Fermi superfluids: molecules and Cooper pairs

Interactions between Fermi atoms can form **two-particle bound states** (or pair) states.These dimers arise because of two **separate** reasons:

1. Two-body potential has a bound state. As a result, **molecules** can form in a gas of Fermi atoms.

2. An **attractive** interaction in a Fermi gas always leads to the formation of **Cooper pairs**, strictly as a many-body effect. This was first shown by **Bardeen, Cooper, and Schrieffer** (BCS) in 1957 in their theory of **superconductivity in an electron gas(metals).**

Overview

These **bound states** in **interacting** Fermi gases are **Bosonic** in nature and hence can **Bose condense**, just like Bose atoms can. As a result, in our discussion of trapped Fermi gases, the well-known description of Bose condensate will appear once again, except that it now describes a **molecular Bose condensate** or a **Cooper pair condensate,** immersed in the gas of unpaired Fermi atoms.

In the **extreme limit**, all N Fermi atoms can form N/2 bound states.This is the **BEC limit** of an interacting Fermi gas. It is effectively a Bose-condensed gas of N/2 **molecules**, each with mass M = 2m.

Gross-Pitaevskii(GP) equation for **molecules**

If all the molecules are Bose-condensed, they are **also** described by the GP equation of motion. Each molecule feels the **Hartree mean field** of all the other molecules in the condensate:

$$V_H(r,t) = \int dr' v(r - r') n_c(r', t)$$

The **condensate molecules** are described by Φ(r,t) which satisfies the familiar GP "Schrodinger-like" wave equation

$$i\hbar \frac{\partial \Phi}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2m} + V_{tr}(r) + V_H(r,t) \right] \Phi$$

where the condensate **local density** is $n_c(\mathbf{r}, t) = |\Phi(\mathbf{r},t)|^2$.

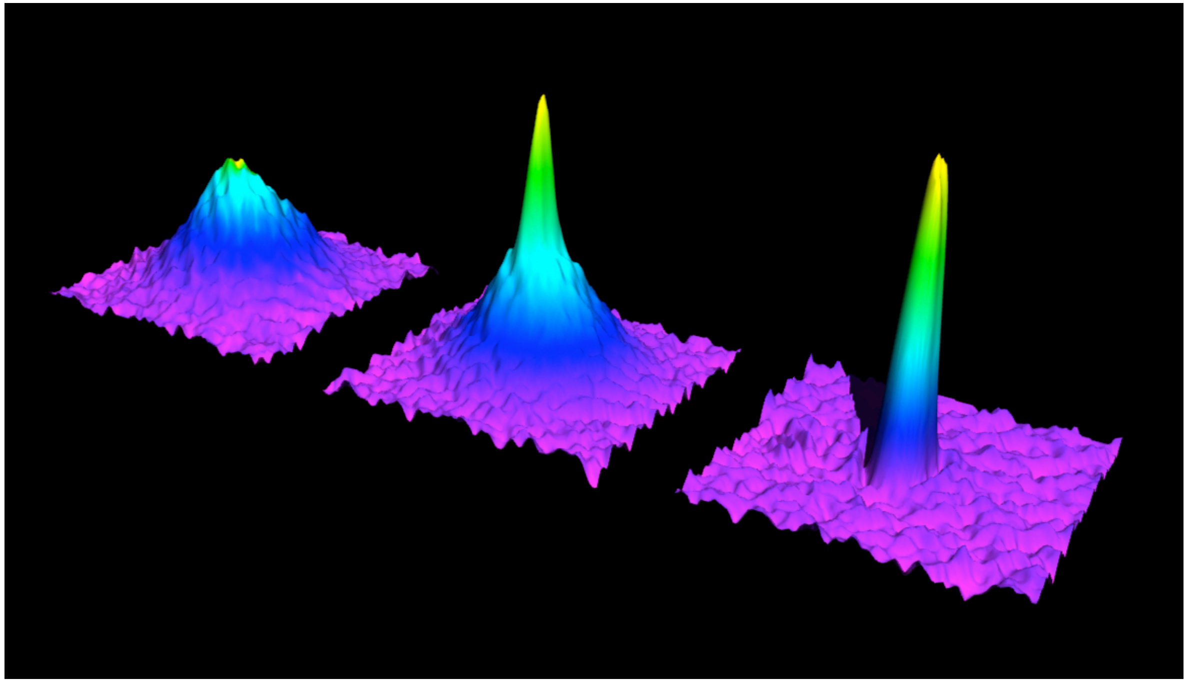
In the s-wave interaction between molecules, we have

$$V_H(r,t) = \frac{4\pi\hbar^2 a_M}{M} n_c(r,t)$$

where now $\mathbf{M = 2m}$ and $\mathbf{a_M = 0.\ 6a_F}$ (Petrov *et al*, PRL, 2004).

The density of Bosons in a trap as the temperature goes from above T_{BEC} to below

$T > T_c$ $\quad$ $T = T_c$ $\quad$ $T \ll T_c$



The peak on the **right** is almost a **pure atom condensate.** (from *MPI*, *Munich*)

One sees the characteristic **bi-modal density profile**, with a broad **thermal cloud of non-condensate atoms** and a sharp **condensate peak.** A **molecular BEC** has the **same features**, as we shall see.

Interesting as this pure molecular BEC is , new physics occurs when some Fermi atoms have not paired up to form molecules. As mentioned earlier, the other extreme is the BCS superfluid phase, where Cooper pairs play the role of the molecules. This leads us to the crossover between the BCS and BEC phases of superfluid Fermi gases. The rest of these lectures will discuss this crossover in more detail.

Great progress in studying this BCS-BEC crossover has been achieved in the last 15 months, both by experimentalists and theorists. It is the most important discovery in ultracold atoms since BEC in 1995.

NOTE: For clarity, I will often discuss the results for a **uniform** Fermi gas. The physics is similar for a trapped Fermi gas. The actual calculations are done for a **trapped gas**.

Selected references to the BCS-BEC crossover literature

Creation of molecules:

Regal et al (JILA-Jin), Nature, **424**, 47(2003)

Strecker et al(Rice-Hulet), PRL, **91**, 0804026 (2003)

Molecular BEC:

Greiner et al(JILA-Jin), Nature, **426**, 537(2003)

Jochim et al(Innsbruck-Grimm), Science, **302**, 2101(2003)

BCS superfluid phase:

Regal et al(JILA-Jin),PRL, **92**, 040403(2004)

Collective oscillations of condensate:

Kinast et al(Duke-Thomas), PRL, **92**,150402(2004)

Bartenstein et al(Innsbruck-Grimm), PRL, **92**, 203201(2004)

Single-particle Fermi excitations:

Chin et al(Innsbruck-Grimm) , Science, **305**,1128(2004)

For theory references, see:

Ohashi and Griffin, cond-mat/0410220

Chen, Stajic, tan and Levin, cond-mat/0404274

Why work with a two-component Fermi gas?

- At ultra-low temperatures, atoms have very low momentum and hence only the **lowest partial wave** contributions from the interaction need be kept.

- Only the **s-wave scattering** contribution is large, but this does not arise between identical Fermions because of the Pauli principle. However, it can occur between atoms with **different** values of m_F (denoted by **spin**$\Uparrow$ and **spin** $\Downarrow$).

- This s-wave scattering allows rapid **thermalization** and hence cooling of the two-component Fermi gas. Bose atoms are also used for "sympathetic" cooling.

Interacting quantum gases

At **ultralow** temperatures, a **tremendous** simplification occurs because the atoms have such low energy. Only the **lowest partial wave scattering** contribution to the interatomic potential between two atoms is not **frozen out**.

Thus for two identical Bose atoms or two Fermi atoms in **different** hyperfine states, we need only can keep the ***l* = 0 partial wave,** ie, the **s-wave** scattering length **a** . Moreover, standard **two-body scattering theory** in quantum mechanics shows that one can replace the **real interatomic** potential with an effective short-range pseudopotential:

$$v_{\uparrow\downarrow}(r-r') = \frac{4\pi\hbar^2 a_{\uparrow\downarrow}}{m}\delta(r-r') \equiv -U\delta(r-r')$$

The s-wave scattering length **a** is the **only** parameter needed to describe the interactions in ultracold **Bose gases** as well as in two-component **Fermi gases.** This is one of the reasons why cold gases are so interesting.

Using this pseudopotential for the s-wave interaction between spin up and spin down atoms, the interaction energy is

$$V = \sum \int dr \int dr' \psi_{\downarrow}^{+}(r)\psi_{\uparrow}^{+}(r')v_{\uparrow\downarrow}(r-r')\psi_{\uparrow}(r')\psi_{\downarrow}(r)$$

$$= -U \int dr \psi_{\downarrow}^{+}(r)\psi_{\uparrow}^{+}(r)\psi_{\uparrow}(r)\psi_{\downarrow}(r)$$

$$= -U \sum_{p,q} c_{p\downarrow}^{+} c_{-p\uparrow}^{+} c_{-q\uparrow} c_{q\downarrow}$$

$$\boxed{\psi_{\alpha}(r) = \sum_{p} e^{ip.r} c_{p\alpha}}$$

NB: We use the convention that an **attractive bare potential** corresponds to U > 0. This is the case of interest in **Fermi superfluid gases.**

This simplified form of the interaction is no good for **high** energy processes and one has to introduce a **renormalized interaction** to get rid of these problems.

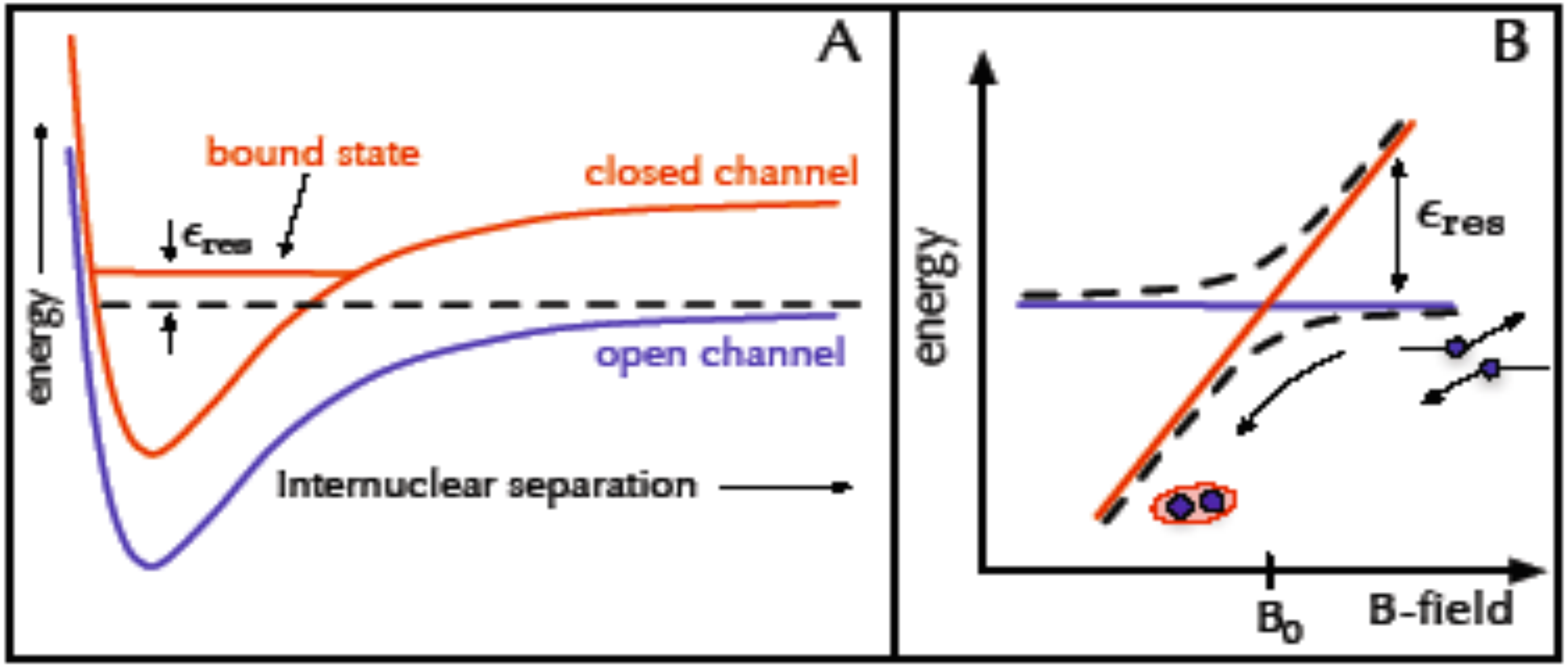
What are Feshbach Resonances?

- One of the most exciting recent topics in ultracold atoms has been the realization of the usefulness of **Feshbach resonances** in the **atomic scattering cross-section**.These are a **two-body** phenomenon and exist in both **Bose** and **Fermi** gases. However, they are most useful in Fermi gases.

- Such resonances arise when two colliding atoms have a total **kinetic energy** very close to the bound state energy level of a molecular potential (the so-called closed channel). In the literature, this **molecular bound state energy** is often denoted by **2ν** .

- The effective s-wave scattering length a_S has a resonance when **$2\nu = 0$** . The energy of the bound state molecular level can be shifted (**tuned**) by a small external magnetic field B.

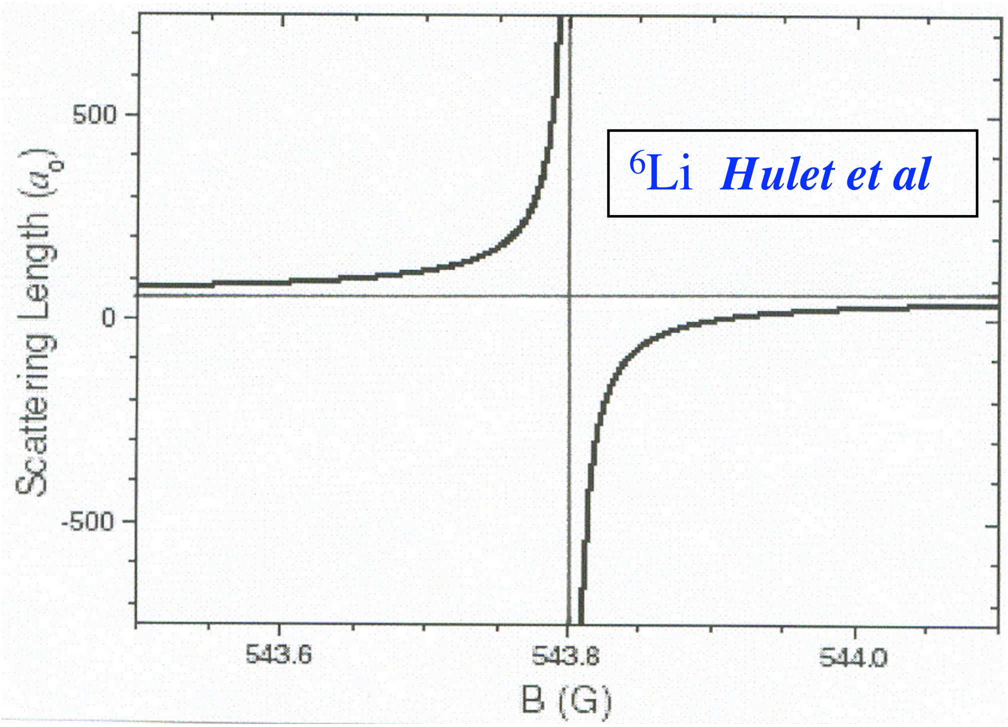
Two fermions in open channel strongly couple to a bound state, with energy $\varepsilon_{res} = 2\nu$.



Two body physics of how dimer states can be created.
Process is reversible (adiabatic).

From Jamie Williams et al,
New Journ. Phys. 6, 123 (2004)

Feshbach resonance: two body physics



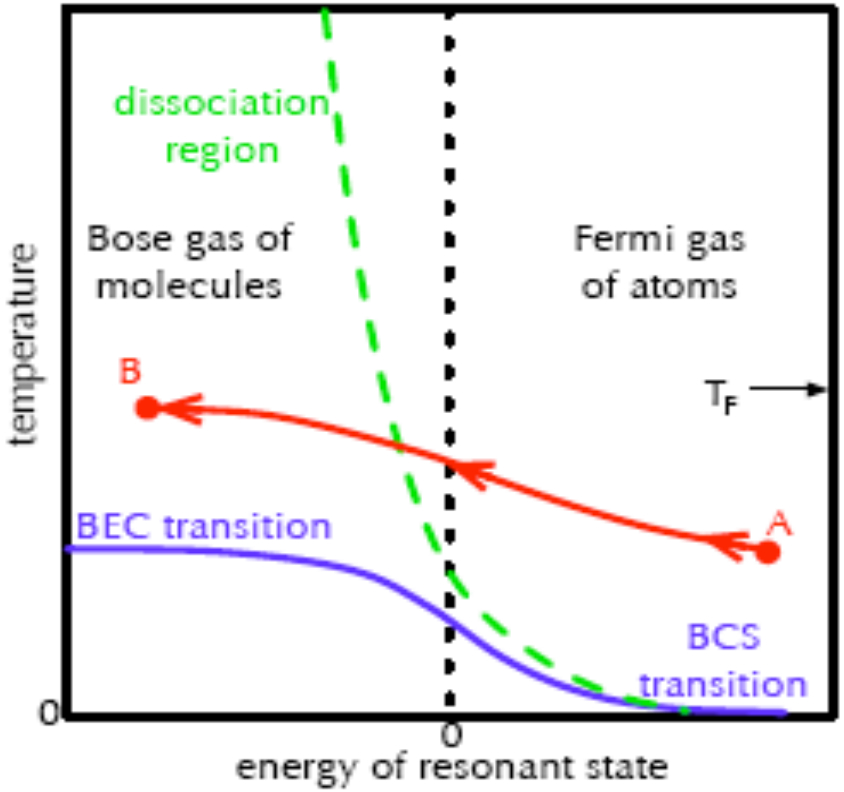
Molecules only form when $a_{2b} > 0$. This is equivalent to $2\nu < 0$ or $B < B_0$.

$$2\nu \propto B - B_0$$

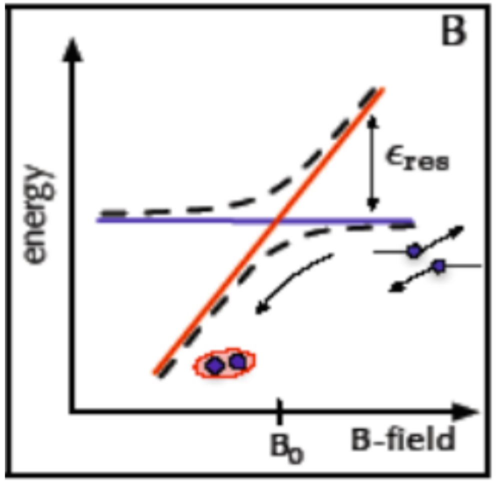
$$-\frac{4\pi\hbar^2 a_{2b}}{m} \equiv U + \frac{g^2}{2\nu}$$

--->

$$a_S = a_{bg}\left(1 + \frac{w}{B_0 - B}\right)$$



$2\nu \propto B - B_0$

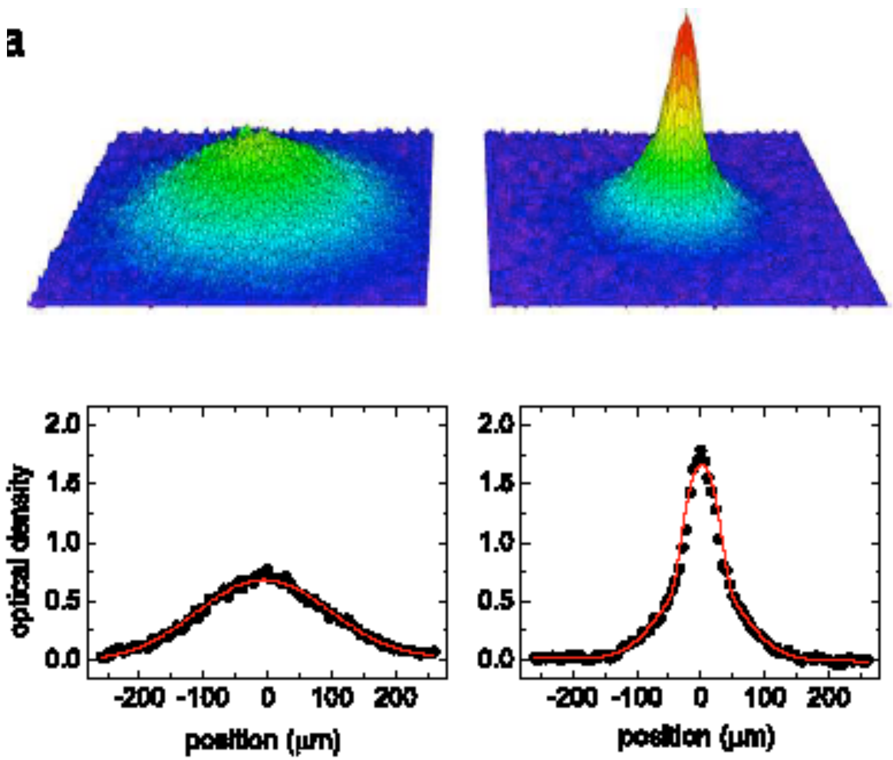


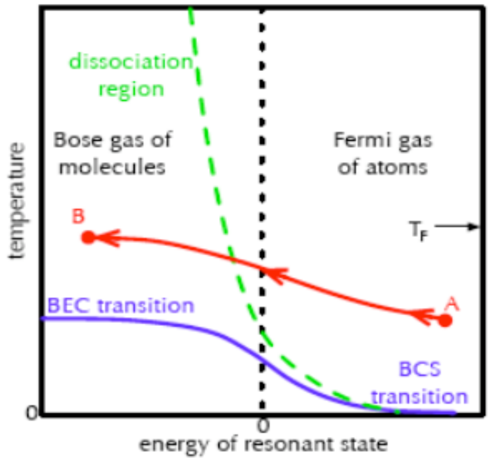
The **blue curve** represents the **phase boundary** into the **superfluid state of bound pairs**- to be discussed later.

From Williams et al, 2004

A molecular Bose condensate formed by SLOWLY ramping the magnetic field from just above ($a_s < 0$) to just below ($B - B_0 = -0.56G$) the resonance ($a_s > 0$).

$T = 0.19T_F$ $N_C = 0\%$ $T = 0.06T_F$ $N_C = 12\%$





$2\nu \propto B - B_0$

© Geoffrey Wheeler
Deborah Jin, Markus Greiner and Cindy Regal (left to right)

The density profile of the free Fermi atoms is not shown. The molecular condensate has the same profile as an atomic BEC, except M = 2m.

Greiner, Regal and Jin, Nature, Nov.7, 2003

Second topic: BCS theory of superconductors

A two component Fermi gas (electrons in metals, ^{3}He atoms, alkali atoms) with an attractive interaction Is unstable to the **formation of a bound state of two Fermions** (of "opposite" spin). This Cooper pair is a many-body effect, and only arises in a **degenerate Fermi gas** . It does **NOT** depend on the **interatomic potential** having a "bound state".

Once these Cooper pairs **(Bosons)** form at T_{BCS} , they produce a Cooper pair condensate. The remaining Fermi atoms swim around in this **condensate soup**, and develop a gap $\boldsymbol{\Delta}$ in their **single particle** energy spectrum.

$$H-\mu N=\sum_{p,\sigma}(\varepsilon_{p,\sigma}-\mu)c^{+}_{p,\sigma}c_{p,\sigma}-U\sum_{p,q}c^{+}_{p\uparrow}c^{+}_{-p\downarrow}c_{-q\downarrow}c_{q\uparrow}$$

$$\Rightarrow\Rightarrow\qquad\approx\sum_{p,\sigma}(\varepsilon_{p,\sigma}-\mu)c^{+}_{p,\sigma}c_{p,\sigma}-\sum_{p}(\Delta c^{+}_{p\uparrow}c^{+}_{-p\downarrow}+h.c.)$$

$$\Delta=U\sum_{q}\langle c_{-q\downarrow}c_{q\uparrow}\rangle\equiv U\phi_C$$

Cooper pairs

This is the essence of the famous BCS-Gorkov theory of superconductivity in an interacting Fermi gases with an attractive interaction - U. The order parameter ϕ_C describes bound states of two Fermions, which are Bose-condensed into the same state. Remark:This MFA theory ignores Cooper pairs outside of the condensate.

This BCS mean field approximation can be diagonalized by the Bogoliubov transformation,

$$H_{BCS} - \mu N = \sum_{p,\alpha} E_p \alpha^{+}_{p\alpha} \alpha_{p\alpha} + const.$$

where the BCS quasiparticles have an energy given by the famous expression $E_p = \sqrt{(\varepsilon_p - \mu)^2 + \Delta^2}$

$$E_q = \left[(\varepsilon_q - \mu)^2 + \Delta^2 \right]^{1/2}$$

$$E_p = \sqrt{(\varepsilon_p - \mu)^2 - \Delta^2}$$

One can work out the equivalent quasiparticles for Fermions in a parabolic trap(see *Ohashi& Griffin*).

Physics and math of BCS-Bogoliubov quasiparticles

One diagonalizes the BCS-Gorkov mean field Hamiltonian using the famous **Bogoliubov transformation**

$$c_{p\uparrow} = u_p \alpha_{p\uparrow} + v_{-p} \alpha^{+}_{-p\downarrow}$$

$$c_{p\downarrow} = u_p \alpha_{p\downarrow} - v_{-p} \alpha^{+}_{-p\uparrow}$$

The **α, α**$^{+}$ quasiparticle operators to satisfy Fermi anti-commutation relations,such as

$$\left[\alpha_{p\uparrow}, \alpha^{+}_{q\uparrow}\right]_{+} = \delta_{p,q}$$

As a result, the Bogoliubov amplitudes ***u*** and ***v*** must satisfy the normalization condition

$$\left|u_{p\uparrow}\right|^2 + \left|v_{p\uparrow}\right|^2 = 1$$

We have reduced problem to a gas of **non-interacting** Fermi quasiparticles. Our favorite easy problem!

Calculation gives the following explicit expressions for the Bogoliubov u and v coefficients

$$u_p^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_p - \mu}{E_p}\right) \qquad v_p^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_p - \mu}{E_p}\right)$$

where the BCS quasiparticle **excitation energy** is

$$E_p = \left[\left(\varepsilon_p - \mu\right)^2 + \Delta^2\right]^{1/2}$$

It should be emphasized that **destroying** an atom is very strange in a BCS superconductor, since it involves **destroying** a quasiparticle excitation and at the same time **creating** a quasiparticle:

$$c_{p\uparrow} = u_p \alpha_{p\uparrow} + v_{-p} \alpha_{-p\downarrow}^{+}$$

Similarly, a quasiparticle (α^+) is a **coherent** superposition of a **particle** (c^+) and a **hole** (c) :

The self-consistent equations for the BCS gap Δ

Clearly, we have two quantities we need to calculate using our quasiparticle solution, namely the chemical potential μ and the energy gap **Δ.** The **number equation** is

$$N \equiv \sum_{q,\alpha} \left\langle c^+_{q\alpha} c_{q\alpha} \right\rangle = \sum_q \left[\left| u_q \right|^2 \left\langle \alpha^+_{q\uparrow} \alpha_{q\uparrow} \right\rangle_{Bog} + \left| v_{-q} \right|^2 \left\langle \alpha_{-q\downarrow} \alpha^+_{-q\downarrow} \right\rangle_{Bog} \right]$$

using the fact that $\langle \alpha\alpha \rangle = 0$ and $\langle \alpha^+ \alpha^+ \rangle = 0$. Since the quasiparticles are non-interacting Fermions, $\langle \alpha^+ \alpha \rangle = f(\mathrm{E})$ is the **Fermi distribution function** for quasiparticles. Thus

$$N = N_F = \sum_q \left[1 - \frac{\varepsilon_q - \mu}{E_q} + 2 \frac{\varepsilon_q - \mu}{E_q} f(E_q) \right]$$

This is the number equation, giving ***N*** **as a function of μ and Δ** (you should verify it).

The self-consistent BCS gap equation

We recall that the Cooper pair order parameter was defined as

$$\Delta \equiv U \sum_q \left\langle c_{-q\downarrow} c_{q\uparrow} \right\rangle \equiv U \phi_C$$

This can again be **easily calculated** by writing c and c$^+$ in terms of Bogoliubov quasiparticles, just as we did for the density,

$$\Delta = U \sum_q u_q v_q \left[\left\langle \alpha^+_{q\uparrow} \alpha_{q\uparrow} \right\rangle + \left\langle \alpha^+_{q\downarrow} \alpha_{q\downarrow} \right\rangle - 1 \right]$$

$$= U \sum_q u_q v_q \left(2 f(E_q) - 1 \right) \; = U \sum_q \frac{\Delta}{2E_q} \left(2 f(E_q) - 1 \right)$$

One last thing we have to do is **renormalize** the bare attractive interaction U to remove problems at high momentum.This turns out to be given by the two-body s-wave scattering length a.

The renormalized two-body pseudopotential for s-wave scattering is given by

$$U_{2b} = \frac{-U}{1 - U \sum_{q \le q_c} \frac{1}{2\varepsilon_q}} \equiv -\frac{4\pi\hbar^2 a_{2b}}{m}$$

This **defines** the correct scattering length a_{2b}. Now the gap equation can be re-written in terms of $\boldsymbol{U_{2b}}$,or equivalently $\boldsymbol{a_{2b}}$

$$1 = -\frac{4\pi\hbar^2 a_{2b}}{m} \sum_q \left[\frac{1 - 2f(E_q)}{2E_q} - \frac{1}{2\varepsilon_q} \right]$$

where the quasiparticle energy is

$$E_q = \left[\left(\varepsilon_q - \mu \right)^2 + \Delta^2 \right]^{1/2}$$

Now the integrand in the gap equation is **well behaved** at large momentum.

To summarize, the standard BCS theory reduces to two coupled equations for the number of fermions *N* and the gap function Δ (*aka* the order parameter)

$$1 = -\frac{4\pi\hbar^2 a_{2b}}{m}\sum_q \left[\frac{1-2f(E_q)}{2E_q} - \frac{1}{2\varepsilon_q}\right]$$

$$N = N_F = \sum_q \left[1 - \frac{\varepsilon_q - \mu}{E_q} + 2\frac{\varepsilon_q - \mu}{E_q} f(E_q)\right]$$

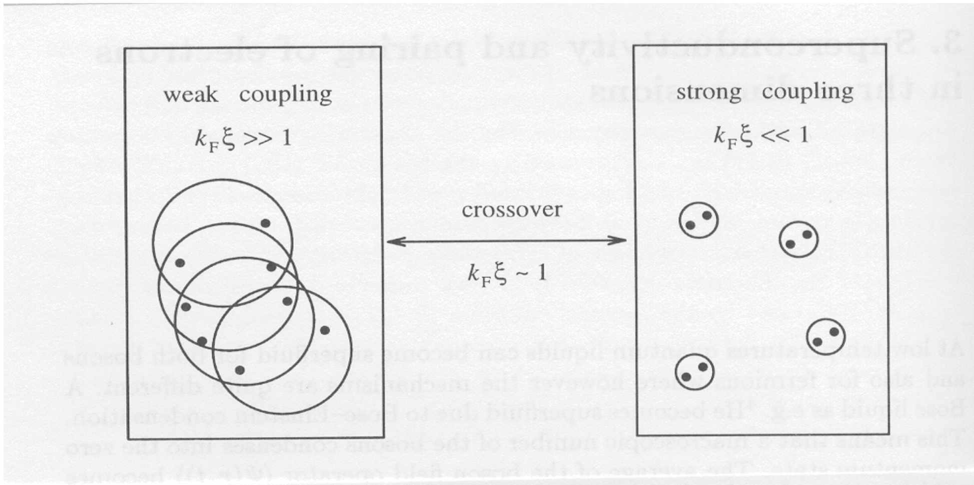
In standard **weak coupling** limit (when $k_F|a_{2b}| << 1$) one can show there is no solution of the gap equation unless a_{2b} is **negative.** In this weak coupling BCS limit, one finds that $\mu \cong \varepsilon_F$. Also the BCS **transition temperature** is given by

$$T_{BCS} = T_F \exp\left(-\frac{\pi}{2k_F|a_{2b}|}\right) << T_F$$

The BCS-BEC Crossover -1980s

As the magnitude of the attractive interaction is increased, the Cooper pairs become more tightly bound and eventually we pass over to a region described as a dilute gas of small Cooper pair molecules. This is the famous BCS-BEC crossover, first studied in Eagles in 1969 and in the 1980s by Leggett (at T=0) and Nozieres (at T_c). At the same time, the spectral weight of the Fermi atoms decreases , as they combine to form Cooper pairs.

BCS



BEC

From Haussmann,1993

Formally this BCS-BEC crossover can be studied by using the **full number and gap equations**, considering $k_F a_{2b}$ as an adjustable parameter (Leggett, 1980) and let the the solutions tell us what happens!

It turns out that the dimensional parameter $(k_F a_{2b})^{-1}$ covers the range

$$-\infty \rightarrow \frac{1}{k_F a_{2b}} \rightarrow +\infty$$

BCS **BEC**

as the bare attractive interaction is steadily increased. These original calculations **did not address how** you could vary the value of the s-wave scattering length. **Feshbach resonances** allow you to do this easily in trapped atomic Fermi gases!! A whole new window on the physical world has opened up.

A crucial bit of physics is left out of the BCS number and gap equations

When we think about it, our BCS equations **implicitly assume** that all the Cooper pairs are Bose condensed in the same $q_{CM} = 0$ state. In our number equation, we only calculated the contribution of the free Fermi atoms.

But it turns out that as the value of a_{2b} becomes > 0, the Cooper pairs become stable two-particle states and can **occupy finite momentum states**.Thus T is increased, more and more Cooper pairs leave the condensate. In this improved theory, T_C will correspond to where the **Cooper pair condensate is depleted**,
just like any other Bose gas! Nozieres (1985) was the first to calculate the **superfluid transition temperature** across the
BCS-BEC crossover, as a_{2b} is varied, taking this depletion into account.

The method used by Nozieres and Schmitt-Rink (1985) replace the BCS number equation by calculating the number of Fermions using the **thermodynamic identity**

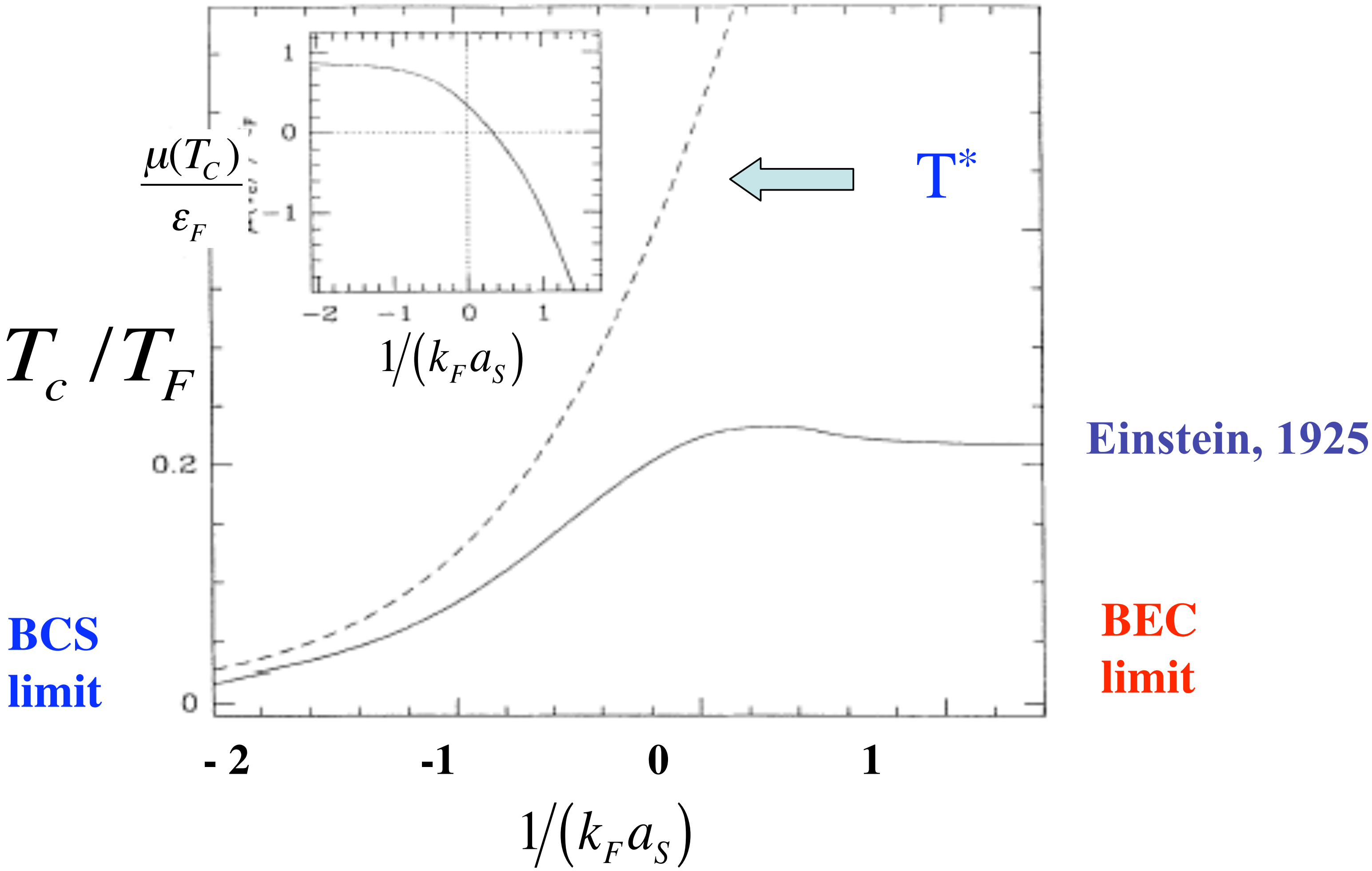
$$N \equiv -\frac{\partial \Omega}{\partial \mu}$$

where the thermodynamic potential Ω(μ,T) of the interacting Fermi gas is given by

Ω(μ,T) = free energy of a **Fermi gas of atoms**
+free energy of **fluctuations in the particle-particle channel**. These correspond to the formation of **bound states** of two atoms (Cooper pairs) with finite centre of mass monentum.

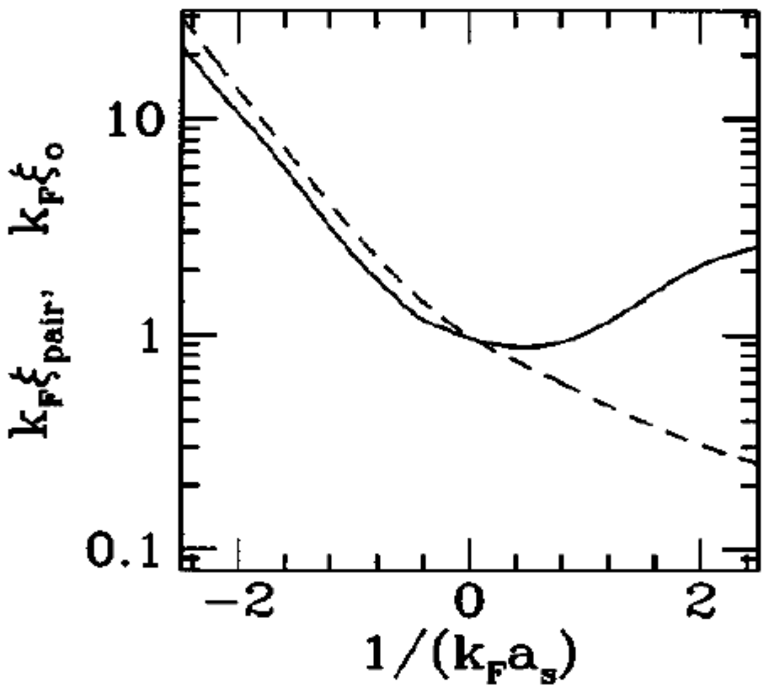
Left out in BCS⇒

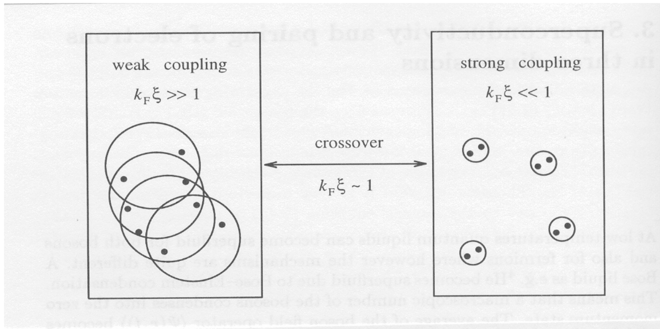
Including this **Cooper pair gas** changes μ very much.



T_C is the BCS-BEC superfluid phase transition temperature. T^* shows where the bound states **breakup** or ionize. Note that the **weak coupling** T_{BEC} result corresponds to the breakup of Cooper pairs, not depletion.

Sa de Melo , Randeria and Engelbrecht, PRL, 1993



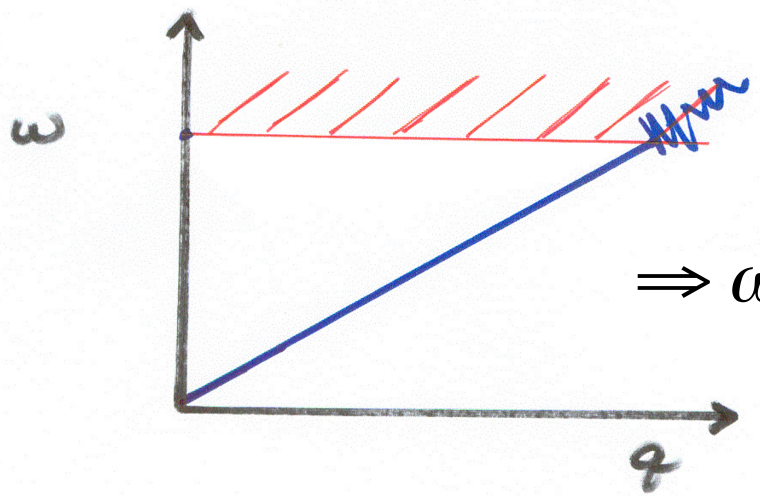


$$\frac{1}{k_F} \propto n^{-1/3} \approx d$$

Dashed line - - - - shows the smooth **decrease** in size of the bound state pair as we go from **BCS to BEC region.**

Engelbrecht, Randeria and Sa de Melo, PRB, 1997

The two-particle continuum starts at **2Δ**.The **Anderson-Bogoliubov** (1958) collective mode can exist undamped within this energy gap. It is an oscillation of the **Cooper pair condensate**



⇒ **2Δ**

$$\Rightarrow \omega = \frac{v_F}{\sqrt{3}} q$$

This is for a uniform BCS superfluid. The analogous Anderson-Bogoliubov modes have been recently worked out for a trapped Fermi superfluid.