THEORETICAL ASPECTS OF THE BCS-BEC CROSSOVER

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Summary:

- Trapped Fermi atoms: **Fano-Feshbach resonances** $\Longrightarrow$ atomic scattering length a_F tuned from negative to positive values across resonance

- **Theoretical issue** : single- vs multi-channel Hamiltonian

- **Broad and narrow** Fano-Feshbach resonances of ^6Li at (about) 822G and 543G

- **Multi-channel calculation** for molecular ^6Li

- Effective **single-channel Hamiltonian** sufficient to reproduce all relevant features of scattering problem *and* to realize BCS-BEC crossover !

♣ **BCS-BEC crossover:** Evolution

from Cooper pairing (Fermi character)
to condensation of composite bosons (Fermi degrees of freedom quenched).

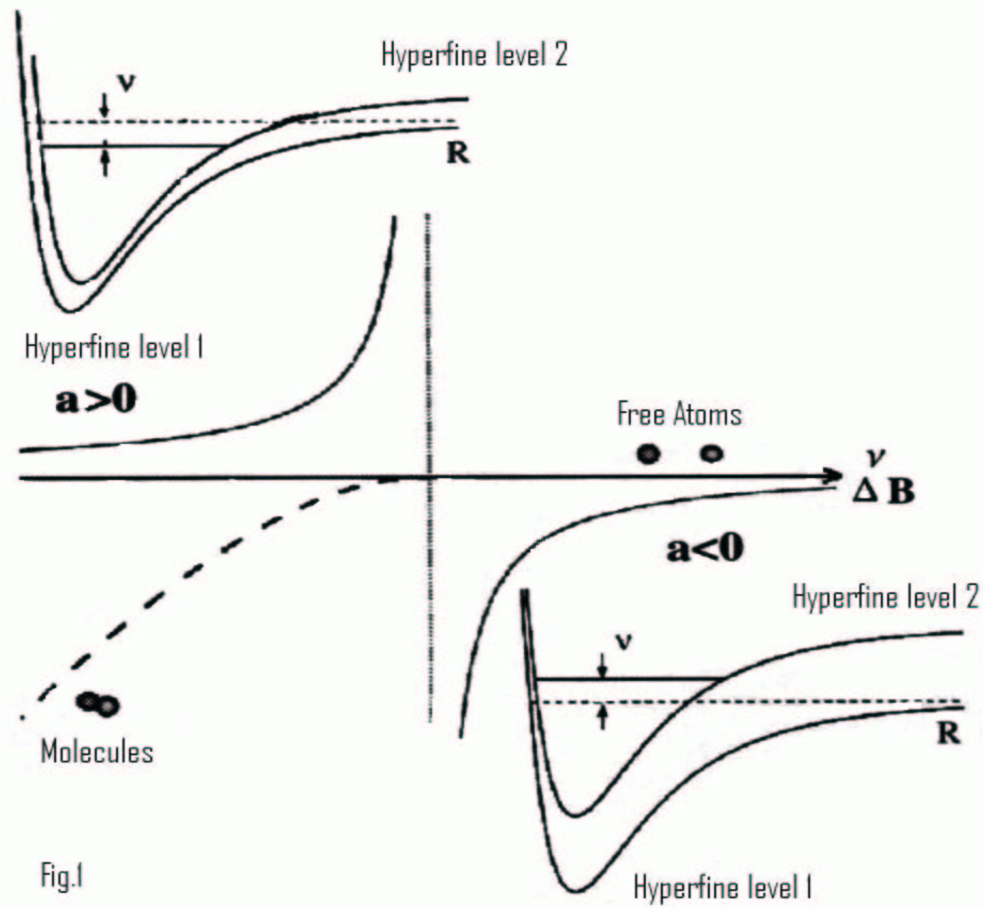
- Recent **experimental advances** with trapped Fermi atoms have enhanced interest in this problem.

- Trapped Fermi gases are **ideal testing ground** for theories $\Longleftarrow$ only few degrees of freedom !

- Attractive interaction between fermions provided by **Fano-Feshbach resonance** $\Longleftarrow$ mixing of channels with different (electronic and nuclear) spins.

- Fano-Feshbach resonance: resonant state becomes true bound state **by varying the applied magnetic field** $\Longrightarrow$ a_F changes sign and provides a mechanism to **cross over** from BCS to BEC.

$\boxed{\textbf{FIG. 1}}$



Hyperfine level 2
ν
R
Hyperfine level 1
a>0
Free Atoms
ν
Δ B
a<0
Hyperfine level 2
ν
R
Molecules
Hyperfine level 1

Fig.1

♣ **Two-body problem :**

• Onset of bound state when $a_F > 0$ can be described by **point-contact interaction** $v(\mathbf{r}) = v_0 \delta(\mathbf{r})$ (suitable regularization required) $\Longrightarrow$

a_F is the sole relevant parameter !

• However, presence of (at least) two channels in a Fano-Feshbach resonance $\Longrightarrow$

fermions are transferred from scattering channels into resonance channel to form a boson

$\Longrightarrow$ should two-body Hamiltonian require this boson as an essential ingredient ?

$$\Longrightarrow$$

♣ Ensuing **many-body Hamiltonian** would be built on the mixing of these two (scattering and resonant) channels

$\Longleftrightarrow$ fermions and bosons in thermal equilibrium would be present at the same time

$$\Longrightarrow$$

theory of "**resonance superfluidity**" (Timmermans et al.; Holland et al.; Griffin et al.).

♣ **Two model many-body Hamiltonians** :

- fermions only

$$\mathrm{H_f} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \;+\; v_0 \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow}$$

$(\sigma = \uparrow, \downarrow)$

- with mixing of fermions and bosons

$$\mathrm{H_{f\,b}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} + \mathrm{U} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow}$$

$$+\; \nu \sum_{\mathbf{q}} b^\dagger_{\mathbf{q}} b_{\mathbf{q}} \;+\; \left(\mathrm{g} \sum_{\mathbf{k}\mathbf{q}} b^\dagger_{\mathbf{q}}\; c_{\mathbf{q}/2-\mathbf{k}\downarrow}\, c_{\mathbf{q}/2+\mathbf{k}\uparrow} \;+\; \mathrm{H.c.} \right)$$

$c \;\longleftrightarrow\;$ fermions $\qquad\qquad b \;\longleftrightarrow\;$ bosons

♣ **Question** :

• What is the **"minimal" theoretical model** to describe the BCS-BEC crossover with trapped Fermi atoms ?

• Is it necessary to use **a fermion-boson model** $\longleftrightarrow$ $\mathrm{H}_{\mathrm{f\,b}}$ with (at least) two channels ?

• Would rather be enough to use **a fermion-only model** $\longleftrightarrow$ H_{f} , with a single channel and a point-contact interaction ?

This question needs to be answered **before** trying to interpret the experimental results.

Main point :

both experimental realization of BCS-BEC crossover with trapped Fermi atoms

and theoretical use of single- or multi-channel models **depend on the "width"** of Fano-Feshbach resonance

(two aspects strictly related to each other).

♣ To **answer** above question $\Longrightarrow$
perform detailed numerical calculation $\Longrightarrow$
extract relevant information to be fed into physics of BCS-BEC crossover

[S. Simonucci, P. Pieri, and G.C. S., cond-mat/0407600]

- For definiteness: **broad and narrow** Fano-Feshbach resonances of ^6Li at about 822G and 543G (selected to realize BCS-BEC crossover experimentally)

- Multi-channel calculation by Born-Oppenheimer scheme

- Nuclear wave equation solved for s-wave
(it contains hyperfine and Zeeman couplings).

- **Low-energy sector** spanned by five channels:

singlet $^1\Sigma_g^+$ with spin configurations $|0,0>_e \; |0,0>_n$ and $|0,0>_e \; |2,0>_n$ (**resonance channels**)

triplet $^3\Sigma_u^+$ with spin configurations $|1,1>_e \; |1,\bar{1}>_n$, $|1,0>_e \; |1,0>_n$, and $|1,\bar{1}>_e \; |1,1>_n$
(**scattering channels**)

♣ **Representative outcomes** of calculation :

- Molecular energy curves $\boxed{\textbf{FIG. 2}}$
- Scattering length vs magnetic field $\boxed{\textbf{FIG. 3}}$

Several quantities can be extracted from calculation:

(i) Binding energy $\mathbf{E_b}$ compared to $\epsilon_0 = (Ma_F^2)^{-1}$

(ii) Radius $\bar{\mathbf{R}}$ of bound wave function compared to $a_F/\sqrt{2}$

(iii) Radius $\bar{\mathbf{R}}_\mathbf{2}$ of component in resonance channel

(iv) Wave-function projection $|\mathbf{w_1}|^\mathbf{2}$ in scattering channel

(v) Projection $< \phi_{\rm c\,p} | \mathbf{w_1} >$ onto bound wave function $\phi_{\rm c\,p} = \sqrt{2/a_F}\, \exp(-R/a_F)$ for contact potential

(vi) "Effective range" $\mathbf{r_0}$ obtained from scattering amplitude $f(k) = (g(k) - ik)^{-1}$ with $g(k) = -a_F^{-1} + \mathbf{r_0} k^2/2$.

$\boxed{\textbf{Table I}}$

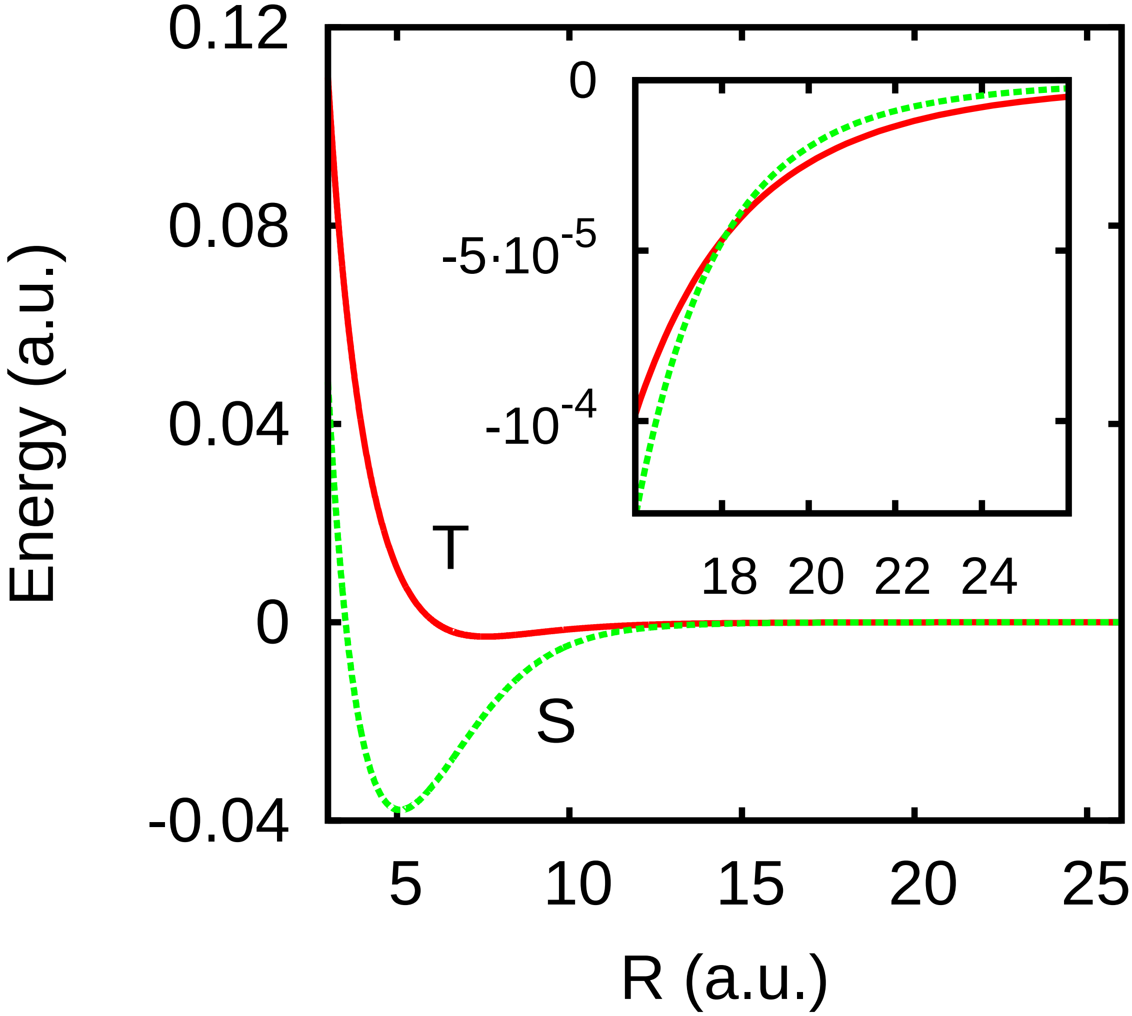


Fig.2. Molecular energy curves for the singlet (S) and triplet (T) states of lowest energy vs the nuclear separation R. The inset shows the details of the crossing at $R = 18$ a.u..

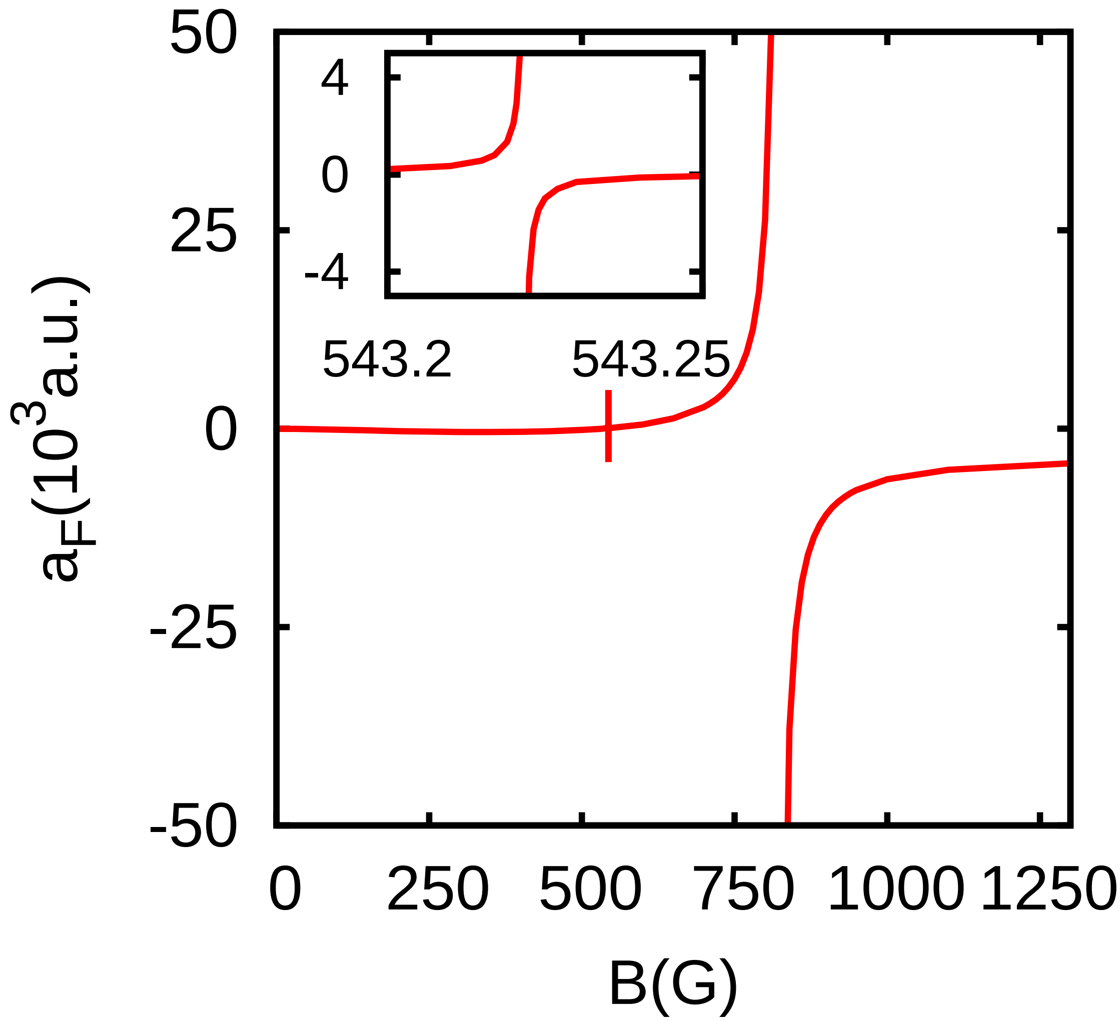


Fig.3. Scattering length a_F vs magnetic field B. The inset shows the details of the narrow resonance at about $543G$.

B (G)	a_F	E_b/ϵ_0	$\sqrt{2}\bar{R}/a_F$	$\bar{R}_2/\bar{R}$	$\lvert w_1\rvert^2$	$\langle\phi_\mathrm{cp}\lvert w_1\rangle$	r_0
650	1.29	1.068	1.00053	.039	.99669	.972	.085
750	6.26	1.014	1.00004	.008	.99986	.994	.087
800	26.2	1.003	1.00024	.002	.99998	.999	.088
850	-25.3						.088
1100	-5.17						.090
1300	-4.35						.090
.2200	2.09	.0425	1.148	.022	.062	.194	-121
.2210	4.85	.0581	1.517	.007	.134	.289	-121
.2216	41.7	.9066	.5853	.002	.304	.550	-124
.2218	-34.3						-125
.2220	-10.7						-127
.2225	-4.22						-126

Table I. Comparison of the molecular calculation with the effective single-channel model, for the broad resonance at about $822G$ and for the narrow resonance at about $543G$. For the narrow resonance, only decimal digits after $543G$ are reported in the first column. Both a_F and r_0 are in 10^3a.u..

♣ **For broad resonance** $\Longrightarrow$

effective single-channel model with contact potential reproduces all results of multi-channel calculation !

In particular, note that:

- $\mathbf{E_b}/\epsilon_\mathbf{0}$, $\mathbf{\bar{R}}/\mathbf{a_F}/\sqrt{\mathbf{2}}$, $|\mathbf{w_1}|^\mathbf{2}$, and $< \phi_{\mathrm{c\,p}}|\mathbf{w_1} > \ \simeq 1$

- Extension $\mathbf{\bar{R}_2}$ of boson (introduced in resonance-superfluidity theory) $<<$ extension $\mathbf{\bar{R}}$ of internal wave function of composite boson

- $\mathbf{r_0}/\mathbf{a_F} << 1$.

♣ **Important point for BCS-BEC crossover**

is to complement the above analysis by :

- **Fermi wave vector** k_F characteristic of the trap

- Minimum **experimental accuracy** of magnetic field.

♣ **Reasoning goes as follows** :

Dimensionless parameter $(k_F a_F)^{-1}$ **exhausts BCS-BEC crossover** within $\approx$ 1 about unitarity limit $(k_F a_F)^{-1} = 0$ irrespective of theoretical model !

$$\Longleftarrow$$

BCS $(a_F < 0)$ and **BEC** $(a_F > 0)$ regimes reached for $k_F|a_F| << 1$, while in **crossover region** $k_F|a_F| \approx \infty$

To span crossover $\Longrightarrow$ identify **three values** of $(\mathbf{k_F\, a_F})^{-1}$ (say, $-1.0, 0.0, 1.0$), by tuning magnetic field across FF resonance

$$\text{———————} \circ \text{———————} \circ \text{———————} \circ \text{———————}>$$

$$-1.0 \qquad\qquad 0.0 \qquad\qquad 1.0 \quad (\mathbf{k_F\, a_F})^{-1}$$

For experiments with broad resonance (at $822G$) $k_F = 2 - 3 \times 10^{-4}$ a.u. $\Longrightarrow$

above values of $(k_F a_F)^{-1} \longleftrightarrow B = (1300, 822, 730)\, G$

separated by $\delta B \gtrsim 100G$ **much larger** than minimum experimental accuracy !

• For these values of B $\Longrightarrow$

single-channel model with contact potential **totally appropriate** for two-body scattering !!!

$\boxed{\textbf{(see Table I)}}$

♣ **Situation reversed for narrow resonance at (about) 543G** :

above values of $(k_F a_F)^{-1}$ $\longleftrightarrow$

$$B = (543.2225, 543.2217, 543.2209)\, G$$

separated by $\delta B \simeq 0.001 G$ **fifty times smaller** than minimum experimental accuracy !!!

$$\Longrightarrow$$

No way of realizing BCS - BEC crossover with narrow resonance of ^6Li !

♣ **In addition ,** $\mathbf{r_0\, k_F} < 10^{-2}$
for the broad resonance

$$\Longrightarrow$$

energy dependence of scattering properties (over and above that resulting for contact potential)
is **irrelevant** !!!

$$\Longrightarrow$$

"resonance superfluidity" theory **not required** .

♣ **To complete the mapping**

onto single - channel model $\Longrightarrow$ identify **effective spin states** $|\uparrow>_{\text{eff}}$ and $|\downarrow>_{\text{eff}}$.
From molecular calculation , for broad resonance wave function is (essentially) a triplet both for electrons and nuclei $\Longrightarrow$

$$|\uparrow>_{\text{eff}} \qquad \longleftrightarrow \qquad |1/2, -1/2>_e \ |1, 0>_n$$

$$|\downarrow>_{\text{eff}} \qquad \longleftrightarrow \qquad |1/2, -1/2>_e \ |1, 1>_n$$

♣ **Question : Why are these resonances "broad" and "narrow" relative to each other?**

• Out of five channels spanning low energy , **two singlets** $^1\Sigma_g^+$ with spin

$$|0,0>_e|0,0>_n \quad \text{and} \quad |0,0>_e|2,0>_n$$

interact mostly with **triplet** $^3\Sigma_u^+$ with spin

$$|1,\bar{1}>_e|1,1>_n$$

• $\boxed{\textbf{Figure 4}}$

magnetic field dependence of energy of last singlet

bound state (with 38 nodes) **(dashed line)**

relative to

threshold of triplet channel **(dotted line)**

(when channels are decoupled)

Two curves cross each other at (about) 550G .

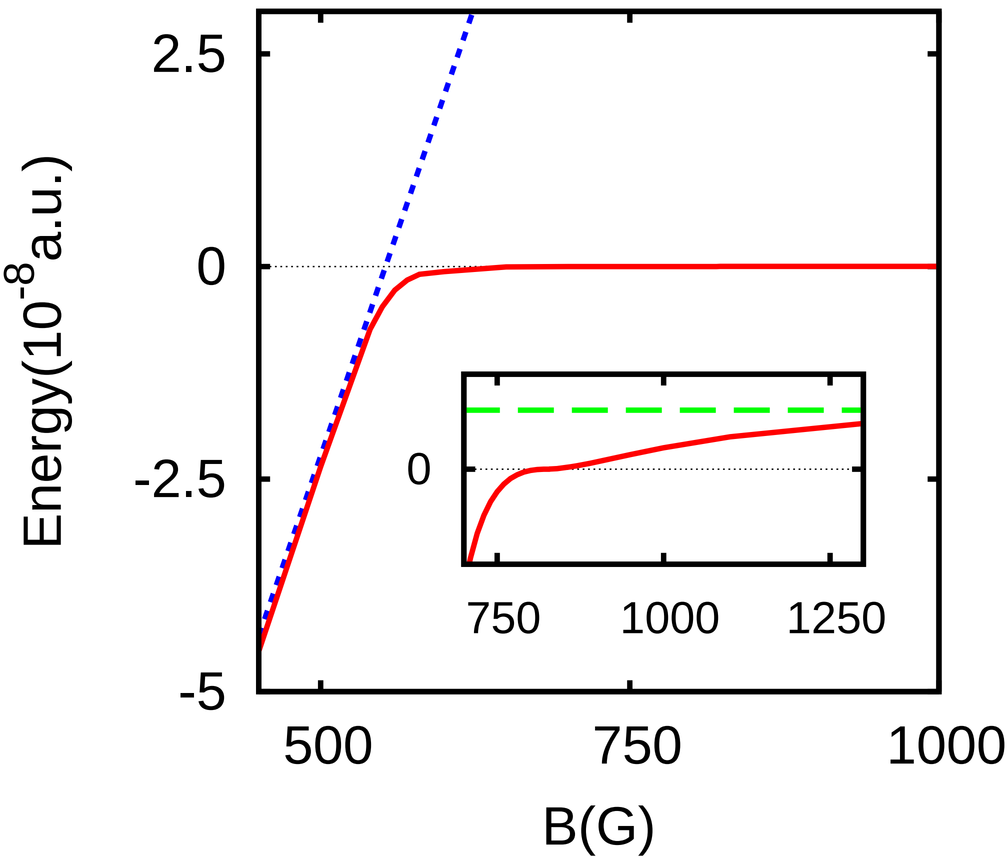


Fig.4. Mechanism for the narrow and broad Fano-Feshbach resonances.

• Triplet channel has **virtual state** at threshold with large (negative) background scattering length ($\mathbf{a}_{\rm bg} \simeq -3790$ a.u.)

• **One** linear combination of two singlet channels **decouples** from triplet virtual state (that one crossing threshold at about 550G)

• **Other** combination which couples with triplet forced to have an **avoided crossing** (when interaction of singlets and triplet is restored)

• Combination which decouples from triplet $\longrightarrow$ mantains singlet character through crossing $\longrightarrow$ **"narrow" resonance** at about 543G

• Combination which couples with triplet $\longrightarrow$ (almost) full triplet character past avoided crossing

• Its **energy broadening** tends asymptotically to broadening $(M\,\mathbf{a}_{\rm bg}{}^2)^{-1}$ of virtual state

$\boxed{\textbf{inset of Fig. 4}}$

$\longrightarrow$ it crosses threshold **slowly** vs magnetic field
$\longrightarrow$ this accounts for **"broad" nature of resonance** at about 822G .

♣ **Examples of calculations done with** $\mathrm{H_f}$

(1) Comparison with experimental results for ^6Li :

- Density profiles about unitarity limit $\boxed{\textbf{FIG. 5}}$
- Root-mean-square radius vs $(k_F\, a_F)^{-1}$ $\boxed{\textbf{FIG. 6}}$

[A. Perali, P. Pieri, and G.C. S., PRL **93**, 100404 (2004)]

(2) Comparison with Quantum Monte Carlo results :

- $T = 0$ chemical potential vs $(k_F\, a_F)^{-1}$ $\boxed{\textbf{FIG. 7}}$
- $T = 0$ excitation gap vs $(k_F\, a_F)^{-1}$ $\boxed{\textbf{FIG. 8}}$

[P. Pieri, L. Pisani, and G.C. S., Phys. Rev. B **70**, 094508 (2004)]

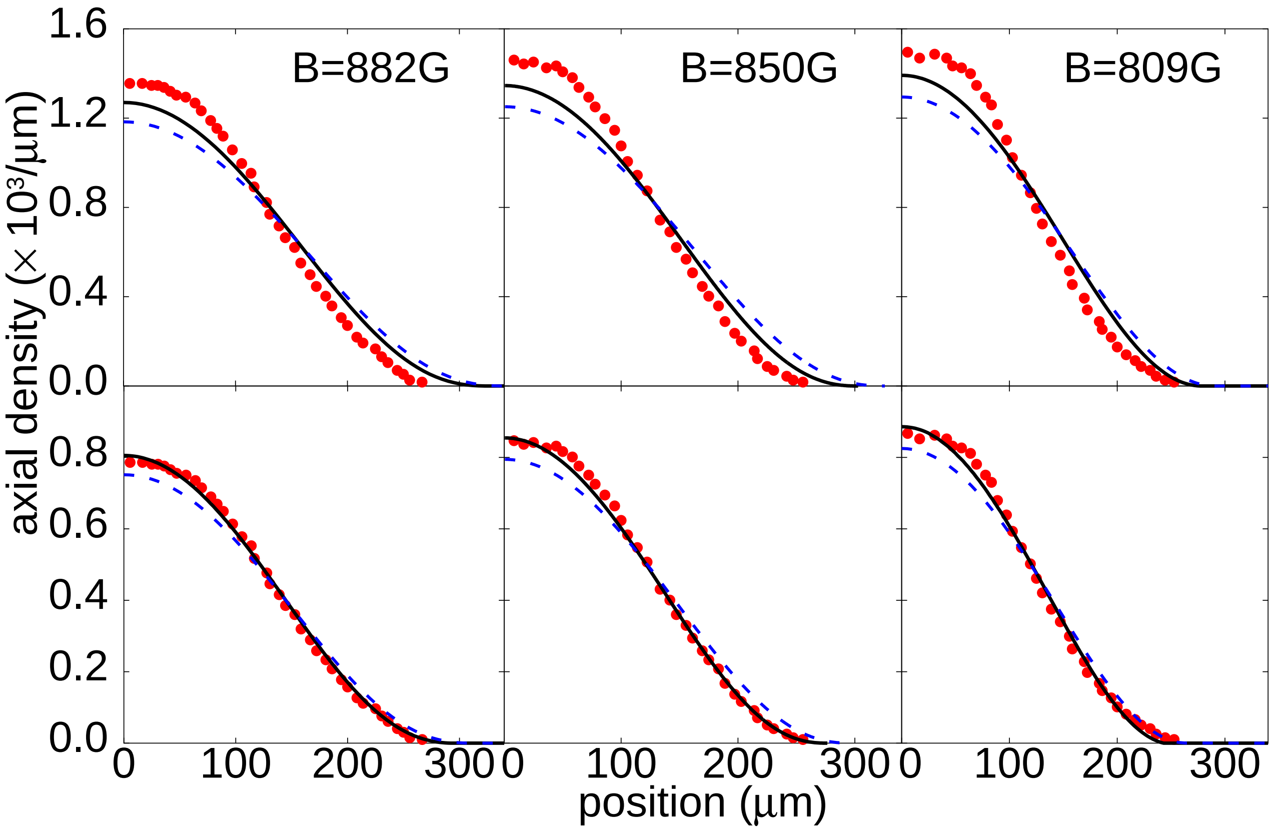


Fig.5. Comparison between experimental and theoretical axial density profiles. Experimental data from [M. Bartenstein *et al.* (2004)] (dots) are shown for three diffeent values of the magnetic field B tuning the FF resonance. Theoretical results at $T = 0$ obtained by our theory (full lines) and by BCS mean field (dashed lines) are shown for the corresponding couplings $(k_F a_F)^{-1}$ given in the text. The upper (lower) panel refers to the estimated number of atoms $N = 4 \times 10^5$ ($N = 2.3 \times 10^5$).

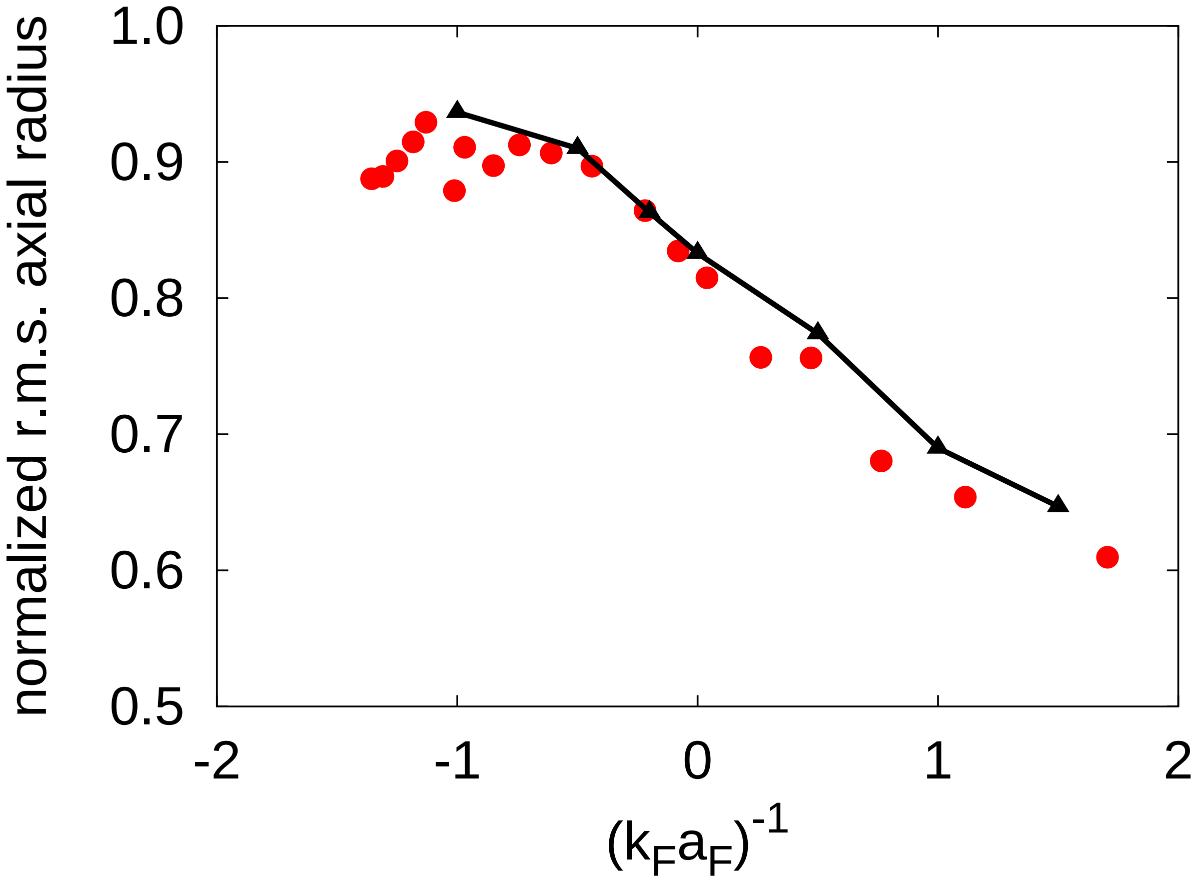


Fig.6. Comparison between experimental (dots) and theoretical (triangles) normalized root-mean square axial radius across the crossover regime. Experimental data are taken from [M. Bartenstein *et al.* (2004)]. The values of $(k_F a_F)^{-1}$ and of the non-interacting root-mean square axial radius used also for the experimental data are obtained with $N = 2.3 \times 10^5$.

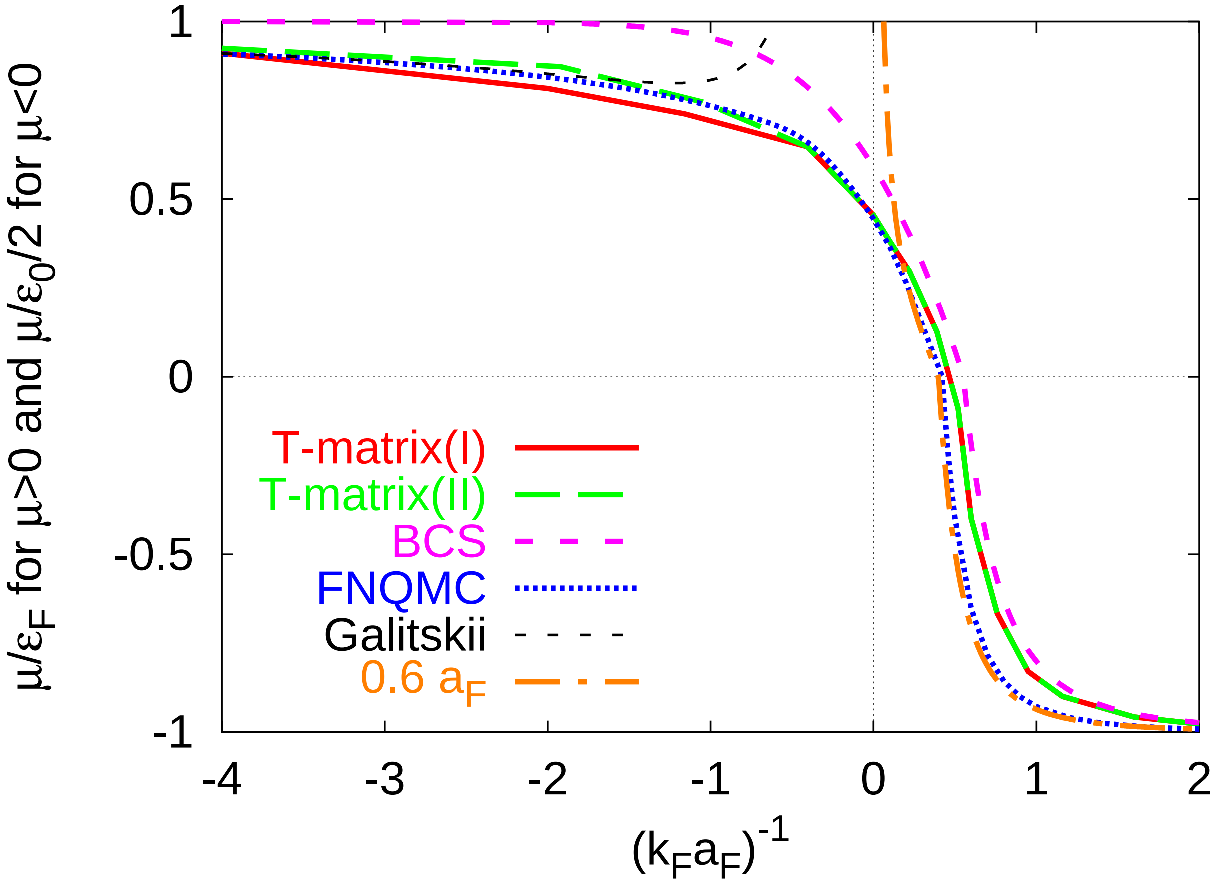


Fig.7. Chemical potential at zero temperature vs coupling parameter $(k_F a_F)^{-1}$. The results of the present theory (T-matrix(I) in the legend) and of its version without inclusion of the self-energy shift Σ_0 (T-matrix(II)) are compared with BCS mean-field (BCS), Fixed-node QMC data (FNQMC) from [Astrakharchik *et al.* (2004)], Galitskii's expression for the dilute Fermi gas (Galitskii) and the asymptotic expression for strong-coupling, using the result $a_B = 0.6 a_F$.

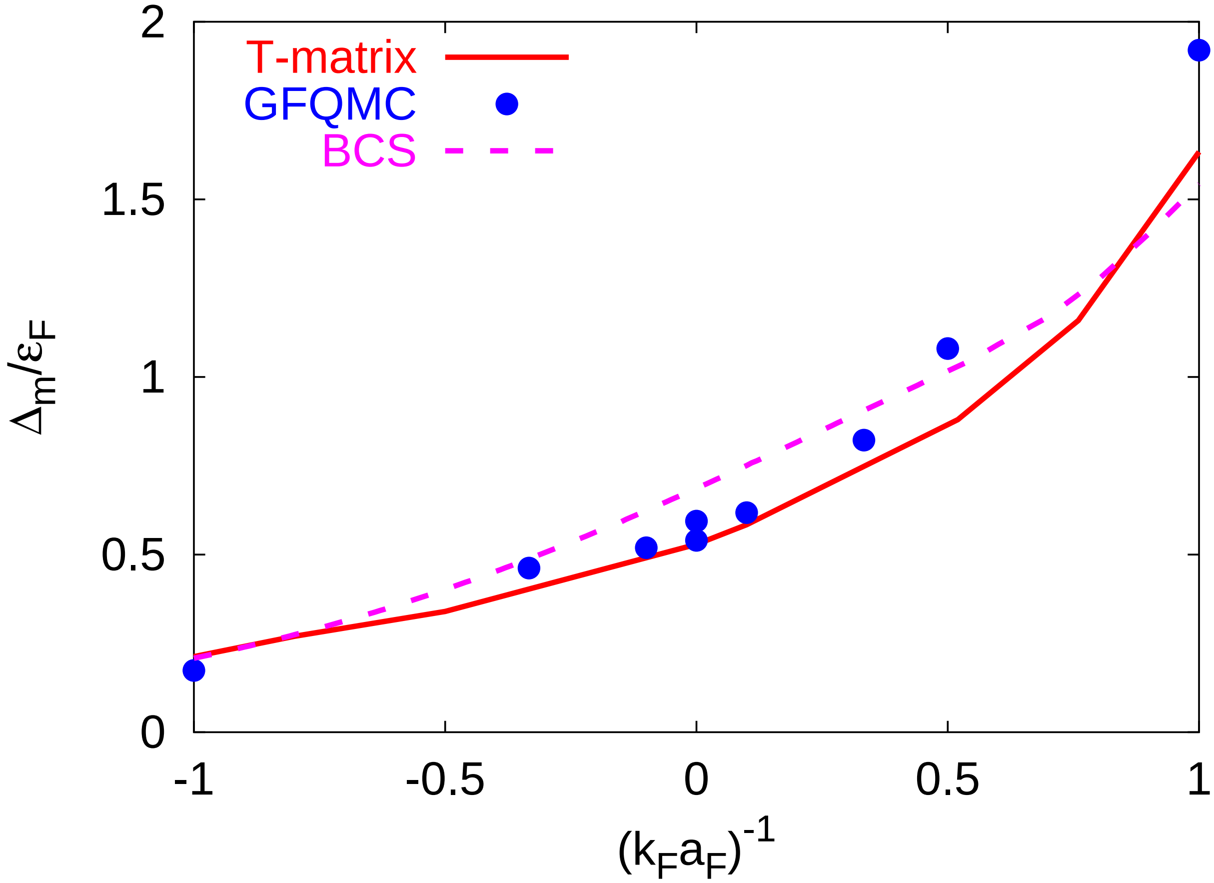


Fig.8. Excitation gap $\Delta_{\rm m}$ at zero temperature vs coupling parameter $(k_F a_F)^{-1}$. The results of the present theory (T-matrix) are compared with the Green's function QMC data (GFQMC) from [Carlson *et al.* (2004)] and with BCS mean-field (BCS).

Conclusions :

- **Experiments** : to realize BCS-BEC crossover with trapped Fermi atoms using FF resonances , watch out for values of

$\mathbf{k_F}$ (characteristic of the trap)

minimum experimental accuracy of B

- **Theory** : when FF resonance is ok to realize BCS-BEC crossover $\Longrightarrow$ **effective single-channel** Hamiltonian with contact interaction can be used

- **In practice**, it appears that "resonance superfluidity" theory is **not required** .

- **Excellent comparison with**

(i) Experimental data for ^6Li

(ii) Quantum Monte Carlo results .