6. Fermi gases with tunable interaction

6.1 Motivations

* experimental progress since 2002:
  - → stable, long-lived spin $\frac{1}{2}$ Fermi gases in the strongly interacting regime
  - → scattering length a tuned with Feshbach resonance [Thomas, Salomon, Jin, Ketterle, Grimm, Hulet]
  - → BEC - BCS cross-over can be studied [Early theory: Leggett, Nozières, Schmitt-Rink, Randeria]
* the unitary regime can be obtained:

$$f_k^{s\text{ wave}} = \frac{-1}{u(k)+ik} \qquad u(k) \in \mathbb{R}$$

$$f_k^{\text{unitary}} = \frac{-1}{ik} \qquad \text{universal!}$$

in practice $u(k) \simeq \frac{1}{a} - \frac{1}{2}k^2 r_e$ so have

- "$a = \infty$" $\quad (k|a| \gg 1)$
- $k|r_e| \ll 1$

OK for fermions on broad Feshbach resonances because

k remains $\sim k_F$, $k_F \equiv (6\pi^2 \rho_\uparrow)^{1/3}$

[for bosons, Efimov effect : effective 3-body attraction

k may go up to $1/|r_e|$]

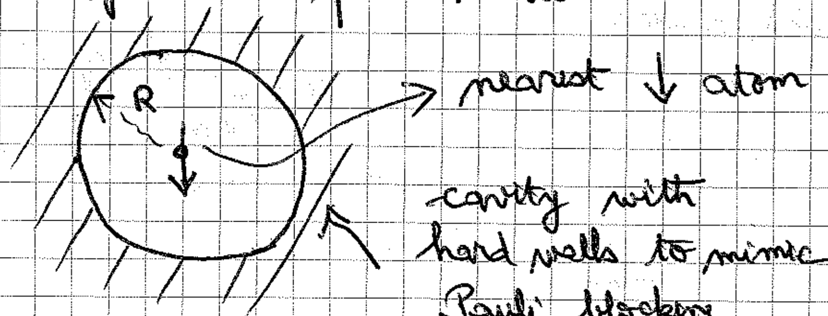
* current hot topic : $N_\uparrow \neq N_\downarrow$

Here we take $N_\uparrow = N_\downarrow$, $\rho_\uparrow = \rho_\downarrow$.

6.2 A toy model : various macroscopic branches

Imagine you are a spin $\uparrow$ atom :

[Pricoupenko]



$R \propto 1/k_F$

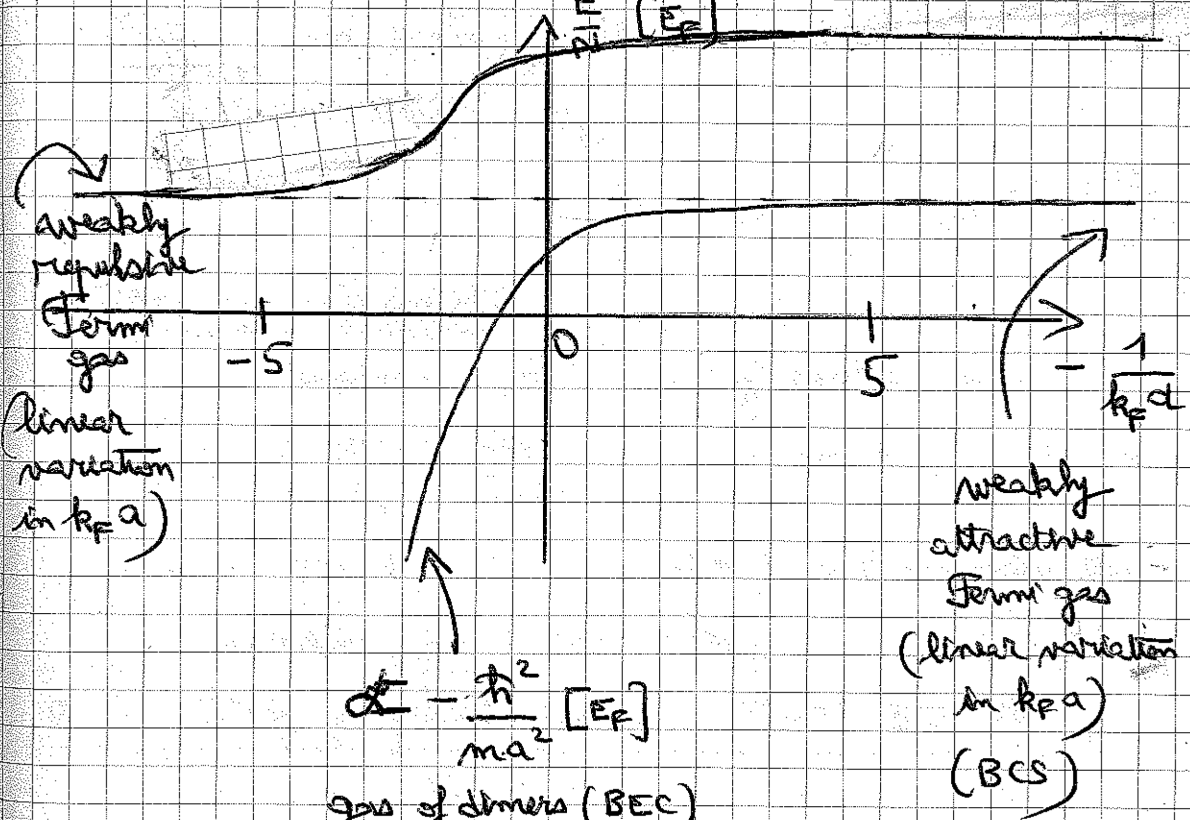
$$\varepsilon \phi(\vec{r}) = -\frac{\hbar^2}{m} \Delta \phi(\vec{r}) \text{ with}$$

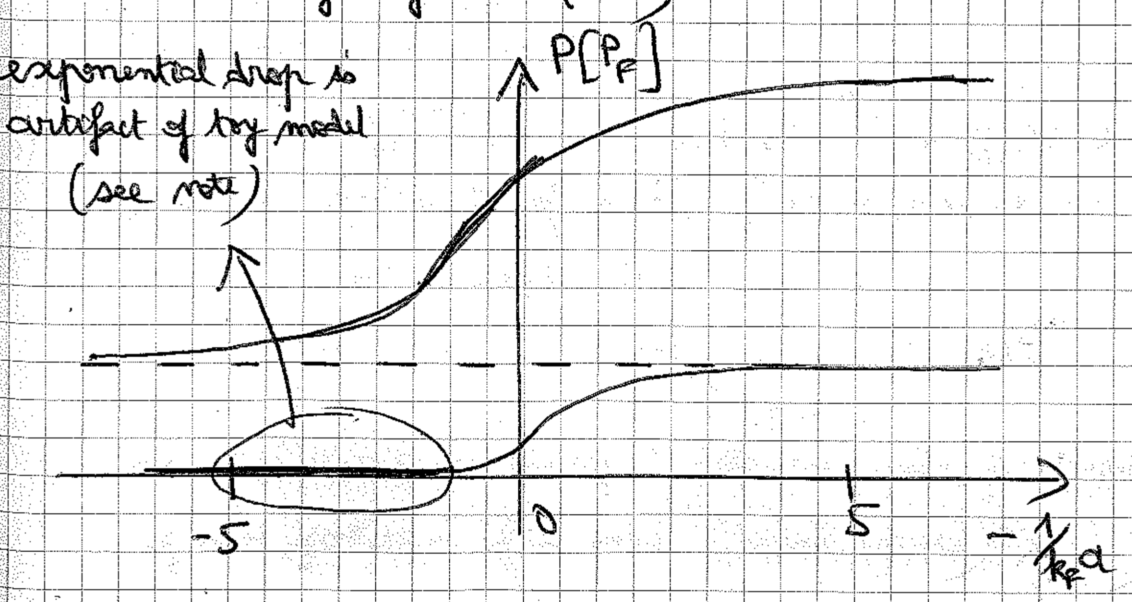
$$\rightarrow \phi(R) = 0$$

$$\rightarrow \phi(r) \underset{r\to 0}{=} A\left(\frac{1}{r} - \frac{1}{a}\right) + O(r^2)$$

Then gas energy $E \propto N\varepsilon$

gas pressure $P = -\partial_V E$ $\quad (V = N/\rho)$


$\frac{E}{N}$ $[E_F]$
weakly repulsive Fermi gas
(linear variation in $k_F a$)
-5
0
5
$-\frac{1}{k_F a}$
weakly attractive Fermi gas
(linear variation in $k_F a$)
(BCS)
$\simeq -\frac{\hbar^2}{m a^2}$ $[E_F]$
gas of dimers (BEC)


$P[P_F]$
exponential drop is artifact of toy model
(see note)
-5
0
5
$-1/k_F a$

__Note:__ in reality, dimers interact with scattering length $a_{dim} = 0{,}6\, a$

$$\Rightarrow \quad P \simeq \frac{1}{2} \rho_{dim}^2 \, g_{dim} \qquad g_{dim} = \frac{4\pi\hbar^2 a_{dim}}{2m}$$

__Seen in experiments:__

→ beginning ($a \to 0^+$) of excited branch
[metastable with respect to dimer formation by 3-body collisions]

→ ground branch: adiabatic and reversible transformation from BEC to BCS

6.3 Study of ground branch: $T=0$ BCS theory

a variational theory that predicts

- long range order in
$$g_1^{pair} = \langle [\psi_\uparrow \psi_\downarrow (\vec{r})]^\dagger [\psi_\uparrow \psi_\downarrow (\vec{0})] \rangle$$
i.e. a condensate of pairs [pairs may be non bosonic: not a simple BEC]
- static theory: energy required to break a pair ("gap")
- time dependent theory: collective modes for center of mass oscillations of the pairs (sound waves)

Lattice model

$$H = \sum_{\vec{k} \in D} \sum_{\sigma=\uparrow,\downarrow} \left(\frac{\hbar^2 k^2}{2m} - \mu\right) a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}$$

$$+ \sum_{\vec{r},\sigma} U(\vec{r})\, \psi_\sigma^\dagger \psi_\sigma + g\, l^3 \sum_{\vec{r}} \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow$$

in the low filling limit $k_F l \ll 1$

6.3.1 BCS ansatz

* a coherent state of pairs:

$$|\psi_{BCS}\rangle = e^{\gamma C^\dagger} |0\rangle \qquad \gamma \in \mathbb{C}$$

$$C^\dagger = \sum_{\vec{r}_1, \vec{r}_2} l^6\, \phi(\vec{r}_1, \vec{r}_2)\, \psi_\uparrow^\dagger(\vec{r}_1)\, \psi_\downarrow^\dagger(\vec{r}_2)$$

creates a pair

* Schmidt decomposition of pair wavefunction:

$$\gamma |\phi\rangle = \sum_\alpha \Gamma_\alpha |A_\alpha\rangle \otimes |B_\alpha\rangle$$

$\Gamma_\alpha \geq 0$ $\quad \{|A_\alpha\rangle\}$ orthonormal basis (spinless) particle

$\{|B_\alpha\rangle\}$ other orthonormal basis

$c^\dagger_{\alpha\uparrow}$ creates in $|\uparrow\rangle|A_\alpha\rangle$

$c^\dagger_{\alpha\downarrow}$ creates in $|\downarrow\rangle|B_\alpha\rangle$

$$\gamma C^\dagger = \sum_\alpha \Gamma_\alpha c^\dagger_{\alpha\uparrow} c^\dagger_{\alpha\downarrow}$$

$$|\Psi_{BCS}\rangle^{\text{norm.}} = \left[\prod_\alpha \frac{1+\Gamma_\alpha c^\dagger_{\alpha\uparrow} c^\dagger_{\alpha\downarrow}}{(1+\Gamma_\alpha^2)^{1/2}}\right]|0\rangle$$

$$= \left[\prod_\alpha \left(U_\alpha - V_\alpha c^\dagger_{\alpha\uparrow} c^\dagger_{\alpha\downarrow}\right)\right]|0\rangle$$

* Wick theorem applies:

$$|\Psi_{BCS}\rangle^{\text{norm.}} = e^{\sum_\alpha \theta_\alpha (c^\dagger_{\alpha\uparrow} c^\dagger_{\alpha\downarrow} - h.c.)}|0\rangle$$

with $\quad U_\alpha = \cos\theta_\alpha \qquad V_\alpha = -\sin\theta_\alpha$

squeezed vacuum for fermions

* basic properties:

$$\langle \hat N\rangle = \sum_\alpha \frac{2\Gamma_\alpha^2}{1+\Gamma_\alpha^2}$$

$$\operatorname{Var}\hat N = \sum_\alpha \frac{4\Gamma_\alpha^2}{(1+\Gamma_\alpha^2)^2} \leq 2\langle \hat N\rangle$$

$\simeq$ for all $\Gamma_\alpha \ll 1$

Why $\simeq$ for all $\Gamma_\alpha \ll 1$?

$$\langle [C, C^\dagger]\rangle = 1 - \frac{\sum_\alpha 2\Gamma_\alpha^4/(1+\Gamma_\alpha^2)}{\sum_\alpha \Gamma_\alpha^2} \simeq 1 \quad \text{if all } \Gamma_\alpha \ll 1$$

a coherent state of $N/2$ bosons:

$$\operatorname{Var}(\hat N/2) = \langle \hat N/2\rangle$$

6.3.2 Energy minimization

$$E_H[\gamma\phi] = \frac{\langle \Psi_{BCS} | H | \Psi_{BCS} \rangle}{\langle \Psi_{BCS} | \Psi_{BCS} \rangle}$$

$$\delta |\Psi_{BCS}\rangle = \sum_{\vec{r}_1, \vec{r}_2} \ell^6 \, \delta(\gamma\phi(\vec{r}_1,\vec{r}_2)) \, \psi_\uparrow^\dagger(\vec{r}_1) \psi_\downarrow^\dagger(\vec{r}_2) |\Psi_{BCS}\rangle$$

$$\equiv \delta\hat{X} \; |\Psi_{BCS}\rangle$$

$$\delta E_H = \underbrace{\langle H \delta\hat{X} \rangle - \langle H \rangle \langle \delta\hat{X} \rangle}_{\text{should vanish } \forall \, \delta(\gamma\phi)} + \text{c.c.}$$

Key results:

① $\exists$ quadratic Hamiltonian $\mathcal{H}$ such that

$$\langle H \delta\hat{x} \rangle - \langle H \rangle \langle \delta\hat{x} \rangle = \langle \mathcal{H} \delta\hat{x} \rangle - \langle \mathcal{H} \rangle \langle \delta\hat{x} \rangle \quad \forall \, \delta(\gamma\phi)$$

② $\mathcal{H}$ obtained by Wick contractions:

$$g_0 \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow \Longrightarrow \psi_\uparrow^\dagger \psi_\downarrow^\dagger \; g_0 \langle \psi_\downarrow \psi_\uparrow \rangle + \text{h.c.}$$

$$g_0 \langle \psi_\downarrow \psi_\uparrow \rangle \equiv \Delta(\vec{r}) \quad \text{pairing term}$$

$$+ \psi_\uparrow^\dagger \psi_\uparrow \, g_0 \langle \psi_\downarrow^\dagger \psi_\downarrow \rangle + \uparrow \leftrightarrow \downarrow$$

Hartree mean field term

vanishes for $\ell \to 0$ ($g_0 \to 0$)

(3) eigenstates of quadratic Hamiltonians are BCS states

Consequences:

$$\delta E_H = 0 \; + \; (1) \;\Longrightarrow\; \delta E_{\mathcal{H}} = 0$$

$+$ (3) : $|\Psi_{BCS}\rangle$ is an eigenstate of $\mathcal{H}$

* BCS energy minimization amounts to calculating the ground state of a quadratic hamiltonian $\mathcal{H}[\langle\psi_\downarrow \psi_\uparrow\rangle]$

A self-consistent problem:

$$\langle\psi_\downarrow \psi_\uparrow\rangle_0 = \langle\psi_\downarrow \psi_\uparrow\rangle$$

* one can also take excited states of $\mathcal{H}$:

easy access to pair breaking excitations of the gas

6.3.3 Diagonalisation of a quadratic Hamiltonian

Heisenberg equations of motion for the field are linear:

$$i\hbar\, \partial_t \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow^+ \end{pmatrix} = L^\uparrow \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow^+ \end{pmatrix}$$

$$L^\uparrow = \begin{pmatrix} h & \Delta \\ \Delta^* & -h^* \end{pmatrix}$$ hermitian [here, $h = \frac{p^2}{2m} + U - \mu + g_0 \langle\psi_\uparrow^+ \psi_\uparrow\rangle$]

modal expansion :

$$\begin{pmatrix} \psi_\uparrow(\vec{r}) \\ \psi_\downarrow^\dagger(\vec{r}) \end{pmatrix} = \sum_{\varepsilon_\alpha>0} b_{\alpha\uparrow} \begin{pmatrix} u_\alpha(\vec{r}) \\ v_\alpha(\vec{r}) \end{pmatrix} + b_{\alpha\downarrow}^\dagger \begin{pmatrix} -v_\alpha^*(\vec{r}) \\ u_\alpha^*(\vec{r}) \end{pmatrix}$$

eigenenergy $\varepsilon_\alpha > 0$ eigenenergy $-\varepsilon_\alpha < 0$

$$\mathcal{H} = ct + \sum_{\varepsilon_\alpha>0,\sigma} \varepsilon_\alpha b_{\alpha\sigma}^\dagger b_{\alpha\sigma}$$

In ground state of $\mathcal{H}$:

total density $\quad \rho(\vec{r}) = 2 \sum_{\varepsilon_\alpha>0} |v_\alpha(\vec{r})|^2$

" gap " function

$$\Delta(\vec{r}) = -g_0 \sum_{\varepsilon_\alpha>0} u_\alpha(\vec{r}) v_\alpha^*(\vec{r})$$

6.3.4 Discussion of homogeneous case

spectrum $\quad \varepsilon_k = \left[\left(\frac{\hbar^2 k^2}{2m} - \mu\right)^2 + \Delta^2\right]^{1/2}$

① density : $\quad \rho = \int_{\cancel{D}\ \mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3} \left[1 - \frac{\frac{\hbar^2k^2}{2m} - \mu}{\varepsilon_k}\right]$

② gap equation : $\quad \frac{\Delta}{g_0} = -\int_D \frac{d^3\vec{k}}{(2\pi)^3} \frac{\Delta}{2\varepsilon_k}$

$$\frac{\Delta}{g} = \Delta \int \frac{d^3\vec{k}}{(2\pi)^3} \left[\frac{m}{\hbar^2 k^2} - \frac{1}{2\varepsilon_k}\right]$$

(3) pair wavefunction

$$\phi(\vec{r}_1-\vec{r}_2) \propto \sum_{\vec{k}\in D} \Gamma_{\vec{k}}\, e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}$$

$$\Gamma_k = -\frac{V_k}{U_k} = \frac{-\Delta}{\frac{\hbar^2k^2}{2m}-\mu+E_k}$$

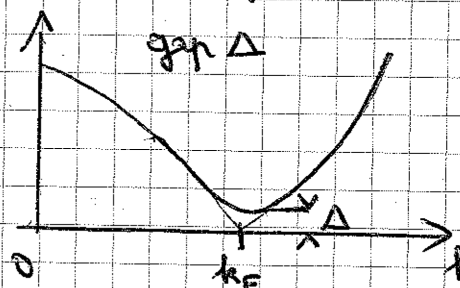
* limit $a\to 0^-$: $\mu>0$, $\Delta\to 0$

$$\int_{\mu-\delta}^{\mu+\delta} dE\, \underbrace{\rho(E)}_{\text{DoS}} \frac{1}{\sqrt{\Delta^2+(E-\mu)^2}} \underset{\Delta\to 0}{\sim} 2\rho(\mu)\ln\frac{2\delta}{\Delta}$$

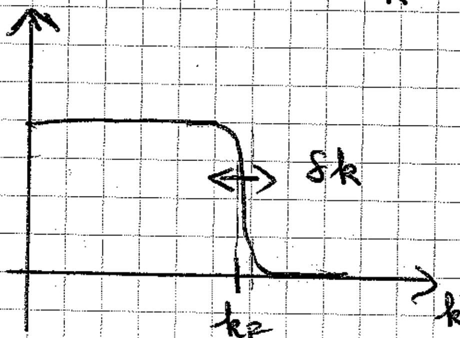
$$\Longrightarrow \quad \Delta \simeq 8e^{-2}\,\mu\, e^{-\pi/2k_F|a|}$$

$\rho \simeq \rho_{\text{ideal gas}}$

gap Δ



momentum distribution V_k^2



⚠ no gap in collective excitations (sound waves)

$$\frac{\hbar k_F \delta k}{m} \simeq \Delta$$

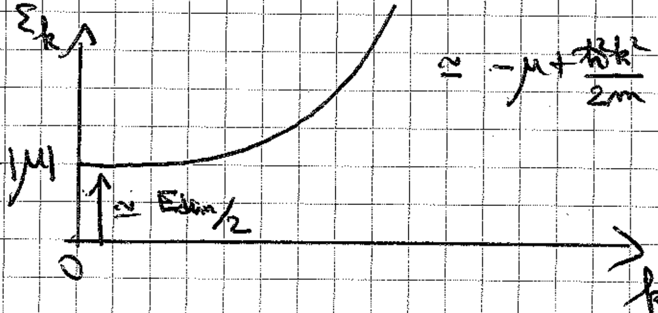
$1/\delta k$ = size of a pair

* limit $a \to 0^+$: $\mu \to -\infty$, $\Delta \to +\infty$ but $\Delta \ll |\mu|$

(2) $\Rightarrow$ $\frac{1}{g} \simeq \int \frac{d^3k}{(2\pi)^3} \frac{m}{\hbar^2 k^2} - \frac{1}{\frac{\hbar^2 k^2}{m} - 2\mu}$

$\mu \simeq -\frac{\hbar^2}{2ma^2} = -E_{dim}/2$ [Remember $\mu = \frac{\mu_{mol}}{2}$]

(1) $\Delta \simeq \frac{2}{\sqrt{3\pi}} (k_F a)^{3/2} \frac{\hbar^2}{ma^2}$ is not the gap



$\simeq -\mu + \frac{\hbar^2 k^2}{2m}$

Δ no gap in collective excitations (sound waves)

(3) $\Gamma_k \simeq \frac{-\Delta}{2\left[\frac{\hbar^2 k^2}{2m} - \mu\right]} \ll 1 \quad \forall k \Rightarrow$ pairs are bosons

$\Phi(\vec{r}_1 - \vec{r}_2) \simeq \frac{1}{L^{3/2}} \Phi_{dim}(|\vec{r}_1 - \vec{r}_2|)$

$\Phi_{dim}(r) \propto \frac{e^{-r/a}}{r}$ (Bethe-Peierls)

* $a \to \infty$:

$\mu = \eta\, \mu_{ideal} = \eta \frac{\hbar^2 k_F^2}{2m}$ $\quad \Delta \propto E_F$, $\mu \propto E_F$

$\eta \lesssim \eta_{BCS} = 0.5906\ldots$

$\eta_{QMC} \simeq 0.4$ (Juillet) confirms fixed node (Pandharipande, Giorgini) and agrees with latest experiments