Fermions

A simple argument:

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



(Salomon, ENS, 2001)



Observing quantum statistics



(Rice, 2001)

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, $k_B T >> \hbar \omega_{ho}$ 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: $\mu \to E_F$; $f(r, p) \to \Theta(p^2/2m + V_{ext} - E_F)$ step function

One gets

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

Same dependence as BEC critical temperature $k_B T_c = 0.94 \hbar \omega_{ho} N^{1/3}$





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...

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

Mixture of two spin states or two species

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

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

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



Same physics of weak coupling superconductors!

Mixture of two spin states or two species

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

with
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a<0 atoms can form bound pairs (bosons) and undergo BCS superfluiditya>0 atoms can form bound molecules (bosons) and undergo BEC.

BEC of molecules a > 0 $k_F \mid a \mid << 1$

When the scattering length *a* is positive, the interaction can produce weakly **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 \underline{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.

Mixture of two spin states or two species

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

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

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

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

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



Mixture of two spin states or two species

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

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

a<0 atoms can form bound pairs (bosons) and undergo BCS superfluiditya>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

BCS-BEC crossover

(in a 2-component Fermi gases)





Experiments



...and many more after 2005.

Also imbalanced spin mixtures (different populations). Also mixtures of different atoms: 40K-87Rb (Florence), 6Li-23Na (MIT), ...



Theory of the BCS-BEC crossover



Important efforts in recent few years to provide improved **many-body schemes** (Holland, Griffin, Timmermans, Strinati), including numerical quantum **Monte Carlo** approaches (Carlson, Giorgini,...)

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.



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



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

$$\mu = (1 + \beta) \frac{\hbar^2}{2m} (6\pi^2 n)^{2/3} \qquad \text{with} \qquad \begin{array}{l} \beta = 0 & \text{Ideal Fermi gas} \\ \beta \neq 0 & \text{Fermi gas at unitarity} \end{array}$$

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

One finds: $\beta \approx -0.6$ (it is negative, reflecting attractive role of the interaction).

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

Uniform gas 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 $\langle \hat{\Psi}^{+}_{\uparrow} \hat{\Psi}_{\uparrow} \rangle \quad \langle \hat{\Psi}^{+}_{\downarrow} \hat{\Psi}_{\downarrow} \rangle \longrightarrow \text{ these would give divergent terms at unitarity}$

One gets the BCS Hamiltonian

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

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

$$\Delta(\mathbf{r}) = -\int d\mathbf{s} \, V(\mathbf{s}) \left\langle \hat{\Psi}_{\downarrow}(\mathbf{r} + \mathbf{s}/2) \hat{\Psi}_{\uparrow}(\mathbf{r} - \mathbf{s}/2) \right\rangle$$
Crucial point: this Hamiltonian can be put in diagonal form by replacing particles with quasi-particles (Bogoliubov transformations)

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

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

 $\hat{\Psi}_{\uparrow}(\mathbf{r}) = \sum_{i} \left[u_{i}(\mathbf{r})\hat{\alpha}_{i} + v_{i}^{*}(\mathbf{r})\hat{\beta}_{i}^{+} \right]$ $\hat{\Psi}_{\downarrow}(\mathbf{r}) = \sum_{i} \left[u_{i}(\mathbf{r})\hat{\beta}_{i} + v_{i}^{*}(\mathbf{r})\hat{\alpha}_{i}^{+} \right]$

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

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

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 (see Giorgini et al. RMP 2008 for details).

Bogoliubov – de Gennes equations

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

$$\begin{pmatrix} H_0(\mathbf{r}) & g\Psi_0^2 \\ -g\Psi_0^{*2}(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \mathcal{E}_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$
Bosons
$$H_0(\mathbf{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu + 2g |\Psi_0(\mathbf{r})|^2$$

Note: in lecture #2 we wrote the same eqs in this form:

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

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

Fermions

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.

VS.

Important difference:

Due to macroscopic occupation of a single state, in BEC the order parameter is obtained expanding the Hamiltonian in $\delta \Psi(\mathbf{r})$ where $\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \delta \Psi(\mathbf{r})$. 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.

Bogoliubov – de Gennes equations

The mean-field theory based on BdG equation

- \bigcirc gives the correct limit of free fermions in external potentials for $a=0^{-1}$
- 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 and negative a.
- E It gives the wrong scattering length for molecule-molecule interaction.

Bogoliubov – de Gennes equations

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \mathcal{E}_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$
 Fermions
$$H_0(\mathbf{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

$$\int d^3r \left[u_i^*(\mathbf{r}) u_j(\mathbf{r}) + v_i^*(\mathbf{r}) v_j(\mathbf{r}) \right] = \delta_{i,j}$$

$$\begin{split} n &= (2/V) \sum_i \int \left| v_i(\mathbf{r}) \right|^2 d\mathbf{r} & \longleftarrow & \text{density} \\ \Delta(\mathbf{r}) &= -g \sum_i u_i(\mathbf{r}) v_i(\mathbf{r})^* & \longleftarrow & \text{order parameter} \end{split}$$

These equations must be solved numerically by means of an iterative procedure in order to ensure self-consistency.

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

$$\int d^3r \left[u_i^*(\mathbf{r}) u_j(\mathbf{r}) + v_i^*(\mathbf{r}) v_j(\mathbf{r}) \right] = \delta_{i,j}$$

$$n = (2/V) \sum_{i} \int |v_i(\mathbf{r})|^2 d\mathbf{r} \qquad \text{density}$$

$$\Delta(\mathbf{r}) = -g \sum_{i} u_i(\mathbf{r}) v_i(\mathbf{r})^* \qquad \text{order parameter}$$

Caveat: a regularization procedure must be used to cure ultraviolet divergence (pseudo-potential, cut-off energy) as discussed by Randeria and Leggett. See also: G. Bruun et al., Eur. Phys. J D 7, 433 (1999), A. Bulgac and Y. Yu, PRL 88, 042504 (2002).

Bogoliubov – de Gennes equations

$$\begin{pmatrix} H_0(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix} = \mathcal{E}_i \begin{pmatrix} u_i(\mathbf{r}) \\ v_i(\mathbf{r}) \end{pmatrix}$$
 Fermions
$$H_0(\mathbf{r}) = -\frac{\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{r}) - \mu$$

In a lattice, the external potential is periodic of period *d* and one can use the Bloch wave decomposition

$$u_{i}(\mathbf{r}) = \tilde{u}_{i}(z)e^{iPz}e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$v_{i}(\mathbf{r}) = \tilde{v}_{i}(z)e^{-iPz}e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$Q = P/\hbar$$

$$\Delta(\mathbf{r}) = e^{i2Qz}\tilde{\Delta}(z)$$
functions of period d



Once BdG equations are solved, one can calculate the energy density e = E/V

$$e = \int d\mathbf{r} \left[\sum_{i} 2(\mu - \epsilon_i) |\tilde{v}_i(z)|^2 + \sum_{i} \Delta(\mathbf{r}) \tilde{u}_i(z) \tilde{v}_i^*(z) \right]$$

From the energy density one can then calculate



I will show some of the results obtained in: Equation of state and effective mass of the unitary Fermi gas in a 1D periodic potential [Phys. Rev. A 78, 063619 (2008)].





when $E_F \ll E_R$:

The lattice favors the formation of molecules (bosons).

The interparticle distance becomes larger than the molecular size.

In this limit, the BdG equations describe a BEC of molecules.

The chemical potential becomes linear in density.





when $E_F \ll E_R$:

The lattice favors the formation of molecules (bosons).

The interparticle distance becomes larger than the molecular size.

In this limit, the BdG equations describe a BEC of molecules.

The chemical potential becomes linear in density.

The system is highly compressible.

The effective mass approaches the solution of the two-body problem.

The effects of the lattice are larger than for bosons!





when
$$E_F \sim E_R$$
:

Both quantities have a maximum, caused by the band structure of the quasiparticle spectrum.

Sound velocity
$$c_s = \sqrt{\kappa^{-1}/m^*}$$



Significant reduction of sound velocity the by lattice !



Density profile of a trapped gas

From the results for $\mu(n)$ and using a local density approximation, we find the density profile of the gas in the harmonic trap + 1D lattice



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

We have just seen an example of BdG calculations: Fermions at unitarity in an optical lattice.

Similar calculations:

Quantized vortex in the BCS-BEC crossover (Sensarma, Randeria, Ho, PRL 2006).



Bogoliubov – de Gennes equations

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

We have just seen an example of BdG calculations: Fermions at unitarity in an optical lattice.

Similar calculations:

Dark soliton in the BCS-BEC crossover (Trento, PRA 2007).



Bogoliubov – de Gennes equations

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

We have just seen an example of BdG calculations: Fermions at unitarity in an optical lattice.

More recently:

Critical velocity of superfluid flow through single barrier and periodic potentials (Trento, just submitted). ELEVENTH J.J. GIAMBIAGI WINTER SCHOOL: The Quantum Mechanics of the XXI Century: Manipulation of Coherent Atomic Matter Buenos Aires, Argentina, July 27th - August 7th, 2009

Mean-field theory of trapped atomic cold gases

Thank you for your attention