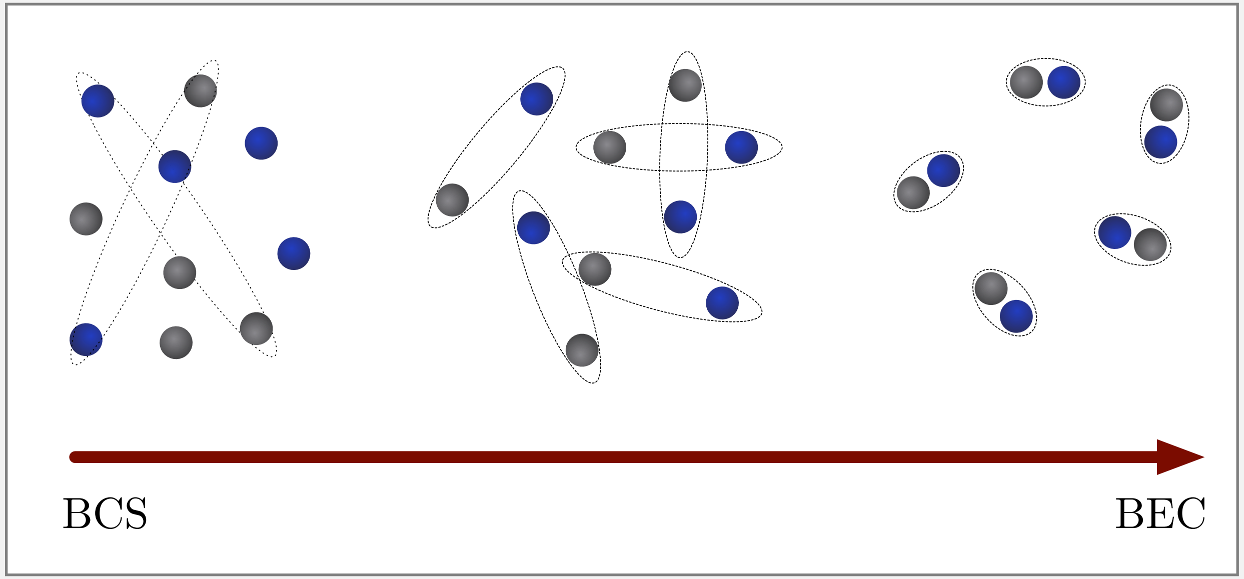
BEC-BCS crossover and beyond

Meera Parish

Monash University (Melbourne)

Introduction

- What is the BCS-BEC crossover?

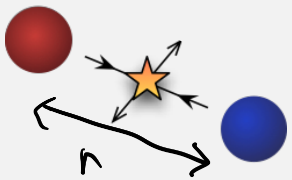


- Why study it?
  - First realization in cold-atom experiments
  - Relevant to a range of systems
    e.g., neutron stars, superconductors, excitons…

Outline of lectures

- Two-body physics
  - Feshbach resonance
- BCS-BEC crossover
  - Ground state & excitations
  - Unitarity
- Finite temperature
- Spin-imbalanced Fermi gas
  - Quantum phase transitions
  - The polaron problem

Two-body physics



- C.O.M. : one-body problem:

$$-\frac{\hbar^2}{2m_r}\nabla^2\psi + V(r)\psi(r) = E\psi(r)$$

$2m_r$ ← reduced mass

$V(r)$ ← rotationally symmetric + short-ranged

⇒ Radial component: $R(r) = u(r)/r$ ⇒

$$\left[-\frac{\hbar^2}{2m_r}\frac{\partial^2}{\partial r^2} + \cancel{\frac{\hbar^2 \ell(\ell+1)}{2m_r r^2}} + V(r)\right]u(r) = Eu(r)$$

← centrifugal barrier

Low energy: $E \ll \frac{\hbar^2}{m_r r_0^2}$

r_0 ⇒ range of interaction

→ Experience $V(r)$ if $\ell = 0$ (s-wave) scattering

For $r > r_0$, we have:

$$u_>''(r) + \frac{2m_r}{\hbar^2}E u_>(r) = 0$$

$$E = \frac{\hbar^2 k^2}{2m_r}$$

↳ General sol'n:

$$u_>(r) = C\sin(kr + \delta_0(k)) \quad (*)$$

$\delta_0(k)$ ← phase shift

[No interactions: $u(r=0) = 0$ {otherwise $\nabla^2\psi$ diverges @ $r=0$}

⇒ $\delta_0 = 0$]

For $r < r_0$, we can ignore E:

$$u_<''(r) - \frac{2m_r}{\hbar^2}V(r)u_<(r) = 0$$

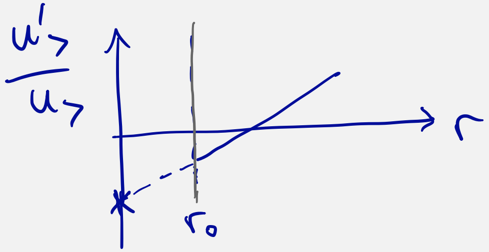
∴ B.C. for sol'n (*) is independent of E:

$$\left.\frac{u_>'}{u_>}\right|_{r=0} = \text{const.} \equiv -1/a$$

scattering length (s-wave)

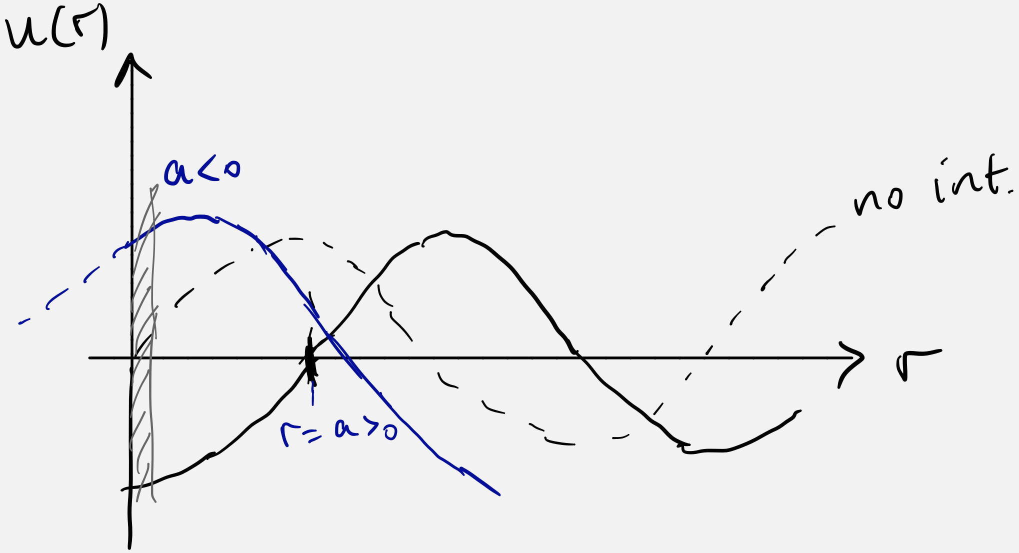
$$\therefore \left.\frac{u'_>}{u_>}\right|_{r=0} = k\cot(kr+\delta_0)\Big|_{r=0} = k\cot(\delta_0)$$

$$= -1/a$$



For $k|a| \ll 1$, $\quad \tan\delta_0 = -ka \simeq \delta_0$

$$\therefore u(r) \simeq C\sin(kr - ka)$$



Now $\psi(r) = \dfrac{u(r)}{r} = C\,\dfrac{\sin(kr+\delta_0)}{r}$

$$= \frac{C}{r}\left[\frac{e^{i(kr+\delta_0)} - e^{-i(kr+\delta_0)}}{2i}\right]$$

$$= \frac{C e^{-i\delta_0}}{2i}\left[e^{i2\delta_0}\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}\right]$$

Compare this with:

$$\Psi(r) = \frac{1}{2ik}\left[(1+2ikf_0(k))\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}\right], \quad r\to\infty$$

$$\therefore 1 + 2ikf_0(k) = e^{2i\delta_0} \qquad [\text{Sakurai}]$$

$$\boxed{f_0(k) = \frac{1}{k\cot\delta_0 - ik} = \frac{1}{-1/a - ik}}$$

Bound states

$\Rightarrow$ Poles of scattering amplitude : $f_0^{-1}(k) = 0$

$$\psi(r) = \psi_{inc} + \underbrace{\psi_{scat}}_{f_0(k)\frac{e^{ikr}}{r}}$$

Also, $k = iQ$ (not $-iQ$) $\rightsquigarrow \dfrac{e^{-Qr}}{r}$

$\hookrightarrow E = \dfrac{\hbar^2 k^2}{2m_r} = -\dfrac{\hbar^2 Q^2}{2m_r} < 0$

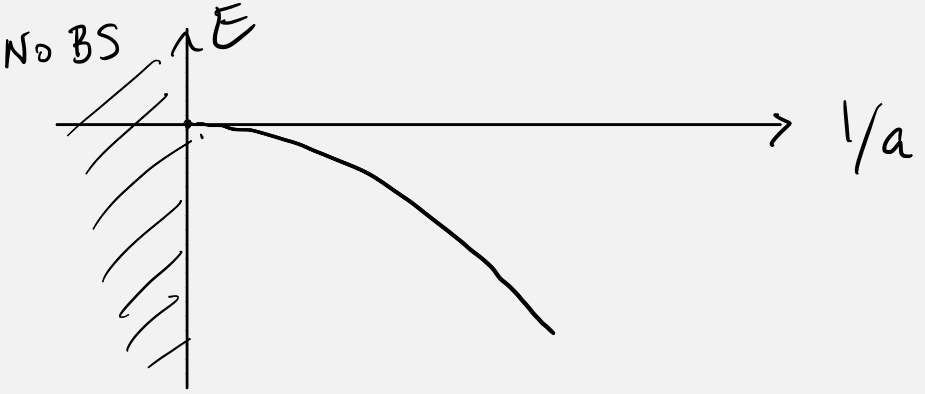
$\therefore$ we have : $-1/a - i(iQ) = 0$

$\therefore Q = 1/a$

$\therefore$ only have bound state when $a > 0$

$$E = -\frac{\hbar^2}{2m_r a^2}$$

$|a| \gg r_0$

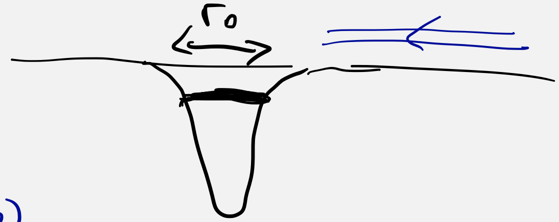


B.S. appears at $1/a = 0$

N.B. Cross section:

$$\sigma(k) \simeq |f_0(k)|^2 = \left|\frac{1}{k}\right|^2$$

$1/a = 0$



⌜Attractive potential with bound state "repels" $(a > 0)$ since scattering states must be orthogonal to bound state⌟

Feshbach resonance

→ Regime: $|a| \gg r_0$

Atom-atom potential depends on electron spin, not nuclear spin:

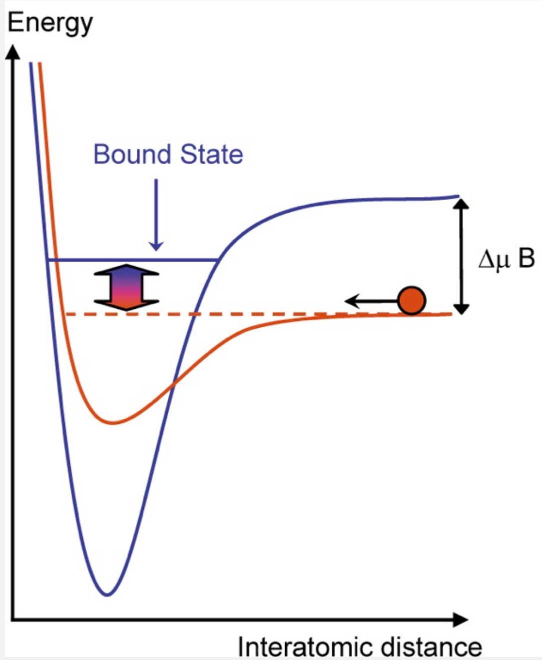
$$V(r) = V_0(r) + V_S(r)\,\hat{S}_1 \cdot \hat{S}_2$$

e^-: hyperfine interaction $S \cdot I$

can couple potentials with different electron spin configurations

+ magnetic field B vary energy difference

$\Rightarrow$ vary scattering length a



• Further reading:

Chin et al. RMP 82, 1225 (2010)

Renormalization

→ Use 2-body problem to replace interaction potential by scattering parameters

- Consider S.E. in operator form:

$$(\hat{H}_0 + \hat{V})|\psi\rangle = E|\psi\rangle$$

General sol'n (Lippmann-Schwinger):

$$|\psi\rangle = |\psi_0\rangle + \underbrace{(E - \hat{H}_0 + i0)^{-1}}_{\text{Green's function } \hat{G}_0(E)} \hat{V}|\psi\rangle$$

$$\left[\hat{H}_0|\psi_0\rangle = E|\psi_0\rangle\right]$$

unscattered wave

Define T matrix: $\hat{V}|\psi\rangle = \hat{T}|\psi_0\rangle$

$$\therefore |\psi\rangle = (1 + \hat{G}_0\hat{T})|\psi_0\rangle \quad (1)$$

Now $|\psi\rangle = |\psi_0\rangle + \hat{G}_0\hat{V}|\psi\rangle$

$$\hookrightarrow (1 - \hat{G}_0\hat{V})|\psi\rangle = |\psi_0\rangle \quad (2)$$

$$\hookrightarrow |\psi\rangle = (1 - \hat{G}_0\hat{V})^{-1}|\psi_0\rangle \quad (1),(2)$$

$$= (1 + \hat{G}_0\hat{T})|\psi_0\rangle$$

$$\therefore 1 + \hat{G}_0\hat{T} = (1 - \hat{G}_0\hat{V})^{-1}$$

$$\Rightarrow (1 - \hat{G}_0\hat{V})(1 + \hat{G}_0\hat{T}) = 1$$

i.e. $\hat{G}_0\hat{T} - \hat{G}_0\hat{V} - \hat{G}_0\hat{V}\hat{G}_0\hat{T} = 0$

$$\therefore \boxed{\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{T}}$$

$$\Rightarrow \boxed{\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{T}}$$ (infinite series)

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \ldots$$

- Related to scattering amplitude:

$$f(\vec{k}', \vec{k}) = -\frac{1}{4\pi}\frac{2m_r}{\hbar^2}\langle \vec{k}' | \hat{T} | \vec{k} \rangle$$

Contact interactions: $\langle \vec{k}' | \hat{V} | \vec{k} \rangle = g$

$$\langle k' | \hat{T}(E) | k \rangle = \langle k' | \hat{V} | k \rangle + \langle k' | \hat{V}\hat{G}_0\hat{V} | k \rangle + \ldots$$

$$= g + \frac{g^2}{\Omega}\sum_q \langle q | \hat{G}_0 | q \rangle + \ldots$$

$$= \left(\frac{1}{g} - \frac{1}{\Omega}\sum_q \langle q | \hat{G}_0 | q \rangle \right)^{-1}$$

$$\hat{G}_0 = \frac{1}{E - H_0}$$

$$f_0(k) = \frac{1}{-1/a - ik}$$

Take $E = 0$: $f = -a$

(3D)

- We have:

$$\frac{1}{g(\Lambda)} + \frac{1}{\Omega}\sum_q^{\Lambda} \frac{1}{q^2/2m_r} = \frac{m_r}{2\pi\hbar^2 a}$$

$\therefore$ $g \sim 1/\Lambda \to 0$ as $\Lambda \to \infty$

[Λ is high momentum cutoff set by range of potential; Ω is system volume]

BCS-BEC crossover

* Consider 2-component Fermi gas $(\uparrow, \downarrow)$
  - → equal populations $(n_\uparrow = n_\downarrow = n)$
    $(\mu_\uparrow = \mu_\downarrow = \mu)$
  - → equal masses $(m_\uparrow = m_\downarrow = m)$
  - → attractive contact interactions

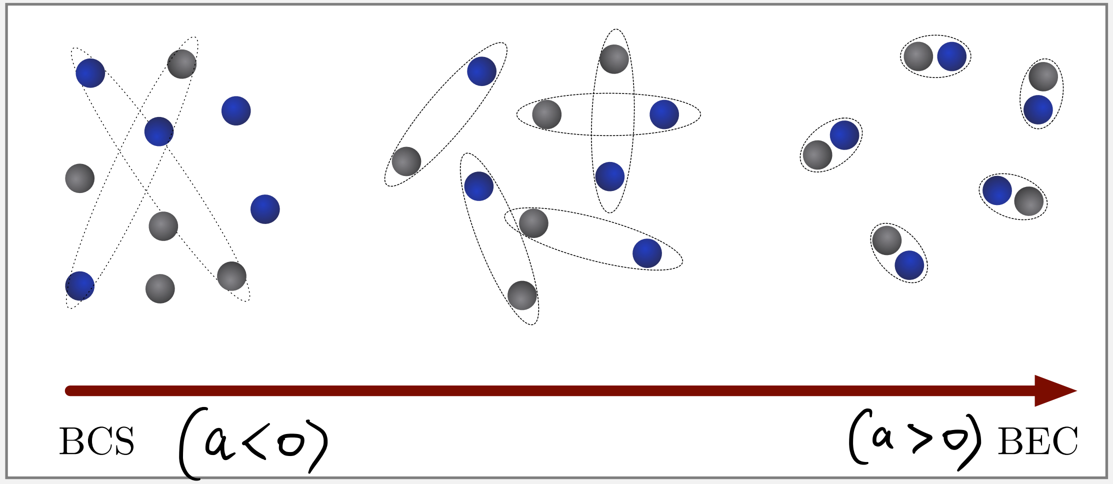
* Hamiltonian:

$$\hat{H} - \mu \hat{N} = \sum_{k,\sigma} (\varepsilon_k - \mu) \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma}$$

$$+ \frac{g}{\Omega} \sum_{k,k',q} c^\dagger_{k+q/2\uparrow} c^\dagger_{-k+q/2\downarrow} c_{-k'+q/2\downarrow} c_{k'+q/2\uparrow}$$

BCS wave function:

$$\boxed{|\psi\rangle = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}) |0\rangle}$$



(i) Variational wave function

- Boson operator $b^\dagger_q = \sum_k \varphi_k c^\dagger_{k+q/2\uparrow} c^\dagger_{-k+q/2\downarrow}$

- BEC limit ⇒ coherent state:

$$|\psi\rangle = N e^{\lambda b^\dagger_0} |0\rangle = N e^{\lambda \sum_k \varphi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}} |0\rangle$$

normalization

$$(c^\dagger_{k\sigma})^2 = 0$$

$$\hookrightarrow |\psi\rangle = N \prod_k (1 + \lambda \varphi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}) |0\rangle$$

MMP, arXiv:1402.5171

⊛ BCS wave function:

$$|\Psi\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle$$

where $v_k/u_k = \lambda \varphi_k$, $N = \prod_k u_k$

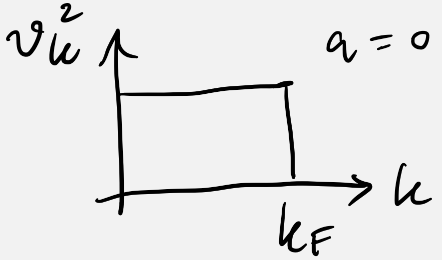
and $u_k^2 + v_k^2 = 1$

⇒ Smoothly connected to coherent state of bosons (BEC)

→ Non-interacting case $(a=0)$:

$$|FS\rangle = \prod_{|k|<k_F} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}|0\rangle$$

Note: $\langle\Psi|c^\dagger_{k\sigma} c_{k\sigma}|\Psi\rangle = v_k^2$



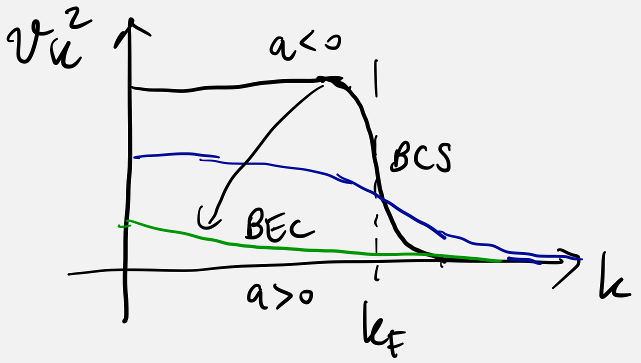
Fermi wave vector:

$$k_F = (6\pi^2 n)^{1/3}$$

$$\left[n = \frac{1}{\Omega}\sum_k v_k^2\right]$$

$$\mu = \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Behavior throughout crossover $(T=0)$:

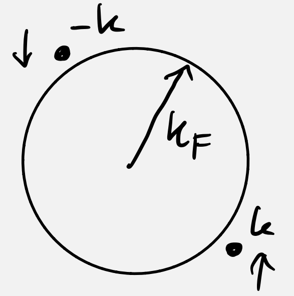


Unitarity $1/a = 0$:

$$\mu = \xi\, \varepsilon_F$$

universal constant

Cooper pair:



⊛ Free energy

Ground-state wave function:

$$|\Psi\rangle = \prod_k \left(u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow}\right)|0\rangle$$

$$F = \langle\Psi|(\hat{H} - \mu\hat{N})|\Psi\rangle$$

$$= 2\sum_k (\varepsilon_k - \mu) v_k^2 + \frac{g}{\Omega}\sum_{k,k'} v_k u_k v_{k'} u_{k'}$$

$$+ \underbrace{\frac{g}{\Omega}\sum_{k,k'} v_k^2 v_{k'}^2}_{\sim g n^2 \longrightarrow 0 \text{ as } g \to 0}$$

$\Rightarrow$ Minimize F w.r.t. u_k, v_k at fixed μ:

$\hookrightarrow u_k^2 + v_k^2 = 1 \Rightarrow v_k = \sin\theta_k$

$u_k = \cos\theta_k$

$\frac{\partial F}{\partial \theta_k} = 0$:

$$2(\varepsilon_k - \mu) u_k v_k + (u_k^2 - v_k^2)\frac{g}{\Omega}\sum_{k'} u_{k'} v_{k'} = 0 \quad (**)$$

Limit $v_k \to 0$, we recover 2-body eq'n:

$$2\varepsilon_k v_k + \frac{g}{\Omega}\sum_{k'} v_{k'} = 2\mu v_k$$

$$\therefore 2\mu \simeq -\varepsilon_B = -\frac{\hbar^2}{m a^2} \quad \text{(BEC limit)}$$

Defining $\Delta = -\frac{g}{\Omega}\sum_k u_k v_k$, $\xi_k = \varepsilon_k - \mu$,

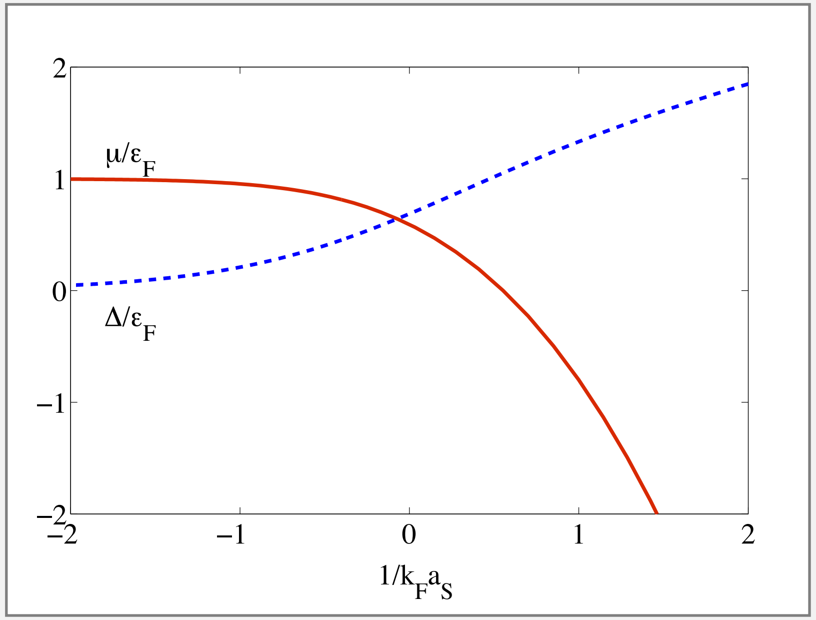
Eq (**) becomes:

$$\frac{u_k v_k}{u_k^2 - v_k^2} = \frac{\Delta}{2\xi_k} = \frac{1}{2}\frac{\sin 2\theta_k}{\cos 2\theta_k}$$

$$\Rightarrow \sin 2\theta_k = \frac{\Delta}{\sqrt{\xi_k^2 + \Delta^2}}, \quad \cos 2\theta_k = \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}}$$

$$\hookrightarrow u_k v_k = \frac{\Delta}{2\sqrt{\xi_k + \Delta^2}}$$

BCS-BEC crossover



BCS limit $1/k_F a \to -\infty$:

$$\mu \simeq \varepsilon_F$$

$$\Delta/\varepsilon_F \simeq \# \, e^{\pi/2k_F a}$$

$$\boxed{\begin{array}{ll} (1) & -\dfrac{1}{g} = \dfrac{1}{\Omega} \displaystyle\sum_k \dfrac{1}{2\sqrt{\xi_k^2 + \Delta^2}} \; ; \; \text{"Gap eq'n"} \\ (2) & n = \dfrac{1}{2\Omega} \displaystyle\sum_k \left(1 - \dfrac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right) \; [\text{Number eq'n}] \end{array}}$$

$$\Delta = -\frac{g}{\Omega} \sum_k u_k v_k = -\frac{g}{\Omega} \sum_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle$$

↳ gives measure of fermion pairing

Replace g with a:

$$\frac{1}{g} + \frac{1}{\Omega} \hat{\sum_k} \frac{1}{2\varepsilon_k} = \frac{m}{4\pi\hbar^2 a} \, ,$$

where $\varepsilon_k = \dfrac{\hbar^2 k^2}{2m}$

(ii) "Mean-field approach"

Assume pairing dominates, such that:

$$\Delta = -\frac{g}{\Omega}\sum_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle$$

↳ zero momentum

Write operators:

$$-\frac{g}{\Omega}\sum_k c^\dagger_{k+q/2\uparrow}\, c^\dagger_{-k+q/2\downarrow} = \Delta\,\delta_{q,0} + \delta\hat{\Delta}_q$$

where $\delta\hat{\Delta}_q = -\Delta\,\delta_{q,0} - \frac{g}{\Omega}\sum_k c^\dagger_{k+q/2\uparrow}\, c^\dagger_{-k+q/2\downarrow}$

↳ assume small

Now expand $\hat{H}_{int}$:

$$\hat{H}_{int} = \frac{\Omega}{g}\sum_q \left|\Delta\delta_{q0} + \delta\hat{\Delta}_q\right|^2$$

$$\simeq \frac{\Omega}{g}\Delta^2 + \Delta\sum_q \delta_{q0}\left(\delta\hat{\Delta}_q + \delta\hat{\Delta}^\dagger_q\right)$$

$$\therefore\ \hat{H}_{int} \simeq -\frac{\Omega}{g}\Delta^2 - \Delta\sum_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - \Delta\sum_k c_{-k\downarrow} c_{k\uparrow}$$

∴ we have mean-field Hamiltonian:

$$\hat{H}_{MF} = -\frac{\Omega}{g}\Delta^2 + \sum_k \Psi^\dagger_k \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta & \mu - \varepsilon_k \end{pmatrix} \Psi_k + \sum_k (\varepsilon_k - \mu)$$

where $\Psi^\dagger_k = (c^\dagger_{k\uparrow}, c_{-k\downarrow})$

Diagonalise using transformation:

$$\begin{pmatrix} \gamma^\dagger_{k\uparrow} \\ \gamma_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix}\begin{pmatrix} c^\dagger_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix}$$

$$\therefore\ \hat{H}_{MF} = -\frac{\Omega}{g}\Delta^2 + \sum_k(\varepsilon_k - \mu - E_k) + \sum_{k\sigma} E_k \gamma^\dagger_{k\sigma}\gamma_{k\sigma}$$

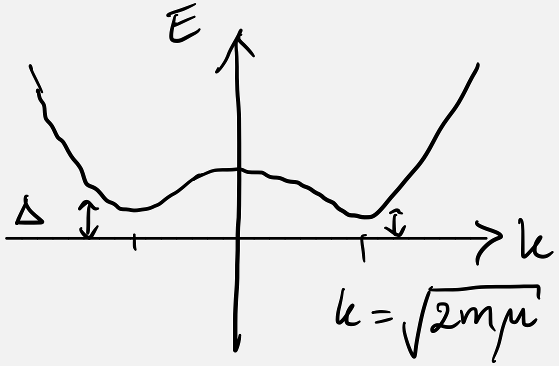
$$\Rightarrow E_k = \sqrt{\xi_k^2 + \Delta^2} > 0$$

- Ground state:

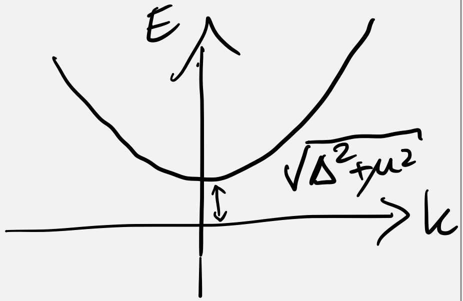
$$\langle \hat{H}_{MF} \rangle = -\frac{\Omega}{g}\Delta^2 + \sum_k \left(\varepsilon_k - \mu - E_k\right)$$

$$\frac{\partial}{\partial \Delta}\langle \hat{H}_{MF} \rangle = 0 \Rightarrow \text{Gap eq'n}$$

- Excitation energy: $E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$



$\mu > 0$



$\mu < 0$

Qualitative change $\underline{@ \ \mu = 0}$ $\Rightarrow$ "crossover point"

MFT: $1/k_F a \simeq 0.55$ (see earlier fig.)

Unitarity $1/k_F a = 0$: universal + scale invariant

$\therefore \mu = \xi \varepsilon_F$, pressure $P = \xi P_{FG}$

non-int gas

where ξ is universal constant.

Best estimate: $\xi \simeq 0.37$ [MIT expt]

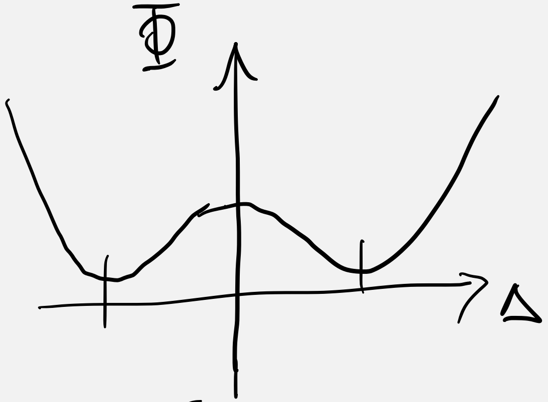
Ku et al Science 2012

(MFT: $\xi \simeq 0.59$)

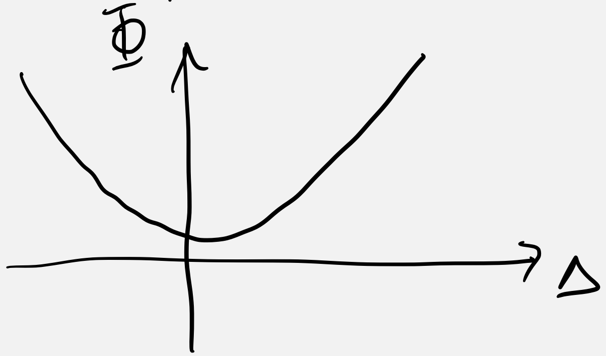
⊛ How can pairing/condensation be destroyed?

- Finite temperature

$$\Phi_{MF} = -\frac{\Omega}{g}\Delta^2 + \sum_k (\varepsilon_k - \mu - E_k) - \frac{2}{\beta}\sum_k \log\left(1+e^{-\beta E_k}\right)$$

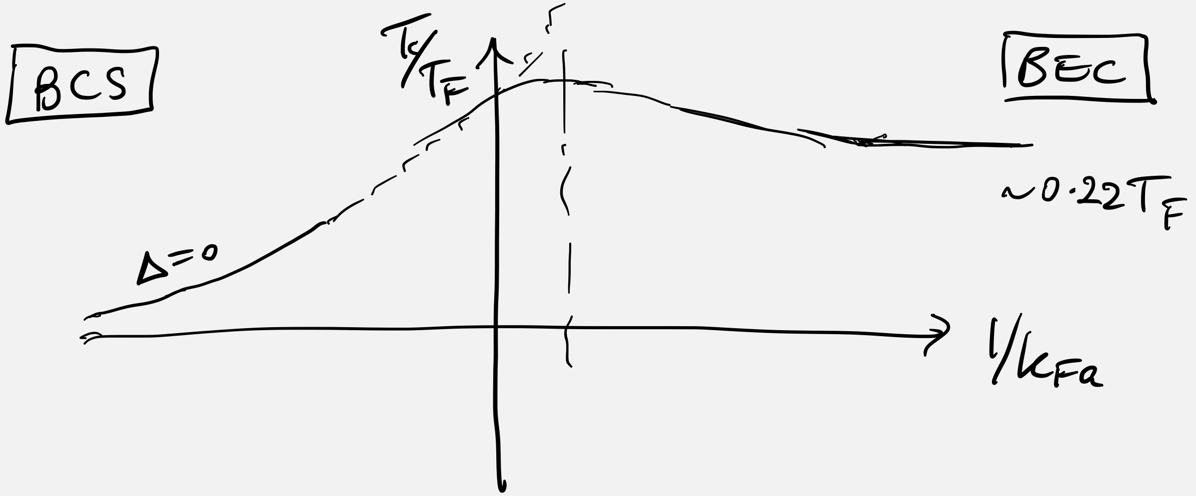


$T < T_c$



$T > T_c$

$\rightarrow$ min. @ $\Delta = 0$



- Spin imbalance