
- formation of molecules with energy $\hbar^2 / ma^2$ on the BEC side $k_F a << 1$
- BEC of molecules interacting with scattering length $a_M = 2a$



Theory of the BCS-BEC crossover

Unitary regime when $k_F |a| >> 1$

At **unitarity** the system is strongly correlated but its properties **do not** depend on the value of scattering length **a** (not even on the sign of a)!

The typical length scale of interaction becomes much larger than the size of the gas itself. It disappears from the description of the system.

Universality

All lengths disappear from the calculation of energy, chemical potential, thermodynamic functions, etc., except the interparticle distance, which is fixed by the total density of the gas *n*.

Theory of the BCS-BEC crossover

Unitary regime when $k_F|a| >> 1$

Universality All lengths disappear from the calculation of energy, chemical potential, thermodynamic functions, etc., except the interparticle distance, which is fixed by the total density of the gas *n*.

Example:
The equation of state of a **unitary uniform gas** at T=0 must exhibit the **same** density dependence as the **ideal Fermi gas** (dimensionality arguments rule out different dependences). Thus

$$\mu = (1+\beta)\frac{\hbar^2}{2m}\left(6\pi^2 n\right)^{2/3}$$

with $\beta = 0$ Ideal Fermi gas
$\beta \neq 0$ Fermi gas at unitarity

Many-body calculations are needed to determine value of β.

Possible comparison with experiments (see experiments on the equation of state at ENS and MIT)

The equation of state can be used to determine density profiles, release energy and collective frequencies in Thomas-Fermi approximation.

Mean-field theory of the BCS-BEC crossover

Two-component Fermi gas as at T=0.
Many-body Hamiltonian written in terms of fermionic operators $\hat{\Psi}^+_\uparrow, \hat{\Psi}^+_\downarrow, \hat{\Psi}_\uparrow, \hat{\Psi}_\downarrow$

$$\hat{H} = \sum_{\sigma=\uparrow,\downarrow}\int d\mathbf{r}\,\hat{\Psi}^+_\sigma(\mathbf{r})\left[-\frac{\hbar^2\nabla^2}{2m_\sigma}-\mu_\sigma\right]\hat{\Psi}_\sigma(\mathbf{r}) + \frac{1}{2}\iint d\mathbf{r}\,d\mathbf{r}'\,\hat{\Psi}^+_\uparrow(\mathbf{r})\hat{\Psi}^+_\downarrow(\mathbf{r}')V(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}_\downarrow(\mathbf{r}')\hat{\Psi}_\uparrow(\mathbf{r})$$

Approximation: **include** the interaction only in **pairing** correlations, treated at mean-field level. **Ignore** direct (Hartree) interaction terms proportional to the averages $\langle\hat{\Psi}^+_\uparrow\hat{\Psi}_\uparrow\rangle$ $\langle\hat{\Psi}^+_\downarrow\hat{\Psi}_\downarrow\rangle$ $\longrightarrow$ these would give divergent terms at unitarity

One gets the BCS Hamiltonian

$$\hat{H}_{BCS} = \sum_{\sigma=\uparrow,\downarrow}\int d\mathbf{r}\,\hat{\Psi}^+_\sigma(\mathbf{r})\left[-\frac{\hbar^2\nabla^2}{2m_\sigma}-\mu_\sigma\right]\hat{\Psi}_\sigma(\mathbf{r}) - \int d\mathbf{r}\left\{\Delta(\mathbf{r})\left[\hat{\Psi}^+_\uparrow(\mathbf{r})\hat{\Psi}^+_\downarrow(\mathbf{r}) - (1/2)\langle\hat{\Psi}^+_\uparrow(\mathbf{r})\hat{\Psi}^+_\downarrow(\mathbf{r})\rangle\right] + H.c.\right\}$$

where $\Delta(\mathbf{r}) = -\int d\mathbf{s}\,V(\mathbf{s})\langle\hat{\Psi}_\downarrow(\mathbf{r}+\mathbf{s}/2)\hat{\Psi}_\uparrow(\mathbf{r}-\mathbf{s}/2)\rangle$ order parameter

$\mathbf{s} = |\mathbf{r}-\mathbf{r}'|$

Mean-field theory of the BCS-BEC crossover

$$\hat{H}_{BCS} = \sum_{\sigma=\uparrow,\downarrow} \int d\mathbf{r}\, \hat{\Psi}^{+}_{\sigma}(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m_\sigma} - \mu_\sigma \right] \hat{\Psi}_{\sigma}(\mathbf{r}) - \int d\mathbf{r} \left\{ \Delta(\mathbf{r}) \left[\hat{\Psi}^{+}_{\uparrow}(\mathbf{r}) \hat{\Psi}^{+}_{\downarrow}(\mathbf{r}) - (1/2) \left\langle \hat{\Psi}^{+}_{\uparrow}(\mathbf{r}) \hat{\Psi}^{+}_{\downarrow}(\mathbf{r}) \right\rangle \right] + H.c. \right\}$$

$$\Delta(\mathbf{r}) = -\int d\mathbf{s}\, V(\mathbf{s}) \left\langle \hat{\Psi}_{\downarrow}(\mathbf{r}+\mathbf{s}/2) \hat{\Psi}_{\uparrow}(\mathbf{r}-\mathbf{s}/2) \right\rangle$$

Crucial point: this Hamiltonian can be put in diagonal form by replacing particles with **quasi-particles** (**Bogoliubov transformations**) !

$$\hat{\Psi}_{\uparrow}(\mathbf{r}) = \sum_i [u_i(\mathbf{r}) \hat{\alpha}_i + v_i^*(\mathbf{r}) \hat{\beta}_i^+]$$
$$\hat{\Psi}_{\downarrow}(\mathbf{r}) = \sum_i [u_i(\mathbf{r}) \hat{\beta}_i + v_i^*(\mathbf{r}) \hat{\alpha}_i^+]$$

$$\hat{H}_{BCS} = (E_0 - \mu N) + \sum_i \varepsilon_i (\hat{\alpha}_i^+ \hat{\alpha}_i + \hat{\beta}_i^+ \hat{\beta}_i)$$

a gas of independent quasi-particles

The quasi-particle operators obey the anti-commutation rules $\left\{ \hat{\alpha}_i, \hat{\alpha}_j^+ \right\} = \left\{ \hat{\beta}_i, \hat{\beta}_j^+ \right\} = \delta_{ij}$

The quasiparticle amplitudes obey $\int d\mathbf{r} [u_i^*(\mathbf{r}) u_j(\mathbf{r}) + v_i^*(\mathbf{r}) v_j(\mathbf{r})] = \delta_{ij}$

Mean-field theory of the BCS-BEC crossover

$$\hat{\Psi}_{\uparrow}(\mathbf{r}) = \sum_i [u_i(\mathbf{r}) \hat{\alpha}_i + v_i^*(\mathbf{r}) \hat{\beta}_i^+]$$
$$\hat{\Psi}_{\downarrow}(\mathbf{r}) = \sum_i [u_i(\mathbf{r}) \hat{\beta}_i + v_i^*(\mathbf{r}) \hat{\alpha}_i^+]$$

The diagonalization of the Hamiltonian gives the equations for the quasi-particle amplitudes. In general, including the case of a Fermi gas in an external potential, these equations have the form

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

Bogoliubov – de Gennes equations

with $H_0(\mathbf{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$

The order parameter can be obtained by means of a self-consistent procedure (a proper regularization of the interaction is needed):

$$\Delta(\mathbf{r}) = -g \sum_i u_i(\mathbf{r}) v_i^*(\mathbf{r})$$

Mean-field theory of the BCS-BEC crossover

Bogoliubov – de Gennes equations

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

Fermions

$$H_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

Note: remarkable similarity with **Bogoliubov** equations for excitations (quasi-particles) in BECs

$$\begin{pmatrix} H_0(\mathbf{r}) & g\Psi_0^2 \\ -g\Psi_0^{*2}(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

Bosons

$$H_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu + 2g\left|\Psi_0(\mathbf{r})\right|^2$$

Note: some slides ago, we wrote the same eqs in this form:

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

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

Mean-field theory of the BCS-BEC crossover

Fermions vs. **Bosons**

Bogoliubov equations for BECs and Bogoliubov-de Gennes for fermions are two implementations of the same idea: Bogoliubov transformation, i.e. , diagonalization of the many-body Hamiltonian by replacing particle operators by quasi-particle operators.

one of the key concepts in many-body theories

Mean-field theory of the BCS-BEC crossover

Fermions vs. **Bosons**

Bogoliubov equations for BECs and Bogoliubov-de Gennes for fermions are two implementations of the same idea: Bogoliubov transformation, i.e. , diagonalization of the many-body Hamiltonian by replacing particle operators by quasi-particle operators.

Important difference:

Due to macroscopic occupation of a single state, in BEC the order parameter is obtained expanding the Hamiltonian in $\delta\hat{\Psi}(\mathbf{r})$ where $\hat{\Psi}(\mathbf{r}) = \Psi_0(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r})$.
At zero-order one has the GP equation for $\Psi_0(\mathbf{r})$.
At first-order one gets the Bogoliubov equations for bosonic excitations.

Conversely, in the BCS-BEC theory for fermions, there is no zero-order. The Bogoliubov-de Gennes equations give the order parameter itself, together with all fermionic excitations (but no bosonic excitations, such as phonons…). The ground state is the vacuum of quasi-particles.

Mean-field theory of the BCS-BEC crossover

Bogoliubov – de Gennes equations

Fermions

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

$$H_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

The mean-field theory based on BdG equation

- ☺ gives the correct limit of free fermions in external potentials for $a=0^-$
- ☺ gives the correct GP equation for a BEC of molecules of mass $2m$ for $a=0^+$
- ☺ gives a smooth crossover from BCS to BEC, including unitarity.
- ☺ it is accurate enough for many purposes.
- ☹ It is misses important corrections to the ideal Fermi gas for small negative a.
- ☹ It gives the wrong scattering length for molecule-molecule interaction.

Mean-field theory of the BCS-BEC crossover

Bogoliubov – de Gennes equations

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$

$$H_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

$$\Delta(\mathbf{r}) = -g\sum_i u_i(\mathbf{r})v_i^*(\mathbf{r})$$ order parameter

$$n(\mathbf{r}) = 2\sum_i |v_i(\mathbf{r})|^2$$ density

Can be solved numerically by iterations

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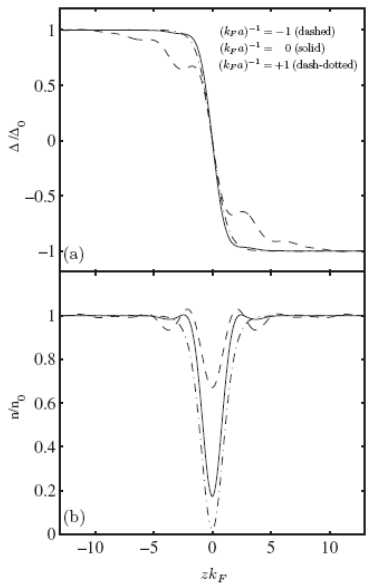
Example:
a dark soliton in a uniform Fermi superfluid

Antezza et al., PRA 76, 043610 (2007)



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As in the case of GP equation, they can be written as equations for the time evolution (time-dependent BsG equations)

Mean-field theory of the BCS-BEC crossover

Time-dependent Bogoliubov – de Gennes equations

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r},t) \\ v_i(\mathbf{r},t) \end{pmatrix} = i\hbar\frac{\partial}{\partial t} \begin{pmatrix} u_i(\mathbf{r},t) \\ v_i(\mathbf{r},t) \end{pmatrix}$$

$$H_0(\mathbf{r}) = -\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

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Also these equations can be solved numerically.

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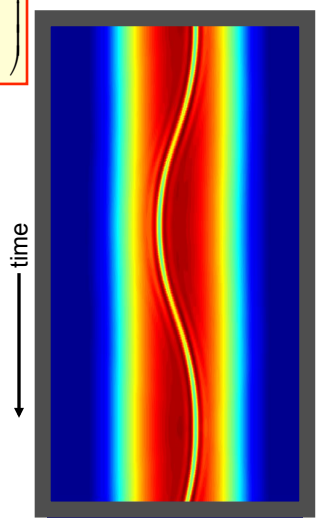
$$n(\mathbf{r},t) = 2 \sum_i |v_i(\mathbf{r},t)|^2$$

Example:
a soliton oscillating in a trapped Fermi gas

Scott et al., PRL 106, 185301 (2011))



Mean-field theory of the BCS-BEC crossover

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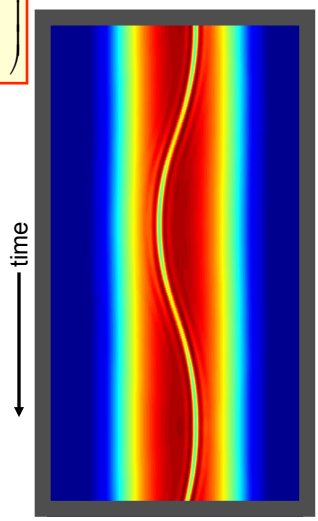
Important remark:
time-dependent BdG include both **bosonic** and **fermionic** degrees of freedom!



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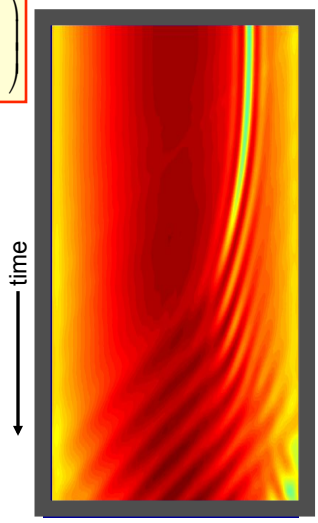
Here a soliton becomes unstable because pair-breaking near the soliton (fermionic excitations) generates phonons (bosonic collective excitations).



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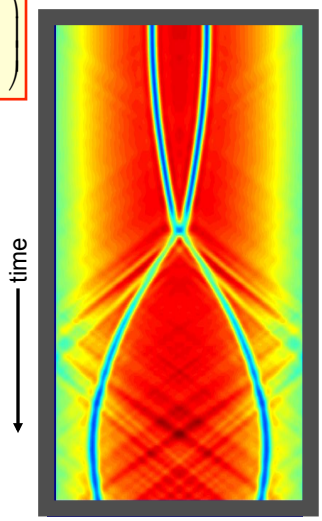
Important remark:
time-dependent BdG include both **bosonic** and **fermionic** degrees of freedom!

Here two solitons collide producing sound waves (bosonic excitations) as a result of inelastic processes induced by the dynamics of fermionic quasiparticles.



Other theories for the BCS-BEC crossover

• Effective GP equation (local chemical potential of Fermi gas replacing the nonlinear term of GP equation; only bosonic degrees of freedom; no pair-breaking)

• Density Functional Theory beyond BdG (free parameters fixed from ab initio calculations)

• Diagrammatic many-body approaches (T-matrix, etc.)

• Exact asymptotic results at unitarity (Tan contact)

• and, of course, Monte Carlo simulations

and others…