Fermionic Pairs and the BCS-BEC Crossover

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1 Introduction

Bose-Einstein Condensation (BEC) is a well known phenomenon for bosons, easily understood from the ideal Bose gas. In contrast, condensation in an ideal Fermi gas is not possible due to the Pauli principle which forbids the ground state to be occupied by more than one fermion. However, BEC is found to occur in an interacting Fermi gas which can be described by assuming only s-wave scattering in the case of a cold, dilute gas. But, there is also another phase in the interacting Fermi gas or rather a limit: it is the so-called BCS limit in which the gas becomes a superfluid, i.e. a fluid without viscosity. The BEC and BCS phases of the interacting Fermi gas can be understood as two opposite limits in the description of the gas. A smooth crossover from one phase to the other is possible by tuning the scattering length of the gas, where the BCS limit is given by an infinite and negative scattering length and the BEC limit by an infinite and positive one. Changing the scattering length can for example be achieved by a so-called magnetic Feshbach resonance [1]. The transition from BEC to BCS is rather a crossover than a phase transition, because it is a smooth transition, i.e. there is no abrupt change in the order of the physical system when going from one limit to the other.

After listing the most significant developments towards a theory of the BCS-BEC crossover, off-diagonal long-range order and its main implication will be presented in the next chapter in order to motivate why to consider BEC of fermions at all and to show that fermionic pairs are required for condensation even from an abstract mathematical point of view. In the third chapter, it will be shown how to obtain the wave function that describes the interacting Fermi gas and the crossover. Lastly, two crucial temperatures which each describe the formation of fermionic pairs and the condensation of such pairs will be derived and the formula for the condensate fraction density derived from off-diagonal long-range order will be given.

1.1 Historic Overview

- 1954: Cooper [2] introduced the nowadays so-called Cooper-pairs, which are bound states of two electrons via phonon interactions on top of a filled Fermi sphere.
- 1957 Barden, Cooper and Schrieffer [3] extended the idea of a single Cooper pair to a many particle wave function which successfully explained superconductivity at the time.
- 1962: Yang [4] conjectured that BEC is possible for fermions, if the second reduced density matrix exhibits off-diagonal long-range order.
- 1980: Leggett [5] assumed fermionic pairs in a Fermi gas with opposite spin and a contact interaction which was the first theory of the BCS-BEC crossover at $T = 0$.
- 1985: Nozières and Schmitt-Rink [6] extended Leggett's theory to temperatures below the critical temperature of Bose-Einstein Condensation
- 2003: Regal, Ticknor, Bohn and Jin [7] realized the first Bose-Einstein condensate of fermions using Potassium-40 atoms.

2 Off-Diagonal Long-Range Order

Off-Diagonal Long-Range Order (ODLRO) is presented here to motivate the possible condensation of fermions and to give a formula for the condensation fraction density. It was first discussed for bosons by Penrose and Onsager [8] in 1956 and extended to fermions by Yang [4] in 1962.

2.1 Reduced Density Matrices and Large Eigenvalues

Starting point is the N-particle density matrix ρ, with normalisation $\mathrm{Tr}(\rho) = 1$. The components of the corresponding first and second reduced density matrices are defined by

$$\begin{aligned} \langle i| \rho_1 |j\rangle &= Tr(a_i \rho a_j^\dagger) \ , \\ \langle ij| \rho_2 |kl\rangle &= Tr(a_i a_j \rho a_l^\dagger a_k^\dagger) \ , \end{aligned} \tag{1}$$

where $\mathrm{a_i^\dagger}$ and $\mathrm{a_i}$ denote the creation and annihilation operators for the state $|i\rangle$. Higher reduced density matrices are defined correspondingly.
Let the largest eigenvalue of ρ_i be denoted by λ_i. Generally, they are obviously bounded by

$$\begin{aligned} \lambda_1 &\leq Tr(\rho_1) = N \ , \\ \lambda_2 &\leq Tr(\rho_2) = N(N-1) \ . \end{aligned} \tag{2}$$

However, in the case of fermions, which obey the Pauli-principle, the above relation specialise to:

$$\begin{aligned} \lambda_1 &\leq 1 \\ \lambda_2 &\leq N \ . \end{aligned} \tag{3}$$

Yang also showed that $\lambda_2 = \mathrm{N}$ can essentially only be reached in one unique way, where fermions form pairs such that the second reduced density matrix of these fermions behaves like the first reduced density matrix of bosons, thus leading to the conjecture that BEC is possible for pairs of fermions. However, he also showed that λ_2 being of order of N is equivalent to the occurrence of ODLRO in ρ_2. Being of order of N can loosely be understood as $\lambda_\mathrm{i} = \mathcal{O}(\mathrm{N}) \equiv \alpha\mathrm{N}$, where α then is the condensate fraction.

2.2 Definition and Relation to Large Eigenvalues

First, consider ODLRO in ρ_1. It can be defined by

$$\langle \mathbf{x}| \rho_1 |\mathbf{y}\rangle > 0 \text{ for } |\mathbf{x} - \mathbf{y}| \to \infty \ , \tag{4}$$

which was shown to be equivalent to $\lambda_1 = \mathcal{O}(\mathrm{N}) \equiv \alpha\mathrm{N}$ for bosons. But, according to equation (3) there can be no ODLRO in ρ_1 for fermions. However, it is possible for ρ_2, where ODLRO can be defined by

$$\langle \mathbf{x}_1\mathbf{x}_2| \, \rho_2 \, |\mathbf{y}_1\mathbf{y}_2\rangle \approx 0 \text{ execpt region around } \mathbf{x} := \mathbf{x}_1 = \mathbf{x}_2 \text{ and } \mathbf{y} := \mathbf{y}_1 = \mathbf{y}_2 \; \forall \, \mathbf{x}, \mathbf{y} \; , \quad (5)$$

which was shown to be the case if and only if $\lambda_2 = \mathcal{O}(\mathrm{N}) \equiv \alpha \mathrm{N}$.

Thus, the occurrence of ODLRO in the second reduced density matrix of N fermions is equivalent to the largest eigenvalue of this matrix being of the order of N and showing BEC of pairs of fermions.

2.3 Condensate Fraction from Off-Diagonal Long-Range Order

The elements of the second reduced density matrix can be calculated following [9]:

$$\langle \mathbf{x}_1\mathbf{x}_2| \, \rho_2 \, |\mathbf{y}_1\mathbf{y}_2\rangle = \langle \Psi^\dagger_\uparrow(\mathbf{x}_1)\Psi^\dagger_\downarrow(\mathbf{x}_2)\Psi_\downarrow(\mathbf{y}_2)\Psi_\uparrow(\mathbf{y}_1)\rangle \; , \quad (6)$$

where $\Psi^\dagger_\sigma(\mathbf{r})$ and $\Psi_\sigma(\mathbf{r})$ are the fermion creation and annihilation operators respectively. Further, following [10], the condensate fraction of fermionic pairs, i.e. half the density of condensed fermions, is given by means of the creation and annihilation operators in momentum space via

$$n_0 = \frac{N_0}{V} = \frac{1}{V} \sum_{\mathbf{k}} |\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle|^2 \quad (7)$$

This gives an applicable formula from which the condensate fraction can be calculated, if one knows how to calculate the so-called pairing field $\langle \mathrm{c}_{\mathbf{k}\uparrow} \mathrm{c}_{-\mathbf{k}\downarrow}\rangle$, which will be presented in chapter 3.

3 The Interacting Fermi Gas

3.1 Cooper Pairs

Cooper actually considered bound states in momentum space of two electrons in a degenerate Fermi gas in order to explain superconductivity, however this concept is more general to fermions in general. Cooper pairs can be understood by considering two fermions on top of a filled, non-interaction Fermi sphere, which describes the occupation of momenta at zero temperature for the ideal Fermi gas and hence its radius in momentum space is given by the Fermi momentum $\mathrm{k_F} = (3\pi^2 n)^{\frac{1}{3}}$.

The binding energy of the Cooper pair can be found by assuming a contact interaction for the fermions forming the pair. A contact interaction of strength U corresponds to hard balls with radius $\mathrm{a_s}$ scattering off each other. In quantum mechanical scattering theory, this corresponds to s-wave scattering in which only wave functions with zero angular momentum (l=0, hence the name s-wave) are considered to describe the scattered particles. This should be sufficient for cold, dilute gases, where typical scattering energies are low. Then, the contact interaction can be related to the scattering length $\mathrm{a_s}$ of s-wave scattering via

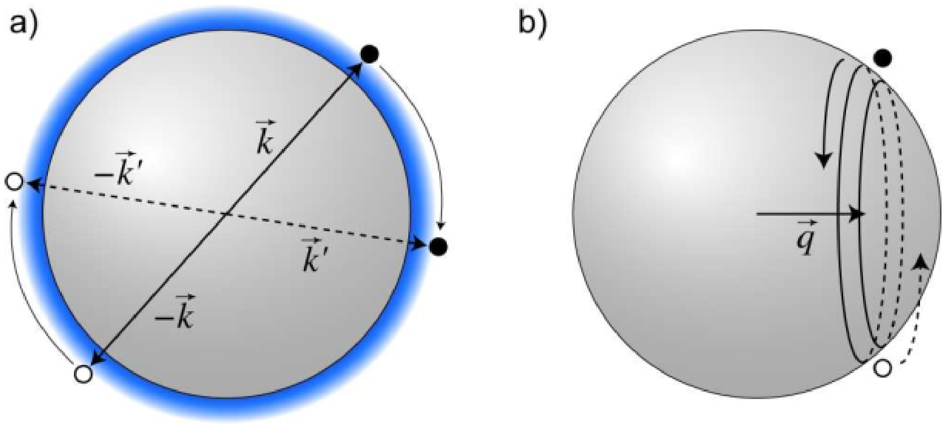

Figure 1: Two interacting fermions are on top of a non-interacting Fermi sphere. Due to their low energy compared to the Fermi energy scattering can only take place in a narrow band above the sphere. a) shows the possible scattered states (blue, the whole sphere) for a pair with vanishing total momentum given. b) shows the possible scattered states (circle on the sphere) for non zero total momentum q. Figure taken from [11].

$$\frac{1}{U} = \frac{m}{4\pi\hbar^2 a_s} - \int \frac{d^3\mathrm{k}}{(2\pi)^3}\frac{1}{2\epsilon_{\mathbf{k}}} \ , \tag{8}$$

where $\epsilon_{\mathbf{k}} = \frac{\hbar^2\mathrm{k}^2}{2\mathrm{m}}$ is the kinetic energy of the fermions. Note that this expression can be properly regularized. It has been shown, that the binding energy is the highest for pairs that have the highest possible number of final scattered states. Following this argument, figure 1 shows that the binding energy is highest for pairs of opposite momenta, which has shown to be

$$E_B = -\frac{8}{e^2}E_F e^{-\pi/k_F|a_s|} \ . \tag{9}$$

This only holds for two interacting fermions on top of a non-interacting Fermi sphere. The situation changes, when interaction for all fermions is switched on, which was studied by Bardeen, Cooper and Schrieffer, who also found the corresponding wave function. In the next section, the relation between fermionic pairs in a BEC and the BCS wave function will be revealed.

3.2 Ground State of the Interacting Fermi Gas

In order to derive the crossover wave function, one can start with the ground state of a BEC of fermionic pairs. This ground state must incorporate the creation of pairs with opposite spin and a function given their relative behaviour. Such a ground state is given by

$$|\Psi\rangle = \int \prod_i d^3 r_i \phi(\mathbf{r}_1 - \mathbf{r}_2)\Psi^\dagger_\uparrow(\mathbf{r}_1)\Psi^\dagger_\downarrow(\mathbf{r}_2)...\phi(\mathbf{r}_{N-1} - \mathbf{r}_N)\Psi^\dagger_\uparrow(\mathbf{r}_{N-1})\Psi^\dagger_\downarrow(\mathbf{r}_N)\,|0\rangle \ , \tag{10}$$

with the fermion creation operator

$$\Psi_\sigma^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \tag{11}$$

and the relative function

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \frac{e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}}{\sqrt{V}} \quad . \tag{12}$$

Of course, the creation and annihilation operators of fermions obey the anti-commutation relations:

$$\begin{aligned} \{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} &= \left\{c_{\mathbf{k}\sigma}^\dagger, c_{\mathbf{k}'\sigma'}^\dagger\right\} = 0 \\ \left\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}^\dagger\right\} &= \delta(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'} \ . \end{aligned} \tag{13}$$

By defining the pair creation operator via

$$b^\dagger = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \ , \tag{14}$$

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

$$|\Psi\rangle = (b^\dagger)^{\frac{N}{2}} |0\rangle \ . \tag{15}$$

The commutation relations of the pair operator b are then given by

$$\begin{aligned} [b,b] &= \sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}\phi_{\mathbf{k}'} \left[c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger, c_{\mathbf{k}'\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger\right] = 0 \\ \left[b^\dagger,b^\dagger\right] &= \sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^*\phi_{\mathbf{k}'}^* \left[c_{-\mathbf{k}\uparrow}c_{\mathbf{k}\downarrow}, c_{-\mathbf{k}'\uparrow}c_{\mathbf{k}'\downarrow}\right] = 0 \\ \left[b,b^\dagger\right] &= \sum_{\mathbf{k}\mathbf{k}'} \phi_{\mathbf{k}}^*\phi_{\mathbf{k}'} \left[c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}, c_{\mathbf{k}'\uparrow}c_{-\mathbf{k}'\downarrow}\right] = \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2(1 - n_{\mathbf{k}\uparrow} - n_{\mathbf{k}\downarrow}) \end{aligned} \tag{16}$$

This shows that b describes the creation and annihilation of bosons (composed of fermionic pairs), if the occupation number densities of the momenta of the fermions $\mathrm{n}_{\mathbf{k}\sigma}$ are vanishing, which means that these occupation number densities have to be distributed very broadly. This is indeed the case deeply in the BEC limit of the interacting Fermi gas as will be shown below (cp. fig. 4). Then $\left[\mathrm{b},\mathrm{b}^\dagger\right] = 1$ for an according normalization of $\phi_{\mathbf{k}}$.

However, it is more convenient to consider the grand canonical ensemble in which the particle number is not conserved but the chemical potential. Starting in the BEC limit, this corresponds to a coherent state of bosons described by the exponential of the same creation operator. Together with normalisation factors C and λ this yields:

$$|\Psi\rangle = C\ exp(\lambda b^\dagger)|0\rangle = C\ \prod_{\mathbf{k}} exp(\lambda\phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle = C\ \prod_{\mathbf{k}}(1 + \lambda\phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle \ . \tag{17}$$

The second equality is explained by looking at how the exponential acts:

$$\begin{aligned}\exp(\lambda\phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle &= \left[1 + \lambda\phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - (\lambda\phi_{\mathbf{k}})^2 (c^\dagger_{\mathbf{k}\uparrow})^2 (c^\dagger_{-\mathbf{k}\downarrow})^2 + \mathcal{O}\big((\lambda\phi_{\mathbf{k}})^3\big)\right]|0\rangle \\ &= \left[1 + \lambda\phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right]|0\rangle \,.\end{aligned} \tag{18}$$

The minus sign comes from commuting the $c^\dagger$ once and all terms with $({c^\dagger}_{\mathbf{k}})^n$ and $n \geq 2$ vanish because of:

$$\begin{aligned}\left\{c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}\sigma}\right\}|0\rangle = 0 \iff c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}\,|0\rangle &= -c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}\,|0\rangle \\ \implies (c^\dagger_{\mathbf{k}\sigma})^n\,|0\rangle &= 0 \;\forall\; n \geq 2 \,.\end{aligned} \tag{19}$$

When performing the product over the exponentials in equation (17), the $c^\dagger$ can always be anti-commuted (while acquiring a minus sign) so that all terms with $({c^\dagger}_{\mathbf{k}})^n$ and $n \geq 2$ vanish for any momentum $\mathbf{k}$, leading to the last equality of equation (17).

Choosing the normalisation factors to be $C = \prod_{\mathbf{k}} u_{\mathbf{k}}$ and $\lambda\phi_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}}$ together with the constrain ${u_{\mathbf{k}}}^2 + {v_{\mathbf{k}}}^2 = 1$ leads to the same form of wave function as derived by Bardeen, Cooper and Schrieffer:

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle \tag{20}$$

This is remarkable: having started with the coherent state of bosons composed of fermionic pairs in the state of a bosonic condensate, one ends up with the BCS wave function! This implies that both regimes are described by the same wave function.

In order to fully determine the the wave function, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ have to be determined. This is done by minimizing the free energy of the system. Therefore, consider the Hamiltonian in the grand canonical ensemble with volume V and a contact interaction U:

$$H - \mu N = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{V} \sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{\mathbf{k}'\downarrow} c_{-\mathbf{k}'\uparrow} \quad ;\; \epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m} \,. \tag{21}$$

The free energy F of the system is then given by

$$F = \langle\Psi|\, H - \mu N\,|\Psi\rangle = 2\sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) v_{\mathbf{k}}^2 + \frac{U}{V} \sum_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \,. \tag{22}$$

In order to minimize the free energy one has to take some sort of derivative and set it to zero. The constraint on $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ allows the parametrization $u_{\mathbf{k}} = \cos(\theta_{\mathbf{k}})$, $v_{\mathbf{k}} = \sin(\theta_{\mathbf{k}})$. Using this, minimizing F by $\frac{\partial F}{\partial \theta_{\mathbf{k}}} = 0$ leads to

$$2(\epsilon_{\mathbf{k}} - \mu) u_{\mathbf{k}} v_{\mathbf{k}} + \frac{U}{V} (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) \sum_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} = 0 \,. \tag{23}$$

Now, defining the gap parameter Δ in the so-called gap equation

$$\Delta = U/V \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -U/V \sum_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} \ , \tag{24}$$

equation (23) becomes

$$2(\epsilon_{\mathbf{k}} - \mu) u_{\mathbf{k}} v_{\mathbf{k}} - (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2)\Delta = 0 \ . \tag{25}$$

The gap Δ is in fact the order parameter which characterises the transition from the Fermi gas to the superfluid phase, i.e. the BCS regime of the interacting Fermi gas. The solution for $\mathrm{u}_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$ in equation (25) is now given defining the energy $\mathrm{E}_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2}$:

$$u_{\mathbf{k}} = \frac{1}{2}(1 + \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}) \ , \ v_{\mathbf{k}} = \frac{1}{2}(1 - \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}) \ . \tag{26}$$

Inserting these expressions for $\mathrm{u}_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$ into the gap equation then yields

$$\Delta = -\frac{U}{V} \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \qquad \Longleftrightarrow \qquad -\frac{1}{U} = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} \equiv \int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{2E_{\mathbf{k}}} \ , \tag{27}$$

where the last equality is understood as a continuous approximation of the sum by an integration over phase space. As mentioned above, the contact interaction U is related to the scattering length via equation (8). Replacing U via this relation then relates the gap to the scattering length:

$$-\frac{1}{U} = \int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{2E_{\mathbf{k}}} \qquad \Longleftrightarrow \qquad -\frac{m}{4\pi\hbar^2 a_s} = \int \frac{d^3\mathrm{k}}{(2\pi)^3} (\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}}) \ . \tag{28}$$

It should also be mentioned that an additional constrain on the system is given by number equation:

$$n = 2 \int \frac{d^3\mathrm{k}}{(2\pi)^3} v_{\mathbf{k}}^2 \ . \tag{29}$$

Here one can identify $\mathrm{n}_{\mathbf{k}} = \mathrm{v}_{\mathbf{k}}^2$ as the occupation number density of momenta. In order to determine the gap and also the chemical potential of the system, it is useful to rewrite the gap and number equations in a dimensionless way using the following standard integrals:

$$I_1 = \int_0^\infty dx \ x^2 \left(\frac{1}{\sqrt{(x^2 - z)^2 + 1}} - \frac{1}{x^2} \right) \tag{30}$$

$$I_2 = \int_0^\infty dx \ x^2 \left(1 - \frac{x^2 - z}{\sqrt{(x^2 - z)^2 + 1}} \right) \ . \tag{31}$$

Using the Fermi energy $\mathrm{E_F} = \frac{\hbar^2 \mathrm{k_F^2}}{2\mathrm{m}}$ and Fermi momentum $\mathrm{k_F} = (3\pi^2 \mathrm{n})^{\frac{1}{3}}$, the gap and number equation can then be written in a dimensionless form:

$$-\frac{1}{\mathrm{k}_F a_s} = \frac{2}{\pi} \sqrt{\frac{\Delta}{E_F}} I_1(\frac{\mu}{\Delta}) \tag{32}$$

$$1 = \frac{3}{2} \left(\frac{\Delta}{E_F} \right)^{\frac{3}{2}} I_2(\frac{\mu}{\Delta}) \ . \tag{33}$$

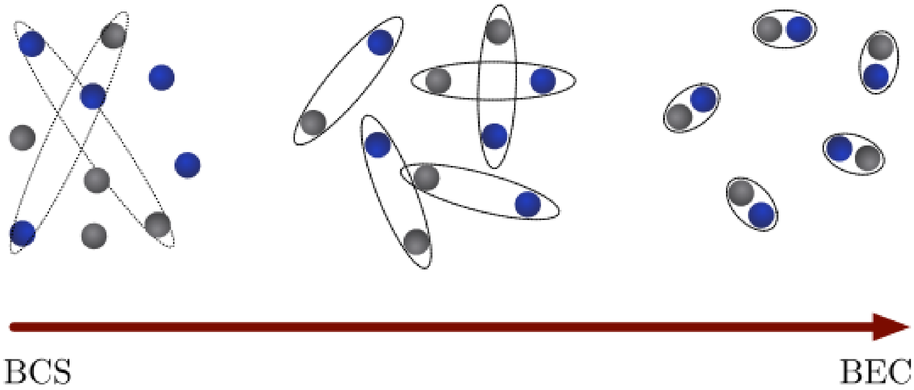

Figure 2: This figure illustrates the size of fermionic pairs in different regimes. In the BEC limit, the size of pairs is much smaller than the typical distance between pairs. In the BCS limit, pairs are strongly overlapping, which leads to properties of a superfluid rather than a condensate. Figure taken from [12].

Further, inserting equation (33) into (32) yields the compact form:

$$-\frac{1}{\mathrm{k}_F a_s} = \frac{2}{\pi}\left(\frac{2}{3I_2(\frac{\mu}{\Delta})}\right)^{\frac{1}{3}} I_1(\frac{\mu}{\Delta}) \tag{34}$$

$$\frac{\Delta}{E_F} = \left(\frac{2}{3I_2(\frac{\mu}{\Delta})}\right)^{\frac{2}{3}} . \tag{35}$$

The gap Δ as a function of the scattering parameter $\frac{1}{\mathrm{k_F a_s}}$ is now obtained by solving gap equation (34) for $\frac{\mu}{\Delta}$ and inserting this expression into the number equation (35). Figure 3 shows the result for the gap and the chemical potential as a function of the scattering parameter and figure 2 gives an intuitive picture of the regimes of the interacting Fermi gas defined by the interaction parameter. Three regimes can be identified via the interaction parameter $1/\mathrm{k_F a_s}$:

$$\text{BCS: } \frac{1}{\mathrm{k}_F a_s} \ll -1 \ , \quad \text{BEC: } \frac{1}{\mathrm{k}_F a_s} \gg 1 \ , \quad \text{BCS-BEC crossover: } -1 < \frac{1}{\mathrm{k}_F a_s} < 1 \ . \tag{36}$$

Also, having obtained Δ, it can be inserted into $\mathrm{n}_{\mathbf{k}} = \mathrm{v}_{\mathbf{k}}^2$. Figure 4 shows $\mathrm{n}_{\mathbf{k}}$ for different scattering parameters, i.e. regimes of the Fermi gas. In the BCS regime it closely resembles a step function, just like the ideal Fermi gas, and it becomes broader and flatter in the BCS-BEC crossover region.

3.3 Low Excitations

In order to understand the behaviour of the interacting Fermi gas for low excitations, i.e. temperatures below the so-called critical temperature, which will be explained later to be the temperature below which condensation takes place, it is more convenient to change the physical picture still describing the same physics. Therefore consider the Bogoliubov

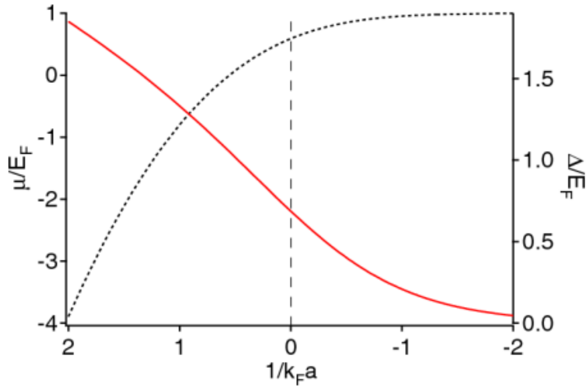

Figure 3: Gap Δ (red line) and chemical potential μ (dotted line) as a function of the scattering parameter. A positive scattering parameter corresponds to the BEC regime and a negative to the BCS regime. Figure taken from [11].

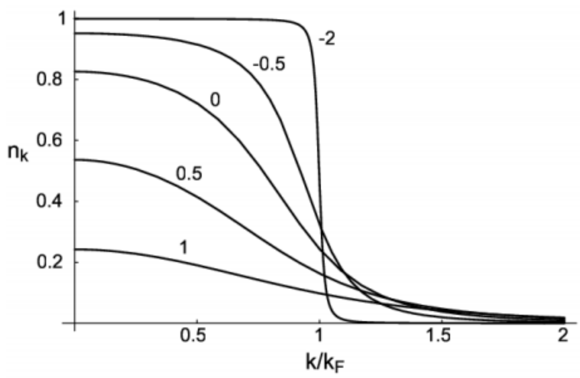

Figure 4: Occupation number density of momenta $\mathrm{n}_{\mathbf{k}} = \mathrm{v}_{\mathbf{k}}^2$ is given for different interaction parameters. Figure taken from [11].

transformation of creation and annihilation operators which leaves the anti-commutation relations unchanged:

$$\begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} = \underbrace{\begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix}}_{\text{Bogoliubov transformation}} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \tag{37}$$

$$\left\{\gamma_{\mathbf{k}\sigma}, \gamma^{\dagger}_{\mathbf{k}'\sigma'}\right\} = \left\{c_{\mathbf{k}\sigma}, c^{\dagger}_{\mathbf{k}'\sigma'}\right\} = \delta(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'} \tag{38}$$

$$\{\gamma_{\mathbf{k}\sigma}, \gamma_{\mathbf{k}'\sigma'}\} = \left\{\gamma^{\dagger}_{\mathbf{k}\sigma}, \gamma^{\dagger}_{\mathbf{k}'\sigma'}\right\} = 0 \ . \tag{39}$$

It is non-trivial to show that these $\mathrm{u}_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$ are actually the same as in the previous derivation of the gap equation. But indeed, the Bogoliubov transformation can be understood as a rotation in a plane and in this case as a rotation in a plane spanned by the c creation and annihilation operators. The γ operators are then linear combinations of the c operators describing fictive or quasi particles. This also justifies the earlier approach to parametrize the $\mathrm{u}_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$ by $\cos(\theta_{\mathbf{k}})$ and $\sin(\theta_{\mathbf{k}})$ respectively.

Applying this transformation to the previous Hamiltonian yields

$$H - \mu N = -V\frac{\Delta^2}{U} + \sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu - E_{\mathbf{k}}) + \sum_{\mathbf{k}} E_{\mathbf{k}}(\gamma^{\dagger}_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow} + \gamma^{\dagger}_{\mathbf{k}\downarrow}\gamma_{\mathbf{k}\downarrow}) \ . \tag{40}$$

At finite temperatures, there will be excitations of quasi particle states which modify the gap equation. In terms of quasi-particles, the so-called paring field becomes:

$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}\rangle = -u_{\mathbf{k}} v_{\mathbf{k}}(1 - \langle\gamma^{\dagger}_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow}\rangle - \langle\gamma^{\dagger}_{\mathbf{k}\downarrow}\gamma_{\mathbf{k}\downarrow}\rangle) \ . \tag{41}$$

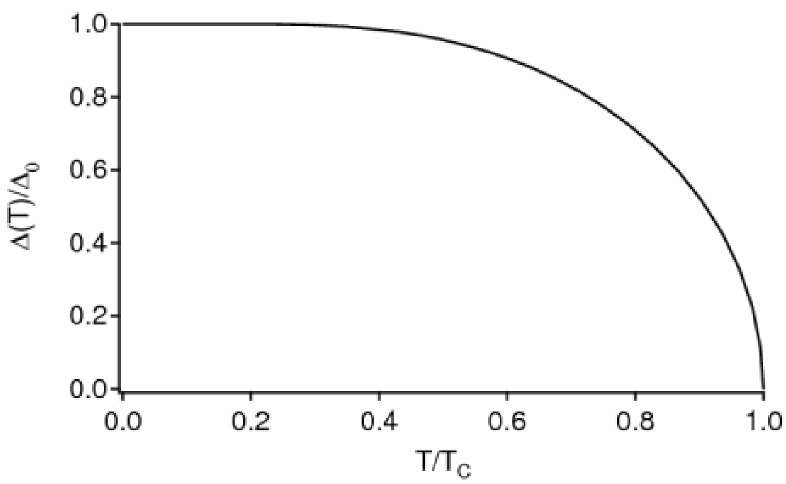

Figure 5: Shown is the gap in units of the gap at zero temperature as a function of temperature in units of the critical temperature below which condensation of fermionic pairs into a BEC occurs. Figure taken from [11].

Since the 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 $\Delta = \sum_\mathbf{k}\langle \mathrm{c}_{\mathbf{k}\uparrow}\mathrm{c}_{-\mathbf{k}\downarrow}\rangle$ becomes temperature dependent ($\beta = 1/\mathrm{k_B T}$):

$$-\frac{m}{4\pi\hbar^2 a_s} = \int\frac{d^3\mathrm{k}}{(2\pi)^3}\left(\frac{1}{2E_\mathbf{k}}tanh(\frac{\beta E_\mathbf{k}}{2}) - \frac{1}{2\epsilon_\mathbf{k}}\right)\,. \tag{42}$$

Solving temperature dependent gap equation yields

$$\Delta(T) \approx \begin{cases}\Delta_0 - \sqrt{2\pi\Delta_0\mathrm{k}_B T}\ exp(-\frac{\Delta_0}{\mathrm{k}_B T}) & \text{for T} \ll T_C\\ \sqrt{\frac{8\pi^2}{7\zeta(3)}}\mathrm{k}_B T_C\sqrt{1-\frac{T}{T_C}} & \text{for } T_C \text{ - T} \gg T_C\ ,\end{cases} \tag{43}$$

where

$$\Delta_0 \coloneqq \frac{8}{e^2}exp(-\frac{\pi}{2\mathrm{k}_F|a_s|}) \tag{44}$$

is the gap at zero temperature. Figure 5 shows the temperature dependent gap below the critical temperature, below which condensation takes place.

4 Fermionic Pair Formation and Condensation

4.1 Pair Formation Temperature

The gap is the order parameter of the Fermi gas characterizing the phase transition from the phase of unpaired fermions to the phase of paired fermions. The temperature $\mathrm{T_{pair}}$ at which fermionic pairs start to form is determined by the condition $\Delta = 0$ which inserted into the temperature dependent gap equation (42) yields an equation for the pairing temperature:

$$-\frac{m}{4\pi\hbar^2 a_s} = \int\frac{d^3\mathrm{k}}{(2\pi)^3}\left(\frac{1}{2(\epsilon_\mathbf{k}-\mu)}tanh(\frac{\beta_{pair}(\epsilon_\mathbf{k}-\mu)}{2}) - \frac{1}{2\epsilon_\mathbf{k}}\right)\,. \tag{45}$$

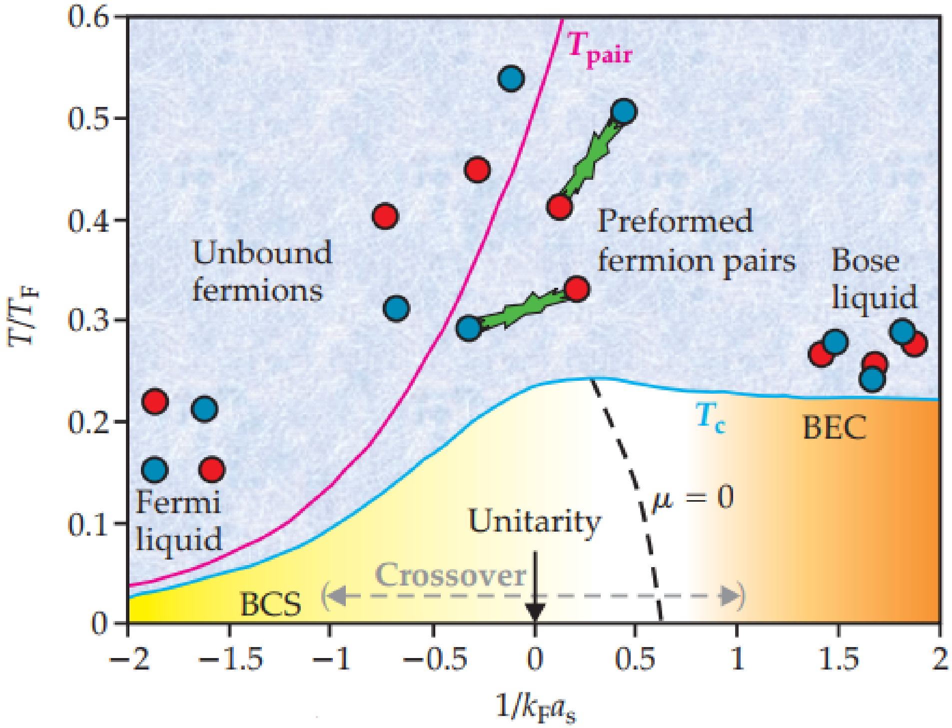

Figure 6: The figure shows T_{pair} and T_C (see [13] for calculation) as functions of the interaction parameter. Figure adopted from [14].

Since the system can be expected to follow the Fermi-Dirac statistic above T_{pair}, the number equation is

$$n = 2 \int \frac{d^3\mathrm{k}}{(2\pi)^3} \frac{1}{1 + exp(\beta_{pair}(\epsilon_{\mathbf{k}} - \mu)} \; . \tag{46}$$

Solving these two equations now allows to calculate T_{pair}. In the BCS regime it can be assumed that $\mu \gg k_B T_{pair}$, hence $\mu \approx E_F$. Solving the above equations with this chemical potential leads to

$$T_{pair}^{BCS} = T_C^{BCS} = \frac{e^\gamma}{\pi} \frac{8}{e^2} exp(-\frac{\pi}{2\mathrm{k}_F |a_s|}) = \frac{e^\gamma}{\pi} \Delta_0 \tag{47}$$

with $e^\gamma \approx 1.78$. In the BCS regime, the pair formation and critical temperature are the same, because in that regime the Fermi fluid constitutes a fluid of strongly overlapping fermion pairs, whose inter-particle spacing is much larger than the average particle distance (cp. fig. 2) and which do not form a condensate in the sense of bosons in a BEC. The overlapping pairs rather exhibit a behaviour similar to superconductivity. In fact, superconductivity can be seen in a more general picture as so-called charged superfluidity and the interacting Fermi gas below the critical temperature forms a superfluid, i.e. a fluid without any viscosity. Experimental evidence for this behaviour was first found in 2005 at MIT by [15] by observing vortices in the superfluid.
In the BEC regime, T_{pair}^{BCS} is given by the so-called Lambert W-function, which is the solution to $x = We^W$ and for $x > 3$ approximated by $W(x) \approx \ln(x - \ln[\ln(x)])$:

$$T_{pair}^{BCS} = \frac{1}{3} \frac{|E_B|}{W[(\frac{\pi}{6})^{\frac{1}{3}} \ \frac{E_B}{2E_F}]} \ . \quad (48)$$

This leads to a very steep increase of T_{pair} towards the BEC regime. Overall, T_{pair} increases exponentially from zero in the BCS regime ($1/k_F a_s \to -\infty$) to very large values in the BEC limit, i.e. in the limit of $1/k_F a_s \to \infty$. This can intuitively be understood as follows: deep in the BEC regime, the very large positive scattering length leads to the formation of very strongly bound fermionic molecules. Hence, the larger the scattering length the larger has to be the energy, i.e. temperature, to break up these molecules which defines the temperature of pair formation.

4.2 Critical Temperature for Condensation

Deeply in BEC regime T_C^{BEC} must simply be given by the well known critical temperature for bosons with molecular density $n_M = n/2$ and mass $m_M = 2m$:

$$T_C^{BEC} = \frac{2\pi\hbar^2}{m_M}(\frac{n_M}{\zeta(\frac{3}{2})})^{2/3} = 0.22 E_F \ . \quad (49)$$

However, there are small positive corrections to this value, when going into the BCS-BEC regime [13]. Since there should be a smooth crossover in T_C from the BCS to the BEC regime, there hence must be a maximum in the crossover regime. Indeed, when doing the complete calculation as in [13], one finds T_C as a function of the interaction parameter as in figure 6. It shows that the maximum for T_C is indeed in the crossover region.

4.3 Condensate Fraction

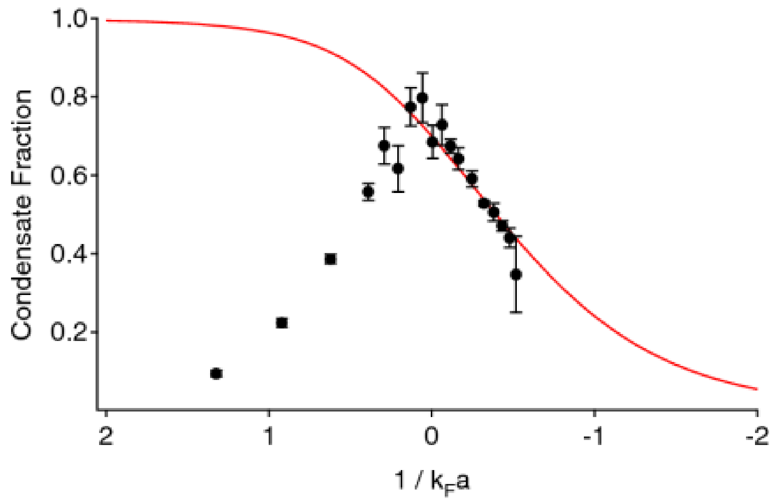

Figure 7: Condensate fraction of fermionic pairs according to equation (50) as a function of the interaction parameter $1/k_F a_s$. Dots and squares give experimental values. The discrepancy in the BEC regime on the left hand side is due to thermal heating during the experiment which leads to a decay of the condensate. Figure taken from [11].

As mentioned in section 2.3, the condensate fraction of fermionic pairs can be calculated from the pairing field $\langle \mathrm{c}_{\mathbf{k}\uparrow}\mathrm{c}_{-\mathbf{k}\downarrow}\rangle$ which also occurs in the definition of the gap equation. Now, taking the temperature dependent gap equation (42), one can see that the pairing field acquires the factor $\tanh(\frac{\beta \mathrm{E}_{\mathbf{k}}}{2})$ and equation (7) for the condensate fraction at arbitrary, low temperatures becomes [10]:

$$n_0 = \frac{1}{V}\sum_{\mathbf{k}} |\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}\rangle|^2 = \sum_{\mathbf{k}} u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 tanh^2(\frac{\beta E_{\mathbf{k}}}{2}) \ . \tag{50}$$

Recall that the interaction parameter $1/\mathrm{k_F a_s}$ is related to the gap which occurs in $\mathrm{E}_{\mathbf{k}}$. Figure 7 gives the condensate fraction as a function of the interaction parameter, hence showing it for the different regimes of the interacting Fermi gas. In the BEC limit, it approaches unity, while it decreases exponentially in the BCS limit. Note: actually there is a more subtle difference in the condensates in both limits. In the BEC limit, the condensate is just a BEC of fermionic pairs. But, towards the BCS limit, there will be a difference between a condensate in the BEC sense and pairs that 'condense' in a superfluid which both occur in the crossover region. Thus, in a more detailed study of the condensate in the BCS regime and the crossover region, one as to distinguish between those two types of 'condensate'.

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