KITP SEMINAR , May 25 , 2004

Molecules vs Cooper pairs in superfluid atomic Fermi gases

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1. Sketch the theory of the **formation and Bose condensation of diatomic molecules** in a model for an interacting **two component** degenerate atomic Fermi gas.

2. Within a simple microscopic model, I will argue that there is **no fundamental difference between a molecular Bose condensate of real molecules and superfluid state composed of Cooper pairs.**

All my work is done in close collaboration with Prof. Yoji Ohashi, University of Tsukuba, Japan

I will discuss four topics:

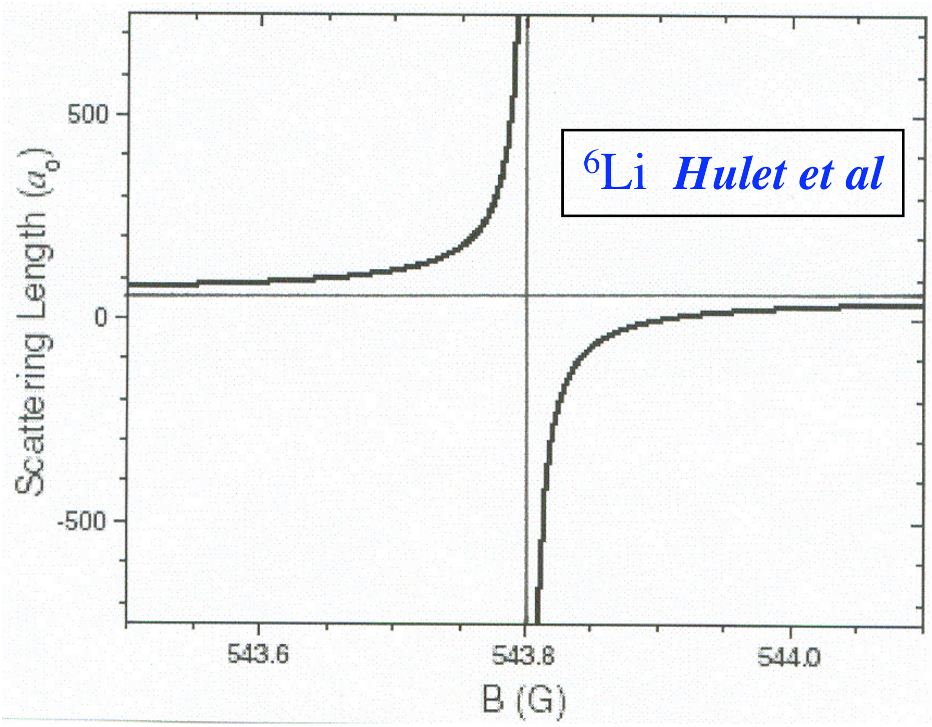
1. **Two body effects** : **Recall what a Feshbach resonance is between two atoms in a vacuum. This is the key in recent experiments involving the formation of diatomic molecules in a Fermi gas.**

2. **Review the BCS theory of superconductivity without a Feshbach resonance. The formation of Cooper pairs in a Fermi gas is due to many-body effects. The BCS quasiparticles are Fermions moving in a Bose condensate of Cooper pairs.**

3. Discuss the transition from the usual BCS state of large overlapping Cooper pairs to a BEC gas with small Cooper pairs. This BCS-BEC crossover arises when one increases the attractive interaction between the atoms.This crossover is the region which is now accessible to experimental study for the first time.

4. Discuss an interacting Fermion-Boson model which incorporates the creation of molecules by a two-body Feshbach resonance and from many-body(BCS) effects. Within this two-channel model, we show there is no fundamental difference between a Bose condensate of molecules and a BCS superfluid phase.

Feshbach resonance: two body physics



Molecules only form when $a > 0$. This is equivalent to $2\square < 0$ or $B < B_0$

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

$$2\square \quad B \square B_0$$

By slowly ramping to just below the resonance (a > 0), long-lived dimer molecules appear which thermalize with the rest of the atoms and form a molecular Bose condensate if the temperature is below T_{BEC} .

BCS theory of superconductors

- **A two component Fermi gas (electrons in metals, ^{3}He atoms or alkali atoms) with an attractive s-wave interaction is unstable to the formation of a bound state (S = 0) of two Fermions . This Cooper pair is a many-body effect, and only arises in a degenerate Fermi gas with a Fermi surface. 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 □ in their single particle energy spectrum.**

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

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

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

Cooper pairs

This is the essence of the famous BCS theory(1957) of superconductivity in interacting Fermi gases with an attractive interaction - *U*. The order parameter Φ_C describes bound states (S = 0) of two Fermions, which are all Bose-condensed into the same state. This MFA does not allow Cooper pairs to be out of the condensate.

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

$$H_{BCS} - \mu N = \sum_{p} E_p \gamma_p^{+} \gamma_p + const.$$

where the BCS quasiparticles have an energy given by

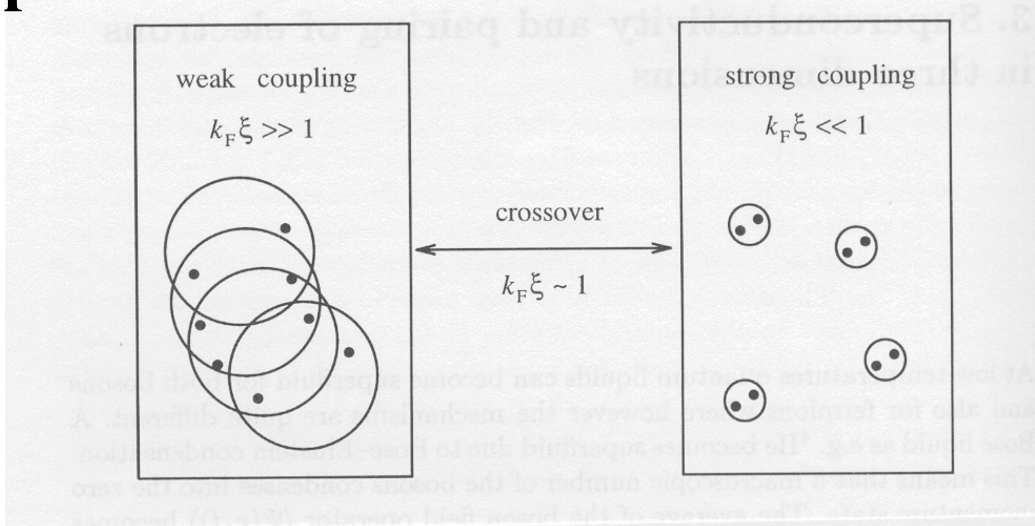
$$E_{qp}(q) = \left[(\varepsilon_q - \mu)^2 + \Delta^2 \right]^{1/2}$$

The energy of unpaired atoms in the superfluid gas is

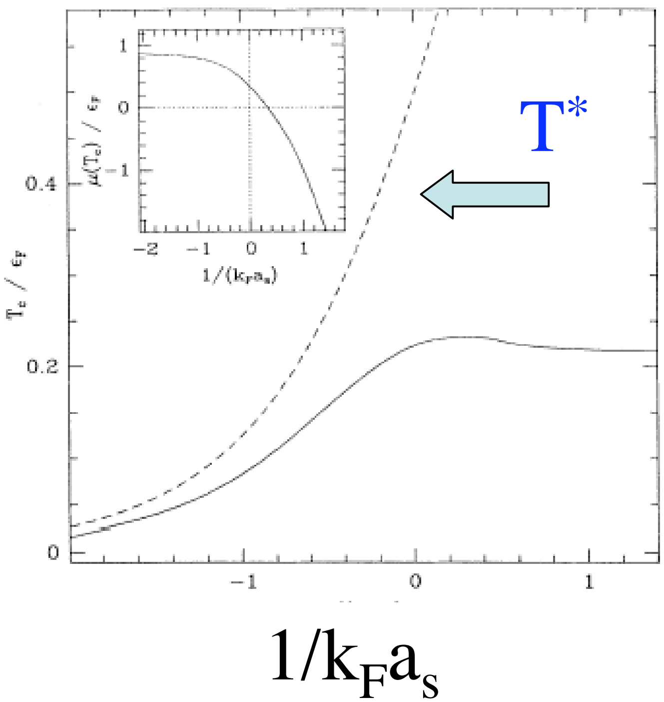
$$\boxed{E_{atom}(q) = \mu + E_{qp}(q)}$$

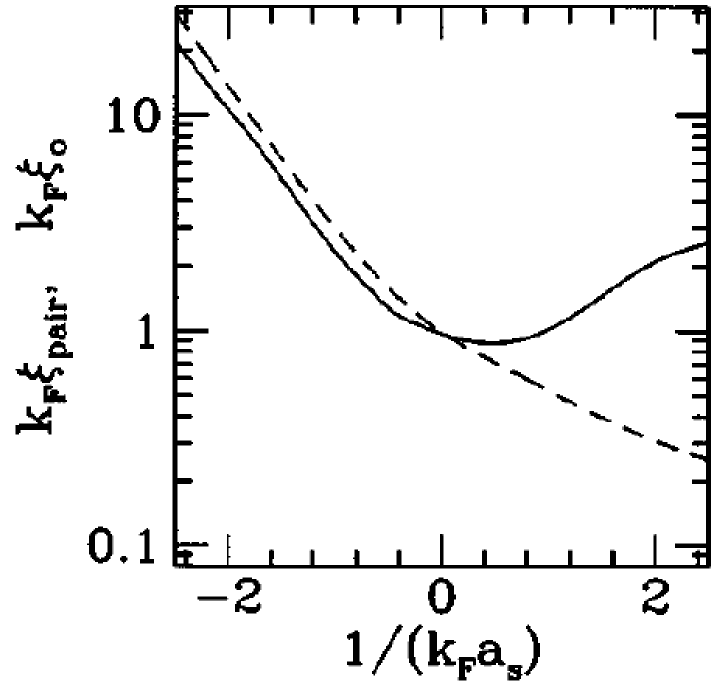
The BCS-BEC Crossover

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 form Cooper pairs.



Haussmann,1993





Engelbrecht, Randeria and Sa de Melo, PRB, 1997

Sa de Melo , Randeria and Engelbrecht, PRL, 1993.

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

In current language, these results are for a single channel.

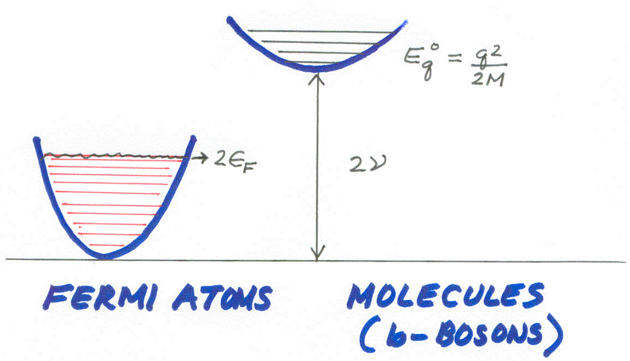
Model for interacting Fermi atoms and molecules - the two channel model.

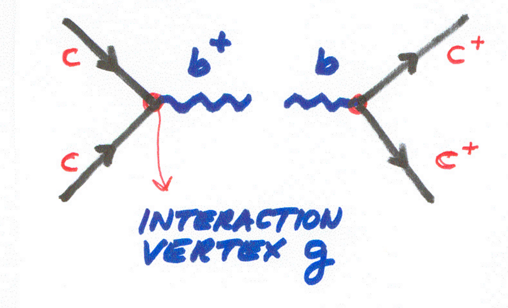
We need a microscopic model that includes:

- ✓ **Feshbach resonance in the two-body potential**
- ✓ **BCS Cooper pair formation**
- ✓ **BCS-BEC crossover as interaction increases**

The model (due to Timmermans, Holland and coworkers) explicitly includes the Fermi atoms, the Bosonic dimers formed from these atoms, and and the Feshbach resonance coupling term. This is now referred to as the two-channel model.

$$\mathcal{H} = \sum_{p\sigma} \varepsilon_p c^\dagger_{p\sigma} c_{p\sigma} + \sum_{q} (E^0_q + 2\nu) b^\dagger_q b_q$$
$$- U \sum_{p,p'} c^\dagger_{p\uparrow} c^\dagger_{-p\downarrow} c_{-p'\downarrow} c_{p'\uparrow} + g_r \sum_{p,q} [b^\dagger_q c_{-p+q/2\downarrow} c_{p+q/2\uparrow} + \text{h.c}].$$





- The atom-molecule interaction is denoted by g_r
- The non-resonant attractive interaction is **- U**

The molecular bound state energy 2ν can be **tuned**.
Molecules(with **finite lifetime**) start to form when $2\nu \leq 2\epsilon_F$ and will **not** be able to **decay** when $2\nu < 0$.

$$N = \langle \sum_{p\sigma} c^{\dagger}_{p\sigma} c_{p\sigma} \rangle + 2 \langle \sum_{q} b^{\dagger}_{q} b_{q} \rangle$$
$$\equiv N_{\mathrm{F}} + 2 N_{\mathrm{B}} .$$

A crucial feature of this Hamiltonian is that the b-molecules are formed from the Fermi atoms. There is thus only one chemical potential, with

$$\mathbf{H - \mu N = H - \mu N_F - 2\mu N_B \text{ , with } \quad \mu_B = 2\mu.}$$

This coupled Hamiltonian modifies the effect of the bare two-body Feshbach resonance. Two atoms are now part of an interacting system in the presence of a filled Fermi sea.

First thing to do is to solve our coupled FB model in a mean field approximation, allowing for Cooper pairs and a Bose condensate of b-molecules:

$$H_{FB} - \mu N = \sum_{p,\sigma} (\epsilon_{p,\sigma} - \mu) c^{+}_{p,\sigma} c_{p,\sigma} + \phi_m^2 (2\nu - 2\mu)$$

$$- U \sum_{p} (\phi_C c^{+}_{p\uparrow} c^{+}_{-p\downarrow} + h.c.) + g \sum_{p} (\phi_m c^{+}_{p\uparrow} c^{+}_{-p\downarrow} + h.c.)$$

ϕ_C **= Cooper pair condensate**

ϕ_m **= Molecular condensate**

Both condensates are dependent on each other. We end up with a BCS-type theory but now with a composite order parameter: $\tilde{\Delta} = U\phi_C - g\phi_m$

$$\tilde{\square} = U\square_C \; \square \; g\square_m$$

This order parameter is the sum of contributions from two mechanisms:

Pair wavefunction = Open (scattering) channel
+ Closed(molecular) channel

However, they are strongly coupled to each other and one determines the other:

$$\square_m = \square \frac{g}{2\square \; \square \; 2\square} \square_C$$

The number of Bose condensed b-molecules is given by $N_b = |\square_m|^2$. The number of Cooper pairs not so easy to calculate.

The composite BCS order parameter reduces to:

$$\tilde{\Box} = U \Box_C \; \Box \; g \Box_m = \Box U + \frac{g^2}{2\Box \, \Box \, 2\Box} \Box \Box_C \equiv U_{eff} \Box_C$$

The physics is clear. The attractive interaction - *U* between the Fermi atoms in the open channel is now renormalized to U_{eff} by the resonant coupling to the b-molecules in the closed channel.

One can speak in terms of a Bose condensate of BCS Cooper pairs or in terms of a molecular BEC of b-molecules, on both sides of the Feshbach resonance.

Note we are now dealing with a renormalized Feshbach resonance for atoms interacting in a superfluid Fermi gas, not two atoms in a vacuum. The b-molecules are described by a propagator

$$D_0(q,\square) = \frac{1}{\square \square \left(E_q^0 + 2\square \square 2\square\right)}$$

For coupling to Cooper pairs with q = 0, $\square$ = 0, this b-molecule propagator reduces to

$$D_o(0,0) = \square \frac{1}{\left(2\square \square 2\square\right)}$$

The b-molecule energy spectrum is also modified by self-energy effects due to coupling to Cooper pairs outside the condensate. This is important at finite T.

It is no surprise that the renormalized energy gap is given by a BCS-type gap equation but now with an enhanced attractive interaction

$$\tilde{\Delta}(T) = \left[U + \frac{g^2}{2\nu - 2\mu}\right] \sum_k \frac{\tilde{\Delta}(T)}{2E_k} \tanh\left(\frac{1}{2}\beta E_k\right)$$

$E_k = \sqrt{[\epsilon_k - \mu]^2 + \tilde{\Delta}^2}$ = BCS quasiparticle spectrum with energy gap at $\tilde{\Delta}$

At $T = T_{BCS}$, $\tilde{\Delta}(T) \to 0$ and above equation reduces to BCS equation for T_{BCS},

$$1 = \left[U + \frac{g^2}{2\nu - 2\mu}\right] \sum_k \frac{\tanh(E_k/2k_B T_{BCS})}{2(\epsilon_k - \mu)}$$

We already see the possibility that T_C will be large. However, □ is very dependent on the value of 2□.

To calculate the chemical potential μ **and** the order parameter $\tilde{\Delta}$ in a **self-consistent way**, one has to include the **fluctuations around the MFA :**

✓ The Cooper pairs **outside** the BCS condensate

- Nozieres and Schmitt-Rink (1985) at T_c .

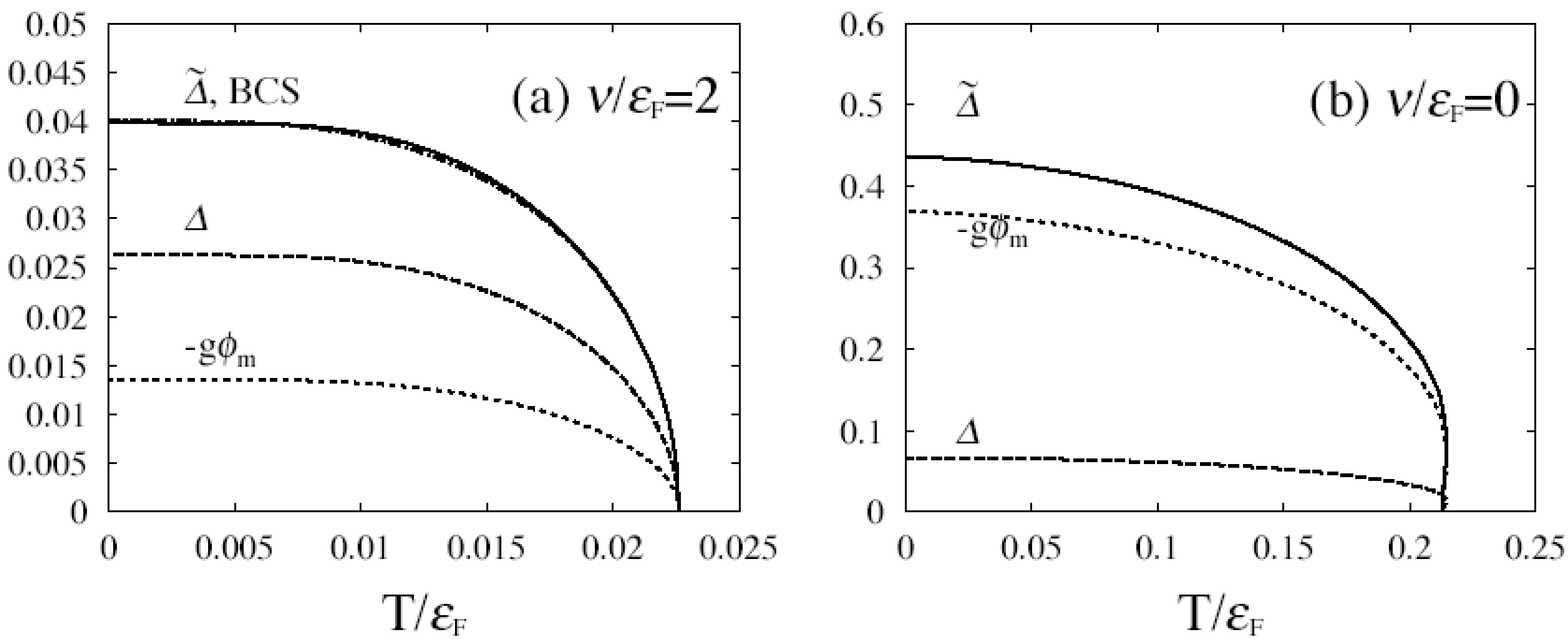
✓ The b-molecules **outside** the molecular condensate

- Ohashi and Griffin (2002) at T_c .

✓ Both effects **below** T_c by Ohashi and Griffin (2003).

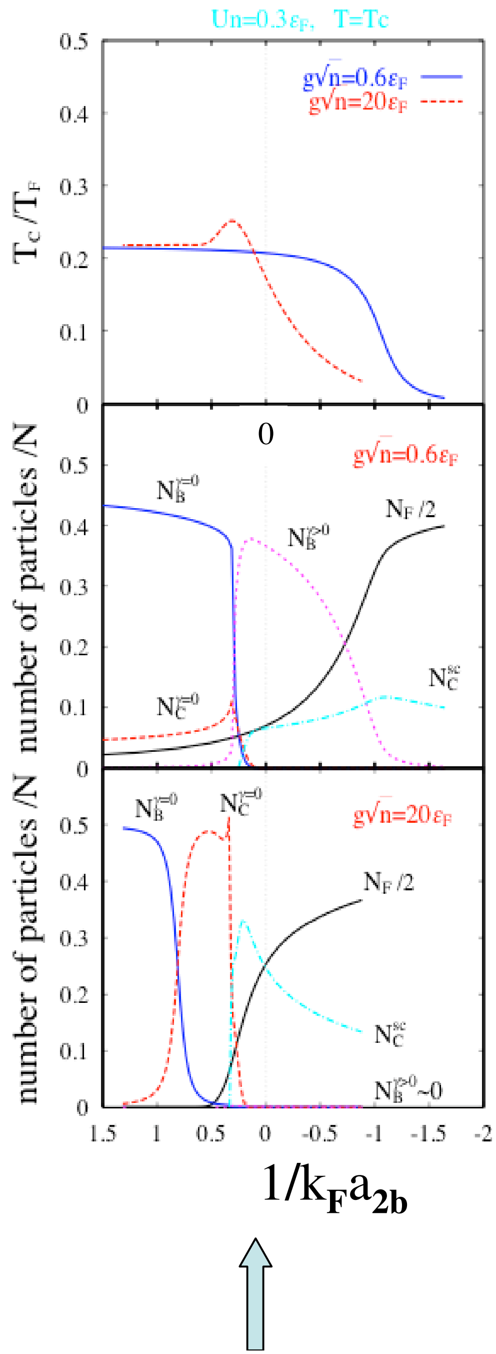
The **number** of b-molecules **and** Cooper pairs is self-consistently adjusted as **2Δ is decreased,**

$$N_F = N_{atoms} + 2N_{Cooper\ pairs} + 2N_{b\text{-}molecules}$$



The relative weight of the b-molecules and the Cooper pairs in the **composite Bose condensate** is shown (uniform gas).

Ohashi and Griffin , PRA, 2003

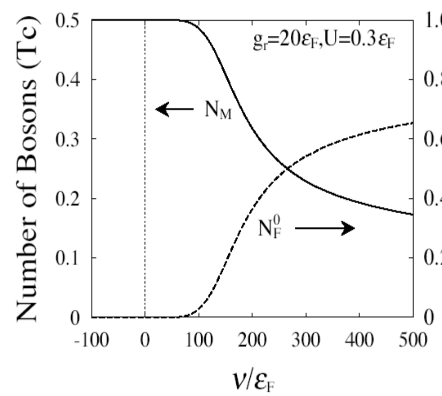


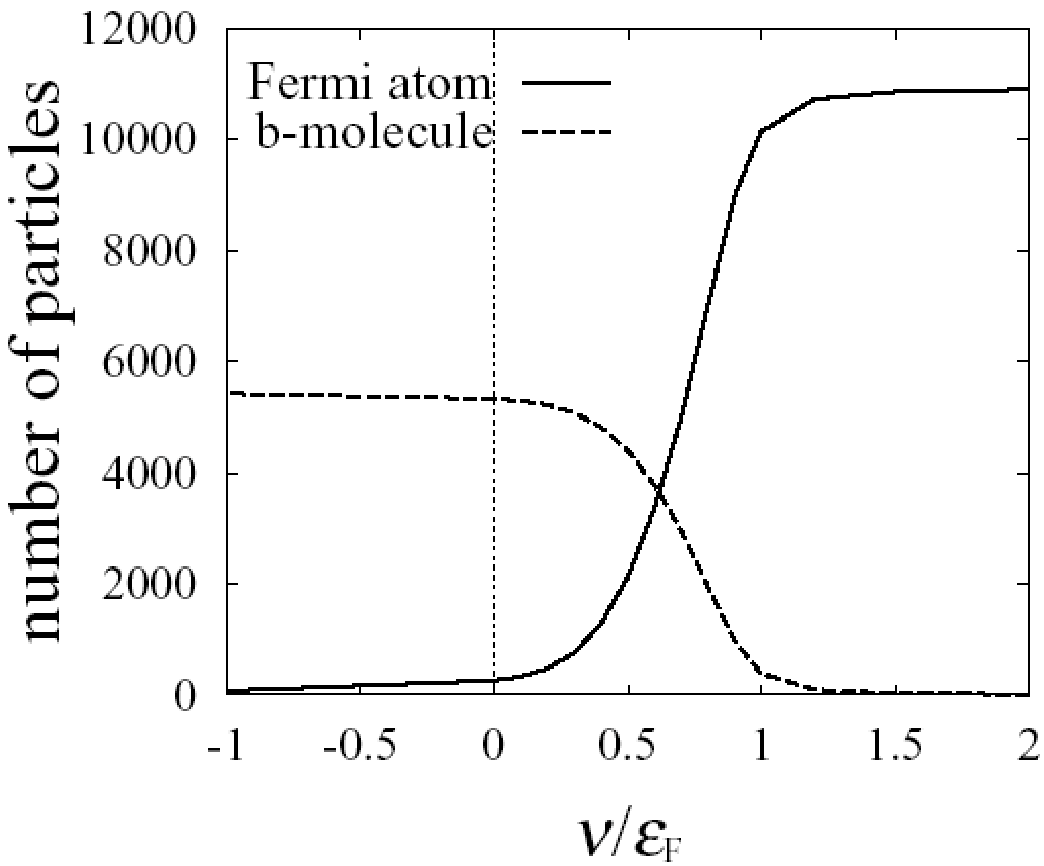
Uniform gas at T_C

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

Narrow resonance

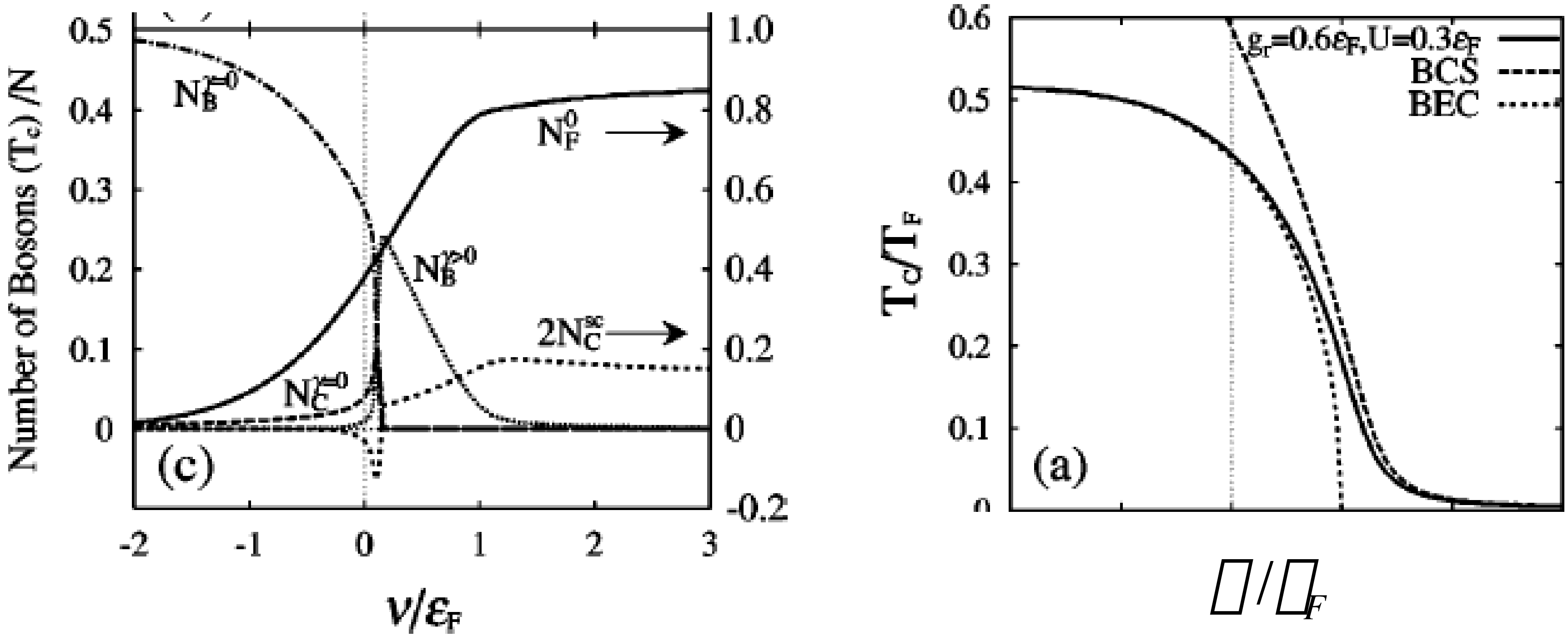
Broad resonance





Trapped gas at T = 0. All b-molecules are in condensate. The Cooper pairs are included in Fermi contribution. For N =10, 900 atoms.

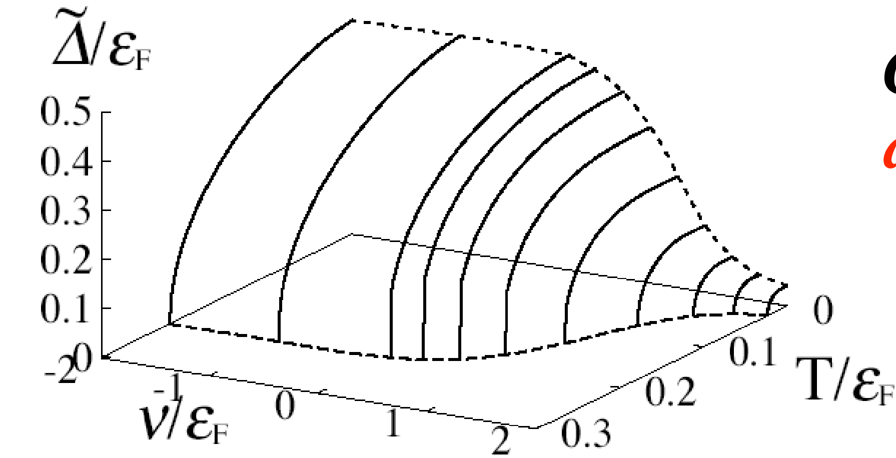
O&G, cond-mat/ 0402031



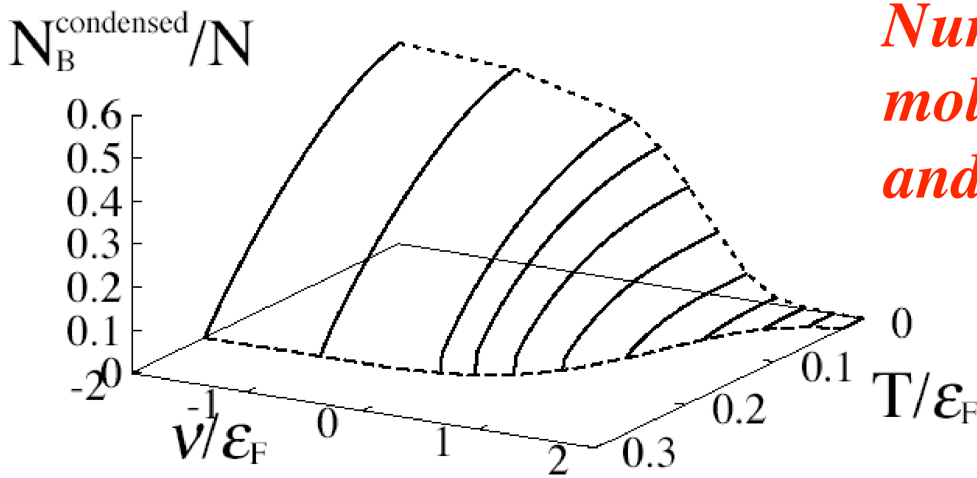
Results for a trapped gas at T_c

Note that T_c/T_F is 0. 5 for a **trapped** gas, not 0. 2

O&G, PRA, 2003



Composite order parameter
as a function of ν and T.



Number of Bose-condensed molecules in the BCS ($\nu > 0$) and BEC ($\nu < 0$) regions.

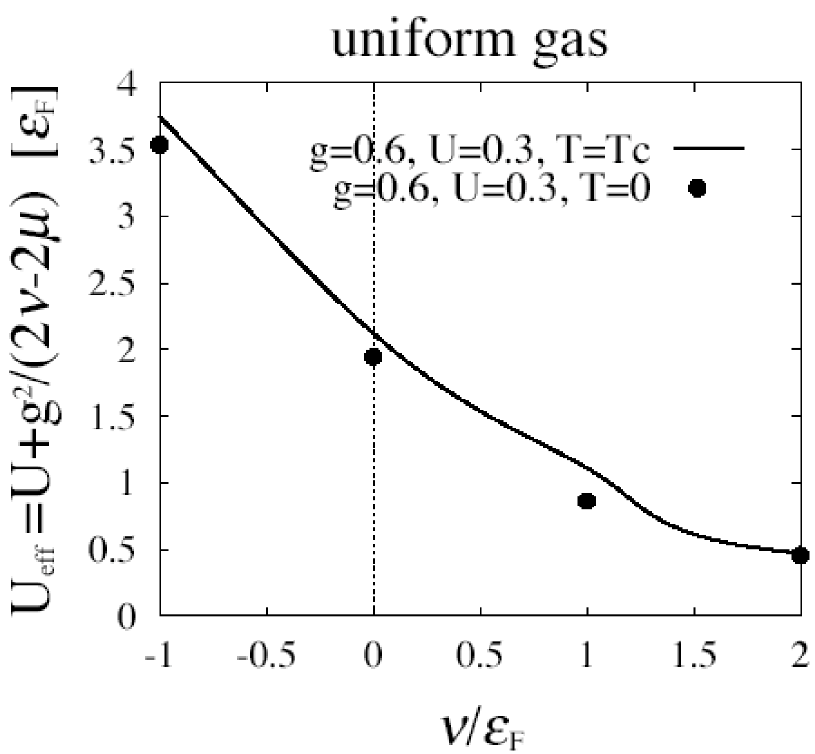
Ohashi & Griffin , PRA, 2003 : Narrow resonance case

The crossover between the two regions is smooth.

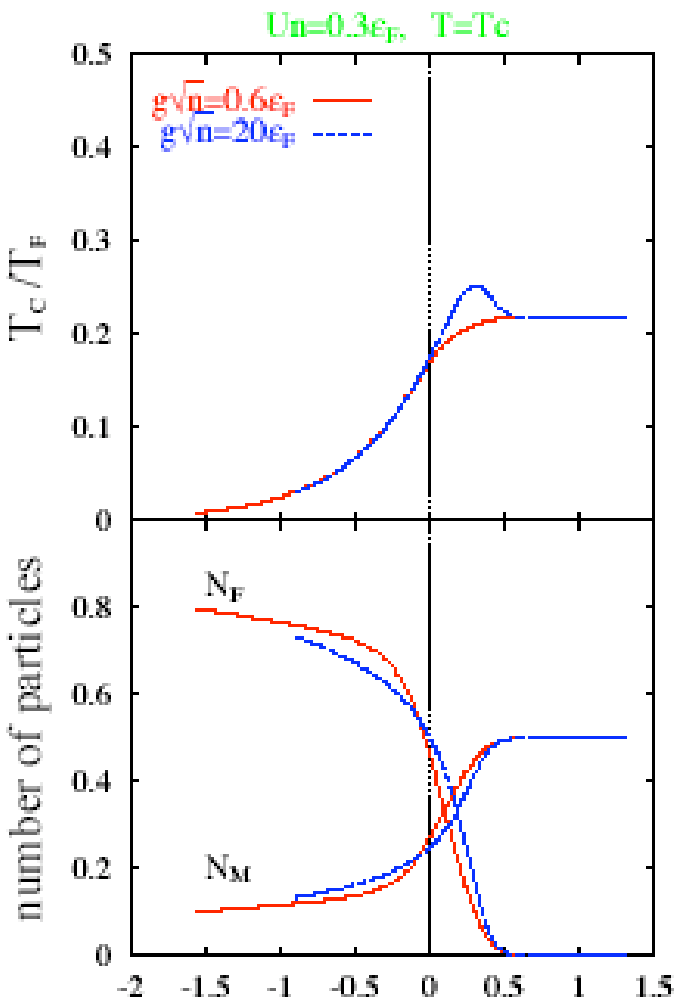
Falco and Stoof (PRL, 2004) have given a **simplified** version of the model worked out by O&G (PRL, 2002). F&S treated the **finite-lifetime** b-molecules which form on the BCS side ($a_{2b} < 0$) as a simple BEC of stable molecules, ignoring the co-existence of Cooper pairs. Comment: It is not clear how experimentalists **distinguish** between long-lived molecules and stable molecules.

In the F&S **poor man's** calculation, there is **sharp transition line** when this BEC of b-molecules ceased to exist in the BCS region (Z =0). The more detailed calculations of O&G show that is **no such abrupt change** and that a BEC of b-molecules and Cooper pairs co-exists on **both sides** of the resonance. However, overall, we view our work as in agreement with that of F&S.

Many-body effects modify the **two-body** Feshbach resonance at 2 = 0 and as result the **effective** attractive interaction is smooth through the crossover, as in the **single channel** pure BCS case originally discussed by Randeria and coworkers.



O&G, *PRA, 2003*



$1/k_F a_{eff}$

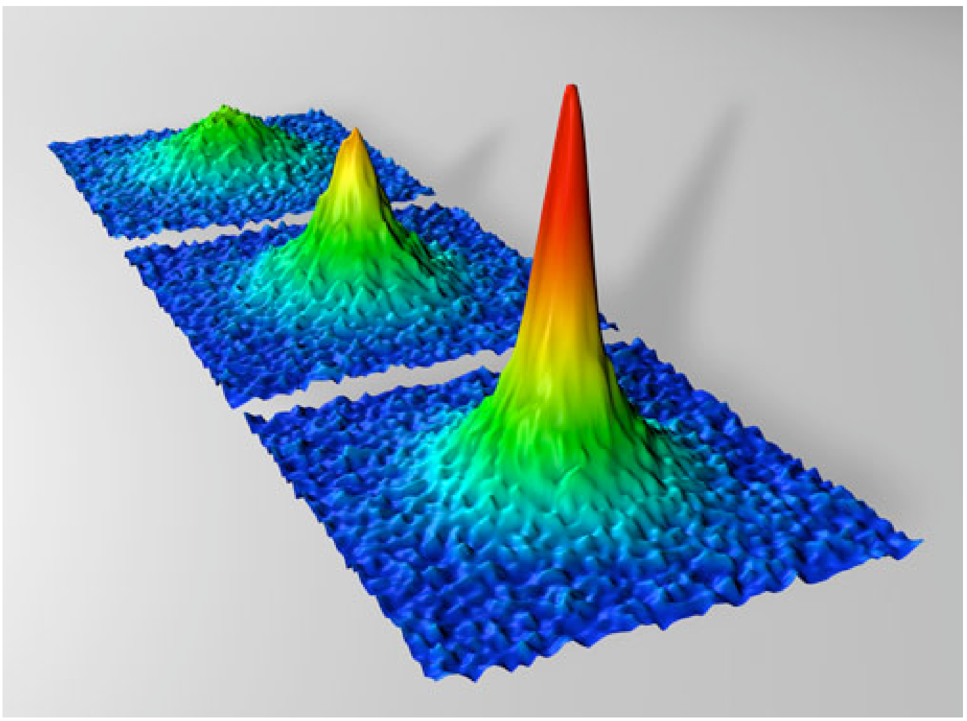
Uniform trap

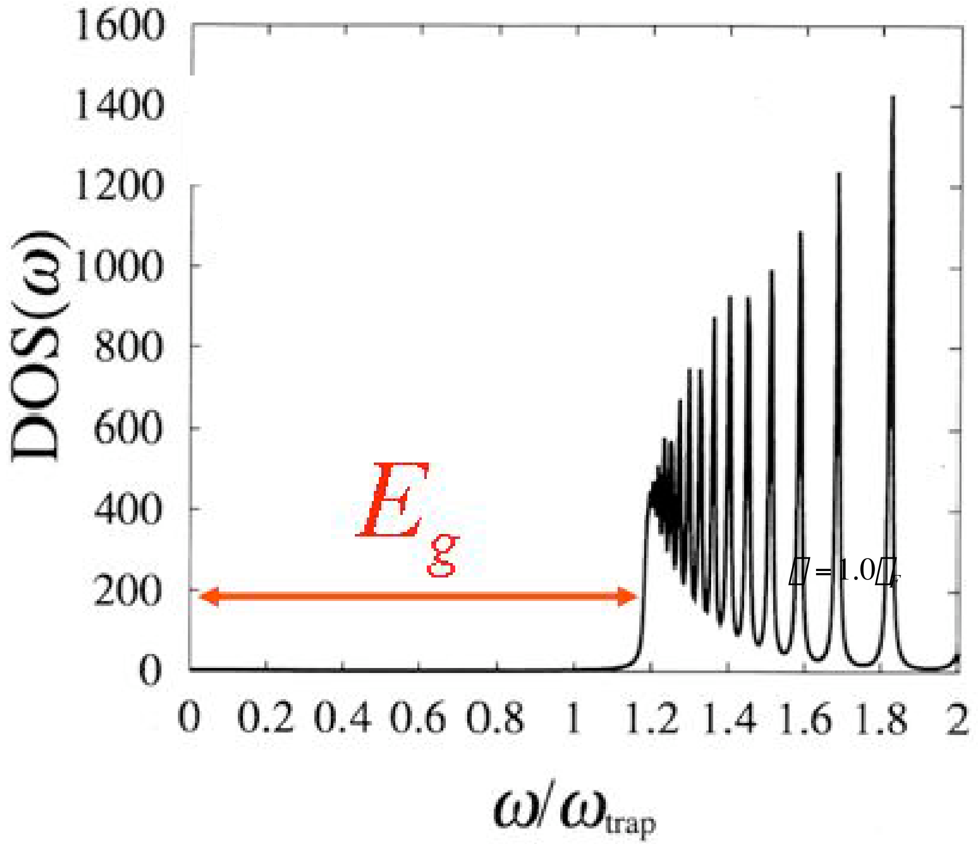
Broad and **narrow** resonance results plotted in terms of $1/a_{eff}$ instead of $1/a_{2b}$.

$$\frac{4\square\hbar^2 a_{eff}}{m} \equiv \square U + \frac{g^2}{2\square\square 2\square}$$

Suggests **universal behavior** when expressed in terms of $\mathbf{1/a_{eff}}$

The recent JILA data in the " BCS region"as defined by $a_{2b} < 0$. The **bimodal profile** clearly shows evidence for the appearance of the Bose condensate of "Cooper" pairs. However, equally exciting is the **first** observation of a **thermal gas of such pairs** (never seen before in BCS superconductors!).





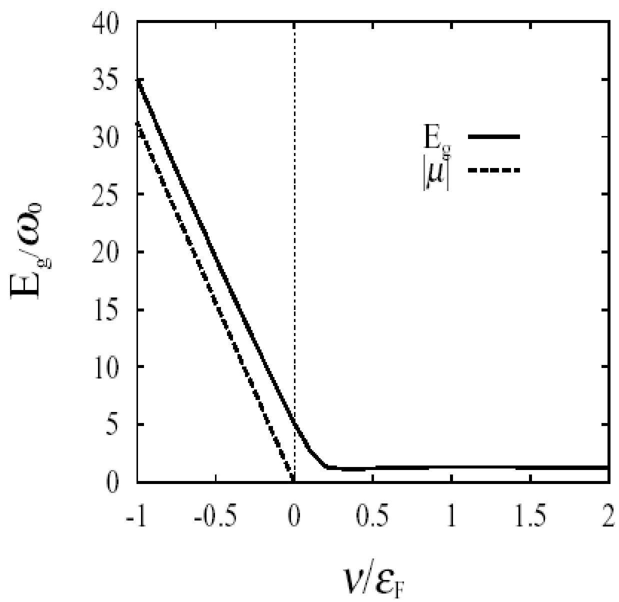
Ohashi and Griffin, cond-mat, Feb, 2004

These results involve solving the de Gennes - Bogoliubov equations for a trapped Fermi gas at T = 0, for □/□$_F$ =1

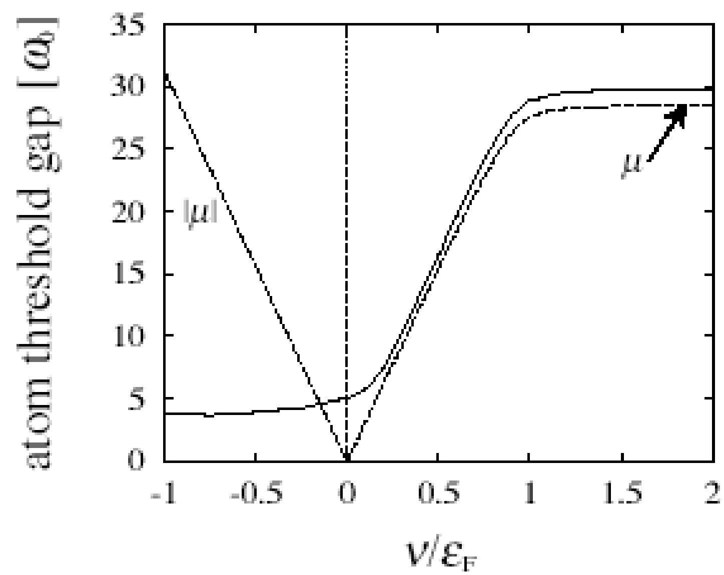
Density of states of **excitations** in a trapped Fermi gas. E_g is the energy gap of BCS excitations. Energy given In units of the isotropic trap frequency.

$$E_{atom}(q) = \square + \left((\square_q \; \square \; \square)^2 + \tilde{\square}^2 \right)^{1/2}$$ ***Uniform gas***

Note that in BCS side **$\square > 0$** while in BEC side **$\square < 0$**



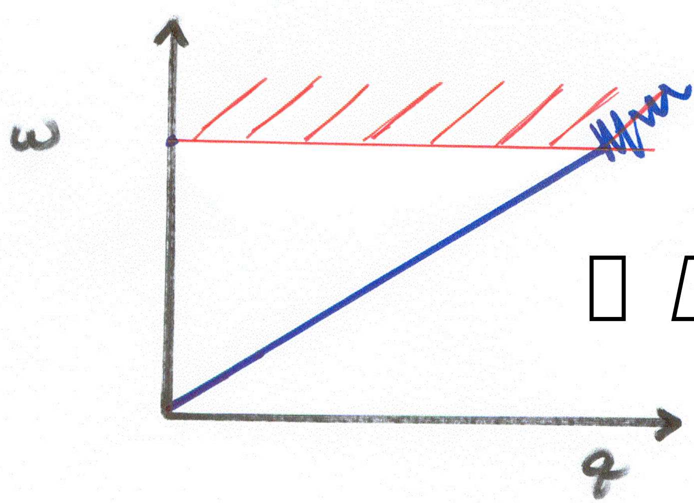
Excitation energy gap



Single atom energy gap

rf-spectroscopy (Jin, Grimm) can be used to measure this single particle gap by **breaking up pairs** (Torma & Zoller, PRL 2000).

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

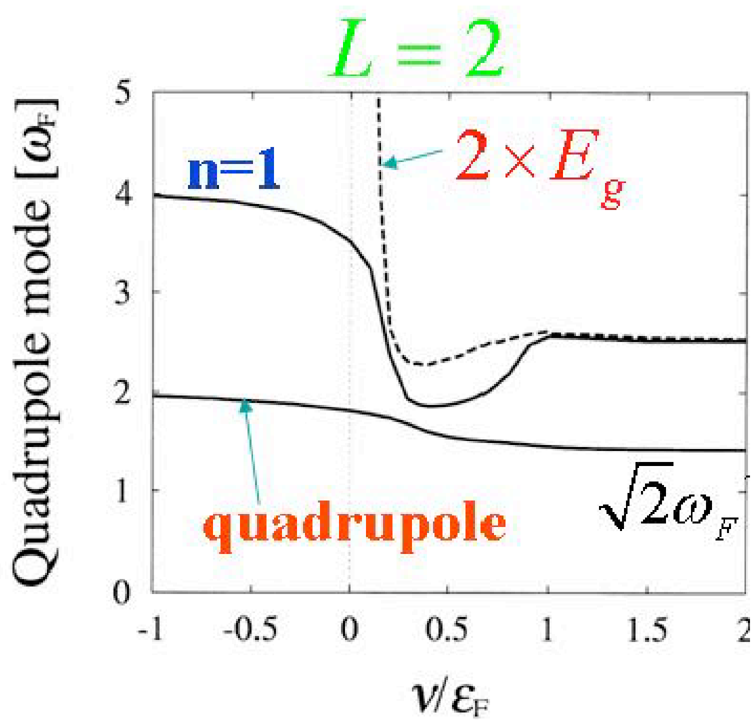


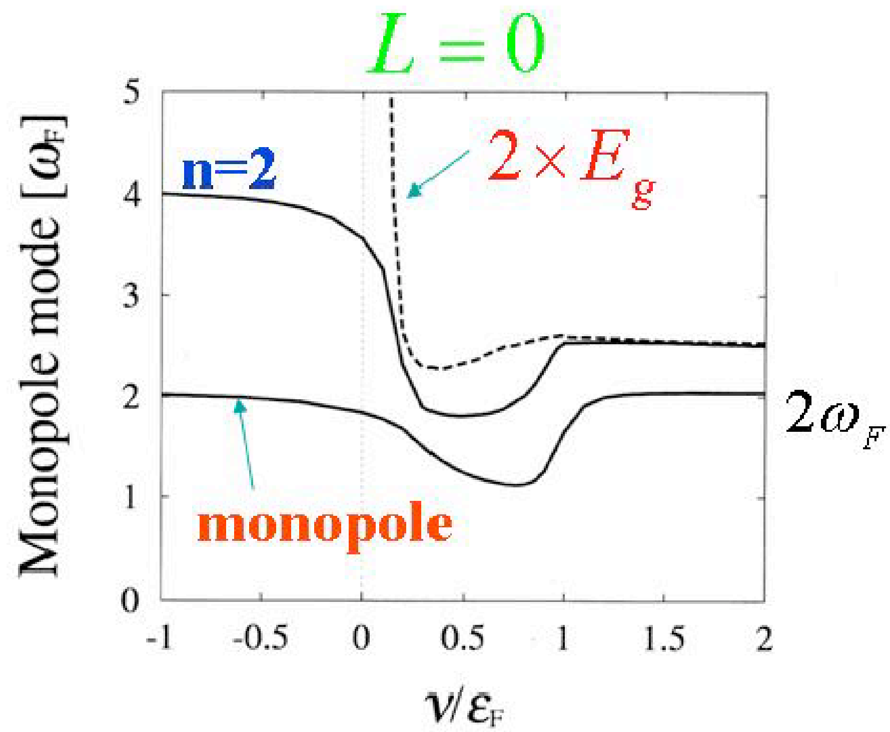
□ 2Δ

$$\square \ \square = \frac{v_F}{\sqrt{3}} q$$

This is for a uniform BCS superfluid. The analogous AB modes have been recently worked out for trapped Fermi atoms, through the BCS-BEC crossover.

Collective modes(collisionless) in a trapped (isotropic) Fermi Gas





Note the interesting **minimum** in the two-particle excitation energygap just above the Feshbach resonance and the resulting **suppression** of the monopole frequency.

O&G, *Fermi Gas Conference, Levico , 2004*

Conclusions

- **There is no qualitative difference between the predictions of single channel and two channel models of the BCS-BEC crossover within a MFA extended to finite temperatures.**

- **There is no fundamental difference between a molecular condensate in the BEC limit and a Cooper pair condensate in the BCS limit . In particular, the single particle excitations have the usual BCS Bogoliubov spectrum and the condensate collective modes behave smoothly through the crossover region.**

- **At this level, we have a good understanding of the BCS-BEC crossover with a Feshbach resonance, building naturally on the original ideas of Eagles, Leggett, Nozieres and Randeria.**

The next step in understanding the two channel model we have been using might be to work explicitly with a three component Fermi gas involving three hyperfine atomic states: a, b and c (Leggett, 2004).

- The **open channel** involves the states **a** and **b**, as before.
- The **closed channel** describing the b-molecules is now described by the states **a** and **c.**