Fermionic pairs and BCS-BEC crossover

Jörg Holsten

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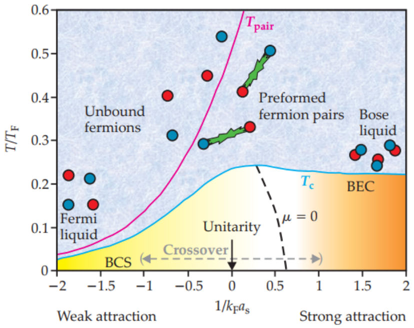


taken from [5]

Overview

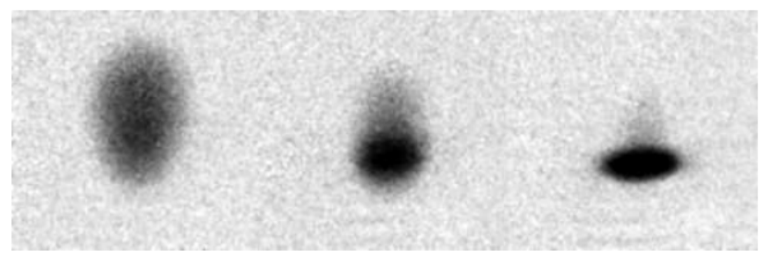
1. Historic Overview
2. Off-Diagonal Long-Range Order
3. Basics of interacting fermi gas and ground state
4. Low excitations
5. Pair formation and condensation temperature

Historic Overview

Historic Overview

- 1954: Cooper-pairs (in momentum space). Bound state of two electrons via phonon interaction on top of filled fermi sphere.
- 1957 Barden, Cooper and Schrieffer extended single Cooper pair to many particle wave function. Succesfully explained superconductivity at the time.
- 1962: Yang conjectures that BEC is possible for fermions if density matrix exhibits off-diagonal long-range order
- 1970's: ^3He-superfluidity discovered. Apparantly fermionic pairs without phonons. BCS more general?
- 1980: Leggett assumed pairs of oppotsite spin and contact interaction $\rightarrow$ first theory of BCS-BEC at $\mathrm{T} = 0$
- 1985: Nozières and Schmitt-Rink extended Leggett's theory to $T \approx T_c$

- 1986: Discovery of high-temperature superconductors. Engelbrecht, Randeria and Sa de Melo extended low temperature theory.
- 2003: first BEC of fermionic pairs at MIT and Innsbrück:



^{6}Li atoms form a condensate at $T \approx 600$ nK. Condensate fraction: 0.75.
Taken from [2]

Off-Diagonal Long-Range Order

Properties of reduced density matrices

N-particle density matrix ρ , $Tr(\rho) = 1$.

- Define reduced density matrices:

$$\langle i|\rho_1|j\rangle = Tr(a_i \rho a_j^\dagger) , \langle ij|\rho_2|kl\rangle = Tr(a_i a_j \rho a_l^\dagger a_k^\dagger) , etc. \quad (1)$$

- Generally, largest eigenvalue λ_i of ρ_i bounded by:

$$\lambda_1 \leq Tr(\rho_1) = N , \lambda_2 \leq Tr(\rho_2) = N(N-1) , etc. \quad (2)$$

- Fermions:

$$\lambda_1 \leq 1 , \lambda_2 \leq N \rightarrow \lambda_2 \approx N \text{ means BEC!} \quad (3)$$

Off-Diagonal Long-Range Order (ODLRO)

Idea corresponds to long-range correlation in (classical) solids!

- Definition of ODLRO:

$$\langle \mathbf{x} | \rho_1 \left| \mathbf{y} \right\rangle > 0 \text{ for } |\mathbf{x} - \mathbf{y}| \to \infty \iff \lambda_1 = \mathcal{O}(N) \equiv \alpha N \tag{4}$$

- For fermions no ODLRO in ρ_1 , but in ρ_2:

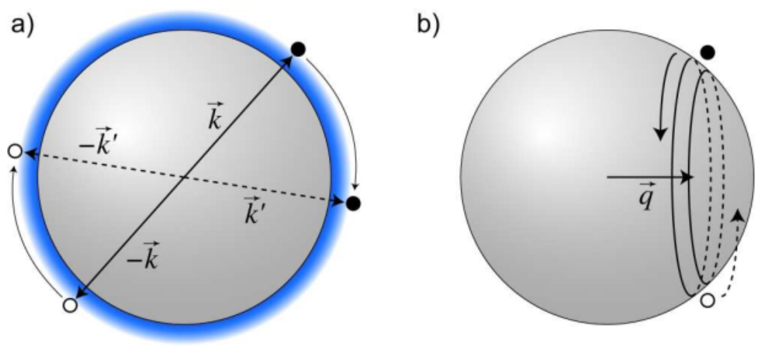
$$\langle \mathbf{x}_1 \mathbf{x}_2 | \rho_2 \left| \mathbf{y}_1 \mathbf{y}_2 \right\rangle \approx 0 \text{ execpt region around } \mathbf{x} := \mathbf{x}_1 = \mathbf{x}_2 \text{ and } \mathbf{y} := \mathbf{y}_1 = \mathbf{y}_2 \ \forall\ \mathbf{x}, \mathbf{y} \iff \lambda_2 = \mathcal{O}(N) \equiv \alpha N \tag{5}$$

→ BEC is simply a form of ODLRO!

Basics of interacting fermi gas and ground state

Cooper pairs

Consider two fermions on top of a filled, non-interacting fermi sphere:



- Scattering takes place in narrow band (blue)
- Binding energy depends on number of possible scattering states
- Largest binding energy for opposite momentum pairs

→ Only consider (k, -k) pairs

taken from [1]

Many body state

- Many body state of fermionic pairs:

$$|\Psi\rangle = \int \prod_i d^3 r_i \phi(\mathbf{r}_1 - \mathbf{r}_2)\Psi_\uparrow^\dagger(\mathbf{r}_1)\Psi_\downarrow^\dagger(\mathbf{r}_2)\ldots\phi(\mathbf{r}_{N-1} - \mathbf{r}_N)\Psi_\uparrow^\dagger(\mathbf{r}_{N-1})\Psi_\downarrow^\dagger(\mathbf{r}_N)\,|0\rangle \tag{6}$$

$$\Psi_\sigma^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \quad \text{and } \phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \frac{e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}}{\sqrt{V}} \tag{7}$$

- Introduce pair creation operator:

$$b^\dagger = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \tag{8}$$

- $|\Psi\rangle$ becomes formally identical to Gross-Pitaevskii ground state of a condensate of bosons:

$$|\Psi\rangle = (b^\dagger)^{\frac{N}{2}}\,|0\rangle \tag{9}$$

State ket

More convinient: grand canonical ensemble → N not fixed, but μ!

- In BEC limit, this corresponds to coherent state of bosons:

$$|\Psi\rangle = C\, exp(\lambda b^\dagger)\,|0\rangle = C \prod_{\mathbf{k}} exp(\lambda \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle = C \prod_{\mathbf{k}} (1 + \lambda \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle \tag{10}$$

Note:

$$\begin{aligned} exp(\lambda \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle &= \left[1 + \lambda \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - (\lambda \phi_{\mathbf{k}})^2 (c^\dagger_{\mathbf{k}\uparrow})^2 (c^\dagger_{-\mathbf{k}\downarrow})^2 + \mathcal{O}\left((\lambda \phi_{\mathbf{k}})^3\right)\right]|0\rangle \\ &= \left[1 + \lambda \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right]|0\rangle \text{ , because} \end{aligned}$$

$$\{c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}\sigma}\}\,|0\rangle = 0 \iff c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}\,|0\rangle = -c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}\,|0\rangle \implies (c^\dagger_{\mathbf{k}\sigma})^n\,|0\rangle = 0 \;\forall\; n \geq 2$$

Final form of state ket

State ket so far: $|\Psi\rangle = C\ \prod_{\mathbf{k}}(1+\lambda\phi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow})\,|0\rangle$

- Choose normalisation $C = \prod_{\mathbf{k}} u_{\mathbf{k}}$, $\lambda\phi_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$ and $u_{\mathbf{k}}{}^2 + v_{\mathbf{k}}{}^2 = 1$:

$$|\Psi_{BCS}\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow})\,|0\rangle \tag{11}$$

- Remarkable: started with coherent state of bosons in BEC, but ended up with BCS wave function!

  $\rightarrow$ same kind of wave function for both limits!
- Next step: determine $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$

Hamiltonian

We will only cosider s-wave scattering! Should be sufficient for cold dilute gases.

- Hamiltonian with contact interaction U:

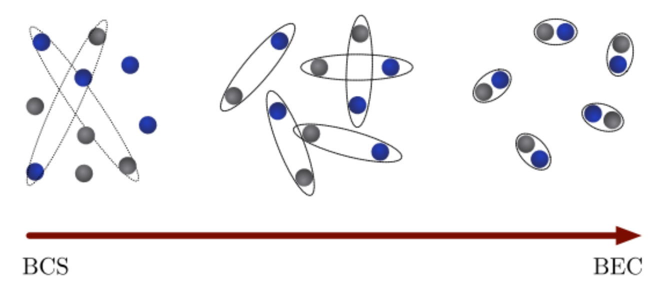
$$H - \mu N = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{V} \sum_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{\mathbf{k}'\downarrow} c_{-\mathbf{k}'\uparrow} \quad ; \; \epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \tag{12}$$

- Contact interaction U characterized by scattering lenght a_s:

$$\frac{1}{U} = \frac{m}{4\pi\hbar^2 a_s} - \int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{2\epsilon_{\mathbf{k}}} \tag{13}$$

$\rightarrow \frac{1}{\mathrm{k}_F a_s}$ defines three regions of the interacting fermi gas:

$$\text{BCS: } \frac{1}{\mathrm{k}_F a_s} \ll -1 \,, \quad \text{BEC: } \frac{1}{\mathrm{k}_F a_s} \gg 1 \,, \quad \text{BCS-BEC crossover: } -1 < \frac{1}{\mathrm{k}_F a_s} < 1 \tag{14}$$



taken from [8]

On BEC side:

- Two body bound state of size a_s

Deriving u and v

In order to derive equations for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, we will minimize the free energy $F = \langle H - \mu N \rangle = \langle \Psi | H - \mu N | \Psi \rangle$:

$$F = \langle \Psi | H - \mu N | \Psi \rangle = 2 \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) |v_{\mathbf{k}}|^2 + \frac{U}{V} \sum_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \tag{15}$$

- ${u_{\mathbf{k}}}^2 + {v_{\mathbf{k}}}^2 = 1$ allows parametrisation:

  $u_{\mathbf{k}} = cos(\theta_{\mathbf{k}})$, $v_{\mathbf{k}} = sin(\theta_{\mathbf{k}})$

- Minimize F by $\frac{\partial F}{\partial \theta_{\mathbf{k}}}$ = 0

$$\Longleftrightarrow 2(\epsilon_{\mathbf{k}} - \mu) u_{\mathbf{k}} v_{\mathbf{k}} + \frac{U}{V} (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) \sum_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} = 0 \tag{16}$$

Introducing gap equation

Minimizing F yields equation for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$:

$$2(\epsilon_{\mathbf{k}}-\mu)u_{\mathbf{k}}v_{\mathbf{k}}-(u_{\mathbf{k}}^2-v_{\mathbf{k}}^2)\Delta = 0\,, \qquad \Delta := -\frac{U}{V}\sum_{\mathbf{k}'} u_{\mathbf{k}'}v_{\mathbf{k}'} = \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle \leftarrow \text{gap equation} \tag{17}$$

- Defining $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+\Delta^2}$, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are then solved by:

$$u_{\mathbf{k}} = \frac{1}{2}\left(1+\frac{\epsilon_{\mathbf{k}}-\mu}{E_{\mathbf{k}}}\right)\,,\ v_{\mathbf{k}} = \frac{1}{2}\left(1-\frac{\epsilon_{\mathbf{k}}-\mu}{E_{\mathbf{k}}}\right) \tag{18}$$

- Inserting $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ into gap equation yields:

$$\Delta = -\frac{U}{V}\sum_{\mathbf{k}}\frac{\Delta}{2E_{\mathbf{k}}} \quad \Longleftrightarrow \quad -\frac{1}{U} = \frac{1}{V}\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k}}} \equiv \int \frac{d^3\mathrm{k}}{(2\pi)^3}\frac{1}{2E_{\mathbf{k}}} \tag{19}$$

Gap equation

- Inserting relation for scattering length leads to:

$$-\frac{1}{U} = \int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{2E_{\mathbf{k}}} \quad \Longleftrightarrow \quad -\frac{m}{4\pi\hbar^2 a_s} = \int \frac{d^3\mathrm{k}}{(2\pi)^3} \left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}}\right) \tag{20}$$

- Additional constrain by number equation:

$$n = 2\int \frac{d^3\mathrm{k}}{(2\pi)^3} v_{\mathbf{k}}^2 \tag{21}$$

- Use standard integrals and ...

$$I_1 = \int_0^\infty dx\, x^2 \left(\frac{1}{\sqrt{(x^2-z)^2+1}} - \frac{1}{x^2}\right) \text{ and } I_2 = \int_0^\infty dx\, x^2 \left(1 - \frac{x^2-z}{\sqrt{(x^2-z)^2+1}}\right) \tag{22}$$

Dimensionless form of gap and number equations

$$I_1 = \int_0^\infty dx\, x^2 \left(\frac{1}{\sqrt{(x^2 - z)^2 + 1}} - \frac{1}{x^2} \right) \text{ and } I_2 = \int_0^\infty dx\, x^2 \left(1 - \frac{x^2 - z}{\sqrt{(x^2 - z)^2 + 1}} \right) \tag{23}$$

- ... and $E_F = \frac{\hbar^2 k_F^2}{2m}$, $k_F = (3\pi^2 n)^{\frac{1}{3}}$ to write:

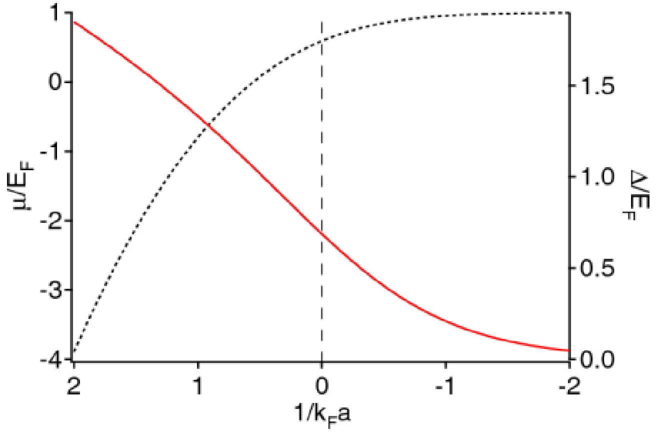
$$-\frac{1}{k_F a_s} = \frac{2}{\pi} \sqrt{\frac{\Delta}{E_F}} I_1\left(\frac{\mu}{\Delta}\right) \;, \qquad 1 = \frac{3}{2} \left(\frac{\Delta}{E_F} \right)^{\frac{3}{2}} I_2\left(\frac{\mu}{\Delta}\right) \tag{24}$$

- Or inserting the second eqn into first:

$$-\frac{1}{k_F a_s} = \frac{2}{\pi} \left(\frac{2}{3 I_2(\frac{\mu}{\Delta})} \right)^{\frac{1}{3}} I_1\left(\frac{\mu}{\Delta}\right) \;, \qquad \frac{\Delta}{E_F} = \left(\frac{2}{3 I_2(\frac{\mu}{\Delta})} \right)^{\frac{2}{3}} \tag{25}$$

$\rightarrow$ by solving first eqn for $\frac{\mu}{\Delta}$ as function of $\frac{1}{k_F a_s}$ and inserting into second eqn gives us the gap Δ!

Gap as function of inverse scattering length

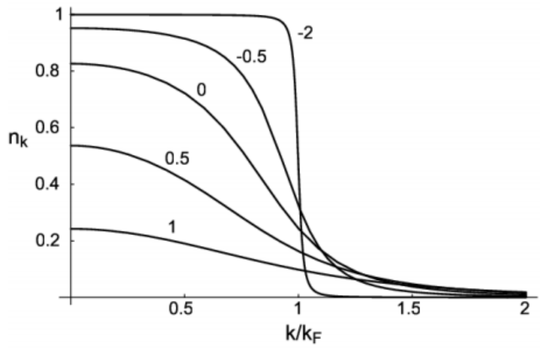


taken from [1]

gap given by red line

Solution of number equation for different regimes

After having obtained Δ, we can insert it into $n_{\mathbf{k}} = v_{\mathbf{k}}^2 = [\frac{1}{2}(1 - \frac{\epsilon_{\mathbf{k}} - \mu}{\sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2}})]^{1/2}$



taken from [1]

Low excitations

Alternativ approach: Mean field and Bogoliubov transformation

- Bogoliubov transformation of operators leaves the anti-commutation relation unchanged:

$$\begin{pmatrix}\gamma_{\mathbf{k}\uparrow}\\ \gamma^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix}=\begin{pmatrix}u_{\mathbf{k}} & -v_{\mathbf{k}}\\ v_{\mathbf{k}} & u_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}c_{\mathbf{k}\uparrow}\\ c^\dagger_{-\mathbf{k}\downarrow}\end{pmatrix} \qquad \Longrightarrow \; \left\{\gamma_{\mathbf{k}\sigma},\gamma^\dagger_{\mathbf{k}'\sigma'}\right\}=\left\{c_{\mathbf{k}\sigma},c^\dagger_{\mathbf{k}'\sigma'}\right\}=\delta(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'} \quad (26)$$

- Mean field + Bogoliubov transformation gives Hamiltonian in terms of quasi-particles states:

$$H-\mu N=-V\frac{\Delta^2}{U}+\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\mu-E_{\mathbf{k}})+\sum_{\mathbf{k}}E_{\mathbf{k}}(\gamma^\dagger_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow}+\gamma^\dagger_{\mathbf{k}\downarrow}\gamma_{\mathbf{k}\downarrow}) \quad (27)$$

→ At finite temperatures there will be excitations of quasi-particle states which modify the gap equation

Low excitations

Recall gap equation: $\Delta = \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$

- In terms of quasi-particles, the so-called paring field becomes:

$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -u_{\mathbf{k}} v_{\mathbf{k}} (1 - \langle \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} \rangle - \langle \gamma^{\dagger}_{\mathbf{k}\downarrow} \gamma_{\mathbf{k}\downarrow} \rangle) \tag{28}$$

- Since quasi-particles follow Fermi-Dirac statistics $\langle \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} \rangle = \frac{1}{1+e^{\beta E_{\mathbf{k}}}}$, the gap equation becomes

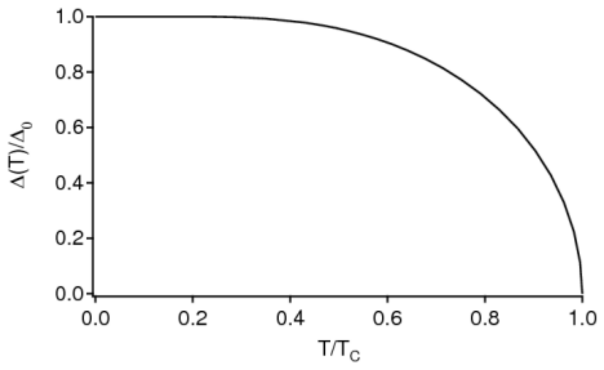
$$-\frac{m}{4\pi\hbar^2 a_s} = \int \frac{d^3 \mathrm{k}}{(2\pi)^3} \left(\frac{1}{2E_{\mathbf{k}}} tanh(\frac{\beta E_{\mathbf{k}}}{2}) - \frac{1}{2\epsilon_{\mathbf{k}}} \right) \tag{29}$$

recall: $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2}$

Solution for $\Delta(T)$ in the BCS regime

Solving temperature dependent gap equation yields with $\Delta_0 := \frac{8}{e^2} exp(-\frac{\pi}{2k_F|a_s|})$:

$$\Delta(T) \approx \begin{cases} \Delta_0 - \sqrt{2\pi\Delta_0 k_B T}\, exp(-\frac{\Delta_0}{k_B T}) & \text{for T} \ll T_C \\ \sqrt{\frac{8\pi^2}{7\zeta(3)}} k_B T_C \sqrt{1 - \frac{T}{T_C}} & \text{for } T_C \text{ - T} \gg T_C \end{cases} \quad (30)$$



taken from [1]

Pair formation and condensation temperature

Temperature of pair formation T^*

We want to know at which temperature T^* fermionic pairs start to form:

- This happens, when the gap vanishes, i.e. $\Delta = 0$, which yields

$$-\frac{m}{4\pi\hbar^2 a_s} = \int \frac{d^3\mathrm{k}}{(2\pi)^3}\left(\frac{1}{2(\epsilon_{\mathbf{k}}-\mu)} tanh(\frac{\beta^*(\epsilon_{\mathbf{k}}-\mu)}{2}) - \frac{1}{2\epsilon_{\mathbf{k}}}\right) \quad (31)$$

- Solve this while keeping the constraint for the number density above T^* given by Fermi-Dirac statistics:

$$n = 2\int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{1+exp(\beta*(\epsilon_{\mathbf{k}}-\mu)} \quad (32)$$

→ These equations allow us to calculate T^*

(Pair formation and critical) temperature

- In BCS regime $\mu \gg k_B T^* \to \mu \approx E_F$:

$$T^*_{BCS} = T_{C,BCS} = \frac{e^\gamma}{\pi}\frac{8}{e^2} exp(-\frac{\pi}{2k_F|a_s|}) \;\; ; e^\gamma \approx 1.78 \tag{33}$$

- T^*_{BEC} involves so-called Lambert W-function → basically T^*_{BCS} continues to increase very steeply into BEC regime
- Deeply in BEC regime $T_{C,BEC}$ is simply given by the well known T_C for bosons with molecular density $n_M = n/2$ and mass $m_M = 2m$:

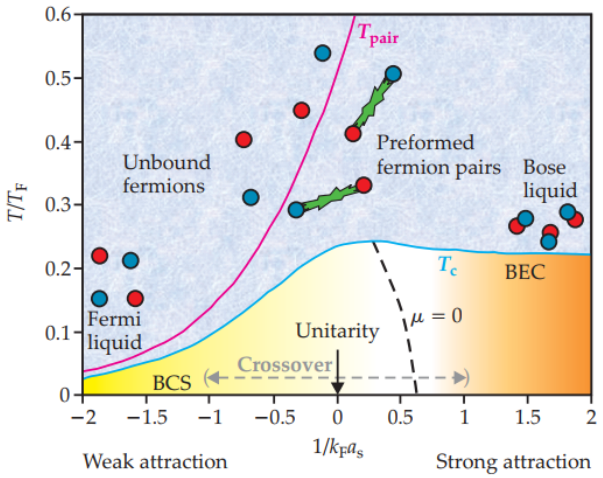
$$T_{C,BEC} = \frac{2\pi\hbar^2}{m_M}(\frac{n_M}{\zeta(\frac{3}{2})})^{2/3} = 0.22E_F \tag{34}$$

- Small corrections if we go into crossover towards BCS:

$$T_C \approx T_{C,BEC}(1 + 1.31 n_M^{1/3} \cdot 0.6 a_s) \tag{35}$$

→ There should be a smooth crossover in T_C from BCS to BEC, hence a maximum between them

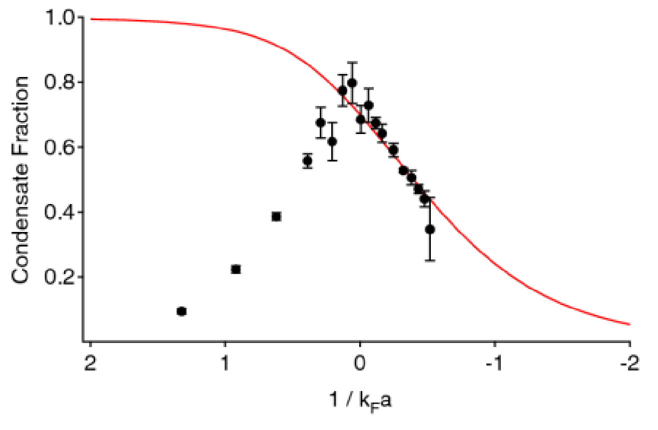
Pair formation and superfluid/condensation temperature



taken from [5]

- We see $\propto exp(-\frac{\pi}{2k_F|a_s|})$ for T^*, T_C in BCS
- and $T_{C,BEC} = 0.22E_F$ with positive corrections towards BCS

Condensate fraction



taken from [1]

- Following ODLRO by Yang:

$$n_0 = \frac{1}{V}\sum_{\mathbf{k}} \left| \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle \right|^2 = \sum_{\mathbf{k}} u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 tanh^2 (\frac{\beta E_{\mathbf{k}}}{2}) \quad (36)$$

- In BEC regime: In experiment condensate decays due to heating

References

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