Molecular bound state and BCS instability

in

atomic Fermi gases

with

Feshbach resonance

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- **Coherent framework** for **many-body effects** with **Feshbach resonance**

- **Normal state** : **Modification** of **molecular threshold** and binding energy by **Fermi sea**

- **Self-consistent** treatment for **equilibrium properties**

with **X. Leyronas**

• Many-body framework for Feshbach resonance

• Work only with **fermions**, **no** 'Feshbach bosons'

(Strinati and coworkers)

Molecules appear **naturally** in the theory

• **Resonance** only through **scattering properties**

of two atoms in vacuum

→ **Exact** description of **two atoms** physics

→ Basic **building block** = **vertex** (as much as possible)

• **Justification** :

Start from true potentials → calculations with all channels →

scattering amplitude

Dilute gas approximation ⇒ lowest order OK

(or perturbative correction in r_{eff} /d)

• can be implemented explicitely for model potentials: well + barrier

$\Rightarrow$ back to "standard" many-body (almost)

- **Pure Feshbach resonance**

- 2 particles in vacuum

$$\boxed{f(\omega) = -\frac{1}{\frac{\omega - \omega_0}{\gamma} + i\,(m\omega)^{1/2}}}$$

ω_0	resonance energy
$\gamma = mw^2/4\pi$	resonance width
$a = -\gamma / \omega_0$	scattering length

- Equivalent to effective range model (Pitaevskii)
- Works well with adjustable $\gamma(B)$ and $a(B)$ (Marcelis et al.)
- Can be improved by $\delta(k) = \delta_{Fes}(k) + \delta_{vs}(k) + \delta_{bg}(k)$ (Marcelis et al.)

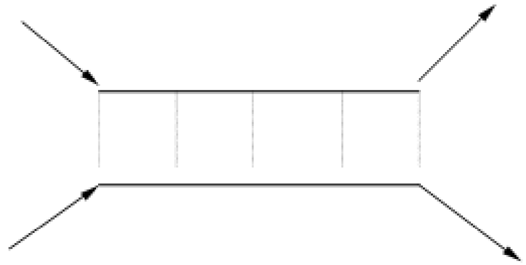
- **Wide** resonance for ^6Li (large γ) start with simple cases first

Low ω $k = (m\omega)^{1/2}$

$$\boxed{f(\omega) = -\frac{1}{a^{-1} + i\,k}} \qquad \varepsilon_b = \frac{1}{ma^2}$$

• Scattering amplitude with Pauli exclusion

-**Pauli exclusion** expected to be **dominant** physical effect



- 2 particles with Fermi sea (at $T \neq 0$)

• Only Pauli exclusion (free fermions propagator)

$\Rightarrow$ " Forbidden " states by Fermi sea

• **Scattering amplitude** depends also on
2 particles total momentum K (weak effect for large momentum)

• $\boxed{K = 0}$

- Adimensional form
  - Energy scale $\mu = k_0^2/2m$ for ω (origin at μ), T, W
  - Wavevector scale k_0
  - $\lambda = -2 a k_0 / \pi = (2/\pi)\, W/\omega_0$ $\quad W = \gamma\, k_0$

  $\overline{W} \sim 10^3$ for ^{6}Li

$$\frac{\pi}{2\,k_0}\,\frac{1}{f(\omega)} = \frac{1}{\lambda} - \frac{\overline{\omega}+2}{\overline{W}} + I(\overline{\omega})$$

$$I(\overline{\omega}) = \int_0^\infty dx \left[\, 1 - \frac{x^2}{x^2 - 1 - \frac{\overline{\omega}}{2}}\ \mathrm{th}\,\frac{x^2-1}{2\,\overline{t}}\,\right]$$

$$\mathrm{Im}\ I(\overline{\omega}) = -\frac{\pi}{2}\left(1+\frac{\overline{\omega}}{2}\right)^{1/2} \mathrm{th}\,\frac{\overline{\omega}}{4\,\overline{t}}$$

- $I(\omega)$ itself does not contain interactions !

• Resonance $\leftrightarrow$ $\mathrm{Im}\, f^{-1}(\omega) = 0$ $\qquad$ $\mathrm{Re}\, f^{-1}(\omega) = 0$

• $\mathrm{Re}\, f^{-1}(\omega,K) \neq \mathrm{Cte}$ $\qquad \leftrightarrow \qquad$ $a_{eff}^{-1}(\omega\ ,K)$

$\Rightarrow$ no resonance $a_{eff}^{-1} = 0$ possible for all atoms at the same time

• Nothing peculiar when $\lambda^{-1} = 0$ is crossed

because negligible for large λ (~ unitary limit)

• OK with experiments which see

nothing peculiar at the (supposed) location of the " Feshbach resonance

- **Normal atomic state instability**

- Useful for understanding superfluid
- Experimentally accessible through fast variation of B

- Ultracold fermionic atomic gas

  No molecules

  - BCS Instability
  - Molecular Instability

$\Rightarrow$ **unexpected links**

- Instabilities for $\boxed{\text{Total momentum } \mathbf{K} = \mathbf{0}}$

- Strongest effects
- Effects disappear progressively for large momentum

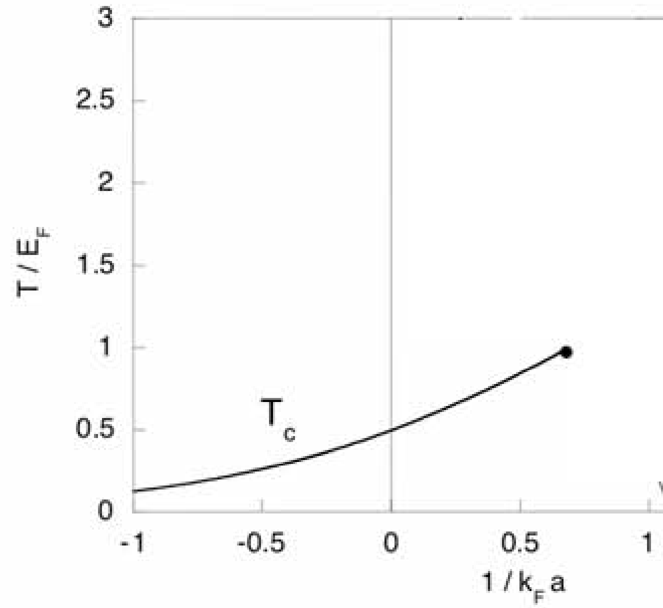
• **BCS instability**

Linked to Pauli exclusion

Resonance $\leftrightarrow$ $\mathrm{Im}\, f^{-1}(\omega) = 0$

$\mathrm{Im}\, I(\omega) = 0 \quad \Rightarrow \quad \omega = 2\,\mu > 0$

$\mathrm{Re}\, f^{-1}(\omega) = 0 \quad ; \quad \mathrm{Re}\, I(\omega) = -1/\lambda$



• Bare interaction only

$\lambda \to 0$

$$\boxed{\frac{T_c}{E_F} = \frac{8\, e^{C-2}}{\pi}\, e^{-1/\lambda}}$$

- Better calculation requires inclusion of fluctuations

• No collapse $\Rightarrow$ BCS instability for $a > 0$

Leggett (80), Sa de Melo *et al* (93), Milstein *et al* (02), Ohashi and Griffin(02)

• Terminal point : $\mu = 0$

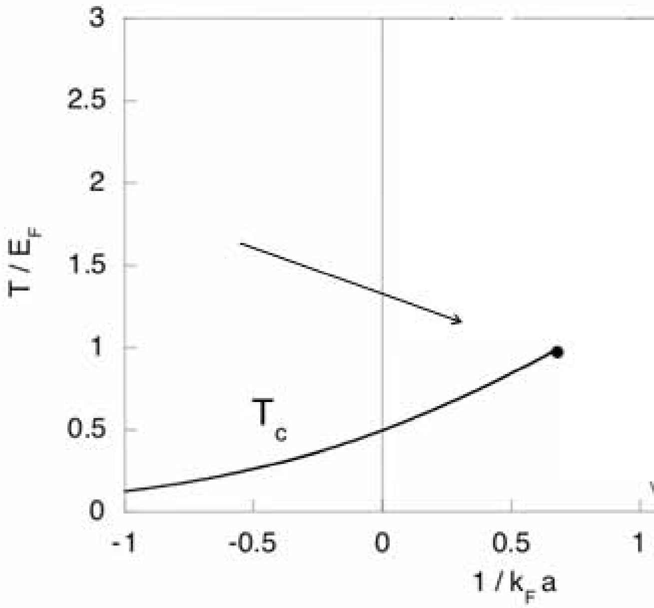
$$\boxed{\frac{T_0}{E_F} = 0{,}99 \qquad \frac{1}{k_F a_0} = 0{,}68}$$

- **Shift of molecular threshold**

Molecular instability :

pole of $f(\omega)$ for real $\omega < 0 \Rightarrow \mathrm{Re}\, I(\omega) = -1/\lambda$

-Molecular instability shifted toward $a > 0$



- **$\mu < 0$ case** (link to classical limit $T \rightarrow \infty$)

(Large) molecules appear for $\omega = -\varepsilon_b = 0$

$$\boxed{\frac{1}{a} = 4\, n\, \Lambda_T^2 = k_F \frac{8}{3\pi} \frac{E_F}{T} \qquad n = \frac{k_F^3}{6\pi^2} \qquad E_F = \frac{k_F^2}{2m}}$$

- **Physical interpretation**

  " Forbidden " states by Fermi sea

  $\Longrightarrow$ Hinder molecular formation

- Terminal point : $\mu = 0$

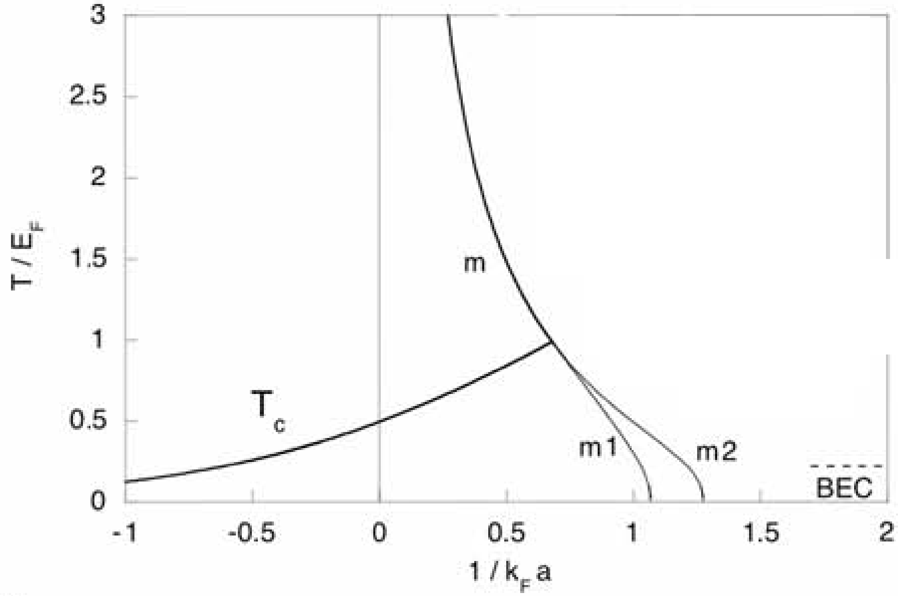
  - Identical to BCS instability

  because both satisfy Im I(ω=0) = 0 and Re I(ω=0) = -1/λ for $\mu = 0$

$$\boxed{\begin{array}{c}\textbf{Find BCS}\\ \text{by following } \textbf{molecular threshold !}\end{array}}$$

- **Molecular instability $\mu \geq 0$ case**

- Superfluid domain !
- Simplest case $T = 0$



$$\boxed{\frac{\pi}{2}\,\frac{1}{k_F a} = 2\, r \,\mathrm{Arctg}\, r - \frac{\pi}{2} r + 2}$$

$r = (|\omega| / 2\,\mu)^{1/2}$

Minimum 1.67 for $r = 0.44 \Rightarrow \omega = -\,0.39\,\mu$

$\Rightarrow$ **Molecular instability** appears for $1/k_F a = 1.06$ with **binding energy** $0.39\, E_F \neq 0$!

- For $1.06 < 1/k_F a < 4/\pi$ **2 poles !**

- For $1/k_F a > 4/\pi$ single **binding energy**

$\Rightarrow$ **standard molecule**

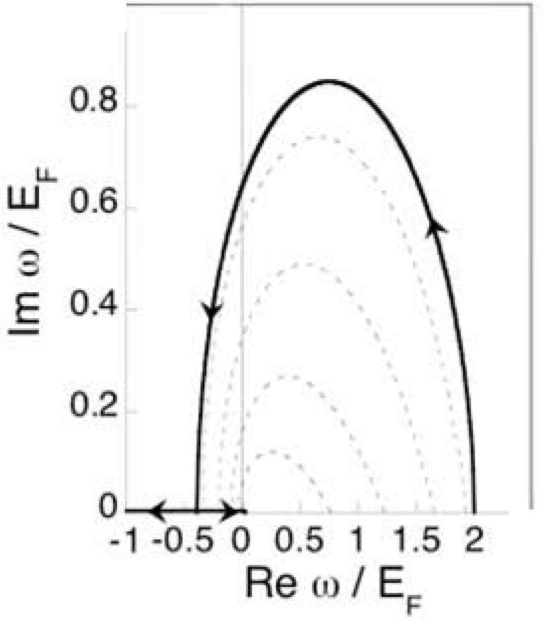
• **Interpretation**

- Pole very near full Fermi sea $\Longrightarrow$

Molecular state of holes (« anti-molecule »)

- Minimum and existence of 2 solutions

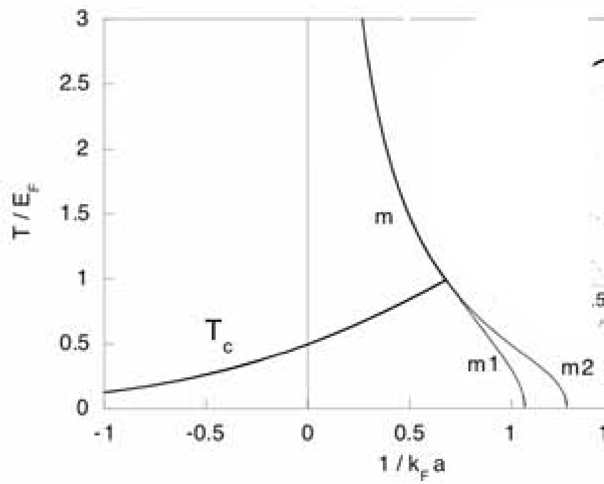
$\leftrightarrow$ term $-(\pi/2)\,(|\omega|/2\mu)^{1/2} \leftrightarrow$ hole density of states



- **Mixed particle-hole nature** **natural** if one follows the evolution of **BCS pole** (mixed particle-hole)

- Forbidden domain ? **Unmixing** domain?

Hole lifetime probably short



• Single pole $\Longrightarrow$

binding energy > **2** E_F > **0**$\leftrightarrow$**existence of BCS**

- Topological **stability** of BCS pole trajectory

$\Longrightarrow$ result quite general

Accident in BEC-BCS transition ?

• Asymetrical picture ~ Cooper problem

- **Equilibrium properties with this vertex**
- **Vertex $\rightarrow$ self-energy $\rightarrow$ n_k $\rightarrow$ density $\rightarrow$ k_F**
- **Recovers known results**

- Large k limit **$T \rightarrow 0$ $a \rightarrow 0_-$ (Belyakov) :**

$$n_k = \left(\frac{2k_F|a|}{3\pi}\right)^2 \frac{k_F^4}{k^4}$$

- Large T limit **virial expansion (Bethe - Uhlenbeck)**
  Interaction contribution (a < 0)

$$\delta n = -\frac{4\sqrt{2}}{\pi}\, a n_0^2 \Lambda_T^3 \int_0^\infty dk\, \frac{e^{-\frac{k^2}{mT}}}{1+k^2a^2}$$

Unitary case OK with Pitaevskii-Stringari, Ho

- Small a limit **$a \to 0_+$**

  $\to$ **Molecules**

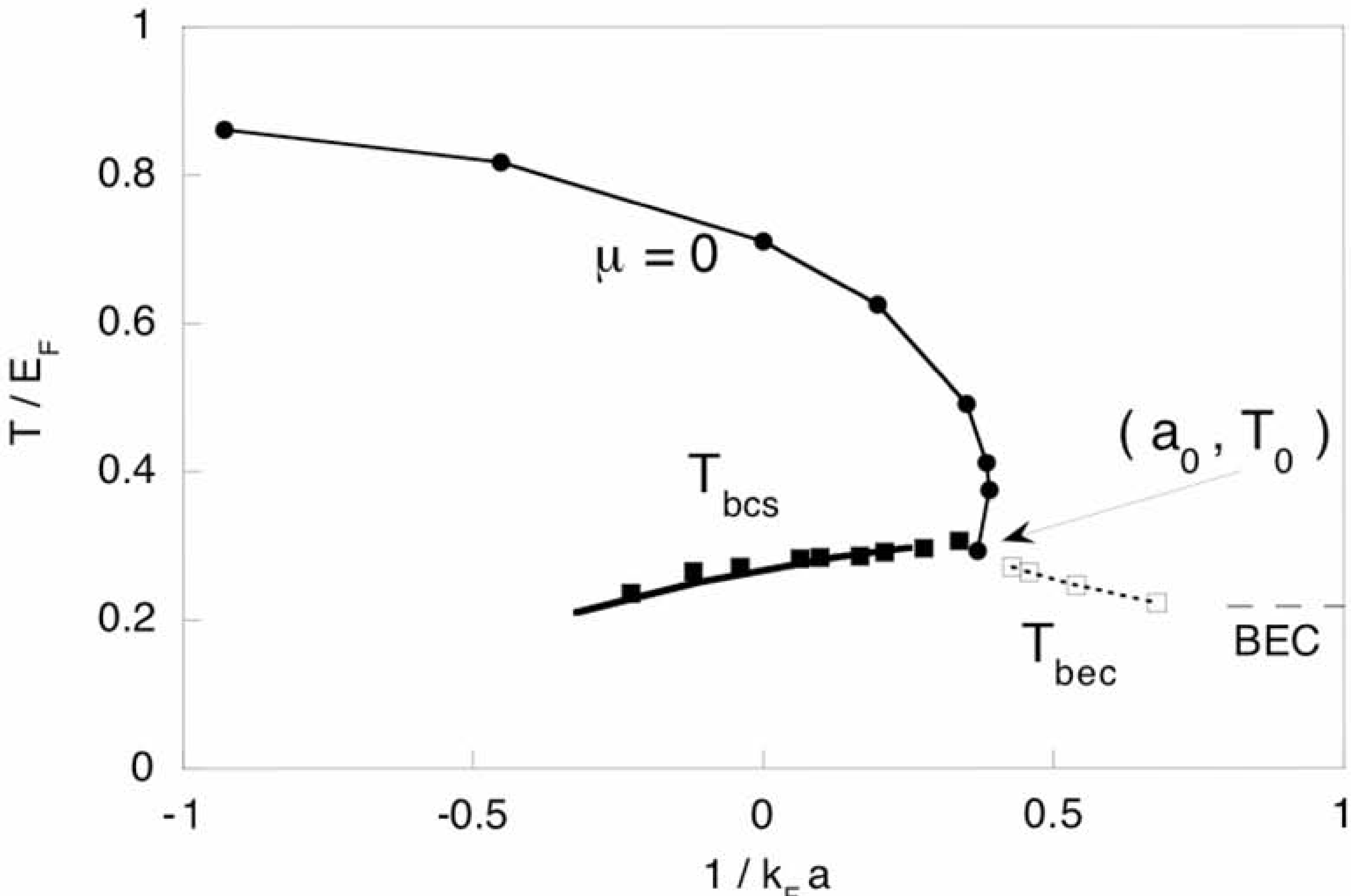
  Small T $\to$ Bose-Einstein condensation

  $$T_{BEC} / E_F = 0.218$$

- Different from Nozières-Schmitt-Rink

  - Full Feshbach resonance can be included
  - Additional diagrams

• $\mu = 0$, T_{BCS} / E_F , T_{BEC} / E_F



• $T=0$ $a^{-1} = 0$ $\beta = -0.39$ — -0.47

• <u>Conclusion</u>

Strong interplay between

Cooper pairs and molecules

Molecular properties

modified by

Fermi sea