

Introduction to physics of ultra cold gases

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Contents

1	General aspects	7
1.1	Introduction	7
1.2	Single particle	8
1.2.1	General aspects	8
1.2.2	Traps	8
1.3	Many particles	9
1.4	Basics of second quantization	11
1.4.1	Bosons	11
1.4.2	Fermions	13
1.4.3	Single particle operator	13
1.4.4	Two particle operator	14
2	Bosons	17
2.1	Free Bose gas	17
2.1.1	General properties	17
2.1.2	Superfluidity in Free Bose Gas condensate	20
2.1.3	BEC in lower dimensions	21
2.2	Trapped Bose gas	22
2.2.1	Box	22
2.2.2	Parabolic trap	23
2.3	Weakly interacting Bose gas	25
2.4	Mean field approximation	30
2.5	BEC in an isotr. harmonic trap at $T=0$	36
2.5.1	Comparison of terms in GP	36
2.5.2	Thomas-Fermi-Regime	38
3	Fermions	47
3.1	Free Fermions	47
3.1.1	General properties	47
3.1.2	Pressure of degenerated Fermi gas	51
3.1.3	Excitations of Fermions at $T=0$	53

3.2	Trapped non-interacting Fermi gas at $T=0$	55
3.3	Weakly interacting Fermi gas	58
3.3.1	Ground state	58
3.3.2	Decay of excitations	62
3.4	Landau-Fermi-Liquid	64
3.4.1	Zero Sound	68
3.5	Bardeen-Cooper-Schrieffer-Theory	70
3.5.1	General treatment	70
3.5.2	BCS Hamiltonian	74
3.6	Andreev reflection	88
A	General energy-momentum relation	90
B	Calculation for section 3.3.1	91
C	Lifetime and Fermis Golden Rule	92
	Bibliography	93

List of Figures

1.1	Interchange of quantum state	15
1.2	Plot of inter atomic potential	16
2.1	Frames of reference	20
2.2	Dispersion in weak interacting BOSE systems	27
2.3	Energy spectra in BOSE condensates	30
2.4	Top view on rotating superfluid liquid	34
2.5	Radial part of the wave function in superfluid BOSE gas	35
2.6	Many vortices in superfluid BOSE gas	35
2.7	Radial wave function in THOMAS-FERMI approximation	40
2.8	Schematic plot of z dependence for negative scattering length	42
3.1	FERMI-DIRAC-Distribution for $T = 0$ and for small T	48
3.2	Excitations of FERMIONS at low temperatures	53
3.3	Schematic view of a trapped particle with large n	55
3.4	Excitations around the FERMI sphere	62
3.5	Spectrum of FERMIONS with COOPER pairing	77
3.6	Pairing gap as function of temperature	82
3.7	Schematic probability flow in BCS	85
3.8	BCS gap	86
3.9	Boundary between superfluid and non superfluid region	88

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Chapter 1

General aspects

1.1 Introduction

The physics of ultra cold gases is interesting, because

- interaction is characterized by a small parameter, so that systems may be analytically analyzed. Usually phenomenological data and experimental data has to be fitted while in this case only the scattering length and the mass m are required as input
- many traps (preparations) and manipulations are possible

The title of this lecture contains two words which have to be defined.

Gases r_0 being the size of the neutral particle (range of interparticle interaction) and n the density, the system is called a gas if

$$r_0 \ll n^{-\frac{1}{3}}, \quad (1.1)$$

i.e. the range of the interparticle interaction is much smaller than the mean interparticle distance. This implies that the interaction is characterized by a small parameter ($\sim r_0 n^{\frac{1}{3}}$).

Ultra cold Classically there is no scale to which ultra cold could be defined. Quantum mechanically the DE BROGLIE wavelength

$$\lambda_D \sim \frac{\hbar}{p} \sim \frac{\hbar}{\sqrt{mk_B T}} \quad (1.2)$$

offers such scale. We call a system ultra cold if

$$\lambda_D \gtrsim n^{-\frac{1}{3}}. \quad (1.3)$$

At this point quantum degeneracy becomes important.

From now on we will set $k_B \equiv 1$.

1.2 Single particle

1.2.1 General aspects

The HAMILTONian is

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + U(\vec{r}) \quad (1.4)$$

where $U(\vec{r})$ is the (Trap)potential. The solutions

$$\varphi_{\nu} : \quad \hat{H}\varphi_{\nu} = \varepsilon_{\nu}\varphi_{\nu} \quad (1.5)$$

are orthogonal and the set of functions $\varphi_{\nu}(\vec{r})$ is complete

$$\int dr \varphi_{\nu}^*(r)\varphi_{\nu'}(r) = \delta_{\nu\nu'} \quad (1.6)$$

$$\sum_{\nu} \varphi_{\nu}^*(\vec{r})\varphi_{\nu}(\vec{r}') = \delta(\vec{r} - \vec{r}'). \quad (1.7)$$

If the particle is free, i.e. $U = 0$ then $\nu \rightarrow p$ and

$$\varphi_p = e^{i\vec{p}\cdot\vec{r}} \quad \varepsilon_p = \frac{p^2}{2m}. \quad (1.8)$$

1.2.2 Traps

General harmonic trap

$$U(\vec{r}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad \text{with solutions} \quad (1.9)$$

$$\psi_{n_x n_y n_z}(\vec{r}) = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z). \quad (1.10)$$

For each space dimension the wave function is of the form

$$\varphi_{n_i}(x_i) = \frac{1}{\sqrt{2^{n_i}(n_i)!\sqrt{\pi}l_0}} e^{-\frac{1}{2}\left(\frac{x_i}{l_0}\right)^2} H_{n_i}\left(\frac{x_i}{l_0}\right). \quad (1.11)$$

Here H_n are the HERMITE polynomials and $l_0 = \sqrt{\frac{\hbar}{m\omega}}$.

Rotationally invariant harmonic trap

$$U(\vec{r}) = \frac{m}{2}(\omega_\rho^2 \rho^2 + \omega_z^2 z^2) \quad \rho = \sqrt{x^2 + y^2} \quad (1.12)$$

This leads to the solution

$$\Psi_{n_\rho m n_z} = \varphi_{n_\rho}(\hat{\rho}) e^{im\phi} \varphi_{n_z}(\hat{z}) \quad \text{with} \quad (1.13)$$

$$\hat{\rho} = \frac{\rho}{\sqrt{\frac{\hbar}{m\omega_\rho}}} i \equiv \frac{\rho}{l_\rho} \quad \hat{z} = \frac{z}{\sqrt{\frac{\hbar}{m\omega_z}}} i \equiv \frac{z}{l_z} \quad (1.14)$$

$$\varphi_{n_z} = \frac{1}{\sqrt{\sqrt{n} 2^{n_z} n_z! l_z}} e^{-\frac{\hat{z}^2}{2}} H_{n_z}(\hat{z}) \quad (1.15)$$

$$\varphi_{n_\rho} = \frac{1}{l_\rho} \sqrt{\frac{n_\rho!}{\pi(n_\rho + |m|)!}} \hat{\rho}^{|m|} e^{-\frac{\hat{\rho}^2}{2}} L_{n_\rho}^{|m|}(\hat{\rho}^2) \quad (1.16)$$

$$\varepsilon_{n_\rho m n_z} = \hbar(\omega_\rho(2n_\rho + |m| + 1) + \omega_z(n_z + \frac{1}{2})). \quad (1.17)$$

Here H are the HERMITE polynomials and L the LAGUERRE polynomials.

Isotropic harmonic trap

$$U(\vec{r}) = \frac{m\omega^2}{2} r^2 \quad (1.18)$$

The dimensionless solutions are

$$\Psi_{nlm} = \varphi_{nl}(\vec{r}) Y_{lm}(\vec{r}) \quad \hat{r} = \frac{r}{\sqrt{\frac{\hbar}{m\omega}}} \equiv r l_0 \quad (1.19)$$

$$\varphi_{nl} = \frac{1}{l_0^{\frac{3}{2}}} \sqrt{\frac{2n!}{\Gamma(n+l+\frac{3}{2})}} \hat{r}^l e^{-\frac{\hat{r}^2}{2}} L_n^{l+\frac{1}{2}}(\hat{r}^2) \quad (1.20)$$

$$\varepsilon_{nlm} = \hbar\omega(2n + l + \frac{3}{2}). \quad (1.21)$$

Here Γ is the EULER gamma (generalized faculty) function.

1.3 Many particles

The HAMILTONIAN is

$$\hat{H} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \Delta_i + U(\vec{r}_i) \right) + \frac{1}{2} \sum_{i \neq j=1}^N U_1(\vec{r}_i - \vec{r}_j). \quad (1.22)$$

The simplest case is the free gas, where $U_1 \equiv 0$. If we label possible single particle states with ν and if each state is occupied by n_ν particles than the total number of particles N is

$$\sum_{\nu} n_{\nu} = N. \quad (1.23)$$

A simple ansatz for the wave function is a product of single particle wave functions:

$$\Psi_{n_1, n_2, \dots}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n) = \varphi_{i_1}(\vec{r}_1) \varphi_{i_2}(\vec{r}_2) \cdots \varphi_{i_n}(\vec{r}_n) \quad (1.24)$$

$$\varepsilon_{n_1, n_2, \dots} = n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots \quad (1.25)$$

This solution satisfies the SCHRÖDINGER equation (1.5) but, in general, it fails to describe the physics of N identical particles¹, because the wave function must change in a specific way under permutations P of any two identical particles. Since $|\psi|^2$ is an observable which is unaffected by the permutation, this leaves two possibilities:

$$P\psi = \pm\psi \quad (1.26)$$

1. "+": *Bosons*

The wave function has to be symmetrized over all possible permutations which exchange particles in different quantum states. This subset of the permutation group is denoted by p' :

$$\Psi_{n_1, n_2, \dots}^{(b)} = \sqrt{\frac{n_1! n_2! \cdots}{N!}} \sum_{p'} \varphi_{\nu_1}(\vec{r}_1) \cdots \varphi_{\nu_n}(\vec{r}_n) \quad (1.27)$$

2. "-": *Fermions*

No two single particles may be in the same state ν . Therefore the sum runs over all possible permutations:

$$\Psi_{n_1, n_2, \dots}^{(f)} = \frac{1}{\sqrt{N!}} \sum_p (-)^p \varphi_{\nu_1}(\vec{r}_1) \cdots \varphi_{\nu_n}(\vec{r}_n) \quad (1.28)$$

Alternatively the wave function can be described by a determinant:

$$\Psi_{n_1, n_2, \dots}^{(f)} = \frac{1}{\sqrt{N!}} \left| \begin{pmatrix} \varphi_{\nu_1}(\vec{r}_1) & \varphi_{\nu_1}(\vec{r}_2) & \cdots & \varphi_{\nu_1}(\vec{r}_n) \\ \varphi_{\nu_2}(\vec{r}_1) & \varphi_{\nu_2}(\vec{r}_2) & \cdots & \varphi_{\nu_2}(\vec{r}_n) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\nu_n}(\vec{r}_1) & \varphi_{\nu_n}(\vec{r}_2) & \cdots & \varphi_{\nu_n}(\vec{r}_n) \end{pmatrix} \right| \quad (1.29)$$

¹i.e. no further quantum numbers like color is present

A general wave function can be written as a linear combination of the above functions

$$\psi^{(b,f)}(\{\vec{r}_i\}) = \sum_{\{p_i\}} C_{\{p_i\}} \psi_{\{p_i\}}^{(b,f)}(\{r_i\}). \quad (1.30)$$

Only the occupations n_i of each single particle state are required. With this information the wave function can be reconstructed. Therefore, a simplified description can be expected if the change from r_i representation to n_i representation is made.

1.4 Basics of second quantization

We have states v_1, v_2, \dots with n_1, n_2, \dots particles. Each state is described by $|n_1, n_2, \dots\rangle$ with the special state vacuum $|0, 0, \dots\rangle \equiv |0\rangle$. The following operators are relevant to these states:

- a_v is the annihilation operator: $n_v \rightarrow n_v - 1$
(Note that $a_v|0\rangle = 0$ for any v)
- a_v^\dagger is the creation operator: $n_v \rightarrow n_v + 1$

Note that these operators annihilate or create particles *in a given quantum state* unlike the operators in first quantization which change the quantum number of one quantum state.

As was already mentioned above, there are two types of particles.

1.4.1 Bosons

In this case we have the following commutation relations:

$$[a_v, a_{v'}^\dagger] = \delta_{vv'} \quad (1.31)$$

$$[a_v, a_{v'}] = [a_v^\dagger, a_{v'}^\dagger] = 0 \quad (1.32)$$

Because states with different v are independent, we consider only one state to understand the consequences of the above generator algebras.

The actions of the operators on the states are as follows:

$$a|0\rangle = 0 \quad (a^\dagger)^n |0\rangle = \alpha_n |n\rangle \quad (1.33)$$

$$\langle 0|a^n = \langle n|\alpha_n \quad (a^\dagger)^{n-1} |0\rangle = \alpha_{n-1} |n-1\rangle \quad (1.34)$$

All states are orthonormal, i.e. $\langle n|m\rangle = \delta_{nm}$. The α_n can be chosen real, as a phase can be absorbed into the definition of the states. It follows

$$\alpha_1^2 = 1 \quad \text{and} \quad (1.35)$$

$$\alpha_n^2 = \langle 0|\mathbf{a}^n (\mathbf{a}^\dagger)^n |0\rangle = \langle 0|\mathbf{a}^{n-1} (1 + \mathbf{a}^\dagger \mathbf{a}) (\mathbf{a}^\dagger)^{n-1} |0\rangle \quad (1.36)$$

$$= \alpha_{n-1}^2 + \langle 0|\mathbf{a}^{n-1} \mathbf{a}^\dagger \mathbf{a} (\mathbf{a}^\dagger)^{n-1} |0\rangle \quad (1.37)$$

$$= \alpha_{n-1}^2 + \langle 0|\mathbf{a}^{n-1} \mathbf{a}^\dagger (1 + \mathbf{a}^\dagger \mathbf{a}) (\mathbf{a}^\dagger)^{n-1} |0\rangle \quad (1.38)$$

$$= 2\alpha_{n-1}^2 + \langle 0|\mathbf{a}^{n-1} (\mathbf{a}^\dagger)^2 \mathbf{a} (\mathbf{a}^\dagger)^{n-2} |0\rangle \quad (1.39)$$

$$= n\alpha_{n-1}^2 + \underbrace{\langle 0|\mathbf{a}^{n-1} (\mathbf{a}^\dagger)^n \mathbf{a}|0\rangle}_{=0} \quad (1.40)$$

$$= n!. \quad (1.41)$$

Therefore each state can be written as

$$|n\rangle = \frac{1}{\sqrt{n!}} (\mathbf{a}^\dagger)^n |0\rangle \quad \text{and} \quad (1.42)$$

$$\mathbf{a}^\dagger |n\rangle = \frac{1}{\sqrt{n!}} \mathbf{a}^\dagger (\mathbf{a}^\dagger)^n |0\rangle = \frac{1}{\sqrt{n!}} \sqrt{(n+1)!} |n+1\rangle \quad (1.43)$$

$$= \sqrt{n+1} |n+1\rangle. \quad (1.44)$$

Analogously we calculate

$$\mathbf{a}|n\rangle = \frac{1}{\sqrt{n!}} \mathbf{a} (\mathbf{a}^\dagger)^n |0\rangle = \frac{1}{\sqrt{n!}} (1 + \mathbf{a}^\dagger \mathbf{a}) (\mathbf{a}^\dagger)^{n-1} |0\rangle \quad (1.45)$$

$$= \frac{1}{\sqrt{n!}} \left\{ \sqrt{(n-1)!} |n-1\rangle + \mathbf{a}^\dagger \mathbf{a} (\mathbf{a}^\dagger)^{n-1} |0\rangle \right\} \quad (1.46)$$

$$= \frac{1}{\sqrt{n!}} \left\{ \sqrt{(n-1)!} |n-1\rangle + \mathbf{a}^\dagger (1 + \mathbf{a}^\dagger \mathbf{a}) (\mathbf{a}^\dagger)^{n-2} |0\rangle \right\} \quad (1.47)$$

$$= \frac{1}{\sqrt{n!}} \left\{ 2\sqrt{(n-1)!} |n-1\rangle + (\mathbf{a}^\dagger)^2 \mathbf{a} (\mathbf{a}^\dagger)^{n-2} |0\rangle \right\} \quad (1.48)$$

$$= \frac{1}{\sqrt{n!}} n \sqrt{(n-1)!} |n-1\rangle = \sqrt{n} |n-1\rangle. \quad (1.49)$$

Defining the particle number operator $\hat{n} = \mathbf{a}^\dagger \mathbf{a}$ we get

$$\hat{n}|n\rangle = \mathbf{a}^\dagger \mathbf{a}|n\rangle = \mathbf{a}^\dagger \sqrt{n} |n-1\rangle = \sqrt{n} \sqrt{n} |n\rangle = n|n\rangle, \quad (1.50)$$

and the energy operator is therefore $\epsilon_n = \epsilon \mathbf{a}^\dagger \mathbf{a}$.

1.4.2 Fermions

The operators a_v and a_v^\dagger obey anticommutation relations

$$\{a_v, a_{v'}^\dagger\} = \delta_{vv'} \quad (1.51)$$

$$\{a_v, a_{v'}\} = \{a_v^\dagger, a_{v'}^\dagger\} = 0 \quad \text{PAULI Principle.} \quad (1.52)$$

Again, considering for simplicity the one state problem, it is easy to see that the occupation number N can only be 0 (the vacuum state) or 1 (PAULI principle):

$$a|0\rangle = 0 \quad a|1\rangle = |0\rangle \quad a^\dagger|0\rangle = |1\rangle \quad \text{with} \quad (1.53)$$

$$\hat{H} = \varepsilon a^\dagger a \quad \hat{n} = a^\dagger a \quad (1.54)$$

1.4.3 Single particle operator

We can now define the field operators as

$$\hat{\psi}(\vec{r}) = \sum_v a_v \varphi_v(\vec{r}) \quad (1.55)$$

$$\hat{\psi}^\dagger(\vec{r}) = \sum_v a_v^\dagger \varphi_v^*(\vec{r}). \quad (1.56)$$

Here v runs over all states and the $\varphi_v(\vec{r})$ are the amplitudes (probabilities) at \vec{r} for a particle to be in the state v . They have the following (anti-)commutation relations:

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}') \right]_{\pm} = \sum_{vv'} \varphi_v(\vec{r}) \varphi_{v'}^*(\vec{r}') \left[a_v, a_{v'}^\dagger \right]_{\pm} \quad (1.57)$$

$$= \sum_v \varphi_v(\vec{r}) \varphi_v^*(\vec{r}') = \delta(\vec{r} - \vec{r}') \quad (1.58)$$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}') \right]_{\pm} = \left[\hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}') \right]_{\pm} = 0 \quad (1.59)$$

By using the field operators $\hat{\psi}(\vec{r})$ and $\hat{\psi}^\dagger(\vec{r})$ various quantum mechanical operators can easily be transformed from the space representation (\vec{r} -representation) into the occupation number representation (n -representation).

For a *Single particle operator*

$$\hat{F}_1 = \sum_{i=1}^N f(\vec{r}_i) \quad (1.60)$$

(Examples:

$$n(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i) \quad \text{density} \quad (1.61)$$

$$\hat{H}_1 = \sum_i \left\{ -\frac{\hbar^2}{2m} \Delta_i + U(\vec{r}_i) \right\} \text{Single particle HAMILTONian} \quad (1.62)$$

we have

$$\hat{F}_1 = \int d^3r \hat{\psi}^\dagger(\vec{r}) f(\vec{r}) \hat{\psi}(\vec{r}) = \sum_{\mathbf{v}\mathbf{v}'} \langle \mathbf{v}' | f | \mathbf{v} \rangle \mathbf{a}_{\mathbf{v}'}^\dagger \mathbf{a}_{\mathbf{v}} \quad (1.63)$$

$$\langle \mathbf{v}' | f | \mathbf{v} \rangle = \int d^3r' \phi_{\mathbf{v}'}^\dagger(\vec{r}') f(\vec{r}) \phi_{\mathbf{v}}(\vec{r}'). \quad (1.64)$$

Each term in the sum on the r.h.s. of eq. (1.63) describes the transition of a particle from a state \mathbf{v} to a state \mathbf{v}' with amplitude $\langle \mathbf{v}' | f | \mathbf{v} \rangle$.

Examples:

$$\hat{n}(\vec{r}) = \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \quad (1.65)$$

$$\hat{N} = \sum_{\mathbf{v}} \mathbf{a}_{\mathbf{v}}^\dagger \mathbf{a}_{\mathbf{v}} \quad (1.66)$$

$$\hat{H}_1 = \int d^3r \left(\sum_{\mathbf{v}'} \mathbf{a}_{\mathbf{v}'}^\dagger \phi_{\mathbf{v}'}^*(\vec{r}) \right) \left\{ -\frac{\hbar^2}{2m} \Delta + U(\vec{r}) \right\} \left(\sum_{\mathbf{v}} \mathbf{a}_{\mathbf{v}} \phi_{\mathbf{v}}(\vec{r}) \right) \quad (1.67)$$

$$= \int d^3r \left(\sum_{\mathbf{v}'} \mathbf{a}_{\mathbf{v}'}^\dagger \phi_{\mathbf{v}'}^*(\vec{r}) \right) \left(\sum_{\mathbf{v}} \mathbf{a}_{\mathbf{v}} \varepsilon_{\mathbf{v}} \phi_{\mathbf{v}}(\vec{r}) \right) \quad (1.68)$$

$$= \sum_{\mathbf{v}} \varepsilon_{\mathbf{v}} \mathbf{a}_{\mathbf{v}}^\dagger \mathbf{a}_{\mathbf{v}} \quad \text{with} \quad \int d^3r \phi_{\mathbf{v}'}^*(\vec{r}) \phi_{\mathbf{v}}(\vec{r}) = \delta_{\mathbf{v}\mathbf{v}'} \quad (1.69)$$

1.4.4 Two particle operator

$$\hat{F}_i = \sum_{j \neq k} f(\vec{r}_j, \vec{r}_k) \quad (1.70)$$

Example:

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{i \neq j} U_1(\vec{r}_i - \vec{r}_j) \quad (1.71)$$

Now we have

$$\hat{F}_2 = \int d^3r d^3r' \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}') f(\vec{r}, \vec{r}') \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}) \quad (1.72)$$

and the the interaction part of the HAMILTONIAN as example:

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}'_1, \mathbf{v}'_2} \langle \mathbf{v}'_1 \mathbf{v}'_2 | U_1 | \mathbf{v}_1 \mathbf{v}_2 \rangle \mathbf{a}_{\mathbf{v}'_1}^\dagger \mathbf{a}_{\mathbf{v}'_2}^\dagger \mathbf{a}_{\mathbf{v}_2} \mathbf{a}_{\mathbf{v}_1} \quad \text{with} \quad (1.73)$$

$$\langle \mathbf{v}'_1 \mathbf{v}'_2 | U_1 | \mathbf{v}_2 \mathbf{v}_1 \rangle = \int d^3r d^3r' \phi_{\mathbf{v}'_1}^*(\vec{r}) \phi_{\mathbf{v}'_2}^*(\vec{r}') U_1(\vec{r} - \vec{r}') \phi_{\mathbf{v}_2}(\vec{r}') \phi_{\mathbf{v}_1}(\vec{r}) \quad (1.74)$$

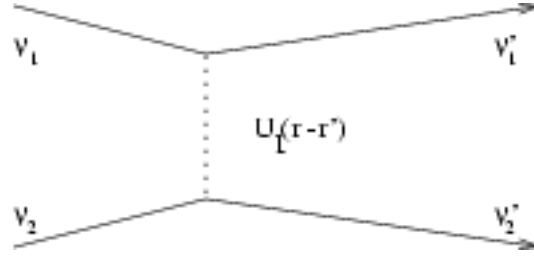


Figure 1.1: Interchange of quantum state

This term describes the scattering of two particles in initial states v_1 and v_2 into final states v_1' and v_2' with an amplitude $\langle v_1' v_2' | U_I | v_2 v_1 \rangle$.

We can now write down the complete HAMILTONoperator in the form:

$$\hat{H} = \sum_{\nu} \varepsilon_{\nu} a_{\nu}^{\dagger} a_{\nu} + \frac{1}{2} \sum_{v_1, v_2, v_1', v_2'} \langle v_1' v_2' | U_I | v_2 v_1 \rangle a_{v_1'}^{\dagger} a_{v_2'}^{\dagger} a_{v_2} a_{v_1} \quad \text{with} \quad (1.75)$$

$$\hat{N} = \sum_{\nu} a_{\nu}^{\dagger} a_{\nu} \quad (1.76)$$

The constraint of fixed N introduces technical difficulties. To avoid them, we introduce the chemical potential μ

$$\hat{H} \rightarrow \hat{H} - \mu \hat{N} \quad (1.77)$$

and keep a fixed \bar{n} . The system can be thought as connected with a reservoir and the chemical potential governs the exchange process. In our calculations we have to replace

$$\varepsilon_{\nu} \rightarrow \varepsilon_{\nu} - \mu \quad (1.78)$$

to take this extra term into account.

If we consider the homogeneous case then ν becomes \vec{p} and

$$\varphi_{\nu} = e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \quad \sum_{\nu} \rightarrow \mathcal{V} \int \frac{d^3 p}{(2\pi\hbar)^3} \quad (1.79)$$

$$\varepsilon_{\nu} = \frac{p^2}{2m} \quad \langle \varphi_{\nu} | \varphi_{\nu'} \rangle \rightarrow (2\pi\hbar)^3 \delta(\vec{p} - \vec{p}'). \quad (1.80)$$

For the time being we set the volume $\mathcal{V} \equiv 1$. Since we consider the homogeneous case \vec{p} is conserved therefore

$$\langle \vec{p}_1' \vec{p}_2' | U_I | \vec{p}_1 \vec{p}_2 \rangle = (2\pi\hbar)^3 \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_1' - \vec{p}_2') g. \quad (1.81)$$

To calculate g we have to switch carefully to the center of mass reference system and use relative coordinates. Then g turns out to be the FOURIER transform of $U_1(\vec{r})$:

$$g = \int d^3r U_1(\vec{r}) e^{i(\vec{p}_1 - \vec{p}_2) \cdot \vec{r} / \hbar}. \quad (1.82)$$

But quantum degenerate cold gases, eqn. (1.1)-(1.3), imply collisions of particles with low momenta (i.e. slow particles, $r_0 p \ll \hbar$). From scattering theory we know that in this regime collisions are characterized by only one parameter, the scattering length a . Therefore, in the BORN approximation,

$$g = \frac{4\pi\hbar^2}{m} a. \quad (1.83)$$

As a result, the HAMILTONIAN takes the form

$$\hat{H} = \sum_{\vec{p}} (\varepsilon_{\vec{p}} - \mu) a_{\vec{p}}^\dagger a_{\vec{p}} + \frac{1}{2} g \sum_{p_1, p_2, p'_1, p'_2} a_{p'_1}^\dagger a_{p'_2}^\dagger a_{p_2} a_{p_1}. \quad (1.84)$$

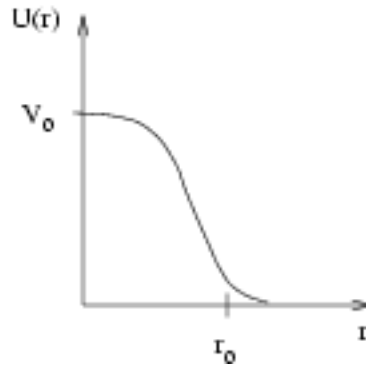


Figure 1.2: Plot of inter atomic potential

Chapter 2

Bosons

2.1 Free Bose gas

2.1.1 General properties

For a free BOSE gas the HAMILTONian is

$$\hat{H} = \sum_{\vec{p}} (\epsilon_{\vec{p}} - \mu) \mathbf{a}_p^\dagger \mathbf{a}_p. \quad (2.1)$$

At high temperature we have classical behavior; we consider only ultra cold gases for which

$$\frac{\hbar}{\sqrt{2mT_Q}} \sim n^{-\frac{1}{3}} \rightsquigarrow T_Q \sim \frac{\hbar^2}{m} n^{\frac{2}{3}}, \quad (2.2)$$

where T_Q is the quantum degeneracy temperature. With this HAMILTONian at $T \searrow 0$ the ground state is identical to the product of the single particle ground states and the fixed average density¹ is given by

$$\bar{n} = \langle \sum_p \mathbf{a}_p^\dagger \mathbf{a}_p \rangle = \langle \sum_p n_p \rangle = \sum_p \frac{1}{\exp(\frac{\epsilon_p - \mu}{T}) - 1} \quad (2.3)$$

$$= \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp(\frac{\epsilon_p - \mu}{T}) - 1}. \quad (2.4)$$

This equation defines μ ; two properties can be derived from it:

1. $\mu \leq \epsilon_0 = 0$ because n must be positive

¹Note that we take the quantum mechanical as well as the statistical average

2. The density of states at energy ε is

$$v(\varepsilon) = \sum_{\vec{p}} \delta(\varepsilon - \varepsilon_p) = \int \frac{d^3 p}{(2\pi\hbar)^3} \delta\left(\varepsilon - \frac{\vec{p}^2}{2m}\right) \quad (2.5)$$

$$= 4\pi \frac{1}{(2\pi\hbar)^3} \int_0^\infty dp p^2 \delta\left(\varepsilon - \frac{p^2}{2m}\right) \quad (2.6)$$

$$= \left(\frac{\sqrt{2m}}{2\pi\hbar}\right)^3 4\pi \int_0^\infty dx \sqrt{x} \delta(\varepsilon - x) \sim \sqrt{\varepsilon} \xrightarrow{T \searrow 0} 0. \quad (2.7)$$

Obviously the ground state is not counted properly.

Analyzing the occupation of each state

$$n_p = \frac{1}{\exp\left(\frac{(\varepsilon_p + |\mu|)}{T}\right) - 1} \quad (2.8)$$

we can distinguish two cases:

1. At a given \vec{p} and μ

$$T \downarrow : n_p \downarrow \quad (2.9)$$

2. At a given \vec{p} and T

$$|\mu| \downarrow : n_p \uparrow \quad (2.10)$$

Therefore, to keep the average density fixed, we have to decrease the modulus of the chemical potential with decreasing temperature:

$$T \downarrow \Rightarrow |\mu| \downarrow \quad (2.11)$$

But $\mu \geq 0$ hence we can define T_C to be the temperature where $\mu = 0$:

$$\bar{n} = \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left(\frac{p^2}{2mT_C}\right) - 1} \quad x^2 = \frac{p^2}{2mT_C} \quad (2.12)$$

$$= (2mT_C)^{\frac{3}{2}} \frac{4\pi}{(2\pi\hbar)^3} \int_0^\infty dx \frac{x^2}{e^{x^2} - 1} \quad (2.13)$$

$$= (2mT_C)^{\frac{3}{2}} \frac{1}{2\pi^2\hbar^3} \int dx x^2 e^{-x^2} \frac{1}{1 - e^{-x^2}} \quad (2.14)$$

$$= (2mT_C)^{\frac{3}{2}} \frac{1}{2\pi^2\hbar^3} \frac{\sqrt{\pi}}{4} \xi\left(\frac{3}{2}\right) = \left(\frac{mT_C}{2\pi\hbar^2}\right)^{\frac{3}{2}} \xi\left(\frac{3}{2}\right) \quad (2.15)$$

Here we have used

$$\int_0^{\infty} dx x^2 e^{-x^2} \sum_{n=0}^{\infty} e^{-nx^2} = \int dx x^2 \sum_{n=1}^{\infty} e^{-nx^2} \quad (2.16)$$

$$= \sum_{n=1}^{\infty} \frac{1}{n^{\frac{3}{2}}} \int_0^{\infty} dy y^2 e^{-y^2} = \xi \left(\frac{3}{2} \right) \frac{1}{4} \sqrt{\pi} \quad (2.17)$$

$$\int_0^{\infty} dy e^{-\alpha y^2} = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \quad (2.18)$$

$$\int_0^{\infty} dy y^2 e^{-\alpha y^2} = -\frac{\partial}{\partial \alpha} \int_0^{\infty} dy e^{-\alpha y^2}. \quad (2.19)$$

Therefore the critical temperature is

$$T_C = (2\pi) \left[\xi \left(\frac{3}{2} \right) \right]^{-\frac{2}{3}} \frac{\hbar^2}{m} \bar{n}^{\frac{2}{3}} = 3.31 \frac{\hbar^2}{m} \bar{n}^{\frac{2}{3}}. \quad (2.20)$$

For $T < T_C$ we can now rewrite

$$\bar{n} = n_0(T) + \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left(\frac{\epsilon_p}{T}\right) - 1} \quad (2.21)$$

$$= n_0(T) + \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left(\frac{p^2}{2mT_C} \frac{T_C}{T}\right) - 1} \quad (2.22)$$

$$= n_0(T) + \underbrace{\left(\frac{T}{T_C} \right)^{\frac{3}{2}} \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left(\frac{p^2}{2mT_C}\right) - 1}}_{\bar{n}} \quad (2.23)$$

$$n_0(T) = n \left[1 - \left(\frac{T}{T_C} \right)^{\frac{3}{2}} \right] \quad (2.24)$$

$$n_p = n_0 (2\pi\hbar)^3 \delta(\vec{p}) + \underbrace{\frac{1}{\exp\left(\frac{p^2}{2mT_C}\right) - 1}}_{\approx \frac{1}{p^2} \ll \delta(\vec{p})}. \quad (2.25)$$

This means, we have a macroscopic occupation of the ground state, i.e. BOSE-EINSTEIN condensation (BEC).

Further properties:

$$E = \sum_p \frac{p^2}{2m} n_p \sim T^{\frac{5}{2}} \quad (2.26)$$

For $T = 0$ all particles are in the ground state with $\epsilon_0 = 0$. But $\mu = 0$ also therefore the energy E_0 of the system is independent of the number of particle and hence unphysical particle number fluctuations are expected. Further

$$\hat{H} = \sum_p (\epsilon_p - \mu) a_p^\dagger a_p \xrightarrow{T < T_C} \sum_p \frac{p^2}{2m} a_p^\dagger a_p \quad (2.27)$$

$$\vec{P} = \sum_p \vec{p} a_p^\dagger a_p. \quad (2.28)$$

This means that the excitations are identified with particles.

2.1.2 Superfluidity in Free Bose Gas condensate

Dissipation means creations of excitations with momentum \vec{p} opposite to the gas velocity due to the interaction of the gas with wall. These excitations decrease the momentum of the gas and stops it after some time. If the medium is superfluid, no such excitations occur. At $T \equiv 0$ no thermal excitations are present, only interactions with the walls are relevant. To find out if those excitations occur, we have check, whether $E_{\text{before}} > E_{\text{after}}$. To describe the situation we have to look at two different frames of reference:

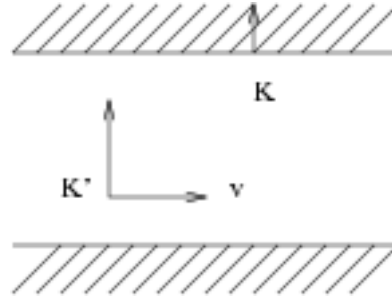


Figure 2.1: Frames of reference

Before $k' : E' = E_0, \vec{P}' = 0$ (no excitations, all particles in ground state with $\vec{p} = 0$)
 $k : E = E_0 + \frac{1}{2}MV^2$

After $E' = E_0 + \epsilon_p, \vec{P}' = \vec{p}_1$ (small)
 $E = E_0 + \frac{1}{2}MV^2 + \epsilon_p + \vec{p} \cdot \vec{V}$

Obviously the total energy decreases (dissipation occurs) if $\vec{p} \downarrow \uparrow \vec{V}$, i.e.

$$\varepsilon_p - pV \leq 0 \quad \Leftrightarrow \quad \varepsilon_p \leq pV. \quad (2.29)$$

This is possible for $V \leq V_C$ with

$$V_C = \min_p \frac{\varepsilon_p}{p} = \min_p \frac{p}{m} = 0. \quad (2.30)$$

For the free BOSE gas dissipation of a flow at $T = 0$ occurs for arbitrary small velocities.

2.1.3 BEC in lower dimensions

In 2D

$$\frac{d^3 p}{(2\pi\hbar)^3} \rightarrow \frac{d^2 p}{(2\pi\hbar)^2} \quad (2.31)$$

$$n = \int \frac{d^2 p}{(2\pi\hbar)^2} \frac{1}{\exp\left(\frac{\varepsilon_p}{T}\right) - 1}. \quad (2.32)$$

This expression diverges at $p \searrow 0$ as $\frac{1}{p}$ therefore $\mu \neq 0$ always. BEC occurs only at $T = 0$, when all particles are in the ground state, i.e. $T_C = 0$.

In 1D no BEC occurs (even at $T = 0$).

However superfluidity in 2D is possible (if we switch on interaction, see below).

2.2 Trapped Bose gas

2.2.1 Box

In a box with $\mathcal{V} = L^3$, N particles and infinite potential at the walls the wave function of one particle is of the form

$$\psi(\vec{r}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\left(\frac{\pi}{L}n_x x\right) \sin\left(\frac{\pi}{L}n_y y\right) \sin\left(\frac{\pi}{L}n_z z\right) \quad (2.33)$$

$$\varepsilon_{\vec{n}} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \quad p_i = \frac{\pi}{L}n_i \quad (2.34)$$

$$\varepsilon_0 = \frac{3}{2} \frac{\hbar^2 \pi^2}{mL^2} \quad \varepsilon_1 = \frac{6}{2} \frac{\hbar^2 \pi^2}{mL^2} \sim T_C N^{-\frac{2}{3}} \quad (2.35)$$

$$T_C = 3.31 \frac{\hbar^2}{m} \left(\frac{N}{L^3}\right)^{\frac{2}{3}} = 3.31 \frac{\hbar^2 N^{\frac{2}{3}}}{mL^2} \rightsquigarrow \varepsilon_0 \sim T_C N^{-\frac{2}{3}} > 0 \quad (2.36)$$

$$N = \sum_{\vec{n}} \frac{1}{\exp\left(\frac{\varepsilon_{\vec{n}} - \mu}{T}\right) - 1}. \quad (2.37)$$

Since N has to remain finite even for $T \rightarrow 0$, $\varepsilon_n - \mu \sim T$ has to hold (at least for low T). To look at this we assume that

$$\varepsilon_0 - \mu \ll \varepsilon_1 - \varepsilon_0 \quad (2.38)$$

$$\varepsilon_n - \mu = \varepsilon_n - \varepsilon_0 + \underbrace{\varepsilon_0 - \mu}_{\approx 0} \approx \varepsilon_n - \varepsilon_0. \quad (2.39)$$

Using this assumption we get

$$N \approx \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{T}\right) - 1} + \sum'_n \frac{1}{\exp\left(\frac{\varepsilon_n - \varepsilon_0}{T}\right) - 1} \quad (2.40)$$

$$= \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{T}\right) - 1} + \int d^3n \frac{1}{\exp\left(\frac{\varepsilon_n - \varepsilon_0}{T}\right) - 1} \quad (2.41)$$

$$\approx \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{T}\right) - 1} + \frac{\mathcal{V}}{(2\pi\hbar)^3} \int d^3p \frac{1}{\exp\left(\frac{p^2}{2mT}\right) - 1} \quad (2.42)$$

$$= \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{T}\right) - 1} + \mathcal{V} n \left(\frac{T}{T_C}\right)^{\frac{3}{2}} \quad N = \mathcal{V} n. \quad (2.43)$$

In (2.41) we substituted $\Delta n_x = 1 \Rightarrow \Delta p_x = \frac{\hbar\pi}{L}$ with

$$\int dn_x dn_y dn_z = \left(\frac{L}{\pi\hbar}\right)^3 \int_{p>0} d^3 p = \frac{\mathcal{V}}{(2\pi\hbar)^3} \int_p d^3 p. \quad (2.44)$$

In (2.42) we note, that only terms with $p \gg \varepsilon_0$ are important. From (2.43) we get

$$\frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{T}\right) - 1} = N \left[1 - \left(\frac{T}{T_C}\right)^{\frac{3}{2}} \right] = N_0 \quad (2.45)$$

$$\Leftrightarrow \quad \varepsilon_0 - \mu = T \ln \left(1 + \frac{1}{N \left[1 - \left(\frac{T}{T_C}\right)^{\frac{3}{2}} \right]} \right) \quad (2.46)$$

$$= \frac{T}{N} \frac{1}{\left[1 - \left(\frac{T}{T_C}\right)^{\frac{3}{2}} \right]} \quad (2.47)$$

which is macroscopically small for $T \ll T_C$. This justifies our assumption above². For the number of particles in the first excited state we get at $\varepsilon_1 - \varepsilon_0 \ll T \ll T_C$

$$N_1 = \frac{1}{\exp\left(\frac{\varepsilon_1 - \mu}{T}\right) - 1} \approx \frac{1}{\exp\left(\frac{\varepsilon_1 - \varepsilon_0}{T}\right) - 1} \approx \frac{T}{\varepsilon_1 - \varepsilon_0} \quad (2.48)$$

$$\sim \frac{T}{T_C} N^{\frac{2}{3}} \gg 1 \quad \text{but} \quad (2.49)$$

$$\frac{N_1}{N_0} \sim N^{-\frac{1}{3}} \frac{T}{T_C} \quad N_1 \ll N_0. \quad (2.50)$$

Therefore the occupation of the ground state is macroscopically larger than that of any other state.

2.2.2 Parabolic trap

In an isotropic parabolic trap with N particles and oscillator frequency ω the energy is

$$\varepsilon_{\vec{n}} = \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) \quad \varepsilon_0 = \frac{3}{2} \hbar\omega. \quad (2.51)$$

²actually it only shows that our assumption is self consistent

The same arguments as in 2.2.1 hold true that $\mu \rightarrow \varepsilon_0$ for $T \searrow 0$. Redefining

$$\tilde{\mu} = \mu - \varepsilon_0 = \mu - \frac{3}{2}\hbar\omega \quad \tilde{\mu} \searrow 0 \text{ for } T \searrow 0 \quad (2.52)$$

$$n_x = \frac{T_C}{\hbar\omega} n'_x \quad (2.53)$$

we get

$$N = \sum_{\vec{n}} \frac{1}{\exp(\varepsilon_{\vec{n}} - \mu) - 1} \quad (2.54)$$

$$\approx \int dn_x dn_y dn_z \frac{1}{\exp\left(\frac{\hbar\omega}{T_C}(n_x + n_y + n_z)\right) - 1} \quad \text{for } T \searrow 0 \quad (2.55)$$

$$= \left(\frac{T_C}{\hbar\omega}\right)^3 \int d^3 n' \frac{1}{\exp(n'_x + n'_y + n'_z) - 1} \quad (2.56)$$

$$= \left(\frac{T_C}{\hbar\omega}\right)^3 \sum_{n=1}^{\infty} \int d^3 n' e^{-n(n'_x + n'_y + n'_z)} \quad (2.57)$$

$$= \left(\frac{T_C}{\hbar\omega}\right)^3 \sum_{n=1}^{\infty} \int dn'_x e^{-nn'_x} \int dn'_y e^{-nn'_y} \int dn'_z e^{-nn'_z} \quad (2.58)$$

$$= \left(\frac{T_C}{\hbar\omega}\right)^3 \sum_{n=1}^{\infty} \frac{1}{n^3} = \left(\frac{T_C}{\hbar\omega}\right)^3 \xi(3). \quad (2.59)$$

Solving this for the critical temperature we get

$$T_C = \hbar\omega N^{\frac{1}{3}} \xi(3)^{-\frac{1}{3}} = 0.94 N^{\frac{1}{3}} \hbar\omega \gg \hbar\omega. \quad (2.60)$$

Quantitatively the critical temperature for a trapped gas can be obtained from the same type of arguments as in the homogeneous case:

$$\lambda_D \sim \frac{\hbar}{\sqrt{mT}} \sim \bar{n}^{-\frac{1}{3}} \quad (2.61)$$

Since for a classical oscillator potential and kinetic energy have the same magnitude and the latter is related via (1.2) to temperature we can estimate the size of the cloud as

$$\frac{m\omega^2 R^2}{2} \sim \frac{T}{2} \quad \Rightarrow R \sim \frac{1}{\omega} \sqrt{\frac{T}{m}} \quad (2.62)$$

$$\rightsquigarrow \bar{n} = \frac{N}{R^3} \quad \Rightarrow T_C \sim \hbar\omega N^{\frac{1}{3}}. \quad (2.63)$$

2.3 Weakly interacting Bose gas

If we consider a unit volume at $T = 0$ the HAMILTONian reads

$$\hat{H} = \sum_p \varepsilon_p \mathbf{a}_p^\dagger \mathbf{a}_p + \frac{1}{2}g \sum_{\vec{p}_1 + \vec{p}_2 = \vec{p}_3 + \vec{p}_4} \mathbf{a}_{p_3}^\dagger \mathbf{a}_{p_4}^\dagger \mathbf{a}_{p_2} \mathbf{a}_{p_1}. \quad (2.64)$$

Since $\varepsilon_p - \varepsilon_0 \approx 0$ we cannot apply perturbation theory because we cannot guarantee $g < \varepsilon_p - \varepsilon_0$. Explicit calculation show divergent terms already in second order. Our solution will also show the invalidity of perturbation theory (cf. (2.111)).

We note that almost all particles are in the ground state, i.e.

$$\mathbf{a}_p^\dagger \mathbf{a}_p \ll n_0 \quad \forall p \neq 0 \quad (2.65)$$

$$\mathbf{a}_0^\dagger \mathbf{a}_0 = n_0 \gg 1 \quad (2.66)$$

$$\mathbf{a}_0 \mathbf{a}_0^\dagger = \underbrace{1 + n_0}_{\approx n_0} \gg 1. \quad (2.67)$$

This leads to the simplification $\mathbf{a}_0, \mathbf{a}_0^\dagger \approx \sqrt{n_0} \gg 1$. Taking leading terms in n_0 , we can write (2.64) in the form

$$\hat{H} = \sum_p \varepsilon_p \mathbf{a}_p^\dagger \mathbf{a}_p + \frac{1}{2}gn_0^2 + \frac{1}{2}gn_0 \sum_{\vec{p} \neq 0} \left\{ \mathbf{a}_p \mathbf{a}_{-p} + \mathbf{a}_{-p}^\dagger \mathbf{a}_p^\dagger + 4\mathbf{a}_p^\dagger \mathbf{a}_p \right\}. \quad (2.68)$$

The remaining momenta have to be equal in the last sum because of conservation of total momentum.

Remembering that

$$n_0 = n - \sum_p n_p \quad (2.69)$$

we can rewrite (2.68) with the considered accuracy as

$$\hat{H} = \frac{1}{2}gn^2 + \sum_{p \neq 0} \varepsilon_p \mathbf{a}_p^\dagger \mathbf{a}_p + \frac{1}{2}gn \sum_{\vec{p} \neq 0} \left\{ 2\mathbf{a}_p^\dagger \mathbf{a}_p + \mathbf{a}_{-p}^\dagger \mathbf{a}_p^\dagger + \mathbf{a}_p \mathbf{a}_{-p} \right\} \quad (2.70)$$

$$\stackrel{!}{=} E_0 + \sum_{p \neq 0} \omega_p \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p \quad (2.71)$$

which is a HAMILTONoperator for quasi particles in a harmonic potential. To find the relation between these quasi-particles and our original (or base) operators we assume according to BOGOLYUBOV

$$\tilde{\mathbf{a}}_p = u_p \mathbf{a}_p + v_p \mathbf{a}_{-p}^\dagger \quad u_p^* = u_p \quad u_p = u_{-p} \quad (2.72)$$

$$\tilde{\mathbf{a}}_p^\dagger = u_p \mathbf{a}_p^\dagger + v_p \mathbf{a}_{-p} \quad v_p^* = v_p \quad v_p = v_{-p} \quad (2.73)$$

and require them to obey the BOSE commutators:

$$\left[\tilde{\mathbf{a}}_p, \tilde{\mathbf{a}}_{p'} \right] = \left[\tilde{\mathbf{a}}_p^\dagger, \tilde{\mathbf{a}}_{p'}^\dagger \right] = 0 \quad \left[\tilde{\mathbf{a}}_p, \tilde{\mathbf{a}}_{p'}^\dagger \right] = \delta_{pp'} \quad (2.74)$$

Using this we get

$$\begin{aligned} \left[\tilde{\mathbf{a}}_p, \tilde{\mathbf{a}}_{p'}^\dagger \right] &= u_p u_{p'} \underbrace{\left[\mathbf{a}_p, \mathbf{a}_{p'}^\dagger \right]}_{\delta_{pp'}} + u_p v_{p'} \underbrace{\left[\mathbf{a}_p, \mathbf{a}_{-p'} \right]}_0 \\ &\quad + v_p v_{p'} \underbrace{\left[\mathbf{a}_{-p}^\dagger, \mathbf{a}_{p'}^\dagger \right]}_0 + v_p v_{p'} \underbrace{\left[\mathbf{a}_{-p}^\dagger, \mathbf{a}_{-p'} \right]}_{-\delta_{pp'}} \end{aligned} \quad (2.75)$$

$$= \delta_{pp'} (u_p^2 - v_p^2) \Rightarrow u_p^2 - v_p^2 = 1. \quad (2.76)$$

This equation is solved if we set

$$u_p = \cosh(\phi_p) \quad v_p = \sinh(\phi_p). \quad (2.77)$$

The inverse relations are then given by

$$\mathbf{a}_p = u_p \tilde{\mathbf{a}}_p - v_p \tilde{\mathbf{a}}_{-p}^\dagger \quad (2.78)$$

$$\mathbf{a}_p^\dagger = u_p \tilde{\mathbf{a}}_p^\dagger - v_p \tilde{\mathbf{a}}_{-p}. \quad (2.79)$$

If we now define $\tilde{\epsilon}_p = \epsilon_p + gn$ and insert (2.78) and (2.79) into the HAMILTONIAN (2.70) we get

$$\hat{H} = \frac{1}{2} gn^2 + \sum_{p \neq 0} \left\{ \tilde{\epsilon}_p \mathbf{a}_p^\dagger \mathbf{a}_p + \frac{1}{2} gn \left(\mathbf{a}_p^\dagger \mathbf{a}_{-p}^\dagger + \mathbf{a}_{-p} \mathbf{a}_p \right) \right\} \quad (2.80)$$

$$\begin{aligned} &= \frac{1}{2} gn^2 + \sum_{p \neq 0} \left\{ \tilde{\epsilon}_p \left[u_p^2 \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p + v_p^2 \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_{-p}^\dagger - u_p v_p \left(\tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_{-p}^\dagger + \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_p \right) \right] \right. \\ &\quad \left. + \frac{1}{2} gn \left[u_p^2 \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_{-p}^\dagger + v_p^2 \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_p - v_p u_p \left(\tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p + \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_{-p}^\dagger \right) \right] \right. \\ &\quad \left. + u_p \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_p + v_p^2 \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_{-p}^\dagger - u_p v_p \left(\tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p + \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_{-p}^\dagger \right) \right\} \end{aligned} \quad (2.81)$$

$$\begin{aligned} &= \underbrace{\frac{1}{2} gn^2 + \sum_{p \neq 0} \{ \tilde{\epsilon}_p v_p^2 - gn v_p u_p \}}_{E_0} \\ &\quad + \sum_{p \neq 0} \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p \left[\tilde{\epsilon}_p (u_p^2 + v_p^2) - 2gn u_p v_p \right] \\ &\quad + \sum_{p \neq 0} \left(\tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_{-p}^\dagger + \tilde{\mathbf{a}}_{-p} \tilde{\mathbf{a}}_p \right) \underbrace{\left[-\tilde{\epsilon}_p u_p v_p + \frac{1}{2} gn (u_p^2 + v_p^2) \right]}_{=0}. \end{aligned} \quad (2.82)$$

Thus ϕ_p has to be chosen such that

$$gn(u_p^2 + v_p^2) - 2\tilde{\epsilon}_p u_p v_p = 0. \quad (2.83)$$

The simplest way to find the angle ϕ from this equation is to use the relation

$$4u_p^2 v_p^2 = (u_p^2 + v_p^2)^2 - \underbrace{(u_p^2 - v_p^2)^2}_{=1}. \quad (2.84)$$

We get as the result

$$u_p^2 = \frac{1}{2} \left[\frac{\tilde{\epsilon}_p}{\omega_p} + 1 \right] \quad v_p^2 = \frac{1}{2} \left[\frac{\tilde{\epsilon}_p}{\omega_p} - 1 \right] \quad (2.85)$$

$$\omega_p^2 = \tilde{\epsilon}_p^2 - (gn)^2 \quad \tilde{\epsilon}_p = \epsilon_p + gn \quad (2.86)$$

with the HAMILTONIAN

$$\hat{H} = \frac{1}{2} gn^2 + \frac{1}{2} \sum_{p \neq 0} (\omega_p - \tilde{\epsilon}_p) + \sum_{p \neq 0} \omega_p \tilde{a}_p^\dagger \tilde{a}_p \quad \text{with} \quad (2.87)$$

$$\omega_p^2 = \tilde{\epsilon}_p^2 - (gn)^2 = (\tilde{\epsilon}_p - gn)(\tilde{\epsilon}_p + gn) = \epsilon_p(\epsilon_p + 2gn) \quad (2.88)$$

$$= \frac{p^2}{2m} \left(\frac{p^2}{2m} + 2gn \right). \quad (2.89)$$

For $p \rightarrow 0$ we have $\omega \sim p$.

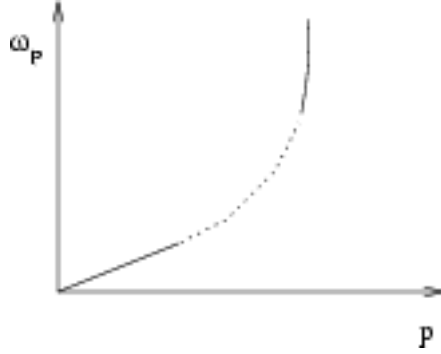


Figure 2.2: ω_p as function of p

More precisely, if we define³

$$p_c^2 = mgn \quad v^2 = \frac{gn}{m} \quad (2.90)$$

³In this context we assume $n \approx n_0$

we get

$$\omega_p = \begin{cases} vp & p \ll p_c \\ \frac{p^2}{2m} + gn & p \gg p_c. \end{cases} \quad (2.91)$$

Reconsidering the requirement for superfluidity (2.30) we get

$$v_c = \min_p \left(\frac{\omega_p}{p} \right) = v \neq 0. \quad (2.92)$$

If $p \ll p_c$ i.e.

$$\omega_p = \frac{p_c}{m} p \quad \text{for } p \ll p_c \quad (2.93)$$

we get

$$\omega_p - \tilde{\epsilon}_p = \frac{\omega_p^2 - \tilde{\epsilon}_p^2}{\omega_p + \tilde{\epsilon}_p} = -\frac{(gn_0)^2}{\omega_p + \tilde{\epsilon}_p} \approx \begin{cases} \frac{(gn_0)^2}{gn_0} = gn_0 & p \leq p_c \\ \frac{(gn_0)^2}{2\epsilon_p} = (gn_0)^2 \frac{m}{p^2} & p \geq p_c \end{cases} \quad (2.94)$$

$$E_0 = \frac{1}{2}gn_0^2 - \frac{1}{2}(gn_0)^2 \sum_p \frac{m}{p^2} - \frac{1}{2} \sum_p \left\{ \frac{(gn_0)^2}{\omega_p + \tilde{\epsilon}_p} - (gn_0)^2 \frac{m}{p^2} \right\} \quad (2.95)$$

$$= \frac{1}{2}n_0^2 \underbrace{\left\{ g - g^2 \sum_p \frac{m}{p^2} \right\}}_{\text{independent of } n} - \frac{(gn_0)^2}{2} \sum_p \left\{ \frac{1}{\omega_p + \tilde{\epsilon}_p} - \frac{m}{p^2} \right\} \quad (2.96)$$

$$= \frac{1}{2}n_0^2 \Gamma - \frac{(gn_0)^2}{2} \sum_p \left\{ \frac{1}{\omega_p + \tilde{\epsilon}_p} - \frac{m}{p^2} \right\}. \quad (2.97)$$

Here Γ is the quantum mechanical scattering amplitude defined by

$$\Gamma = g - g \sum_p \frac{m}{p^2} \Gamma \quad \text{and} \quad (2.98)$$

$$\Gamma = \frac{4\pi\hbar^2}{m} a. \quad (2.99)$$

The solution is solved iteratively:

$$\Gamma = g - g^2 \sum_p \frac{m}{p^2} + \dots \quad (2.100)$$

The sum (2.97) is convergent with the dominant contribution coming from $p \leq p_c$. Looking at each term of E_0 we get

$$\sum_{p \leq p_c} \frac{1}{\omega_p + \tilde{\epsilon}_p} \approx \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\omega_p + \epsilon_p} \approx \frac{1}{\hbar^3} \int_{p \leq p_c} d^3 p \frac{1}{gn_0} \sim \frac{p_c^3}{gn_0 \hbar^3} \quad (2.101)$$

$$= \frac{mp_c}{\hbar^3} \quad (2.102)$$

$$\sum_{p \leq p_c} \frac{m}{p^2} \sim \frac{m}{\hbar^3} \int_{p \lesssim p_c} \frac{d^3 p}{p^2} \sim \frac{mp_c}{\hbar^3}. \quad (2.103)$$

Using this the second term of (2.97) for E_0 can be estimated (up to some numerical constant C resp. \tilde{C} , c.f. (2.106)) as

$$E_0 \sim \frac{2\pi\hbar^2}{m} an_0^2 - C \frac{1}{2} (gn_0)^2 \frac{mp_c}{\hbar^3} \quad (2.104)$$

$$= \frac{2\pi\hbar^2 an_0^2}{m} \left(1 - \tilde{C} \sqrt{a^3 n_0}\right). \quad (2.105)$$

Here $\sqrt{a^3 n_0}$ is our old small parameter (cf. (1.1) with $a \sim r_0$).

The exact calculation leads to

$$E_0 = \frac{2\pi\hbar^2}{m} an^2 \left[1 + \frac{128}{15} \sqrt{\frac{a^3 n}{\pi}}\right]. \quad (2.106)$$

Note, that the equation contains n , not n_0 .

Lastly the number of particles outside the condensate (i.e. $p \neq 0$) in the ground state considering $\tilde{\alpha}_p|0\rangle = 0$ is

$$\langle \sum_{p \neq 0} \alpha_p^\dagger \alpha_p \rangle = \sum_{p \neq 0} v_p^2 = \frac{1}{2} \sum_{p \neq 0} \frac{\tilde{\epsilon}_p - \omega_p}{\omega_p} = \frac{1}{2} \sum_{p \neq 0} \frac{\tilde{\epsilon}_p^2 - \omega_p^2}{\omega_p(\tilde{\epsilon}_p + \omega_p)} \quad (2.107)$$

$$= \frac{(gn)^2}{2} \sum_{p \neq 0} \frac{1}{\omega_p(\tilde{\epsilon}_p + \omega_p)} \approx \frac{(gn)^2}{2} \sum_{p \lesssim p_c} \frac{1}{vpgn} \quad (2.108)$$

$$\approx gn \frac{1}{v} \frac{p_c^3}{(2\pi\hbar)^3} \frac{1}{p_c} \approx gn \frac{1}{v} \frac{p_c^2}{\hbar^3} \sim n\sqrt{na^3} \quad \text{with} \quad (2.109)$$

$$g = \frac{4\pi\hbar^2 a}{m}. \quad (2.110)$$

This result ($\sim a^{\frac{3}{2}}$ is not possible by perturbation because in perturbation only integer powers of the interaction constant are possible).

By exact calculations we get

$$\langle \sum \mathbf{a}_p^\dagger \mathbf{a}_p \rangle = \frac{8}{3} n \sqrt{\frac{na^3}{\pi}} = n' \ll n \quad \text{with} \quad (2.111)$$

$$a \sim r_0 \ll n^{-\frac{1}{3}}. \quad (2.112)$$

Using the definition of g (1.83) we calculate the chemical potential in leading order using (2.105) or (2.106)

$$\mu = \frac{\partial E_0}{\partial n} \approx \frac{\partial E_0}{\partial n_0} = gn_0 \approx ng > 0 \quad (2.113)$$

because (cf. (2.69))

$$n_0 = n \left(1 - \frac{8}{3} \sqrt{\frac{na^3}{\pi}} \right) \approx n. \quad (2.114)$$

This is valid for the ground state at $T = 0$ and no excitations present.

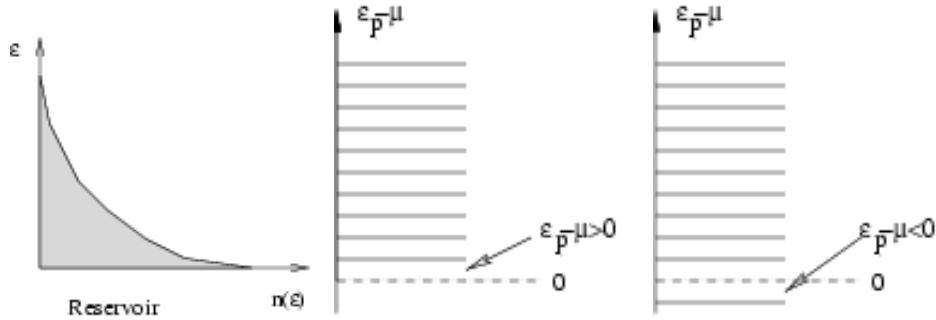


Figure 2.3: Energy spectra in BOSE condensates. If in the free case $\varepsilon - \mu$ would become zero \bar{n} (2.4) cannot be fixed. If a repulsive interaction is present, the average number of particles can be fixed because $E_{\text{int}} \sim an^2$

2.4 Mean field approximation

Again we note, that

$$\mathbf{a}_p \mathbf{a}_p^\dagger \rightarrow n_p + 1 \gg 1 \quad \text{and} \quad (2.115)$$

$$\mathbf{a}_p^\dagger \mathbf{a}_p \rightarrow n_p \gg 1. \quad (2.116)$$

If we are interested only in quantities proportional to n , we can neglect $[\mathfrak{a}_p, \mathfrak{a}_p^\dagger] = 1$. Our theory then becomes a classical field description:

$$\hat{\Psi}(\vec{r}) \rightarrow \Psi(r) = \sqrt{n(r)} e^{i\Phi(r)} \quad \text{with} \quad (2.117)$$

$$\Psi^\dagger \Psi = n(r). \quad (2.118)$$

This works only if the classical field is slowly varying or by using FOURIERtransformation the momenta are small (slow motion). The reason behind this is, that n and Φ behave similar to p and x in ordinary space. The wave function can always be multiplied with a phase without changing the physics:

$$\psi_v(\vec{r}) \rightarrow e^{i\phi} \psi_v(\vec{r}) \quad \text{single particle} \quad (2.119)$$

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) \rightarrow e^{iN\phi} \Psi(\vec{r}_1, \dots, \vec{r}_N) \quad (2.120)$$

This implies the operators $\hat{N} = -i\frac{\partial}{\partial\phi}$ and $\hat{\phi} = \phi$ which leads to

$$[\hat{\phi}, \hat{N}] = i \quad \Rightarrow \quad \Delta N \Delta \phi \geq 1. \quad (2.121)$$

But in a sufficiently large volume ΔV one may have $\Delta N \gg 1$ (but still $\frac{\Delta N}{N} \ll 1$). Therefore, it follows from (2.121), that in this case $\Delta\phi \ll 1$. As a result, for such a volume \bar{N} and $\bar{\phi}$ are well defined quantities. By dividing our system into blocks with volume $\Delta\mathcal{V}$, we can define \bar{N} and $\bar{\phi}$ for each block and these quantities vary slowly from block to block.

If we consider the thermodynamic limit, i.e. $N \rightarrow \infty$ while $\frac{N}{\mathcal{V}}$ remains fixed we get

$$\langle N-1 | \hat{\Psi}(\vec{r}) | N \rangle = \Psi(\vec{r}) \quad \text{and} \quad -i\hbar \frac{\partial}{\partial t} \hat{\Psi} = [\hat{H}, \hat{\Psi}] \quad (2.122)$$

$$\Rightarrow -i\hbar \frac{\partial}{\partial t} \Psi = \lim_{\dots} \langle N-1 | (\hat{H} \hat{\Psi} - \hat{\Psi} \hat{H}) | N \rangle \quad (2.123)$$

$$= \lim_{\dots} \langle N-1 | (E(N-1) \hat{\Psi} - \hat{\Psi} E(N)) | N \rangle \quad (2.124)$$

$$= \lim_{\dots} \underbrace{(E(N-1) - E(N))}_{=:-\mu} \langle N-1 | \hat{\Psi} | N \rangle \quad (2.125)$$

$$= -\mu \Psi. \quad (2.126)$$

This differential equation can be solved by

$$\Psi(\vec{r}, t) = e^{-i\frac{\mu t}{\hbar}} \Psi(\vec{r}). \quad (2.127)$$

If we replace \hat{H} by $\hat{H}' = \hat{H} - \mu$ we absorb this trivial phase in our HAMILTONIAN.

This leads to⁴ the GROSS-PITAJEWSKI equation (GP):

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \Delta \psi + (g|\psi|^2 - \mu) \psi \quad (2.128)$$

Here $|\psi|^2 = n \approx n_0$. Therefore we will not distinguish between n and n_0 .

If we are looking for a stationary, homogeneous solution, then all derivatives (in GP) become zero and if $\psi \neq 0$ we find

$$\mu = gn. \quad (2.129)$$

Setting the possible phase to 0, we can describe small fluctuations around the ground state by a wave function

$$\psi = \sqrt{n_0} + \delta\psi(\vec{r}, t). \quad (2.130)$$

Substituting this wave function into the GP (2.128), taking only terms up to linear order in $\delta\psi$ and using (2.129) we get

$$i\hbar \frac{\partial}{\partial t} \delta\psi = -\frac{\hbar^2}{2m} \Delta \delta\psi + gn_0 (\delta\psi + \delta\psi^*). \quad (2.131)$$

To solve this, we make the ansatz

$$\delta\psi(\vec{r}, t) = A \exp(i(\frac{\vec{p} \cdot \vec{r}}{\hbar} - \omega t)) + B^* \exp(-i(\frac{\vec{p} \cdot \vec{r}}{\hbar} - \omega t)) \quad (2.132)$$

and insert it into (2.131):

$$\hbar\omega A = (\varepsilon_p + gn_0)A + gn_0 B \quad (2.133)$$

$$-\hbar\omega B^* = (\varepsilon_p + gn_0)B^* + gn_0 A^* \quad (2.134)$$

Solving this for ω we get $\omega_p = \sqrt{\tilde{\varepsilon}_p^2 - (gn_0)^2}$ and $\tilde{\varepsilon}_p = \varepsilon_p + gn_0$ again.

Calculating the expectation value and remembering (2.129) we get a functional for ψ :

$$E\{\psi\} = \int d^3r \left(\frac{\hbar^2}{2m} |\nabla \psi|^2 + \frac{1}{2} g |\psi|^4 - \mu |\psi|^2 \right) \quad (2.135)$$

$$= \int d^3r \left(\frac{\hbar^2}{2m} |\nabla \psi|^2 + \frac{1}{2} g (|\psi|^2 - n_0)^2 - \frac{1}{2} gn_0^2 \right) \quad (2.136)$$

Since the functional does not depend on a *space independent* Φ , i.e. $E\{\psi\} = E\{e^{i\Phi}\psi\}$ we can choose a phase. For the previous calculations $\Phi = 0$. Once the phase is chosen, the symmetry is broken, because

$$\psi_0 \neq e^{i\Phi} \psi_0 \quad (2.137)$$

If Φ is a slowly varying function, then the functional will not change much.

⁴not shown here

Theorem 1 (Goldstone) *If a global continuous symmetry is spontaneously broken (the ground state is not invariant under symmetry operations) then there exists a soft mode, i.e. a ω_p with $\omega_p \xrightarrow{p \rightarrow 0} 0$.*

We have such a situation. If $p \rightarrow 0$ then $\varepsilon_p \rightarrow 0$ and therefore $\omega_p \rightarrow 0$. This leads (2.131) to $B = -A$ and a purely imaginary change in the phase:

$$\delta\psi = Ae^{i(\cdot)} - A^*e^{-i(\cdot)} \quad (2.138)$$

$$= i\varepsilon\sqrt{n_0}\Phi(\vec{r}, t) \quad \text{and (2.130) becomes} \quad (2.139)$$

$$\psi(\vec{r}, t) = \sqrt{n_0} + i\varepsilon\sqrt{n_0}\Phi(\vec{r}, t) \approx \sqrt{n_0}e^{i\varepsilon\Phi} \quad (2.140)$$

If we substitute this solution into the definition of the probability flow (=superfluid flow) we get

$$\vec{j} = n\vec{v}_s = -\frac{i\hbar}{2m}(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi) \quad (2.141)$$

$$= n\frac{\hbar}{m}\nabla\Phi \quad \text{with } \psi(\vec{r}, t) = \sqrt{n(\vec{r}, t)}e^{i\Phi(\vec{r}, t)}. \quad (2.142)$$

Here \vec{v}_s is the velocity of the superfluid flow. It is a potential flow:

$$\vec{v}_s = \frac{\hbar}{m}\vec{\nabla}\Phi \quad (2.143)$$

therefore the rotation $\nabla \times \vec{v}_s = 0$. If we compare this to solid body rotation with

$$\vec{v}_{\text{SB}} = \vec{\Omega} \times \vec{r} \quad \text{we get} \quad (2.144)$$

$$\nabla \times \vec{v}_{\text{SB}} = 2\vec{\Omega} \neq 0. \quad (2.145)$$

Therefore the fluid must stay at rest even if the vessel is rotated.

On the other hand

$$E_{\text{rot}} = E - (\vec{M} \cdot \vec{\Omega}) \quad (2.146)$$

and thus rotation must occur (M becomes nonzero) if Ω is large enough.

To solve this we keep $\nabla \times \vec{v}_s = 0$ everywhere except for a line where

$$\psi|_{\text{line}} = 0. \quad (2.147)$$

Calculating

$$\oint \vec{v}_s \cdot d\vec{l} = \text{const} = 2\pi\Gamma = \frac{\hbar}{m} \oint \nabla\Phi d\vec{l} = \frac{\hbar}{m} \delta\Phi = \frac{\hbar}{m} 2\pi k. \quad (2.148)$$

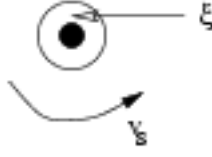


Figure 2.4: Top view on rotating superfluid liquid

Here Γ is the vorticity or circulation and $k \in \mathbb{Z}$ the circulation quantum number. With $\vec{v}_s \sim \vec{e}_\phi$ and $d\vec{l} = \vec{e}_\phi r d\phi$ we get for the critical velocity

$$v_s = \frac{\hbar k}{m r}. \quad (2.149)$$

This expression becomes infinite for $r \rightarrow 0$ (while being nice for $r \rightarrow \infty$) therefore superfluidity has to break down at some distance $r \sim \xi$ with

$$v_s = v_c = \frac{p_c}{m} = \frac{1}{m} \sqrt{mgn_0} = \sqrt{\frac{gn_0}{m}}. \quad (2.150)$$

For $k = 1$ we get

$$\xi \sim \frac{\hbar}{mv_c} = \frac{\hbar}{p_c} = \frac{\hbar}{\sqrt{mgn_0}}. \quad (2.151)$$

By using (2.151), (1.83) and (1.1) we get for a number of particles in a volume ξ^3 the macroscopic value

$$n\xi^3 \sim \frac{1}{\hbar^2} \frac{1}{\sqrt{an^{\frac{1}{3}}}} \gg 1. \quad (2.152)$$

and therefore, the length ξ is much larger than the average interparticle distance. If L is the length of one vortex, we now get for the energy of the vortex

$$\frac{E(k)}{L} = \frac{1}{2} \int d^2r \rho v_s^2 = \frac{1}{2} nm \left(\frac{\hbar k}{m} \right)^2 \int \frac{d^2r}{r^2} \quad (2.153)$$

$$= \pi nm \left(\frac{\hbar k}{m} \right)^2 \int_\xi^R \frac{dr}{r} = \pi n \frac{\hbar^2}{m} k^2 \ln \left(\frac{R}{\xi} \right) \quad (2.154)$$

and for the angular momentum

$$\frac{M(k)}{L} = \int d^2r \rho v_s r = mn \frac{\hbar}{m} k 2\pi \int_\xi^R dr r \approx \pi n \hbar k R^2. \quad (2.155)$$

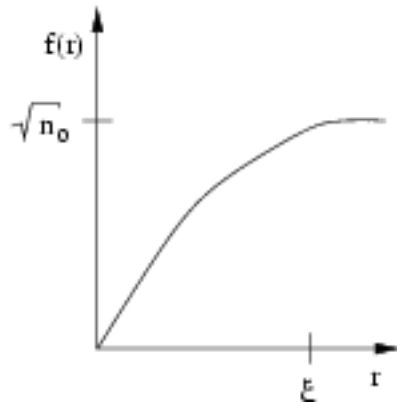


Figure 2.5: Radial part $f(r)$ of the wave function in superfluid BOSE gas

Conclusions:

If M is fixed then we either have k repeated vortices or one vortex with circulation k^5 . Since $kE(1) < E(k)$ it is energetically favorable to have vortices with $k = 1$ only.

The critical velocity, when at least one vortex exists, is with

$$E_{\text{rot}} = E - (\vec{M} \cdot \vec{\Omega}_C) \stackrel{!}{=} 0 \quad (2.156)$$

$$\Omega_C = \frac{E(1)}{M(1)} = \frac{\hbar}{mR^2} \ln\left(\frac{R}{\xi}\right). \quad (2.157)$$

Ω_C is very small, usually $\Omega \gg \Omega_C$ and many vortices exist. They repel each other and a lattice is created where phonons can be observed.

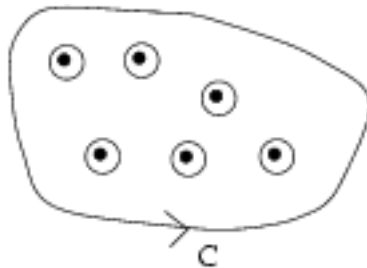


Figure 2.6: Many vortices in superfluid BOSE gas

⁵or a proper combination of both

If we compare our superfluid rotation with solid body rotation we get with $k = 1$

$$\oint \vec{v}_S d\vec{l} = \frac{\hbar}{m} \oint \nabla \Phi d\vec{l} = \frac{2\pi\hbar}{m} N_v = \frac{2\pi\hbar}{m} n_v S_c \quad (2.158)$$

$$\oint \vec{v}_{s.b.} d\vec{l} = \int d^2s \nabla \times \vec{v}_{s.b.} = 2\Omega S_c. \quad (2.159)$$

Here N_v and n_v are the number and density of vortices respectively and S_c the area enclosed in the calculation. Substituting both equation we get

$$n_v = \frac{m\Omega}{\hbar\pi}. \quad (2.160)$$

The velocity around one vortex is

$$\vec{v}_s = \frac{\hbar}{m} \frac{\vec{e}_z \times \vec{r}}{r^2} \quad (2.161)$$

and the total velocity is the superposition of each velocity

$$\vec{v}_s(\vec{r}) = \sum_i \frac{\hbar}{m} \frac{\vec{e}_z \times (\vec{r} - \vec{r}_i)}{|\vec{r} - \vec{r}_i|^2}. \quad (2.162)$$

2.5 BEC in an isotr. harmonic trap at $T=0$

2.5.1 Comparison of terms in GP

$$\hat{H} = \int d^3r \hat{\psi}^\dagger \left\{ -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right\} \hat{\psi} + \frac{1}{2}g \int d^3r \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \quad (2.163)$$

$$U(\vec{r}) = \frac{m\omega^2}{2} r^2 \quad g = \frac{4\pi\hbar^2}{m} a \quad (2.164)$$

A macroscopic number of particles is in the ground state of the trap and the condensate wave function can be written as

$$\Phi(\vec{r}, t) = \left(\lim_{N \rightarrow \infty} \right) \langle N-1 | \psi | N \rangle = \varphi(\vec{r}, t) e^{-i\frac{\mu t}{\hbar}} \quad (2.165)$$

Here the braces around the limit denote that we always take the leading terms in N only. The exponential wave function carries only the trivial time dependences which arises from the different number of particles. We now get the time dependent GP (cf. (2.128)) with potential.

$$i\hbar \frac{\partial}{\partial t} \varphi = \left\{ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U(r) \right\} \varphi + g|\varphi|^2 \varphi \quad (2.166)$$

The ground state must be a stationary state. We can choose φ real because if φ contained a non trivial space dependent phase $\phi(r)$ this would cause a gas flow and therefore an increase of energy (cf. (2.142)) Thus, the equation of the ground state wave function $\varphi(\vec{r})$ reads

$$-\frac{\hbar^2}{2m}\nabla^2\varphi + U(\vec{r})\varphi + g\varphi^3 = \mu\varphi \quad (2.167)$$

$$n(\vec{r}) = \varphi^2 \quad \int d^3r \varphi^2(\vec{r}) = N \quad (2.168)$$

Solving this equation we get μ .

The simplest case is the non-interacting gas, i.e. $g = 0$:

$$\mu = \varepsilon_0 = \frac{3}{2}\hbar\omega \quad (2.169)$$

$$\varphi = \sqrt{N}\varphi_0(\vec{r}) = \sqrt{N}\frac{1}{\sqrt{l_0^3\pi^{\frac{3}{2}}}}e^{-\frac{r^2}{2l_0^2}} \quad l_0 = \sqrt{\frac{\hbar}{m\omega}} \quad (2.170)$$

If we are looking at weak interaction, we can assume the wave function to still have a similar form. Before proceeding, we have to define the term "weak". For this purpose the ratio between kinetic and potential to interaction energy has to be considered. More precisely

$$E_{\text{kin}} \sim E_{\text{pot}} \sim \hbar\omega N \quad (2.171)$$

$$E_{\text{int}} \sim \frac{1}{2}g \int d^3r \varphi^4 = \frac{1}{2}g \int d^3r n^2(r) \approx g\bar{n}N = g\frac{N}{l_0^3}N \quad (2.172)$$

$$= 4\pi\frac{\hbar^2}{m} \frac{a}{l_0} \frac{N^2}{\frac{\hbar}{m\omega}} \sim \hbar\omega N \left(N\frac{a}{l_0} \right) \quad \text{thus} \quad (2.173)$$

$$\frac{E_{\text{int}}}{E_{\text{kin}}} \sim N\frac{a}{l_0} \quad (2.174)$$

This ratio describes how important interaction is for the ground state wave function.

In the experiment we have $l_0 \sim 1\mu\text{m}$ and

$$^{23}\text{Na}: a=2.75 \text{ nm} \quad ^{87}\text{Rb}: a=5.77 \text{ nm} \quad ^6\text{Li}: a=-1.45 \text{ nm} \quad (2.175)$$

This yields $\frac{a}{l_0} \sim 10^{-3}$. Therefore we can consider the interaction to be small if $N < 1000$ otherwise we have to consider the interaction right from the beginning. On the other hand we still have a gas as our criteria shows:

$$\bar{n}a^3 \ll 1 \quad \Rightarrow \quad \frac{N}{l_0^3}a^3 = \left(N\frac{a}{l_0} \right) \left(\frac{a}{l_0} \right)^2 \ll 1 \quad (2.176)$$

Our system is gaseous while $N < 1000^3 = 10^9$.

2.5.2 Thomas-Fermi-Regime

Repulsive Interaction

This regime is specified by

$$N \frac{a}{l_0} \gg 1 \quad (2.177)$$

Since we are dealing with a trapped gaseous system we assume the system to occupy a volume R^3 with

$$R \gg l_0 \quad (2.178)$$

As described in (2.174) we have

$$E_{\text{kin}} \ll E_{\text{int}} \sim g \bar{n} N = g \frac{N}{R^3} N = g \frac{N^2}{R^3} \quad (2.179)$$

$$\mu = \frac{\partial E}{\partial N} \approx \frac{\partial E_{\text{int}}}{\partial N} \sim g \frac{N}{R^3} \quad (2.180)$$

Because of $E \approx E_{\text{int}}$ (definition of THOMAS-FERMI regime) and $\mu = \frac{\partial E}{\partial N}$ we get

$$\frac{m\omega^2 R^2}{2} \sim \mu = g \frac{N}{R^3} \quad (2.181)$$

$$\Leftrightarrow R^5 \sim g \frac{N}{m\omega^2} \sim \frac{\hbar^2 a}{m} \frac{N}{m\omega^2} \sim Na \left(\frac{\hbar}{m\omega} \right)^2 = Na l_0^4 \quad (2.182)$$

$$= l_0^5 \left(N \frac{a}{l_0} \right) \quad (2.183)$$

$$\Rightarrow R \sim l_0 \left(N \frac{a}{l_0} \right)^{\frac{1}{5}} \gg l_0 \quad (2.184)$$

Therefore we justify (2.178)⁶.

$$\mu = g \frac{N}{R^3} \sim \frac{\hbar^2 a}{m} \frac{N}{l_0^3} \left(N \frac{a}{l_0} \right)^{-\frac{3}{5}} \sim \hbar\omega N \frac{a}{l_0} \left(N \frac{a}{l_0} \right)^{-\frac{3}{5}} \quad (2.185)$$

$$= \hbar\omega \left(N \frac{a}{l_0} \right)^{\frac{2}{5}} \gg \hbar\omega \quad (2.186)$$

$$E_{\text{kin}} \sim \frac{\hbar^2}{2mR^2} N = \frac{\hbar^2}{2ml_0^2} N \left(N \frac{a}{l_0} \right)^{-\frac{2}{5}} = \hbar\omega N \left(N \frac{a}{l_0} \right)^{-\frac{2}{5}} \quad (2.187)$$

⁶Note however, that $2 \lesssim \left(N \frac{a}{l_0} \right)^{\frac{1}{5}} \lesssim 3$ in real experiments.

Comparing this to $E_{\text{int}} = \mu N$ we get

$$\frac{E_{\text{kin}}}{\mu N} \sim \left(N \frac{a}{l_0} \right)^{-\frac{4}{3}} \ll 1 \quad (2.188)$$

which is consistent with (2.179). This means the kinetic energy per particle is $\ll \hbar\omega$.

For numerical calculations it is convenient to use the dimensionless GP. To achieve this we set

$$r = l_0 \tilde{r} \quad \mu = \hbar\omega \tilde{\mu} \quad \varphi = \sqrt{\frac{N}{l_0^3}} \tilde{\varphi} \quad (2.189)$$

If we insert this into the GP (2.167) we get

$$\left\{ -\frac{\hbar^2}{2m l_0^2} \nabla_{\tilde{r}}^2 + \frac{m\omega^2}{2} l_0^2 \tilde{r}^2 \right\} \tilde{\varphi} + \frac{4\pi\hbar^2 a N}{m l_0^3} \tilde{\varphi}^3 = \hbar\omega \tilde{\mu} \tilde{\varphi} \quad (2.190)$$

$$\left\{ -\frac{\hbar\omega}{2} \nabla_{\tilde{r}}^2 + \frac{\hbar\omega}{2} \tilde{r}^2 \right\} \tilde{\varphi} + 4\pi\hbar\omega \frac{Na}{l_0} \tilde{\varphi}^3 = \hbar\omega \tilde{\mu} \tilde{\varphi} \quad (2.191)$$

$$\left\{ -\frac{1}{2} \nabla_{\tilde{r}}^2 + \frac{1}{2} \tilde{r}^2 \right\} \tilde{\varphi} + 4\pi \frac{Na}{l_0} \tilde{\varphi}^3 = \tilde{\mu} \tilde{\varphi} \quad (2.192)$$

If we are looking for the stationary ground state solution we can neglect all derivatives in (2.167) because the ground state is time independent and the kinetic terms are negligible and get

$$\frac{m\omega^2 r^2}{2} \varphi + g\varphi^3 = \mu \varphi \quad (2.193)$$

$$\varphi^2(r) = \frac{1}{g} \left(\mu - \frac{m\omega^2 r^2}{2} \right) \Leftrightarrow r \leq R = \frac{1}{\omega} \sqrt{\frac{2\mu}{m}} \quad (2.194)$$

and 0 otherwise.

Only at R numerical calculations show slight difference to our approximation.

Using this, we get

$$N = \int d^3r \varphi^2(r) = \frac{1}{g} \int_0^R d^3r \left(\mu - \frac{m\omega^2 r^2}{2} \right) \quad (2.195)$$

$$= \frac{\mu}{g} \int_0^R d^3r \left(1 - \frac{r^2}{R^2} \right) \quad (2.196)$$

$$= \frac{\mu}{g} R^3 4\pi \int_0^1 dx x^2 (1-x^2) = 4\pi \frac{\mu}{g} R^3 \left(\frac{1}{3} - \frac{1}{5} \right) \quad (2.197)$$

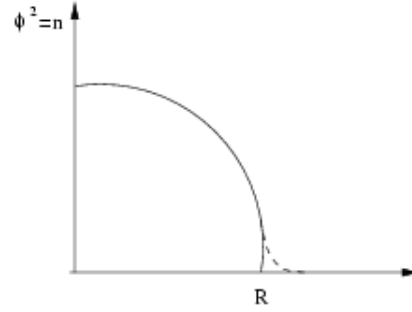


Figure 2.7: $\phi^2 = n$ in THOMAS-FERMI regime. The dashed line indicates the numerical solution for the radial wave function.

$$= 4\pi \frac{\mu m}{4\pi\hbar^2 a} \frac{1}{\omega^3} \left(\frac{2\mu}{m}\right)^{\frac{3}{2}} \frac{2}{15} \quad (2.198)$$

$$= (2\mu)^{\frac{5}{2}} \frac{1}{\sqrt{ma}\omega^3\hbar^2 15} \quad (2.199)$$

$$= \frac{1}{15} \left(\frac{2\mu}{\hbar\omega}\right)^{\frac{5}{2}} \frac{\sqrt{\hbar}}{a\sqrt{m\omega}} = \frac{1}{15} \left(\frac{2\mu}{\hbar\omega}\right)^{\frac{5}{2}} \frac{l_0}{a} \quad (2.200)$$

$$\mu = \frac{1}{2} \hbar\omega \left[15N \frac{a}{l_0}\right]^{\frac{2}{5}} \quad (2.201)$$

Attractive Interaction

If we now consider the regime $a < 0$ we expect a collapse of the free system. If the system is in a trap, the energy levels are discrete and an equilibrium (more precisely, a long living metastable state) is possible. More quantitative (2.171) and (2.173)

$$E_{\text{kin}} = \hbar\omega N \quad (2.202)$$

$$E_{\text{int}} \sim g\bar{n}N = -\hbar\omega N^2 \frac{|a|}{l_0} \quad (2.203)$$

IF N is small the kinetic term can still be dominant thus preventing the collapse, i.e.

$$N \frac{a}{l_0} < 1 \quad (2.204)$$

is necessary.

To get a more quantitative picture we introduce a parameter z to describe possible solutions and start out with the ground state wave function of the harmonic oscillator

$$\varphi(r) = \sqrt{N} \frac{1}{\sqrt{l_0^3 z^3 \sqrt{\pi^3}}} e^{-\frac{r^2}{2l_0^2 z^2}} \quad (2.205)$$

The energy is now a function of z :

$$E(z) = E_0(z) + E_{\text{int}}(z) \quad (2.206)$$

$$E_0(z) = \int d^3r \varphi \left\{ -\frac{\hbar^2}{2m} \nabla^2 + \frac{m\omega^2 r^2}{2} \right\} \varphi \quad (2.207)$$

$$= \frac{\hbar\omega}{2} \frac{N}{\pi^{\frac{3}{2}}} \int d^3r' e^{-\frac{r'^2}{2}} \left\{ -z^{-2} \nabla_{r'}^2 + z^2 r'^2 \right\} e^{-\frac{r'^2}{2}} \quad (2.208)$$

$$= \frac{\hbar\omega}{2} \frac{N}{\pi^{\frac{3}{2}}} \int d^3r' e^{-\frac{r'^2}{2}} \left\{ z^{-2} \underbrace{\left(-\nabla_{r'}^2 - r'^2 \right)}_{\rightarrow 0} + (z^2 + z^{-2}) r'^2 \right\} e^{-\frac{r'^2}{2}} \quad (2.209)$$

$$= \frac{\hbar\omega}{2} N (z^2 + z^{-2}) \frac{1}{\pi^{\frac{3}{2}}} \int d^3r' e^{-r'^2} r'^2 \quad (2.210)$$

$$= \frac{\hbar\omega}{2} N (z^2 + z^{-2}) \frac{4\pi}{\pi^{\frac{3}{2}}} \underbrace{\int_0^\infty dr' r'^4 e^{-r'^2}}_{\frac{3\sqrt{\pi}}{8}} \quad (2.211)$$

$$= \hbar\omega N \frac{3}{4} (z^2 + z^{-2}) \quad (2.212)$$

Analogously we calculate

$$E_{\text{int}} = \frac{1}{2} g \int d^3r \varphi^4 = \dots = \frac{1}{\sqrt{2\pi}} \hbar\omega N \left(N \frac{a}{l_0} \right) \frac{1}{z^3} \quad (2.213)$$

Therefore,

$$E(z) = \hbar\omega N \left\{ \frac{3}{4} (z^2 + z^{-2}) - \underbrace{\frac{1}{\sqrt{2\pi}} \left(N \frac{a}{l_0} \right) \frac{1}{z^3}}_{\xi} \right\} \quad (2.214)$$

Minima of this function can be obtained from this equations

$$\frac{E'(z)}{\hbar\omega N} = \frac{3}{2} (z - z^{-3}) + 3\xi \frac{1}{z^4} = \frac{3}{2z^4} \left\{ z^5 - z + 2\xi \right\} \stackrel{!}{=} 0 \quad (2.215)$$

$$\Leftrightarrow 0 \stackrel{!}{=} z(z^4 - 1) + 2\xi \quad (2.216)$$

In the limit $\xi \ll 1$ we get

$$z_1 \approx 2\xi + O(z^4) \quad (2.217)$$

$$z_2 = 1 - \frac{1}{2}\xi \quad (2.218)$$

The minimum value z_* of the expression $z(z^4 - 1)$ obeys the equation

$$(z^5 - z)' = 5z^4 - 1 \quad (2.219)$$

Thus the minimum occurs at

$$z_* = \frac{1}{5^{1/4}} \quad (2.220)$$

and equals

$$m := z_*(z_*^4 - 1) = -\frac{4}{5^{5/4}} \quad (2.221)$$

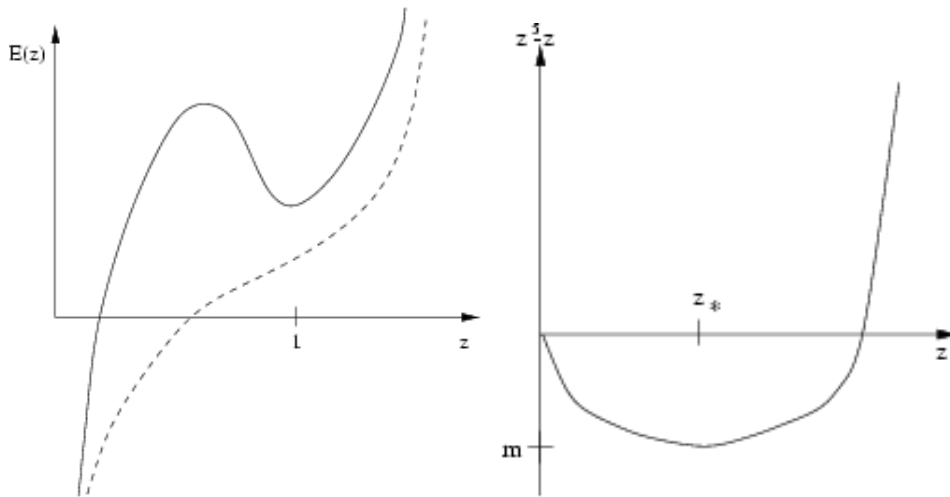


Figure 2.8: $E(z)$ for different values of ξ ; "- -" $2\xi < m$ and "-" $2\xi > m$

Therefore a solutions of (2.215) or (2.216) exists only if

$$2\xi > m = \frac{4}{5^{1/4}} \quad (2.222)$$

As a result the critical value of N is:

$$N_c \frac{|a|}{l_0} = \sqrt{2\pi} \frac{2}{5^{5/4}} = 0.671 \quad \text{in approximation} \quad (2.223)$$

$$= 0.575 \quad \text{numerically in GP} \quad (2.224)$$

Hydrodynamic approach

From superfluid ^4He we expect that hydrodynamics may be applicable for our system as well. The important variables in hydrodynamics are density and velocity (which is $\frac{\hbar}{m}\nabla\Phi$ in our case cf. (2.143)). We are still considering the THOMAS-FERMI-Regime (2.177). Starting out with the ansatz

$$\psi = \sqrt{n(\vec{r},t)}e^{i\Phi(\vec{r},t)} \quad \vec{v}_s = \frac{\hbar}{m}\nabla\Phi \quad (2.225)$$

we evaluate the the various derivatives:

$$i\hbar\frac{\partial}{\partial t}\psi = i\hbar e^{i\Phi} \left\{ \frac{\partial}{\partial t}\sqrt{n} + i\sqrt{n}\frac{\partial}{\partial t}\Phi \right\} \quad (2.226)$$

$$= i\hbar e^{i\Phi} \left\{ \sqrt{n}\frac{1}{2n}\frac{\partial}{\partial t}n + i\sqrt{n}\frac{\partial}{\partial t}\Phi \right\} \quad (2.227)$$

$$= \psi i\hbar \left(\frac{1}{2n}\frac{\partial n}{\partial t} + i\frac{\partial\Phi}{\partial t} \right) \quad \text{and} \quad (2.228)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = -\frac{\hbar^2}{2m} \left\{ (\nabla^2\sqrt{n})e^{i\Phi} + 2(\nabla\sqrt{n})(\nabla e^{i\Phi}) + \sqrt{n}(\nabla^2 e^{i\Phi}) \right\} \quad (2.229)$$

$$= -\frac{\hbar^2}{2m} \left\{ (\nabla^2\sqrt{n})e^{i\Phi} + \frac{\sqrt{n}}{n}(\nabla n)i(\nabla\Phi)e^{i\Phi} + \sqrt{n}(\nabla(i(\nabla\Phi)e^{i\Phi})) \right\} \quad (2.230)$$

$$= -\frac{\hbar^2}{2m} \underbrace{\sqrt{n}e^{i\Phi}}_{\psi} \left\{ \frac{1}{\sqrt{n}}(\nabla^2\sqrt{n}) + \frac{i}{n}(\nabla n)(\nabla\Phi) + i\nabla^2\Phi - (\nabla\Phi)^2 \right\} \quad (2.231)$$

to stitch the GP (2.166) together:

$$i\hbar \left(\frac{1}{2n}\frac{\partial n}{\partial t} + i\frac{\partial\Phi}{\partial t} \right) = -\frac{\hbar^2}{2m} \left\{ \frac{1}{\sqrt{n}}(\nabla^2\sqrt{n}) - (\nabla\Phi)^2 + \frac{i}{n}(\nabla n)(\nabla\Phi) + i\nabla^2\Phi \right\} - \mu + U(r) + gn \quad (2.232)$$

For the imaginary part we get

$$i\hbar\frac{1}{2n}\frac{\partial n}{\partial t} = -\frac{\hbar^2}{2m}\frac{i}{n}(\nabla n\nabla\Phi + n\nabla^2\Phi) = -i\frac{\hbar^2}{2mn}\nabla(n\nabla\Phi). \quad (2.233)$$

This is the continuity equation:

$$\frac{\partial n}{\partial t} + \nabla(n\vec{v}_s) = 0 \quad (2.234)$$

Evaluating the real part we get

$$-\hbar \frac{\partial \Phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{n}} (\nabla^2 \sqrt{n}) + \frac{m}{2} v_s^2 - \mu + U(r) + gn. \quad (2.235)$$

Differentiating this equation with respect to space coordinates (∇) we get

$$m \frac{\partial \vec{v}_s}{\partial t} + \nabla \left\{ -\frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} + \frac{m}{2} v_s^2 - \mu + U(r) + gn \right\} = 0 \quad (2.236)$$

If we linearize both equations, bearing in mind $N \frac{a}{l_0} \gg 1$, we can neglect $\nabla \sqrt{n}$ because we are in the THOMAS-FERMI regime where kinetic energies are small:

$$n = n_0(\vec{r}) + \delta n(\vec{r}, t) \quad (2.237)$$

$$\vec{v}_s = \frac{\hbar}{m} \nabla \Phi(\vec{r}, t) \quad v_s^2 \approx 0 \quad (2.238)$$

For the ground state we have (2.193)

$$n_0(\vec{r}) = \frac{1}{g} [\mu - U(r)] \quad (2.239)$$

which leads (2.234) and (2.236) to

$$\frac{\partial}{\partial t} \delta n + \nabla(n_0 v_s) = 0 \quad \text{and} \quad (2.240)$$

$$m \frac{\partial}{\partial t} v_s + \nabla \underbrace{(U(r) - \mu + gn_0 + g\delta n)}_{=0} = 0 \quad (2.241)$$

$$\Leftrightarrow m \frac{\partial}{\partial t} v_s + g \nabla \delta n = 0. \quad (2.242)$$

Differentiating again with respect to t we get

$$\frac{\partial^2}{\partial t^2} \delta n + \nabla \left(n_0 \frac{\partial \vec{v}_s}{\partial t} \right) = \frac{\partial^2}{\partial t^2} \delta n + \nabla \left(n_0 (-) \frac{g}{m} \nabla \delta n \right) = 0 \quad (2.243)$$

$$\Leftrightarrow \frac{\partial^2}{\partial t^2} \delta n - \nabla \left(\underbrace{\frac{n_0 g}{m}}_{=c^2} \nabla \delta n \right) = 0 \quad (2.244)$$

This equation can be solved for a harmonic trap ([4]). The energy remains degenerated with respect to angular momentum projection:

$$\omega_{n_r, l} = \omega \sqrt{2n_r^2 + 2n_r l + 3n_r + l} \quad (2.245)$$

$$\omega_{n_r, l}^0 = \omega(2n_r + l) \quad \text{non interacting case} \quad (2.246)$$

The solutions are quite different for the interacting and the non interacting case, e.g. for $n_r = 0$ they are

$$\omega_{0,l} = \omega\sqrt{l} \quad \text{vs.} \quad \omega_{0,l}^0 = \omega l. \quad (2.247)$$

This different behavior can be distinguished in experiments.

High energy solutions

In this case we have to formulate a more general wave function:

$$\psi(\vec{r}, t) = \varphi(\vec{r}) + \psi'(\vec{r}, t) \quad (2.248)$$

Here $\varphi(r)$ is the ground state wave function which can be considered as a real function and $\psi' \ll \varphi$ describes excitations. Inserting this ansatz into the GP (2.166) and linearizing with respect to ψ' we get

$$i\hbar \frac{\partial}{\partial t} \psi' = \left\{ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U(r) \right\} \varphi(r) + \{ \dots \} \psi'(\vec{r}, t) \quad (2.249)$$

$$+ g\varphi^2\varphi + g\varphi^2(2\psi' + \psi'^*) \quad (2.250)$$

$$= \left\{ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U \right\} \psi' + g\varphi^2 (2\psi' + \psi'^*) \quad (2.251)$$

This can be solved with

$$\psi' = u(r)e^{-i\omega t} + v^*(r)e^{i\omega t} \quad (2.252)$$

Inserting this solution into (2.251) we get the following system of equations for u and v :

$$\hbar\omega u = \left\{ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U + 2g\varphi^2 \right\} u + g\varphi^2 v \quad (2.253)$$

$$-\hbar\omega v = \left\{ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U + 2g\varphi^2 \right\} v + g\varphi^2 u \quad (2.254)$$

These are the BOGOLYUBOV-DE GENNES equations. The u_i and v_i are the wave function of the excitations while $\hbar\omega_i$ is the excitation energy.

A different approach for the same problem is to use the BOGOLYUBOV transformation. Since it is more extensive than in (2.3) the solution is only sketched here. We start out again with

$$\hat{\psi}'(\vec{r}) = \sum_i \left\{ u_i(\vec{r}) \tilde{a}_i + v_i^*(\vec{r}) \tilde{a}_i^\dagger \right\} \quad (2.255)$$

and require the new operators to obey

$$[\tilde{\alpha}_i, \tilde{\alpha}_j^\dagger] = \delta_{ij} \quad (2.256)$$

$$[\tilde{\alpha}_i, \tilde{\alpha}_j] = [\tilde{\alpha}_i^\dagger, \tilde{\alpha}_j^\dagger] = 0 \quad (2.257)$$

since we want a canonical transformation which preserves the commutator relations.

Inserting (2.255) into the commutators we get

$$[\hat{\psi}'(\vec{r}), \hat{\psi}'(\vec{r}')] = 0 \quad (2.258)$$

$$\Rightarrow \sum_i \left\{ u_i(\vec{r}) v_i^*(\vec{r}') - v_i^*(\vec{r}) u_i(\vec{r}') \right\} = 0 \quad (2.259)$$

$$[\hat{\psi}'(\vec{r}), \hat{\psi}'^\dagger(\vec{r}')] = \delta(\vec{r} - \vec{r}') \quad (2.260)$$

$$\Rightarrow \sum_i \left\{ u_i(\vec{r}) u_i^*(\vec{r}') - v_i^*(\vec{r}) v_i(\vec{r}') \right\} = \delta(\vec{r} - \vec{r}') \quad (2.261)$$

Using the inverse transformation

$$\tilde{\alpha}_i = \int d^3 r \left[u_i^* \hat{\psi}'(\vec{r}) - v_i \hat{\psi}'^\dagger(\vec{r}) \right] \quad (2.262)$$

we get

$$\int d^3 r \left[u_i^*(\vec{r}) u_j(\vec{r}) - v_i^*(\vec{r}) v_j(\vec{r}) \right] = \delta_{ij} \quad (2.263)$$

$$\int d^3 r \left[u_i(\vec{r}) v_j(\vec{r}) - v_i(\vec{r}) u_j(\vec{r}) \right] = 0 \quad (2.264)$$

This is a mathematically rather unusual requirement, e.g. looking at (2.263) with $i = j$ we have

$$\int d^3 r \{ |u_i|^2 - |v_i|^2 \} = 1 \quad (2.265)$$

The HAMILTONIAN can be transformed, i.e.

$$\begin{aligned} \hat{H} &= \hat{H}(\varphi) + \int d^3 r \hat{\psi}'^\dagger \left\{ -\frac{\hbar^2}{2m} \nabla^2 + \mu + U + 2g\varphi^2 \right\} \hat{\psi}' \\ &\quad + \frac{1}{2}g \int d^3 r \varphi^2 \left(\hat{\psi}'^\dagger \hat{\psi}'^\dagger + \hat{\psi}' \hat{\psi}' \right) \end{aligned} \quad (2.266)$$

$$\stackrel{!}{=} \hat{H}(\varphi) + \text{const} + \hbar \sum_i \omega_i \tilde{\alpha}_i^\dagger \tilde{\alpha}_i \quad (2.267)$$

if and only if the u_i and v_i obey the BOGOLYUBOV-DE GENNES equations (2.253) and (2.254).

Chapter 3

Fermions

3.1 Free Fermions

3.1.1 General properties

We describe our particles by their momenta \vec{p} and some other quantum numbers α which might represent spin projections or hyper fine states. The other quantum numbers have g possible values (labeled j) in total. For now, our energy depends only on \vec{p} , i.e. we do not consider effects like spin-orbit splitting. In the free gas case we get

$$\varepsilon_p = \frac{p^2}{2m} \quad \text{and} \quad (3.1)$$

$$n_f(\vec{p}, T) = \frac{1}{\exp\left(\frac{\varepsilon_p - \mu}{T}\right) + 1} \quad (3.2)$$

$$n = \int \frac{d^3 p}{(2\pi\hbar)^3} n_f(\vec{p}, T) \quad (3.3)$$

Since n remains fixed the last equation defines $\mu(T)$. At $T = 0$ we call $\mu(T = 0) = \varepsilon_F$ the FERMI energy.

All states with $p \leq p_F = \sqrt{2m\varepsilon_F}$ are occupied. The reason for this is the PAULI principle which allows at most 1 occupation of each single particle quantum state (or at most g particles in an energy level which is g times degenerate):

$$n = g \int \frac{d^3 p}{(2\pi\hbar)^3} \Theta(\varepsilon_F - \varepsilon_p) = \frac{4\pi}{(2\pi\hbar)^3} g \int_0^{p_F} dp p^2 = g \frac{p_F^3}{6\pi^2\hbar^3} \quad (3.4)$$

$$= g \frac{(2m\varepsilon_F)^{\frac{3}{2}}}{6\pi^2\hbar^3} \quad \varepsilon_F = \varepsilon_F(n) \text{ only} \quad (3.5)$$

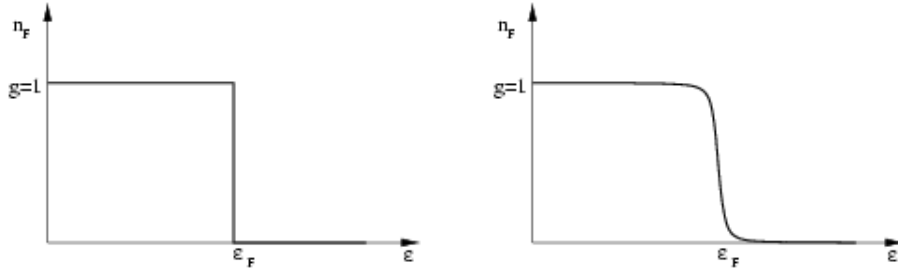


Figure 3.1: FERMI-DIRAC-Distribution at $T = 0$ (left) and at $0 < T \ll \varepsilon_F$ (right)

$$E_0 = g \int \frac{d^3 p}{(2\pi\hbar)^3} \Theta(\varepsilon_F - \varepsilon_p) \frac{p^2}{2m} = n \frac{3}{5} \varepsilon_F \quad (3.6)$$

If we now consider low temperatures, i.e. $0 < T \ll \varepsilon_F$ we get the following distribution:

Here $\mu(T, n) \neq \varepsilon_F$. We rather get

$$n = g \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left(\frac{\varepsilon - \mu}{T}\right) + 1} \quad (3.7)$$

$$= \int_0^\infty d\varepsilon g \int \frac{d^3 p}{(2\pi\hbar)^3} \delta(\varepsilon - \varepsilon_p) \frac{1}{\exp\left(\frac{\varepsilon - \mu}{T}\right) + 1} \quad (3.8)$$

$$= \int_0^\infty d\varepsilon v(\varepsilon) \frac{1}{\exp\left(\frac{\varepsilon - \mu}{T}\right) + 1} \quad (3.9)$$

where the density of states $v(\varepsilon)$ is

$$v(\varepsilon) = g \int \frac{d^3 p}{(2\pi\hbar)^3} \delta\left(\varepsilon - \frac{p^2}{2m}\right) \quad (3.10)$$

$$= g \frac{4\pi}{(2\pi\hbar)^3} \int_0^\infty dp p^2 \delta\left(\varepsilon - \frac{p^2}{2m}\right) \quad (3.11)$$

$$= \frac{g}{2\pi^2 \hbar^3} m \sqrt{2m} \int_0^\infty d\left(\frac{p^2}{2m}\right) \sqrt{\frac{p^2}{2m}} \delta\left(\varepsilon - \frac{p^2}{2m}\right) \quad (3.12)$$

$$= g \frac{m}{2\pi^2 \hbar^3} \sqrt{2m\varepsilon} = g \frac{mp(\varepsilon)}{2\pi^2 \hbar^3} \quad (3.13)$$

Looking again at figure (3.1) we see, that only the region around ε_F is of interest. Since $v(\varepsilon)$ is analytic and smooth for ε close to ε_F we can generally consider for

every analytic function $f(\varepsilon)$:

$$\int_0^\infty d\varepsilon f(\varepsilon) \frac{1}{\exp\left(\frac{\varepsilon-\mu}{T}\right) + 1} = \int_{-\mu}^\infty d\xi f(\mu + \xi) \frac{1}{\exp\left(\frac{\xi}{T}\right) + 1} \quad (3.14)$$

$$\begin{aligned} &= \int_0^\infty d\xi f(\mu + \xi) \frac{1}{\exp\left(\frac{\xi}{T}\right) + 1} \\ &\quad + \int_0^\mu d\xi f(\mu - \xi) \frac{1}{\exp\left(\frac{-\xi}{T}\right) + 1} \end{aligned} \quad (3.15)$$

$$\begin{aligned} &= \int_0^\infty d\xi f(\mu + \xi) \frac{1}{\exp\left(\frac{\xi}{T}\right) + 1} + \int_0^\mu d\xi f(\underbrace{\mu - \xi}_\varepsilon) \\ &\quad - \int_0^\mu d\xi f(\mu - \xi) \frac{1}{\exp\left(\frac{\xi}{T}\right) + 1} \end{aligned} \quad (3.16)$$

$$\approx \int_0^\mu d\varepsilon f(\varepsilon) \quad (3.17)$$

$$+ \int_0^\infty d\xi \frac{1}{\exp\left(\frac{\xi}{T}\right) + 1} [f(\mu + \xi) - f(\mu - \xi)]$$

$$\approx \int_0^\mu d\varepsilon f(\varepsilon) + 2f'(\mu) \int_0^\infty d\xi \frac{\xi}{\exp\left(\frac{\xi}{T}\right) + 1} \quad (3.18)$$

$$= \int_0^\mu d\varepsilon f(\varepsilon) + 2T^2 f'(\mu) \int_0^\infty dx \frac{x}{e^x + 1} \quad (3.19)$$

$$= \int_0^\mu d\varepsilon f(\varepsilon) + \frac{\pi^2}{6} T^2 f'(\mu) \quad (3.20)$$

Here we defined $\xi = \varepsilon - \mu$ and used

$$\frac{1}{e^{-x} + 1} = 1 - \frac{1}{e^x + 1} \quad \text{for (3.15)} \quad (3.21)$$

$$\mu \gg T \Rightarrow \mu \approx \infty \text{ last term in (3.16)} \quad (3.22)$$

$$\int_0^\infty dx x \sum_{n=1}^\infty (-1)^{n+1} e^{-nx} = \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n^2} \quad (3.23)$$

$$= \sum_{n=1}^\infty \frac{1}{n^2} - 2 \sum_{k=1}^\infty \frac{1}{(2k)^2} \quad (3.24)$$

$$= \frac{1}{2} \sum_{n=1}^\infty \frac{1}{n^2} = \frac{\pi^2}{12} \quad \text{in (3.19)} \quad (3.25)$$

Using this so called SOMMERFELD expansion we can now calculate the particle density n :

$$n = \int_0^{\mu(T)} d\varepsilon v(\varepsilon) + \frac{\pi^2}{6} T^2 \left. \frac{dv}{d\varepsilon} \right|_{\varepsilon=v} = \int_0^{\varepsilon_F + \delta\mu} d\varepsilon v(\varepsilon) + \frac{\pi^2}{6} T^2 \left. \frac{dv}{d\varepsilon} \right|_{\varepsilon=v} \quad (3.26)$$

$$\approx \underbrace{\int_0^{\varepsilon_F} d\varepsilon v(\varepsilon)}_n + \delta\mu v(\varepsilon_F) + \frac{\pi^2}{6} T^2 \left. \frac{dv}{d\varepsilon} \right|_{\varepsilon=v} \quad (3.27)$$

which means

$$\Leftrightarrow \delta\mu v(\varepsilon_F) + \frac{\pi^2}{6} T^2 \left. \frac{dv}{d\varepsilon} \right|_{\varepsilon=\varepsilon_F} = 0 \quad \text{and} \quad (3.28)$$

$$(3.13): \quad \left. \frac{dv}{d\varepsilon} \right|_{\varepsilon=\varepsilon_F} = \frac{1}{2\varepsilon_F} v(\varepsilon_F) \quad (3.29)$$

which leads to the shift in the chemical potential

$$\delta\mu = -\frac{\pi^2}{12} \frac{T^2}{\varepsilon_F} = -\varepsilon_F \frac{\pi^2}{12} \left(\frac{T}{\varepsilon_F} \right)^2 \quad (3.30)$$

Using this, we can now calculate the energy using (3.20) with $f(\varepsilon) = \varepsilon v(\varepsilon)$

$$E(T) = \int_0^\infty d\varepsilon v(\varepsilon) \varepsilon \frac{1}{\exp\left(\frac{\varepsilon-\mu}{T}\right) + 1} \quad (3.31)$$

$$= \int_0^{\mu=\varepsilon_F + \delta\mu} d\varepsilon v(\varepsilon) \varepsilon + \frac{\pi^2}{6} T^2 \left. \frac{d}{d\varepsilon} (\varepsilon v(\varepsilon)) \right|_{\varepsilon=v} \quad (3.32)$$

$$= \underbrace{\int_0^{\varepsilon_F} d\varepsilon v(\varepsilon) \varepsilon}_{E_0} + \delta\mu (\varepsilon_F v(\varepsilon_F)) + \frac{\pi^2}{6} T^2 \left\{ v(\varepsilon_F) + \varepsilon_F \left. \frac{\partial v}{\partial \varepsilon} \right|_{\varepsilon=\varepsilon_F} \right\} \quad (3.33)$$

$$= E_0 + \frac{\pi^2}{6} T^2 v(\varepsilon_F) + \varepsilon_F \underbrace{\left[\delta\mu v(\varepsilon_F) + \frac{\pi^2}{6} T^2 \left. \frac{\partial v}{\partial \varepsilon} \right|_{\varepsilon=\varepsilon_F} \right]}_{=0 \text{ (3.28)}} \quad (3.34)$$

Can we understand this solution physically ? We have $Tv(\epsilon)$ states available for excitation with energy of the order of T , which is exactly what the calculation gives in 0th order.

The specific heat is

$$c_{\gamma} = \frac{dE}{dT} = \frac{\pi^2}{3} v(\epsilon_F) T \quad (3.35)$$

unlike the BOSE gas where $c_{\gamma} \sim T^3$.

3.1.2 Pressure of degenerated Fermi gas

For classical gases

$$p = nT \quad (3.36)$$

holds meaning at $T = 0$ pressure vanishes. For quantum gases (BOSE as well as FERMI)

$$p = \frac{2}{3} \frac{E}{\gamma} \quad (3.37)$$

holds. Refer to appendix (A) for the derivation of (3.37). Here $E = E(T)$ for the quantum system considered. For FERMIons we get using (3.4) and (3.6)

$$p = \frac{2}{3} n \frac{3}{5} \epsilon_F = \frac{2}{5} n \frac{p_F^2}{2m} = \frac{1}{5} \frac{n}{m} \left(\frac{6\pi\hbar^3 n}{g} \right)^{\frac{2}{3}} \quad (3.38)$$

$$= \frac{1}{5m} \left(\frac{6\pi\hbar^3}{g} \right)^{\frac{2}{3}} n^{\frac{5}{3}} \neq 0 \quad (3.39)$$

This pressure is sometimes called FERMI-Pressure. It stabilizes the nucleons against strong interaction as well as neutron stars against gravitational forces.

If we look at high temperatures $T \gg \epsilon_F$ we should get the classical behavior plus some quantum corrections. To get the classical behavior we have to require

$$e^{\frac{|\mu|}{T}} \gg 1 \quad \text{and } \mu \text{ negative} \quad (3.40)$$

To calculate the classical behavior we note that independently of the statistics of the particle we have

$$e^{\frac{\epsilon + |\mu|}{T}} \gg 1 \quad \text{for large } T \quad (3.41)$$

and for FERMIONS

$$n_f(\varepsilon) = \frac{1}{\exp\left(\frac{\varepsilon-\mu}{T}\right) + 1} = \frac{1}{\exp\left(\frac{\varepsilon+|\mu|}{T}\right) + 1} \quad (3.42)$$

$$\approx e^{-\frac{|\mu|}{T} - \frac{\varepsilon}{T}} \left(1 - e^{-\frac{|\mu|+\varepsilon}{T}}\right) \quad (3.43)$$

Bearing in mind, that we work with a fixed n we get

$$n = g \int \frac{d^3 p}{(2\pi\hbar)^3} n_F \approx g \int \frac{d^3 p}{(2\pi\hbar)^3} e^{\frac{\mu}{T} - \frac{\varepsilon}{T}} \left(1 - e^{\frac{\mu}{T} - \frac{\varepsilon}{T}}\right) \quad (3.44)$$

$$= \frac{g}{2\pi\hbar^3} m\sqrt{2m} \int d\varepsilon \sqrt{\varepsilon} e^{\frac{\mu}{T} - \frac{\varepsilon}{T}} \left(1 - e^{\frac{\mu}{T} - \frac{\varepsilon}{T}}\right) \quad (3.45)$$

$$= \frac{gm\sqrt{2m}}{2\pi^2\hbar^3} T^{\frac{3}{2}} e^{\frac{\mu}{T}} \int dx \sqrt{x} e^{-x} \left(1 - e^{\frac{\mu}{T} - x}\right) \quad (3.46)$$

$$= \frac{gm\sqrt{2m}}{2\pi^2\hbar^3} T^{\frac{3}{2}} e^{\frac{\mu}{T}} \frac{\sqrt{\pi}}{2} \left(1 - e^{\frac{\mu}{T}} \frac{1}{2\sqrt{2}}\right) \quad (3.47)$$

Here we used the definition of the Γ -Function

$$\Gamma(z) = \int_0^{\infty} dt t^{z-1} e^{-t} \quad (3.48)$$

with its properties

$$\Gamma(1+z) = z\Gamma(z) \quad \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \quad (3.49)$$

Therefore our assumption (3.40) must hold true for the last term in (3.47) to be small. Neglecting the last term we solve for the chemical potential in the lowest order (BOLTZMANN case)

$$e^{\frac{\mu_B}{T}} = \frac{n}{g} \frac{2}{\sqrt{\pi}} \frac{2\pi^2\hbar^3}{m\sqrt{2m}} \frac{1}{T^{\frac{3}{2}}} = \frac{n}{g} \left(\frac{2\pi}{mT}\right)^{\frac{3}{2}} \hbar^3 \quad (3.50)$$

$$\sim \left(\frac{\varepsilon_F}{T}\right)^{\frac{3}{2}} \ll 1 \quad (3.51)$$

Similarly we can calculate the first correction to the classical equation for the pressure:

$$p = \frac{2}{3} \int_0^{\infty} d^3 p v(\varepsilon) n_f(\varepsilon) \varepsilon \quad (3.52)$$

$$= \frac{2}{3} \frac{m\sqrt{2m}}{2\pi^2\hbar^3} g \int_0^{\infty} d\varepsilon \varepsilon^{\frac{3}{2}} e^{\frac{\mu}{T} - \frac{\varepsilon}{T}} \left(1 - e^{\frac{\mu}{T} - \frac{\varepsilon}{T}}\right) \quad (3.53)$$

$$= \frac{2}{3} g \frac{m\sqrt{2m}}{2\pi^2\hbar^3} e^{\frac{\mu}{T}} T^{\frac{5}{2}} \int_0^{\infty} dx x^{\frac{3}{2}} e^{-x} \left(1 - e^{-x} e^{\frac{\mu}{T}}\right) \quad (3.54)$$

$$= \frac{2}{3} g \frac{m\sqrt{2m}}{2\pi^2\hbar^3} T^{\frac{5}{2}} e^{\frac{\mu}{T}} \Gamma\left(\frac{5}{2}\right) \left(1 - e^{\frac{\mu}{T}} \frac{1}{4\sqrt{2}}\right) \quad (3.55)$$

$$= g \frac{m\sqrt{2m}}{2\pi^2\hbar^3} T^{\frac{5}{2}} e^{\frac{\mu}{T}} \frac{\sqrt{\pi}}{2} \left(1 - e^{\frac{\mu}{T}} \frac{1}{4\sqrt{2}}\right) \quad (3.56)$$

$$= T g \frac{m\sqrt{2m}}{2\pi^2\hbar^3} T^{\frac{3}{2}} e^{\frac{\mu}{T}} \frac{\sqrt{\pi}}{2} \left(1 - \frac{1}{2\sqrt{2}} e^{\frac{\mu}{T}} + \frac{1}{4\sqrt{2}} e^{\frac{\mu}{T}}\right) \quad (3.57)$$

$$= T n + T g \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \frac{\sqrt{\pi}}{2} T^{\frac{3}{2}} \frac{1}{4\sqrt{2}} e^{2\frac{\mu}{T}} \quad (3.58)$$

$$= T n + T \frac{n}{4\sqrt{2}} \frac{n}{g} \frac{2}{\sqrt{\pi}} \frac{2\pi^2\hbar^3}{m\sqrt{2m}} \frac{1}{T^{\frac{3}{2}}} \quad (3.59)$$

$$= nT \left(1 + \left(\frac{\pi}{mT}\right)^{\frac{3}{2}} \frac{n\hbar^3}{2g}\right) \quad (3.60)$$

For $T \nearrow \infty$ the correction vanishes of course. Note, that this increase in pressure is due to *only* the FERMI statistics as no interaction was considered. The correction is of the order of $\left(\frac{\epsilon_F}{T}\right)^{\frac{3}{2}}$. In the case of BOSons a similar term appears but it is subtracted from the classical value.

3.1.3 Excitations of Fermions at T=0

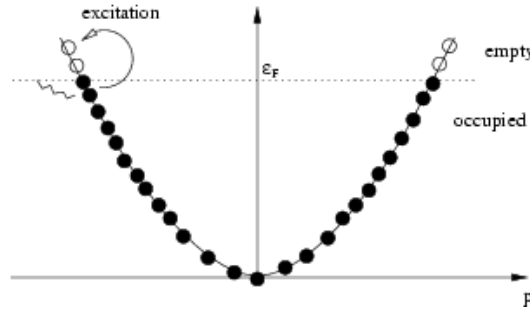


Figure 3.2: Small excitations at the FERMI surface (left)

If we look for excitations at $T = 0$ the system is in its ground state before the excitation. Afterwards one particle is above the FERMI surface leaving a hole below the FERMI surface. Condense matter physicists call this a "particle hole pair". Since we currently consider no interaction the particle and hole are uncorrelated and can be treated separately. Even if interaction is considered the correlation between particle and hole can be usually neglected since their number is small (for $T \ll \epsilon_F$) and, therefore they are "far away".

particle excitations We add a particle into a state \vec{p} with $|\vec{p}| > p_F$. This gives the excitation energy

$$\varepsilon_p = E_0(N) + \frac{p^2}{2m} - E_0(N+1) \quad (3.61)$$

$$= \frac{p^2}{2m} - \underbrace{(E_0(N+1) - E_0(N))}_{=\mu=\varepsilon_F} = \frac{p^2}{2m} - \frac{p_F^2}{2m} > 0 \quad (3.62)$$

hole excitations We remove a particle from a state \vec{p} with $|\vec{p}| < p_F$. This gives the excitation energy

$$\varepsilon_p = E_0(N) - \frac{p^2}{2m} - E_0(N+1) = \frac{p_F^2}{2m} - \frac{p^2}{2m} > 0 \quad (3.63)$$

The energy gain is therefore in both cases

$$\varepsilon = \left| \frac{p^2}{2m} - \frac{p_F^2}{2m} \right| > 0 \quad (3.64)$$

Obviously you can get the same result for a particle hole pair if you simply calculate the energy difference before ($p_2 < p_F$) and after ($p_1 > p_F$) the excitation

$$\delta\varepsilon = \frac{p_1^2}{2m} - \frac{p_2^2}{2m} = \left(\frac{p_1^2}{2m} - \frac{p_F^2}{2m} \right) + \left(\frac{p_F^2}{2m} - \frac{p_2^2}{2m} \right) = \varepsilon_1 + \varepsilon_2 \quad (3.65)$$

We can also discuss this in operator language. If we define

$$\tilde{\mathbf{a}}_p^\dagger = u_p \mathbf{a}_p^\dagger + v_p \mathbf{a}_{-p} \quad (3.66)$$

with

$$u_p = \begin{cases} 1 & p > p_F \\ 0 & p < p_F \end{cases} \quad v_p = \begin{cases} 0 & p > p_F \\ 1 & p < p_F \end{cases} \quad (3.67)$$

where u adds a particle and v adds a hole we can rewrite the HAMILTONIAN (1.84 with $g = 0$) as

$$\hat{H}' = \sum_p \left(\frac{p^2}{2m} - \mu \right) \mathbf{a}_p^\dagger \mathbf{a}_p = E'_0 + \sum_p \left| \frac{p^2}{2m} - \mu \right| \tilde{\mathbf{a}}_p^\dagger \tilde{\mathbf{a}}_p \quad (3.68)$$

E'_0 is the energy of the ground state and the energy of excitations is always positive (which was not satisfied before the transformation). Of course the new operators obey

$$\tilde{\mathbf{a}}_p |g\rangle = 0 \quad (3.69)$$

where $|g\rangle$ is the ground state (filled FERMI sphere).

3.2 Trapped non-interacting Fermi gas at T=0

We consider the isotropic case ($U(r)$) and large number of particle ($N \gg 1$). The energy depends only on the quantum numbers n and l and does not depend on the projection of the angular momentum, i.e.

$$\varepsilon_v = \varepsilon_{nl} \quad (3.70)$$

$$\varepsilon_v = \hbar\omega(2n + l + \frac{3}{2}) \quad \text{for } U_1 \equiv 0 \quad (3.71)$$

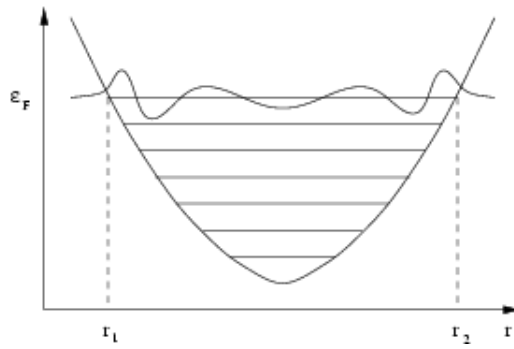


Figure 3.3: Schematic view of a trapped particle with large n

Since the system is rotational invariant, we have

$$\psi_{nlm} = \frac{\chi_{nl}}{r} Y_{lm}(\vec{r}) \quad (3.72)$$

Here $Y_{lm}(\vec{r})$ are the spherical harmonic functions and χ obeys the radial SCHRÖDINGER equation

$$\frac{d^2 \chi_{nl}}{dr^2} + \kappa_{nl}^2(r) \chi_{nl}(r) = 0 \quad \text{with} \quad (3.73)$$

$$\kappa_{nl}^2(r) = 2m(\varepsilon_{nl} - U(r)) - \frac{\hbar^2 l(l+1)}{r^2} \quad (3.74)$$

Since $N \gg 1$ we know that only particles with $n \gg 1$, i.e. those near the FERMI surface, can be excited. We can therefore apply WKB approximation.

If we call the classical turning points r_1 and r_2 we can approximate the radial wave function as

$$\chi_{nl}(r) = \frac{c_{nl}}{\sqrt{p_{nl}}} \cos \left\{ \int_{r_1}^{r_2} dr' p_{nl}(r') - \frac{\pi}{4} \right\} \quad \text{for } r_1 < r < r_2 \quad (3.75)$$

$$p_{nl}(r) = \sqrt{2m(\varepsilon_{nl} - U(r)) - \hbar^2 \frac{(l + \frac{1}{2})^2}{r^2}} \quad (3.76)$$

This regime ($n \gg 1$ but l arbitrary) is called THOMAS-FERMI regime. To calculate the density profile we use the semi-classical BOHR quantization requirement

$$\int_{r_1}^{r_2} dr' p_{nl}(r') = \pi \hbar \left(n + \frac{1}{2} \right) \quad (3.77)$$

First we want to calculate the normalization coefficient c_{nl} :

$$\int d^3r |\psi_{nlm}|^2 = 1 = \int dr \frac{|\chi_{nl}|^2}{r^2} r^2 = \int_0^\infty dr |\chi|^2 \quad \text{thus} \quad (3.78)$$

$$1 = \int_{r_1}^{r_2} dr \frac{c_{nl}^2}{p_{nl}(r)} \cos^2 \{ \dots \} \quad (3.79)$$

$$= c_{nl}^2 \int_{r_1}^{r_2} dr \frac{1}{p_{nl}} \frac{1}{2} (1 + \cos[2 \{ \dots \}]) \quad (3.80)$$

$$\approx \frac{c_{nl}^2}{2} \int_{r_1}^{r_2} dr \frac{1}{p_{nl}} \quad (3.81)$$

Since the integral over strongly oscillating terms almost vanishes we can neglect the second term in (3.80). To calculate the other term we differentiate (3.77) in respect to n . Since the integrand $p_{nl}(r)$ vanishes at the limits of the integration we only have to differentiate the integrand, i.e. differentiating in respect to the upper bound gives

$$\frac{\partial r_2}{\partial n} \frac{\partial}{\partial r_2} \int_{r_1}^{r_2} dr p_{nl}(r) = \frac{\partial r_2}{\partial n} p_{nl}(r_2) = 0 \quad (3.82)$$

Therefore we have

$$\pi \hbar = m \frac{\partial \epsilon_{nl}}{\partial n} \int_{r_2}^{r_1} \frac{dr}{\sqrt{2m(\epsilon_{nl} - U(r)) - \frac{\hbar^2(l+\frac{1}{2})^2}{r^2}}} \quad (3.83)$$

$$= m \frac{\partial \epsilon_{nl}}{\partial n} \int_{r_2}^{r_1} dr \frac{1}{p_{nl}(r)} \quad (3.84)$$

$$\Rightarrow \frac{c_{nl}^2}{2} = \frac{m}{\pi \hbar} \frac{\partial \epsilon_{nl}}{\partial n} \quad (3.85)$$

Note that the normalization coefficient is formally independent of the potential (which is of course relevant through the energy eigenvalues ϵ).

To calculate n we note, that

$$\sum_{m=-l}^l |Y_{lm}(\vec{r})|^2 = \frac{2l+1}{4\pi} \quad (3.86)$$

$$\sum_n \frac{\partial \epsilon_n}{\partial n} f(\epsilon_n) = \int dn \frac{\partial \epsilon}{\partial n} f(\epsilon) = \int d\epsilon f(\epsilon) \quad (3.87)$$

Now the particle density profile is

$$n(r) = g \sum_{\nu} |\psi_{\nu}(\vec{r})|^2 \quad (3.88)$$

$$= g \sum_{nlm} |Y_{lm}(\vec{r})|^2 \frac{1}{r^2} \frac{c_{nl}^2}{p_{nl}} \cos^2 \{ \} \quad (3.89)$$

$$\approx \frac{g}{4\pi} \sum_{nl} \frac{2l+1}{r^2} \frac{c_{nl}^2}{p_{nl}(r)} \frac{1}{2} \quad (3.90)$$

$$= \frac{g}{4\pi} \sum_{nl} \frac{2l+1}{r^2} \frac{m}{\pi\hbar} \frac{\partial \epsilon_{nl}}{\partial n} \frac{1}{\sqrt{2m(\epsilon_{nl} - U(r)) - \hbar^2 \frac{(l+\frac{1}{2})^2}{r^2}}} \quad (3.91)$$

$$= g \frac{m}{4\pi\hbar} \sum_l \frac{2l+1}{r^2} \sum_n \frac{\partial \epsilon_{nl}}{\partial n} \frac{1}{\sqrt{\dots}} \quad (3.92)$$

$$= g \frac{m}{4\pi\hbar} \sum_l \frac{2l+1}{r^2} \int_{\epsilon_l(r)}^{\epsilon_F} d\epsilon \frac{1}{\sqrt{\dots}} \quad (3.93)$$

$$= g \frac{1}{4\pi\hbar} \sum_l \frac{2l+1}{r^2} \sqrt{2m(\epsilon_{nl} - U) - \hbar^2 \frac{(l+\frac{1}{2})^2}{r^2}} \Big|_{\epsilon_l(r)}^{\epsilon_F} \quad (3.94)$$

$$= g \frac{1}{4\pi\hbar} \sum_l \frac{2l+1}{r^2} \sqrt{2m(\epsilon_F - U) - \hbar^2 \frac{(l+\frac{1}{2})^2}{r^2}} \quad (3.95)$$

$$= g \frac{1}{4\pi\hbar^3} \int_0^{x_{\max}(r)} dx \sqrt{2m(\epsilon_F - U(r)) - x} \quad (3.96)$$

$$= g \frac{1}{4\pi\hbar^3} \left(-\frac{2}{3} \right) (2m\epsilon_F - U(r) - x)^{\frac{3}{2}} \Big|_0^{x_{\max}(r)} \quad (3.97)$$

$$= \frac{g}{6\pi^2 \hbar^2} (2m(\epsilon_F - U(r)))^{\frac{3}{2}} \quad (3.98)$$

at $T = 0$. The summation/integration limits have always to be chosen such that p remains real.

This result means that if we redefine

$$\frac{p_F^2(r)}{2m} + U(r) = \epsilon_F \quad (3.99)$$

we get locally the same result as in the non trapped case

$$n(r) = g \frac{p_F^3(r)}{6\pi^2 \hbar^3} \quad (3.100)$$

but now with *local* FERMI momentum.

3.3 Weakly interacting Fermi gas

3.3.1 Ground state

Again we work in second quantization and assume there to be g different types of FERMIONS, i.e.

$$\hat{\psi}_j(\vec{r}) \quad j = 1, \dots, g \text{ with} \quad (3.101)$$

$$\left\{ \hat{\psi}_j(\vec{r}), \hat{\psi}_{j'}(\vec{r}') \right\} = \left\{ \hat{\psi}_j^\dagger(\vec{r}), \hat{\psi}_{j'}^\dagger(\vec{r}') \right\} = 0 \quad (3.102)$$

$$\left\{ \hat{\psi}_j(\vec{r}), \hat{\psi}_{j'}^\dagger(\vec{r}') \right\} = \delta_{jj'} \delta(\vec{r} - \vec{r}') \quad (3.103)$$

This means that for each type of FERMION each state is either occupied once or is not occupied at all, which is of course the PAULI principle.

The HAMILTONIAN now reads

$$\begin{aligned} \hat{H} &= \sum_j \int d^3r \hat{\psi}_j^\dagger(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \hat{\psi}_j(\vec{r}) \\ &\quad + \frac{1}{2} \sum_{jj'} \int d^3r d^3r' \underbrace{\hat{\psi}_j^\dagger(\vec{r}) \hat{\psi}_j(\vec{r})}_{\hat{n}_j(\vec{r})} U_1(\vec{r} - \vec{r}') \underbrace{\hat{\psi}_{j'}^\dagger(\vec{r}') \hat{\psi}_{j'}(\vec{r}')}_{\hat{n}_{j'}(\vec{r}')} \end{aligned} \quad (3.104)$$

$$\begin{aligned} &= \sum_j \int d^3r \hat{\psi}_j^\dagger(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \hat{\psi}_j(\vec{r}) \\ &\quad + \frac{1}{2} \sum_{jj'} \int d^3r d^3r' \hat{\psi}_{j'}^\dagger(\vec{r}') \hat{\psi}_j^\dagger(\vec{r}) U_1(\vec{r} - \vec{r}') \hat{\psi}_j(\vec{r}) \hat{\psi}_{j'}(\vec{r}') \end{aligned} \quad (3.105)$$

We use the following assumption:

$$U_1 = V_0 \delta(\vec{r} - \vec{r}') \quad (3.106)$$

This means we consider only short range interactions. This is reasonable because we consider gases with $r_0 p_F \ll 1$ and $p_F \sim \text{density}^{-\frac{1}{3}}$ ((1.1) and (1.3)). We wrote p_F here instead of p because only momenta $p \sim p_F$ are relevant for any physical process.

Using this we get

$$\begin{aligned}\hat{H} &= \sum_j \int d^3r \hat{\psi}_j^\dagger(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \hat{\psi}_j(\vec{r}) \\ &\quad + \frac{1}{2} V_0 \sum_{j \neq j'} \int d^3r \hat{\psi}_{j'}^\dagger(\vec{r}) \hat{\psi}_j^\dagger(\vec{r}) \hat{\psi}_j(\vec{r}) \hat{\psi}_{j'}(\vec{r})\end{aligned}\quad (3.107)$$

$$\begin{aligned}&= \sum_j \int d^3r \hat{\psi}_j^\dagger(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \hat{\psi}_j(\vec{r}) \\ &\quad + V_0 \sum_{j < j'} \int d^3r \hat{\psi}_{j'}^\dagger(\vec{r}) \hat{\psi}_j^\dagger(\vec{r}) \hat{\psi}_j(\vec{r}) \hat{\psi}_{j'}(\vec{r})\end{aligned}\quad (3.108)$$

where we have to exclude the case of $j = j'$ due to the PAULI principle. If we have a spatial homogeneous system we can write our wave function as

$$\hat{\psi}_j(\vec{r}) = \sum_{\vec{p}} \alpha_{\vec{p},j} e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \quad (3.109)$$

In this case we also have momentum conservation, i.e.

$$\vec{p}_1 + \vec{p}_2 = \vec{p}_3 + \vec{p}_4 \quad (3.110)$$

This will be denoted by a tick at the appropriate summations.

$$\hat{H} = \sum_{j,\vec{p}} \frac{p^2}{2m} \alpha_{\vec{p},j}^\dagger \alpha_{\vec{p},j} + V_0 \sum_{p_1 p_2 p_3 p_4} \sum_{j < j'}' \alpha_{p_4 j'}^\dagger \alpha_{p_3 j}^\dagger \alpha_{p_1 j} \alpha_{p_2 j'} \quad (3.111)$$

In this expression we obviously see that if we have only one type of FERMIONS the interaction term vanishes. This is because we consider only s-wave scattering (i.e. lowest order). If we consider for example the two particle wave function which has to fulfill the PAULI principle

$$\varphi(1,2) = \varphi_{ij}(\vec{r}_1 - \vec{r}_2) = -\varphi_{ji}(\vec{r}_2 - \vec{r}_1) \quad (3.112)$$

If we look at the state with a given relative angular momentum l of these two particles we have

$$\varphi_{ij}(\vec{r}_1 - \vec{r}_2) = (-1)^l \varphi_{ij}(\vec{r}_2 - \vec{r}_1) \quad \text{leading to} \quad (3.113)$$

$$\varphi_{ij}(\vec{r}_1 - \vec{r}_2) = -(-1)^l \varphi_{ji}(\vec{r}_1 - \vec{r}_2) \quad (3.114)$$

Thus we have two cases to consider

$$l = 0, 2, \dots \quad \varphi_{ij} = -\varphi_{ji} = \frac{1}{\sqrt{2}} (|i\rangle|j\rangle - |j\rangle|i\rangle) \quad (3.115)$$

$$l = 1, 3, \dots \quad \varphi_{ij} = \varphi_{ji} = \frac{1}{\sqrt{2}} (|i\rangle|j\rangle + |j\rangle|i\rangle) \quad (3.116)$$

This means we have to have $g \geq 2$ for even relative angular momentum (3.115) and $g \geq 1$ for odd relative angular momentum (3.116). Since we consider only $l = 0$ we therefore need at least two types of FERMIONS to have a non vanishing interaction.

Returning to the non interacting HAMILTONIAN we get the ground state energy

$$E_g = \sum_{j, \vec{p}} \frac{p^2}{2m} \langle a_{pj}^\dagger a_{pj} \rangle = \sum_{j, \vec{p}} \frac{p^2}{2m} n_{pj} = \sum_j n_j \frac{3}{5} \varepsilon_F = n \frac{3}{5} \varepsilon_F \quad (3.117)$$

Here we used (3.6) and considered the ordinary case for which E does not depend on j . Treating the interaction as a perturbation we get

$$E_1 = V_0 \sum_{p_i} \sum'_{j' < j} \langle a_{p_4 j'}^\dagger a_{p_3 j'}^\dagger a_{p_1 j} a_{p_2 j'} \rangle \quad (3.118)$$

$$= V_0 \sum_{j' < j} \sum_{p_1 p_2} \langle a_{p_2 j'}^\dagger a_{p_2 j'} \rangle \langle a_{p_1 j}^\dagger a_{p_1 j} \rangle \quad (3.119)$$

$$= V_0 \sum_{j' < j} \sum_{p_1 p_2} n_{p_2 j'} n_{p_1 j'} = V_0 \frac{g(g-1)}{2} n_1 n_2 = V_0 \frac{1}{2} \frac{g-1}{g} n^2 \quad (3.120)$$

In (3.118) the operators create two particles and two holes. The resulting state will usually be orthogonal to the ground state, unless $p_4 = p_2$ and $p_3 = p_1$. We further assume that $n_1 = n_2 = \dots = \frac{n}{g}$ which is true of course only if *no external fields* are present.

In second order we get

$$E_2 = \sum_e \frac{|\langle e | \hat{H}_{\text{int}} | g \rangle|^2}{E_g - E_e} \quad (3.121)$$

Here $|g\rangle$ is the ground state and $|e\rangle$ is any state possible with two holes ($p_1 j$ and $p_2 j'$) and two particles ($p_3 j$ and $p_4 j'$).

$$E_g - E_e = -\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m} \quad (3.122)$$

As required for any energy difference in respect to the ground state, (3.122) is negative. Now (3.121) becomes (cf. appendix (B))

$$E_2 = -V_0^2 \sum_{j < j'} \sum_{p_i} n_{p_1 j} n_{p_2 j'} \frac{(1 - n_{p_3 j})(1 - n_{p_4 j'})}{\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m}} \quad (3.123)$$

In respect to $p_1, p_2 < p_F$ we have no problem to integrate (sum up). The conservation of momentum fixes p_4 . p_3 however can take any value larger than p_F . The third sum (or integral)

$$\int_{p_F}^{\infty} d^3 p_3 \frac{1}{p_3^2} \quad (3.124)$$

does not converge. To eliminate this divergency, we can use the same technique as in section (2.3) page 28 and use BORN approximation¹:

$$\frac{4\pi\hbar^2 a}{m} = V_0 - V_0 \sum_{p_3 p_4} \frac{1}{\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m}} \frac{4\pi\hbar^2 a}{m} \quad (3.125)$$

$$\Rightarrow V_0 \approx \frac{4\pi\hbar^2 a}{m} + \left(\frac{4\pi\hbar^2 a}{m} \right)^2 \sum_{p_3 p_4} \frac{1}{\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m}} \quad (3.126)$$

Inserting this expression for V_0 into (3.120) and (3.123) we can get rid of the divergent sums

$$E_1 + E_2 = \frac{4\pi\hbar^2 a}{m} \sum_{j < j'} \sum_{p_1 p_2} n_{p_1 j} n_{p_2 j'} \quad (3.127)$$

$$- \left(\frac{4\pi\hbar^2 a}{m} \right)^2 \sum_{j < j'} \sum_{p_i} n_{p_1 j} n_{p_2 j'} \frac{[(1 - n_{p_3 j})(1 - n_{p_4 j'}) - 1]}{\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m}}$$

$$[\dots] = 1 - n_{p_3 j} - n_{p_4 j'} + n_{p_3 j} n_{p_4 j'} - 1 = \{n_{p_3 j} n_{p_4 j'}\} - n_{p_3 j} - n_{p_4 j'}$$

The addend of (3.127) with $\{\dots\}$ is symmetric if $p_1 p_2$ is interchanged with $p_3 p_4$. On the other hand the denominator is *antisymmetric* under interchange. Since the sum runs over all p_i it has to vanish thus preventing the ultraviolet divergence since now three out of 4 momenta are inside the sphere and the fourth momentum is fixed.

$$E_1 + E_2 = \frac{4\pi\hbar^2 a}{m} \sum_{j < j'} \sum_{p_1 p_2} n_{p_1 j} n_{p_2 j'} + \left(\frac{4\pi\hbar^2 a}{m} \right)^2 \sum_{j < j'} \sum_{p_i} n_{p_1 j} n_{p_2 j'} \frac{(n_{p_3 j} + n_{p_4 j'})}{\frac{p_4^2 + p_3^2 - p_1^2 - p_2^2}{2m}} \quad (3.128)$$

¹The summation runs over two momenta as we have two particles in the intermediate state

$$= n \frac{3}{5} \varepsilon_F (g-1) \left\{ \frac{5}{9} \lambda + \frac{11-2\ln(2)}{21} \lambda \right\} \quad (3.129)$$

Here λ is the Gas Parameter

$$\lambda = \frac{2ap_F}{\pi\hbar} = \frac{mp_F}{2\pi^2\hbar^3} \frac{4\pi\hbar^2 a}{m} = v_j(\varepsilon_F) V_0 \ll 1 \quad (3.130)$$

where v_j is the density of states.

3.3.2 Decay of excitations

We want to discuss the life time of excitations, i.e. the inverse scattering time τ . We discuss the regime of $T \ll \varepsilon_F$.

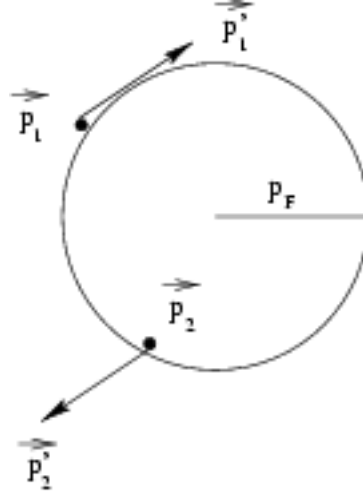


Figure 3.4: Schematic plot of excitations and scattering around the FERMI sphere

The excitations 1 and 2 can "collide", i.e. interaction occurs. The lifetime of the excitation 1 is according to FERMIS Golden Rule (appendix C)

$$\frac{1}{\tau} \sim a^2 \int d^3 p_2 d^3 p'_1 d^3 p'_2 \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_{1'} - \varepsilon_{2'}) \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_{1'} - \vec{p}_{2'}) \times n(\vec{p}_2)(1 - n(\vec{p}_{1'}))(1 - n(\vec{p}_{2'})) \quad (3.131)$$

The first line is the classical value while the second line takes the quantum statistics into account.

$$\left. \begin{array}{l} \varepsilon_{1'} + \varepsilon_{2'} = \varepsilon_1 + \varepsilon_2 > 2\varepsilon_F \\ \varepsilon_F < \varepsilon_1 \lesssim \varepsilon_F + T \end{array} \right\} \Rightarrow \varepsilon_F - T \lesssim \varepsilon_2 < \varepsilon_F, \quad (3.132)$$

i.e. the differences $\varepsilon_1 - \varepsilon_F$ and $\varepsilon_F - \varepsilon_2$ are positive and of the order of temperature T . First we expand the energy momentum relation near the FERMI energy:

$$\varepsilon(p) \approx \varepsilon_F + v_F(p - p_F) \quad \text{for } p \approx p_F \quad (3.133)$$

$$\delta\varepsilon \sim T \Rightarrow \delta p v_F \sim T \Rightarrow \delta p \sim \frac{T}{v_F} \quad (3.134)$$

We can now calculate the fraction of particles involved in the collisions by dividing the number of particles in the shell in momentum space of width $\frac{T}{v_F}$ by the total number of particles:

$$\frac{p_F^2 \delta p}{p_F^3} = \frac{\delta p}{p_F} \sim \frac{T}{v_F p_F} = \frac{T}{\varepsilon_F} \ll 1 \quad (3.135)$$

If we now look at the final states we have

$$2\varepsilon_F < \varepsilon_{1'} + \varepsilon_{2'} \lesssim 2\varepsilon_F + T \quad \text{with (3.132)} \quad (3.136)$$

$$\varepsilon_F < \varepsilon_{1'} \lesssim \varepsilon_F + T. \quad (3.137)$$

Without the PAULI principle the outgoing particles could have any energy allowed, i.e. between 0 and $2\varepsilon_F + T$. But with FERMI statistics being taken into account we have only a fraction $\frac{T}{\varepsilon_F} \ll 1$ of final states available. Thus (3.131) becomes²

$$\frac{1}{\tau} \sim na^2 v_F \left(\frac{T}{\varepsilon_F} \right)^2 \xrightarrow{T \rightarrow 0} 0. \quad (3.138)$$

The first three terms are the classical value, while the fraction is caused by the PAULI principle. The square originates in the fact that FERMI statistics imposes restrictions on the possible momenta of the incoming and outgoing particles.

At $T = 0$ calculation shows

$$\frac{1}{\tau(\varepsilon)} \sim na^2 v_F \left(\frac{\varepsilon}{\varepsilon_F} \right). \quad (3.139)$$

The energy of the excited particles obeys

$$\varepsilon_{\text{ex.}} \sim T \gg \Im \varepsilon_{\text{ex.}} \sim \frac{1}{\tau}. \quad (3.140)$$

Therefore the imaginary part of the excitation spectrum is much less than the real part and hence the excitations are well-defined.

²The exact and rather lengthy derivation is not included here

3.4 Landau-Fermi-Liquid

First we considered the non interacting FERMI gas where we have the filled FERMI sphere as ground state and we were capable of describing all properties for $T \ll \varepsilon_F$ causing excitations (particle transitions) near ε_F . If we now switch on the interaction adiabatically the behavior of the system remains similar to the previous one. In the interacting system a particle disturbs locally the surrounding particles. If we consider the particle together with the disturbance as a new particle (quasiparticle) we can transfer our previous discussion of the non interacting case to the interacting case. This procedure is called LANDAU conjecture and it can be justified by using a more complicated approach based on GREEN functions technique.

We are not interested in the general $E - p$ dependency but only near the FERMI surface as we have seen that the most important physics takes place there. We describe the ground state of an interacting (normal) FERMI system as a FERMI sphere filled with quasiparticles. The number of the quasiparticles is the same as the number of particles by the above conjecture, thus

$$g \frac{p_F^3}{6\pi^2 \hbar^3} = n = n_{qp} \quad (3.141)$$

This means the FERMI momentum also remains the same.

This FERMI liquid approach is experimentally favorably because as – we will show now – the description boils down to a few, experimentally accessible parameters.

If we briefly assume we have only one type of FERMIION we can relate the change in energy of the system to a change in the distribution function as

$$\delta E = \sum_{\vec{p}} \varepsilon(\vec{p}) \delta n_{\vec{p}} \quad (3.142)$$

which provides the definition of $\varepsilon(\vec{p})$ for quasiparticles. LANDAU introduced the f function which determines the change of the energy of the quasiparticle $\varepsilon(\vec{p})$ due to the change in the distribution function:

$$\delta \varepsilon(\vec{p}) = \sum_{\vec{p}'} f_{\vec{p}\vec{p}'} \delta n_{\vec{p}'} \quad (3.143)$$

The LANDAU f -function is a direct consequence of interparticle interaction and, as we will see, it actually governs collective behavior of the system.

We can now expand the energy-momentum relationship around the most interest-

ing point, the FERMI momentum:

$$\varepsilon(\vec{p}) = \mu + \vec{v}_F(\vec{p} - \vec{p}_F) \quad \text{with} \quad (3.144)$$

$$\mu = \frac{p_F^2}{2m} + \text{interaction} \quad (3.145)$$

$$v_F = \frac{p_F}{m^*} \quad (3.146)$$

$$m^* = m + \text{interaction} \quad (3.147)$$

Thus the complicated energy-momentum relation is substantially simplified since only momenta $p \approx p_F$ are important. As expected, the energy depends only on the absolute value of the momentum.

If we compare this result with our previous discussions ((3.117) and (3.120)) in the weakly interacting range

$$E = E_0 + \frac{4\pi\hbar^2 a}{m} \frac{1}{2} \sum_{j \neq j'} \sum_{\vec{p}\vec{p}'} n_{\vec{p}j} n_{\vec{p}'j'} \quad (3.148)$$

$$E_0 = \sum_{\vec{p}} \sum_j \frac{p^2}{2m} n_{\vec{p}j} \quad (3.149)$$

we have

$$\varepsilon_j(\vec{p}) = \frac{p^2}{2m} + \frac{4\pi\hbar^2 a}{m} \sum_{\vec{p}'j \neq j'} n_{\vec{p}'j'} = \frac{p^2}{2m} + \frac{4\pi\hbar^2 a}{m} \sum_{j \neq j'} n_j \quad (3.150)$$

which means that

$$\mu = \varepsilon(p_F) = \frac{p_F^2}{2m} + \frac{4\pi\hbar^2 a}{m} \sum_{j \neq j'} n_j \quad m^* = m \quad (3.151)$$

and therefore

$$\frac{\partial \varepsilon_j(p)}{\partial n_{\vec{p}j}} = f_{\vec{p}j\vec{p}'j'} = \begin{cases} 0 & j' = j \\ \frac{4\pi\hbar^2 a}{m} & j' \neq j \end{cases} \quad (3.152)$$

in first order in the interaction. If we also consider second order terms we get rather complicated terms with non trivial f , lengthy expressions and $m^* \neq m$.

The effective mass m^* can be measured experimentally e.g. in the specific heat (cf. (3.35) and (3.13)).

$$c = \frac{\pi^2}{3} v(\mu) T \quad \text{with} \quad (3.153)$$

$$v(\mu) = \frac{m^* p_F}{2\pi^2 \hbar^3} g \quad (3.154)$$

In our regime of low temperatures $c_{\mathcal{V}} = c_p$ and we thus do not have to distinguish between them.

We now want to calculate the effective mass m^* via the f -function for general FERMION liquid. The liquid moves with the velocity \vec{v} in the laboratory system thus generates the current

$$\vec{j} = mn\vec{v} = \sum_{\vec{p}j} \vec{p} \tilde{n}_{\vec{p}j} \quad (3.155)$$

The distribution function in the frame of the moving liquid relates to the distribution function in the laboratory \tilde{n} as follows

$$\tilde{n}_{\vec{p}j} = n_j(\varepsilon(\vec{p}) - \vec{p} \cdot \vec{v}) = n(\varepsilon(\vec{p})) + \delta n_{\vec{p}j} \quad (3.156)$$

$$\delta n_{\vec{p}j} = \frac{\partial n_{\vec{p}j}}{\partial \varepsilon} \delta \varepsilon \quad \delta \varepsilon = -\vec{p} \cdot \vec{v} + \text{interaction} \quad (3.157)$$

The distribution function of FERMIONS is a step function at $T = 0$ thus its derivative is a δ -function. The current now reads

$$\vec{j} = \sum_{\vec{p}j} \vec{p} \left(n_j(\varepsilon(\vec{p})) + \delta n_{\vec{p}j} \right) = \sum_{\vec{p}j} \vec{p} \frac{\partial n_{\vec{p}j}}{\partial \varepsilon} \delta \varepsilon(\vec{p}) \quad (3.158)$$

The first term in the summation vanishes because the filled FERMION sphere is rotational invariant and the summation runs over all momenta.

$$\frac{\partial n_{\vec{p}j}}{\partial \varepsilon} = -\delta(\varepsilon(p) - \mu) = -\frac{1}{v_F} \delta(p - p_F) \quad (3.159)$$

$$\vec{j} = \sum_{\vec{p}j} \vec{p} \left(-\frac{1}{v_F} \delta(p - p_F) \right) \delta(\varepsilon(\vec{p})) \quad (3.160)$$

$$= -\frac{1}{v_F} \frac{p_F^2}{(2\pi\hbar)^3} p_F g 4\pi \int \frac{d\Omega}{4\pi} \vec{e} \delta \varepsilon(p_F \vec{e}) \quad (3.161)$$

$$= -\frac{g}{v_F} \frac{p_F^3}{2\pi^2 \hbar^3} \int \frac{d\Omega}{4\pi} \vec{e} \delta \varepsilon(p_F \vec{e}) = -\frac{3}{v_F} n \int \frac{d\Omega}{4\pi} \vec{e} \delta \varepsilon(p_F \vec{e}) \quad (3.162)$$

In (3.162) we used (3.141). Looking at the shift in energy assuming $p_F(j) \equiv p_F \forall j$ we get

$$\delta \varepsilon(\vec{p}) = -\vec{p} \cdot \vec{v} + \sum_{\vec{p}'j'} f_{\vec{p}j\vec{p}'j'} \delta n_{\vec{p}'j'} \quad (3.163)$$

$$= -\vec{p} \cdot \vec{v} + \sum_{\vec{p}'j'} f_{\vec{p}j\vec{p}'j'} \frac{\partial n_{\vec{p}'j'}}{\partial \varepsilon} \delta \varepsilon(\vec{p}') \quad (3.164)$$

$$= -\vec{p} \cdot \vec{v} - \frac{1}{v_F} \sum_j \int \frac{d^3 p'}{(2\pi\hbar)^3} f_{\vec{p}j\vec{p}'j'} \delta(p - p_F) \delta\varepsilon(\vec{p}') \quad (3.165)$$

$$= -\vec{p} \cdot \vec{v} - \underbrace{\frac{1}{v_F} \frac{p_F^2}{(2\pi\hbar)^3} 4\pi}_{(3.146) \text{ and } (3.154)} \sum_j \int \frac{d\Omega'}{4\pi} f_{\vec{p}j p_F \vec{e}' j'} \delta\varepsilon(p_F \vec{e}') \quad (3.166)$$

$$= -\vec{p} \cdot \vec{v} - \int \frac{d\Omega'}{4\pi} \sum_j v_{j'}(\mu) f_{\vec{p}j p_F \vec{e}' j'} \delta\varepsilon(p_F \vec{e}') \quad (3.167)$$

This is interesting only for $|\vec{p}| = |\vec{p}_F|$ and we can write using $\vec{p}_F = p_F \vec{e}$

$$\delta\varepsilon(p_F \vec{e}) = -p_F \vec{e} \cdot \vec{v} - \int \frac{d\Omega'}{4\pi} F(\vec{e}\vec{e}') \delta\varepsilon(p_F \vec{e}') \quad \text{with} \quad (3.168)$$

$$F(\vec{e} \cdot \vec{e}') = \sum_j v_{j'}(\mu) f_{p_F \vec{e} j p_F \vec{e}' j'} \quad (3.169)$$

$$= \sum_{l=0}^{\infty} (2l+1) F_l P_l(\vec{e} \cdot \vec{e}') \quad (3.170)$$

Here P_l are the LEGENDRE-Polynomials.

To solve this we make the ansatz

$$\delta\varepsilon(p_F \vec{e}) = A p_F \vec{e} \cdot \vec{v} \quad A = \text{const} \quad (3.171)$$

$$A \vec{e} \cdot \vec{v} = -\vec{e} \cdot \vec{v} - A \int \frac{d\Omega'}{4\pi} \sum_{l=0}^{\infty} (2l+1) F_l P_l(\vec{e} \cdot \vec{e}') \underbrace{\vec{e}' \cdot \vec{v}}_{P_1(\vec{e}' \cdot \vec{v})} \quad (3.172)$$

$$= -\vec{e} \cdot \vec{v} - A F_1 \vec{e} \cdot \vec{v} \quad (3.173)$$

$$A = -\frac{1}{1+F_1} \quad \delta\varepsilon(p_F \vec{e}) = -\frac{p_F \vec{e} \cdot \vec{v}}{1+F_1} \quad (3.174)$$

Thus the current becomes

$$\vec{j} = -\frac{3}{v_F} n \left[-\frac{p_F}{1+F_1} \right] \int \frac{d\Omega}{4\pi} \vec{e}(\vec{e} \cdot \vec{v}) \quad (3.175)$$

$$= \frac{3}{v_F} n \frac{p_F}{1+F_1} \frac{1}{3} \vec{v} = n \frac{m^*}{1+F_1} \vec{v} \quad (3.176)$$

$$\Rightarrow m^* = m(1+F_1) \quad \text{with} \quad \int \frac{d\Omega}{4\pi} \vec{e}_i \vec{e}_j = \frac{1}{3} \delta_{ij} \quad (3.177)$$

where F_1 is usually positive. The value of F_1 has to be derived from an appropriate model or from measurement. Only for very few systems – e.g. FERMI gases – direct calculation is possible.

We now want to discuss some non trivial examples.

3.4.1 Zero Sound

Using a semi-classical approach we can describe small density fluctuations $\delta n_j \ll n$ around the ground state (equilibrium) as

$$n_j(\vec{p}, \vec{r}, t) = n_j(\vec{p}) + \delta n_j(\vec{p}, \vec{r}, t). \quad (3.178)$$

The kinetic equation for $n_j(\vec{p}, \vec{r}, t)$ reads

$$\frac{\partial n_j}{\partial t} + \vec{v} \nabla_r n_j + (-\nabla_r \varepsilon_j) \nabla_{\vec{p}} n_j = I_{\text{coll}} \rightarrow 0 \quad (3.179)$$

where the collisional term vanishes for $T \rightarrow 0$ because $\tau \sim T^{-2} \rightarrow \infty$ which corresponds to the so called collisionless regime, $\omega \tau \gg 1$, where ω is a characteristic frequency. Therefore the kinetic equation in this regime is

$$\frac{\partial n_j}{\partial t} + \vec{v} \nabla_r n_j - \nabla_r \varepsilon_j \nabla_{\vec{p}} n_j = 0. \quad (3.180)$$

The first two terms describe the ballistic motion of particles while the last term acts as a non trivial collective force. This equation has to be solved self-consistently because small fluctuations of density generates the force which in turn changes the density and so on. But first we want to rewrite the equation

$$\nabla_r \varepsilon_j = \nabla_r \left(\varepsilon(p) + \sum_{\vec{p}'j'} f_{\vec{p}j\vec{p}'j'} \delta n_{\vec{p}'j'} \right) = \sum_{\vec{p}'j'} f_{\vec{p}j\vec{p}'j'} \nabla_r \delta n_{\vec{p}'j'} \quad (3.181)$$

$$\frac{\partial \delta n_j}{\partial t} + \vec{v} \nabla_r \delta n_j - \sum_{\vec{p}'j'} f_{\vec{p}j\vec{p}'j'} (-\delta(p - p_F)) (\vec{e} \nabla_r) \delta n_{\vec{p}'j'} = 0 \quad (3.182)$$

$$\frac{\partial \delta n_{\vec{p}j}}{\partial t} + \vec{v} \nabla_r \delta n_{\vec{p}j} + \delta(p - p_F) \sum_{\vec{p}'j'} f_{p_F \vec{e} j \vec{p}'j'} (\vec{e} \nabla_r) \delta n_{\vec{p}'j'} = 0. \quad (3.183)$$

Here we used

$$\frac{\partial n(p)}{\partial \vec{p}} = \frac{\partial n}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \vec{p}} = -\frac{1}{v_F} \delta(p - p_F) \vec{v}_F = -\vec{e} \delta(p - p_F). \quad (3.184)$$

To solve this, we choose the ansatz

$$\delta n_{\vec{p}j} = \delta(p - p_F) \chi(\vec{e}) e^{i(\vec{k} \cdot \vec{r} - \omega t)}. \quad (3.185)$$

Inserting this into (3.183) we get

$$0 = (-i\omega + i\vec{k} \cdot \vec{v})\chi(\vec{e}) + \sum_{\vec{p}'j'} f_{p_F \vec{e} j \vec{p}' j'} i(\vec{e} \cdot \vec{k}) \delta(p - p_F)\chi(\vec{e}') \quad (3.186)$$

$$(\omega - kv_F)\chi(\vec{e}) = \vec{k} \cdot \vec{e} \sum_{\vec{p}'j'} f_{p_F \vec{e} j \vec{p}' j'} \delta(p - p_F)\chi(\vec{e}') \quad (3.187)$$

$$= \vec{k} \cdot \vec{e} \sum_{j'} v_{j'}(\mu) v_F \int \frac{d\Omega'}{4\pi} \chi(\vec{e}') f_{p_F \vec{e} j p_F \vec{e}' j'} \quad (3.188)$$

$$= \vec{k} \cdot \vec{e} \int \frac{d\Omega'}{4\pi} F(\vec{e} \cdot \vec{e}') \chi(\vec{e}') v_F \quad (3.189)$$

$$\chi(\vec{e}) = \frac{v_F \vec{k} \cdot \vec{e}}{\omega - v_F \vec{k} \cdot \vec{e}} \int \frac{d\Omega'}{4\pi} F(\vec{e} \cdot \vec{e}') \chi(\vec{e}'). \quad (3.190)$$

This is difficult to solve. We assume the simplest case, i.e.

$$F(\vec{e} \cdot \vec{e}') = F_0 \quad (3.191)$$

and consider all further deviations as higher order terms. This leads to

$$\chi(\vec{e}) = \frac{v_F \vec{k} \cdot \vec{e}}{\omega - v_F \vec{k} \cdot \vec{e}} F_0 \int \frac{d\Omega'}{4\pi} \chi(\vec{e}') \quad (3.192)$$

$$= \vec{\chi} \frac{v_F \vec{k} \cdot \vec{e}}{\omega - v_F \vec{k} \cdot \vec{e}}. \quad (3.193)$$

If we define $\omega = v_F k s$ with $s = \text{const}$ and $z = \cos(\vec{k} \cdot \vec{e}')$ and integrate both sides of (3.192) over $\frac{d\Omega'}{4\pi}$ we get

$$1 = F_0 \int \frac{d\Omega}{4\pi} \frac{v_F \vec{k} \cdot \vec{e}}{\omega - v_F \vec{k} \cdot \vec{e}} \quad (3.194)$$

$$= F_0 \int_{-1}^1 \frac{dz}{2} \frac{z}{s-z} = \frac{F_0}{2} \int_{-1}^1 dz \left\{ -1 - \frac{s}{z-s} \right\} \quad (3.195)$$

$$= F_0 \left\{ -1 - \frac{s}{2} \ln \left[\frac{(s-1)}{s+1} \right] \right\} \quad (3.196)$$

$$\Leftrightarrow \frac{1}{F_0} + 1 = \frac{s}{2} \ln \left[\frac{1+s}{|1-s|} \right]. \quad (3.197)$$

If $0 < F_0 \ll 1$ the left side became huge therefore s has to be close to 1:

$$s = 1 + \varepsilon \quad \varepsilon \ll 1 \quad (3.198)$$

which leads to

$$\frac{1}{2} \ln \left(\frac{2}{\varepsilon} \right) = \frac{1}{F_0} + 1 \quad (3.199)$$

$$\Rightarrow \varepsilon = \frac{2}{e^2} e^{-\frac{2}{F_0}} \quad (3.200)$$

This is a collective mode in a degenerated collisionless regime (zero sound) with the velocity

$$c_0 = v_F \left(1 + \frac{2}{e^2} e^{-\frac{2}{F_0}} \right) \approx v_F \quad (3.201)$$

compared to sound in the hydrodynamic regime:

$$c_1^2 = \frac{\partial p}{\partial \rho} = \frac{1}{m} \frac{\partial p}{\partial n} = \frac{1}{m} \frac{\partial}{\partial n} \left(\frac{2}{3} n \underbrace{\frac{3}{5} \varepsilon_F}_E \right) \quad (3.202)$$

$$= \frac{1}{m} \frac{\partial}{\partial n} \left(\frac{2}{5} n \frac{1}{2m} \left(\frac{6\pi^2 \hbar^3}{g} n \right)^{\frac{2}{3}} \right) = \frac{1}{m} \frac{5}{3} \frac{1}{5} \frac{1}{m} \left(\frac{6\pi^2 \hbar^3}{g} n \right)^{\frac{2}{3}} \quad (3.203)$$

$$= \frac{1}{3} \left(\frac{p_F}{m} \right)^2 = \frac{v_F^2}{3} \quad \Rightarrow \quad c_1 = \frac{v_F}{\sqrt{3}} \quad (3.204)$$

This is ordinary hydrodynamic sound.

If F_0 was negative s became a complex number with real and imaginary parts being of the same order. Hence, in this case the collective mode is overdamped and of no interest.

3.5 Bardeen-Cooper-Shieffer-Theory

3.5.1 General treatment

If we consider two FERMIONS in vacuum we have a simple quantum mechanical problem. We use the frame of reference where the center of mass is at rest:

$$\vec{P} = \vec{p}_1 + \vec{p}_2 = 0 \quad (3.205)$$

Here we can write the SCHRÖDINGER equation as

$$\left\{ -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + U_1(\vec{r}_1 - \vec{r}_2) \right\} \psi(\vec{r}_1, \vec{r}_2) = E \psi(\vec{r}_1, \vec{r}_2) \quad (3.206)$$

$$\psi(\vec{r}_1, \vec{r}_2) = \sum_{\vec{p}} c_{\vec{p}} e^{i \frac{\vec{p}(\vec{r}_1 - \vec{r}_2)}{\hbar}} \quad (3.207)$$

i.e. we decompose the wave function into plane waves. Inserting this decomposition we get the SCHRÖDINGER equation in momentum space

$$(\varepsilon_1 + \varepsilon_2)c_{\vec{p}} + \sum_{\vec{p}'} U_1(\vec{p} - \vec{p}')c_{\vec{p}'} = Ec_{\vec{p}} \quad (3.208)$$

where

$$\varepsilon_1 = \varepsilon_2 = \frac{p^2}{2m} = \varepsilon_p \quad (3.209)$$

since both particles are identical. Rewriting the SCHRÖDINGER equation once more we have

$$(E - 2\varepsilon_p)c_{\vec{p}} = \sum_{\vec{p}'} U_1(\vec{p} - \vec{p}')c_{\vec{p}'} \quad \text{or} \quad (3.210)$$

$$c_{\vec{p}} = \frac{1}{E - 2\varepsilon_p} \sum_{\vec{p}'} U_1(\vec{p} - \vec{p}')c_{\vec{p}'} \quad (3.211)$$

This discussion is still exact. Now we use a model for the interatomic potential

$$U_1(\vec{p} - \vec{p}') = \begin{cases} V_0 & 0 \leq \varepsilon_p, \varepsilon_{p'} \leq \bar{\omega} \\ 0 & \text{otherwise} \end{cases} \quad (3.212)$$

In ordinary space this expression looks rather strange. Using this model we have

$$c_{\vec{p}} = \frac{1}{E - 2\varepsilon_p} \Theta(\bar{\omega} - \varepsilon_p) V_0 \tilde{\sum}_{\vec{p}'} c_{\vec{p}'} \quad (3.213)$$

The tilde denotes that the sum obeys the constraint

$$\varepsilon_p' \leq \bar{\omega} \quad (3.214)$$

To solve this expression, we sum over all coefficients

$$\tilde{\sum}_{\vec{p}} c_{\vec{p}} = V_0 \tilde{\sum}_{\vec{p}} \frac{1}{E - 2\varepsilon_p} \tilde{\sum}_{\vec{p}'} c_{\vec{p}'} \quad (3.215)$$

$$\Leftrightarrow 1 = V_0 \tilde{\sum}_{\vec{p}} \frac{1}{E - 2\varepsilon_p} \quad (3.216)$$

Since we are looking at an attractive interaction and more specifically for bound states we have

$$V_0 = -|V_0| \quad E = -2\Delta \quad (3.217)$$

where Δ is the binding energy per particle. Using this we have

$$1 = \frac{1}{2} |V_0| \sum_{\vec{p}} \frac{1}{\Delta + \varepsilon_p} \quad (3.218)$$

$$= \frac{1}{2} |V_0| \int_0^{\bar{\omega}} d\varepsilon v(\varepsilon) \frac{1}{\Delta + \varepsilon} \quad (3.219)$$

$$= \frac{1}{2} |V_0| \int_0^{\bar{\omega}} d\varepsilon \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \sqrt{\varepsilon} \frac{1}{\Delta + \varepsilon} \quad (3.220)$$

$$= \frac{1}{2} |V_0| \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \int_0^{\sqrt{\bar{\omega}}} dx \frac{2x^2}{\Delta + x^2} \quad (3.221)$$

$$= |V_0| \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \int_0^{\sqrt{\bar{\omega}}} dx \left(1 - \Delta \frac{1}{\Delta + x^2} \right) \quad (3.222)$$

$$= |V_0| \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \left\{ \sqrt{\bar{\omega}} - \frac{\Delta}{\sqrt{\Delta}} \arctan \left(\frac{\sqrt{\bar{\omega}}}{\sqrt{\Delta}} \right) \right\} \quad (3.223)$$

$$\approx |V_0| \frac{m\sqrt{2m}}{2\pi^2\hbar^3} \left\{ \sqrt{\bar{\omega}} - \frac{\pi}{2} \sqrt{\Delta} \right\} \quad (3.224)$$

$$= |V_0| v(\bar{\omega}) \left\{ 1 - \frac{\pi}{2} \sqrt{\frac{\Delta}{\bar{\omega}}} \right\} \quad (3.225)$$

Here we assumed that $\Delta \ll \bar{\omega}$ and thus the arcus tangent can be approximated as $\frac{\pi}{2}$. Solving this we have

$$\sqrt{\frac{\Delta}{\bar{\omega}}} = \frac{2}{\pi} \left\{ 1 - \frac{1}{|V_0| v(\varepsilon_F)} \right\} > 0 \quad (3.226)$$

Therefore we have threshold (i.e. a minimal $|V_0|$) before a bound state appears. Now we want to consider two FERMIONS on top of a filled and frozen FERMI sphere. Frozen means that we will not consider interactions of the particles inside the FERMI sphere with our two extra particles. In this case we have

$$\varepsilon_p, \varepsilon_{p'} \geq \varepsilon_F \quad (3.227)$$

$$c_{\vec{p}} = \frac{1}{E - 2\varepsilon_p} \sum_{\vec{p}' \geq \vec{p}_F} U_I(\vec{p} - \vec{p}') c_{p'} \quad (3.228)$$

We assume for the potential

$$U_I(\vec{p} - \vec{p}') = \begin{cases} V_0 & \varepsilon_F \leq \varepsilon_p, \varepsilon_{p'} \leq \varepsilon_F + \bar{\omega} \\ 0 & \text{otherwise} \end{cases} \quad (3.229)$$

Now we define

$$\xi_p = \varepsilon_p - \varepsilon_F \geq 0 \quad (3.230)$$

and note that the energy of the ground state is now

$$E = 2\varepsilon_F - 2\Delta \quad (3.231)$$

where Δ is the binding energy per particle.

Again we can rewrite the SCHRÖDINGER equation in our case as

$$c_{\vec{p}} = \frac{\Theta(\bar{\omega} - \xi_p)}{2(\Delta + \xi_p)} |V_0| \sum_{\vec{p}'} \tilde{c}_{\vec{p}'} \quad (3.232)$$

The tilde denotes $\xi_{p'} \leq \bar{\omega}$.

Using the same method with $\Delta \ll \bar{\omega} \ll \varepsilon_F$ as before we get

$$1 = \frac{1}{2} |V_0| \sum_{\vec{p}} \frac{1}{\Delta + \xi_p} = \frac{1}{2} |V_0| \int_0^{\bar{\omega}} d\xi v(\varepsilon_F + \xi_p) \frac{1}{\Delta + \xi_p} \quad (3.233)$$

$$\approx \frac{1}{2} |V_0| v(\varepsilon_F) \ln \left(\frac{\Delta + \bar{\omega}}{\Delta} \right) \approx \frac{1}{2} |V_0| v(\varepsilon_F) \ln \left(\frac{\bar{\omega}}{\Delta} \right) \quad (3.234)$$

In the last step we approximated again $\Delta \ll \bar{\omega}$. solving this for the binding energy Δ we see, that there is *always* a solution regardless of the strength of the potential

$$\Delta = \bar{\omega} e^{-\frac{2}{|V_0|v(\varepsilon_F)}} \quad \text{COOPER 1956} \quad (3.235)$$

This is of course a toy model. The solution including the interaction between all particles – not only between extra ones – has basically the same form except the factor 2 in the numerator of the exponent is replaced by 1.

This result means that FERMIONS with \vec{p} and \vec{p}' become correlated, they form a "COOPER-PAIR".

The shift in energy can be approximated as

$$v_F \Delta p \sim \Delta \Leftrightarrow \Delta p \sim \frac{\Delta}{v_F} \quad (3.236)$$

If we denote the size of the correlation as ξ we can approximate

$$\xi \sim \frac{\hbar}{\Delta p} \sim \frac{\hbar}{\Delta} v_F \sim \frac{\hbar}{p_F} \frac{\varepsilon_F}{\Delta} \gg \frac{\hbar}{p_F} \quad (3.237)$$

This means the the size of the correlation is much larger than the mean interparticle distance. Therefore a mean field theory can be applied for this system.

It turns out that the region of temperatures δT around T_C where fluctuations become important can be estimated as

$$\delta T \sim T_C \left(\frac{\Delta}{\varepsilon_F} \right)^4 \quad (3.238)$$

This is so small that it cannot be found experimentally.

3.5.2 BCS Hamiltonian

The goal is to modify the HAMILTONIAN (3.111) in such a way that the BCS relevant terms are clearly visible while other terms (which are not relevant in this context) are put aside. We assume two types of FERMIONS which we will denote as $+$ and $-$. In this case the interaction part of (3.111) can be written as³

$$\hat{H}_{\text{int}} = V_0 \sum_{p_i} ' \mathbf{a}_{p_3+}^\dagger \mathbf{a}_{p_4-}^\dagger \mathbf{a}_{p_2-} \mathbf{a}_{p_1+} \quad (3.239)$$

We are not interested here in the FERMI-liquid type of renormalisations due to the interaction but only for the terms responsible for the COOPER coupling. Since we neglect all other terms we can write

$$\hat{H}_{\text{int}} = - \sum_p \left\{ \Delta^* \mathbf{a}_{-p-} \mathbf{a}_{p+} + \Delta \mathbf{a}_{p+}^\dagger \mathbf{a}_{p-}^\dagger \right\} + \text{other terms} \quad (3.240)$$

We approximate the operator Δ by its mean field value and note, that the first term destroys a COOPER pair while the second term creates a COOPER pair. Δ has to be calculated as

$$\Delta = -|V_0| \sum_p \langle \mathbf{a}_{-p-} \mathbf{a}_{p+} \rangle \quad (3.241)$$

This is a HARTREE-FOCK type of equation, i.e. (3.240) and (3.241) have to be solved self-consistently.

We can choose Δ real since a space independent phase would be irrelevant and a space dependent phase would cause a probability flow but we are looking for a stationary ground state solution. Thus we have

$$\hat{H}_{\text{eff}} = \sum_{pj} \xi_p \mathbf{a}_{pj}^\dagger \mathbf{a}_{pj} - \Delta \sum_p \left\{ \mathbf{a}_{-p-} \mathbf{a}_{p+} + \mathbf{a}_{p+}^\dagger \mathbf{a}_{-p-}^\dagger \right\} \quad (3.242)$$

$$\xi_p = \frac{p^2}{2m} - \mu \quad \mu = \frac{p_F^2}{2m} \quad (3.243)$$

³for simplicity we now always write p instead of \vec{p}

This case is different to the one encountered in section (2.3) because here we have to calculate \hat{H} and Δ simultaneously.

Again we can make a BOGOLYUBOV transformation

$$\mathbf{a}_{pj} = u_p \tilde{\mathbf{a}}_{pj} + \text{sign}(j) v_p \tilde{\mathbf{a}}_{-p-j}^\dagger = \begin{cases} \mathbf{a}_{p+} = u_p \tilde{\mathbf{a}}_{p+} + v_p \tilde{\mathbf{a}}_{-p-}^\dagger & j = + \\ \mathbf{a}_{p-} = u_p \tilde{\mathbf{a}}_{p-} - v_p \tilde{\mathbf{a}}_{-p+}^\dagger & j = - \end{cases} \quad (3.244)$$

The transformation has to be canonical, thus

$$\left\{ \tilde{\mathbf{a}}_{pj}, \tilde{\mathbf{a}}_{p'j'} \right\} = \left\{ \tilde{\mathbf{a}}_{pj}^\dagger, \tilde{\mathbf{a}}_{p'j'}^\dagger \right\} = 0 \quad (3.245)$$

$$\left\{ \tilde{\mathbf{a}}_{pj}, \tilde{\mathbf{a}}_{p'j'}^\dagger \right\} = \delta_{pp'} \delta_{jj'} \quad (3.246)$$

We again assume the most simple arrangement, i.e.

$$u_p^* = u_p \quad v_p^* = v_p \quad (3.247)$$

and insert the new operators in the FERMI anticommutating relations:

$$\left\{ \mathbf{a}_{pj}, \mathbf{a}_{p'j'} \right\} = \left\{ \mathbf{a}_{pj}^\dagger, \mathbf{a}_{p'j'}^\dagger \right\} = 0 \quad (3.248)$$

$$\left\{ \mathbf{a}_{pj}, \mathbf{a}_{p'j'}^\dagger \right\} = \left\{ u_p \tilde{\mathbf{a}}_{pj} + \text{sign}(j) v_p \tilde{\mathbf{a}}_{-p-j}, \right. \\ \left. u_p \tilde{\mathbf{a}}_{p'j'}^\dagger + \text{sign}(j') v_{p'} \tilde{\mathbf{a}}_{-p'-j'} \right\} \quad (3.249)$$

$$= u_p u_{p'} \delta_{pp'} \delta_{jj'} + \text{sign}(j) \text{sign}(j') v_p v_{p'} \delta_{pp'} \delta_{jj'} \quad (3.250)$$

$$= \delta_{pp'} \delta_{jj'} (u_p^2 + v_p^2) \quad (3.251)$$

Thus we have the requirement that

$$u_p^2 + v_p^2 = 1, \quad (3.252)$$

which means that u_p and v_p have to be expressed as sine and cosine.

Finally the transformed HAMILTONIAN has to have the following form

$$\hat{H}_{\text{eff}} = E_0 + \sum_{pj} \varepsilon_p \tilde{\mathbf{a}}_{pj}^\dagger \tilde{\mathbf{a}}_{pj} \quad (3.253)$$

The coefficients u_p and v_p can be calculated from the dynamics of the system. To this end we calculate

$$\left[\hat{H}_{\text{eff}}, \tilde{\mathbf{a}}_{pj} \right] = \sum_{p'j'} \varepsilon_{p'} \left(\tilde{\mathbf{a}}_{p'j'}^\dagger \tilde{\mathbf{a}}_{p'j'} \tilde{\mathbf{a}}_{pj} - \tilde{\mathbf{a}}_{pj} \tilde{\mathbf{a}}_{p'j'}^\dagger \tilde{\mathbf{a}}_{p'j'} \right) \quad (3.254)$$

$$= - \sum_{p'j'} \varepsilon_{p'} \underbrace{\left(\tilde{\mathbf{a}}_{p'j'}^\dagger \tilde{\mathbf{a}}_{pj} + \tilde{\mathbf{a}}_{pj} \tilde{\mathbf{a}}_{p'j'}^\dagger \right)}_{= \delta_{pp'} \delta_{jj'}} \tilde{\mathbf{a}}_{p'j'} \quad (3.255)$$

$$= - \varepsilon_p \tilde{\mathbf{a}}_{pj} \quad (3.256)$$

The other commutator we do not need to calculate because

$$\left[\hat{H}_{\text{eff}}, \tilde{\mathbf{a}}_{pj}^\dagger \right] = - \left(\left[\hat{H}_{\text{eff}}, \tilde{\mathbf{a}}_{pj} \right] \right)^\dagger = \varepsilon_p \tilde{\mathbf{a}}_{pj}^\dagger \quad (3.257)$$

Now let's use this to calculate the commutator

$$\left[\hat{H}_{\text{eff}}, \mathbf{a}_{pj} \right] = \left[\hat{H}_{\text{eff}}, u_p \tilde{\mathbf{a}}_{pj} + \text{sign}(j) v_p \tilde{\mathbf{a}}_{-p-j}^\dagger \right] \quad (3.258)$$

$$= u_p (-\varepsilon_p) \tilde{\mathbf{a}}_{pj} + \text{sign}(j) v_p \varepsilon_p \tilde{\mathbf{a}}_{-p-j}^\dagger \quad (3.259)$$

$$\stackrel{!}{=} -\xi_p \mathbf{a}_{pj} - \Delta \sum_{p'} \left(\mathbf{a}_{p'+}^\dagger \mathbf{a}_{-p'-}^\dagger \mathbf{a}_{pj} - \mathbf{a}_{pj} \mathbf{a}_{p'+}^\dagger \mathbf{a}_{-p'-}^\dagger \right) \quad (3.260)$$

$$= -\xi_p \mathbf{a}_{pj} - \Delta \sum_{p'} \left\{ \mathbf{a}_{p'+}^\dagger \mathbf{a}_{-p'-}^\dagger \mathbf{a}_{pj} - \left(\delta_{pp'} \delta_{j+} - \mathbf{a}_{p'+}^\dagger \mathbf{a}_{pj} \right) \mathbf{a}_{-p'-}^\dagger \right\} \quad (3.261)$$

$$= -\xi_p \mathbf{a}_{pj} - \Delta \sum_{p'} \left\{ \mathbf{a}_{p'+}^\dagger \mathbf{a}_{-p'-}^\dagger \mathbf{a}_{pj} - \delta_{pp'} \delta_{j+} \mathbf{a}_{-p'-}^\dagger + \mathbf{a}_{p'+}^\dagger \left(\delta_{p-p'} \delta_{j-} - \mathbf{a}_{-p'-}^\dagger \mathbf{a}_{pj} \right) \right\} \quad (3.262)$$

$$= -\xi_p \mathbf{a}_{pj} + \Delta \delta_{j+} \mathbf{a}_{-p-}^\dagger - \Delta \delta_{j-} \mathbf{a}_{-p+}^\dagger \quad (3.263)$$

$$= -\xi_p \mathbf{a}_{pj} + \Delta \text{sign}(j) \mathbf{a}_{-p-j}^\dagger \quad (3.264)$$

$$= -\xi_p \left(u_p \tilde{\mathbf{a}}_{pj} + \text{sign}(j) v_p \tilde{\mathbf{a}}_{-p-j}^\dagger \right) + \Delta \text{sign}(j) \left(u_p \tilde{\mathbf{a}}_{-p-j}^\dagger + \text{sign}(-j) v_p \tilde{\mathbf{a}}_{pj} \right) \quad (3.265)$$

Conferring to (3.259) we get the BOGOLYUBOV-DE GENNES equations:

$$-\varepsilon_p u_p = -\xi_p u_p - \Delta v_p \quad (3.266)$$

$$\varepsilon_p v_p = -\xi_p v_p + \Delta u_p \quad (3.267)$$

which are solved by

$$\varepsilon_p = \sqrt{\Delta^2 + \xi_p^2} \quad (3.268)$$

$$u_p^2 = \frac{1}{2} \left(1 + \frac{\xi_p}{\varepsilon_p} \right) \quad v_p^2 = \frac{1}{2} \left(1 - \frac{\xi_p}{\varepsilon_p} \right) \quad (3.269)$$

The solution is very similar to the BOSE case.

It follows from (3.268) that ε_p is always positive, $\varepsilon_p \geq \Delta > 0$.

The pairing energy is $\Delta \ll \varepsilon_F$ which causes the edges of the FERMI sphere to smear out. The BCS gap in the spectrum can be experimentally observed because

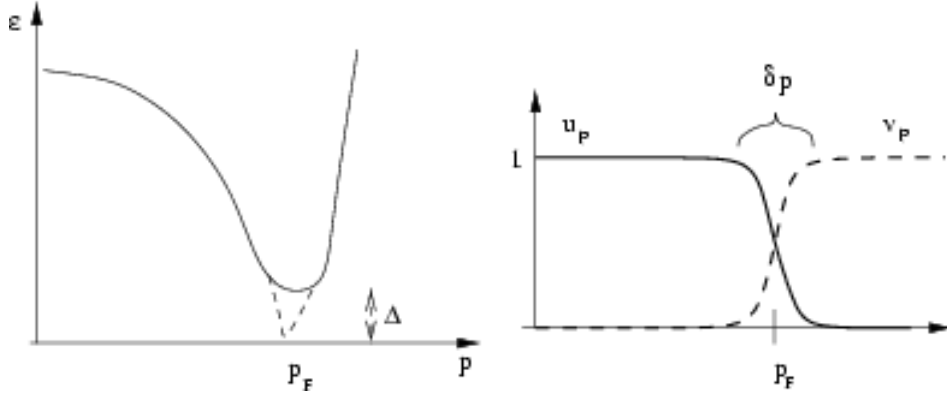


Figure 3.5: Spectrum of FERMIONS with COOPER pairing (left) and plot of u and v as a function of p

the medium is transparent for all external perturbations with frequency $\omega < 2\Delta$ which couple to single particle excitations.

We now want to calculate Δ :

$$\Delta = |V_0| \sum_p \langle (u_p \tilde{a}_{-p-} - v_p \tilde{a}_{p+}^\dagger) (u_p \tilde{a}_{p+} + v_p \tilde{a}_{-p-}^\dagger) \rangle \quad (3.270)$$

$$= |V_0| \sum_p u_p v_p \left(\langle \tilde{a}_{-p-} \tilde{a}_{-p-}^\dagger \rangle - \langle \tilde{a}_{p+}^\dagger \tilde{a}_{p+} \rangle \right) \quad (3.271)$$

$$= |V_0| \sum_p u_p v_p (1 - 2n_p) \quad (3.272)$$

$$= |V_0| \sum_p \frac{1}{2} \frac{\sqrt{\epsilon_p^2 - \xi_p^2}}{\epsilon_p} \tanh\left(\frac{\epsilon_p}{2T}\right) = \Delta |V_0| \sum_p \frac{\tanh\left(\frac{\epsilon_p}{2T}\right)}{2\epsilon_p} \quad (3.273)$$

where we used

$$n_p = \langle \tilde{a}_{p+}^\dagger \tilde{a}_{p+} \rangle = \langle \tilde{a}_{-p-}^\dagger \tilde{a}_{-p-} \rangle = \frac{1}{\exp\left(\frac{\epsilon_p}{T}\right) + 1} \quad (3.274)$$

which is the number of particles involved. Thus we have

$$1 = |V_0| \sum_p \frac{\tanh\left(\frac{\epsilon_p}{2T}\right)}{2\epsilon_p} \quad \epsilon_p = \sqrt{\Delta^2 + \xi_p^2} \quad (3.275)$$

This equation determines $\Delta(T)$. We are mainly interested in the gap near T_C , i.e.

$$1 = |V_0| \sum_p \frac{\tanh\left(\frac{\xi_p}{2T_C}\right)}{2\xi_p} \quad (3.276)$$

which might become problematic for $\xi_p \rightarrow 0$. To solve this, we have to use the scattering length analogous to (3.125) and rewrite the expression as

$$1 = \frac{4\pi\hbar^2|a|}{m} \sum_p \left\{ \frac{\tanh\left[\frac{\xi_p}{2T_C}\right]}{2\xi_p} - \frac{1}{2\frac{p^2}{2m}} \right\} \quad (3.277)$$

$$= \frac{4\pi\hbar^2|a|}{m} \int_{-\varepsilon_F}^{\infty} d\xi v(\xi + \varepsilon_F) \left\{ \frac{\tanh\left[\frac{\xi}{2T_C}\right]}{2\xi_p} - \frac{1}{2(\xi + \varepsilon_F)} \right\} \quad (3.278)$$

$$= \frac{4\pi\hbar^2|a|}{m} \frac{m}{2\pi^2\hbar^3} \int_0^{\infty} dp p^2 \left\{ \frac{\tanh\left[\frac{p^2 - p_F^2}{2m2T_C}\right]}{p^2 - p_F^2} - \frac{1}{p^2} \right\} \quad (3.279)$$

$$= \lambda \int_0^{\infty} dx x^2 \left\{ \frac{\tanh[\alpha(x^2 - 1)]}{x^2 - 1} - \frac{1}{x^2} \right\} \quad (3.280)$$

$$= \lambda \int_0^{\infty} dx \left\{ \tanh[\alpha(x^2 - 1)] - 1 + \frac{\tanh[\alpha(x^2 - 1)]}{x^2 - 1} \right\} \quad (3.281)$$

$$= \lambda \left\{ x(\tanh[\alpha(x^2 - 1)] - 1) \Big|_0^{\infty} - \int dx x \frac{2\alpha x}{\cosh^2[\dots]} \right. \\ \left. + \frac{1}{2} \ln \left| \frac{x-1}{x+1} \right| \tanh(\alpha(x^2 - 1)) \Big|_0^{\infty} \right. \\ \left. - \int_0^{\infty} dx \frac{1}{2} \ln \left| \frac{x-1}{x+1} \right| \frac{2\alpha x}{\cosh^2(\alpha[\dots])} \right\}. \quad (3.282)$$

Here we note, that (3.278) converges. In (3.280) we substituted $p = p_F x$ and used the definition of the gas parameter

$$\lambda = \frac{4\pi\hbar^2|a|}{m} v(\varepsilon_F) = \frac{2|a|p_F}{\pi\hbar} \quad (3.283)$$

The parameter α is defined as

$$\alpha = \frac{\varepsilon_F}{2T_C} \gg 1 \quad (3.284)$$

In the last step, we integrated by part and noted, that the main contribution to the integral comes from the Regime

$$|x^2 - 1| \sim \frac{1}{\alpha} \Rightarrow x \approx 1. \quad (3.285)$$

Using this, we have

$$1 = \lambda \left\{ -\tanh(2\alpha(x-1)) \Big|_0^\infty - \int_0^\infty dx \frac{1}{2} \ln \left| \frac{\alpha(x^2-1)}{\alpha(x+1)^2} \right| \frac{2\alpha x}{\cosh^2(\alpha(x^2-1))} \right\} \quad (3.286)$$

$$= \lambda \left\{ (-2) - \frac{1}{2} \int_{-\infty}^\infty dy \frac{\ln\left(\frac{|y|}{4\alpha}\right)}{\cosh^2(y)} \right\} \quad (3.287)$$

$$= \lambda \left\{ -2 - \int_0^\infty dy \frac{\ln(y) - \ln(4\alpha)}{\cosh^2(y)} \right\} \quad (3.288)$$

$$= \lambda \left\{ -2 + \ln\left(\frac{2\varepsilon_F}{T_C}\right) - \int_0^\infty dy \frac{\ln(y)}{\cosh^2(y)} \right\} \quad (3.289)$$

$$= \lambda \left\{ \ln\frac{2\varepsilon_F}{T_C} - 2 - \ln\left(\frac{\pi}{4\gamma}\right) \right\} = \lambda \ln \left\{ \frac{8\gamma\varepsilon_F}{\pi T_C} e^{-2} \right\} \quad (3.290)$$

Here $\gamma \approx 1.78$ is the EULER constant. Solving for T_C (when $\Delta = 0$) we get

$$T_C = \frac{8\gamma e^{-2}}{\pi} \varepsilon_F e^{-\frac{1}{\lambda}} = 0.61 \varepsilon_F e^{-\frac{1}{\lambda}} \quad (3.291)$$

Now we want to calculate $\Delta = \Delta(T)$. First we look at $T \approx T_C$ i.e.

$$\frac{T_C - T}{T_C} \ll 1 \quad (3.292)$$

We expect $\Delta(T) \ll T_C$. Therefore we can expand (3.268)

$$\varepsilon_p \approx |\xi_p| + \frac{\Delta^2}{2|\xi_p|} \quad (3.293)$$

similar we expand (3.277)

$$1 = \frac{4\pi\hbar^2|a|}{m} \sum_p \left\{ \left(1 + \frac{\Delta^2}{2|\xi_p|} \frac{\partial}{\partial|\xi_p|} \right) \frac{\tanh\left(\frac{|\xi_p|}{2T}\right)}{2|\xi_p|} - \frac{1}{2\frac{p^2}{2m}} \right\} \quad (3.294)$$

$$= \frac{4\pi\hbar^2|a|}{m} \int_{-\varepsilon_F}^\infty d\xi v(\xi + \varepsilon_F) \left\{ \left(1 + \frac{\Delta^2}{2|\xi_p|} \frac{\partial}{\partial|\xi_p|} \right) \frac{\tanh\left(\frac{|\xi_p|}{2T}\right)}{2|\xi_p|} - \frac{1}{2\frac{p^2}{2m}} \right\} \quad (3.295)$$

$$\begin{aligned}
&= \frac{4\pi\hbar^2|a|}{m} \left\{ v(\varepsilon_F) \ln \left(\frac{8\gamma e^{-2}\varepsilon_F}{\pi T} \right) \right. \\
&\quad \left. + \frac{\Delta^2}{2} \int_{-\varepsilon_F}^{\infty} d\xi v(\xi + \varepsilon_F) \frac{1}{\xi} \frac{\partial}{\partial \xi} \frac{\tanh\left(\frac{\xi}{2T}\right)}{2\xi} \right\} \quad (3.296)
\end{aligned}$$

$$\begin{aligned}
&= \lambda \left\{ \ln \left(\frac{8\gamma e^{-2}\varepsilon_F}{\pi T_C} \right) + \ln \left(\frac{T_C}{T} \right) \right\} \\
&\quad + \frac{4\pi\hbar^2|a|}{m} \frac{\Delta^2}{2} v(\varepsilon_F) \int_0^{\infty} d\xi \frac{1}{\xi} \frac{\partial}{\partial \xi} \frac{\tanh\left(\frac{\xi}{2T}\right)}{\xi} \quad (3.297)
\end{aligned}$$

$$= 1 + \lambda \left\{ \ln \left(\frac{T_C}{T} \right) + \frac{\Delta^2}{2T^2} \int_0^{\infty} dx \frac{1}{x} \frac{\partial}{\partial x} \frac{\tanh\left(\frac{x}{2}\right)}{x} \right\} \quad (3.298)$$

In (3.296) we used that the integrand is proportional to $|\xi|^{-3}$ for large $|\xi|$ and that we can replace the lower integration boundary by $-\infty$ because the integrand is therefore strongly localized around 0. In the last step we substituted $\xi = Tx$.

To calculate the last integral, we use the expansion of the hyperbolic tangent:

$$\tanh\left(\frac{x}{2}\right) = 4x \sum_{n=0}^{\infty} \frac{1}{\pi^2(2n+1)^2 + x^2} \quad (3.299)$$

If we use (3.299) to calculate the last addend of (3.298) we get

$$4 \int_0^{\infty} dx \frac{1}{x} \frac{\partial}{\partial x} \sum_{n=0}^{\infty} \frac{1}{\pi^2(2n+1)^2 + x^2} \quad (3.300)$$

$$= 4 \int_0^{\infty} dx \frac{1}{x} \sum_{n=0}^{\infty} \frac{-2x}{(\pi^2(2n+1)^2 + x^2)^2} \quad (3.301)$$

$$= -8 \sum_{n=0}^{\infty} \frac{1}{\pi^3(2n+1)^3} \int_0^{\infty} \frac{dy}{(1+y^2)^2} \quad (3.302)$$

$$= -\frac{8}{\pi^3} \left(1 - \frac{1}{8}\right) \xi(3) \int_0^{\frac{\pi}{2}} \frac{d\phi}{\cos^2(\phi)} \cos^4(\phi) \quad (3.303)$$

$$= -\frac{8}{\pi^3} \frac{7}{8} \frac{\pi}{2} \frac{1}{2} \xi(3) = -\frac{7\xi(3)}{4\pi^2} \quad (3.304)$$

We used the substitutions $x = \pi(2n+1) + y$ and $y = \tan(\phi)$. The sum is calculated analogously to (3.24).

Furthermore we are interested at temperatures T around T_C (3.292) so we can

approximate (3.298) as

$$\ln\left(\frac{T_C}{T}\right) = -\ln\left(1 - \frac{T_C - T}{T_C}\right) \approx \frac{T_C - T}{T_C} \quad (3.305)$$

$$= -\frac{\Delta^2}{2T_C^2} \frac{(-)7\xi(3)}{4\pi^2} = \frac{\Delta^2}{T_C^2} \frac{7\xi(3)}{8\pi^2} \quad (3.306)$$

Thus we have

$$\Delta(T) = \underbrace{\sqrt{\frac{8\pi^2}{7\xi(3)}}}_{\approx 3.06} T_C \sqrt{\frac{T_C - T}{T_C}} \quad (3.307)$$

The pairing energy grows rather rapidly if temperature is lowered. Now we want to look at the other extreme, i.e. $\Delta(T=0) \equiv \Delta_0$. If we subtract (3.275) at $T=0$ from (3.276)

$$\frac{m}{4\pi\hbar^2|a|} = \sum_p \left\{ \frac{1}{2\varepsilon_p} - \frac{1}{\frac{p^2}{m}} \right\} \quad (3.308)$$

$$\frac{m}{4\pi\hbar^2|a|} = \sum_p \left\{ \frac{\tanh\left(\frac{\xi_p}{2T_C}\right)}{2\xi_p} - \frac{1}{\frac{p^2}{m}} \right\} \quad (3.309)$$

we get

$$0 = \sum_p \left\{ \frac{1}{2\varepsilon_p} - \frac{\tanh\left(\frac{\xi_p}{2T_C}\right)}{2\xi_p} \right\} \quad (3.310)$$

$$= \frac{1}{2} \int_{-\varepsilon_F}^{\infty} d\xi v(\xi + \varepsilon_F) \left\{ \frac{1}{\sqrt{\Delta_0^2 + \xi^2}} - \frac{\tanh\left(\frac{\xi}{2T_C}\right)}{\xi} \right\} \quad (3.311)$$

$$\approx \frac{1}{2} v(\varepsilon_F) 2 \int_0^{\infty} d\xi \left\{ \frac{1}{\sqrt{\Delta_0^2 + \xi^2}} - \frac{\tanh\left(\frac{\xi}{2T_C}\right)}{\xi} \right\} \quad (3.312)$$

$$= v(\varepsilon_F) \int_0^{\infty} dx \left\{ \frac{1}{\sqrt{x^2 + \left(\frac{\Delta_0}{2T_C}\right)^2}} - \frac{\tanh(x)}{x} \right\} \quad (3.313)$$

$$= v(\varepsilon_F) \left\{ \left(\ln \left[x + \sqrt{x^2 + \left(\frac{\Delta_0}{2T_C} \right)^2} \right] - \ln(x) \tanh(x) \right) \right|_0^\infty + \int dx \frac{\ln(x)}{\cos^2(x)} \right\} \quad (3.314)$$

$$= v(\varepsilon_F) \left\{ \ln(2) - \ln \left(\frac{\Delta_0}{2T_C} \right) + \ln \left(\frac{\pi}{4\gamma} \right) \right\} \quad (3.315)$$

$$= v(\varepsilon_F) \ln \left(\frac{T_C \pi}{\Delta_0 \gamma} \right) \quad (3.316)$$

In (3.312) we again used that $\{\dots\}$ behaves as $|\xi|^{-3}$ for $|\xi| \rightarrow \infty$ and we again extend the integration from $-\varepsilon_F$ to $-\infty$. Then we substituted $\xi = 2T_C x$. After partial integration we retained the integral (3.289) which solution we inserted. Therefore we have

$$\Delta_0 = \frac{\pi}{\gamma} T_C \approx 1.76 T_C \quad (3.317)$$

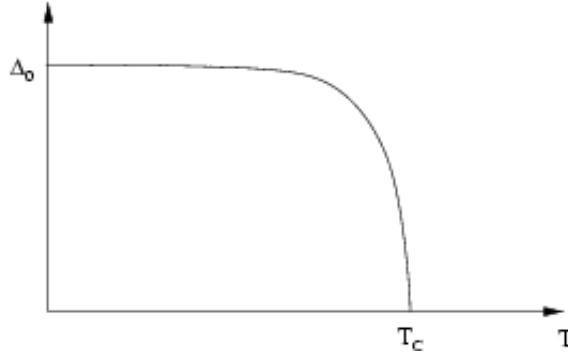


Figure 3.6: Pairing gap as function of temperature

It is important to note, that this is a single particle spectrum, i.e. no collective modes are considered. So if an external field, which acts *only* on single particles, acts with an amplitude less than Δ no excitations occur. The question remains whether other types of excitations with amplitude less than Δ are possible.

The GOLDSTONE theorem (page 33) ensures that at least one branch of gapless excitations exists because the continuous (gauge) symmetry is spontaneously broken in a superfluid phase: the energy (HAMILTONian) is invariant under the gauge transformation $\psi \rightarrow e^{i\phi} \psi$ with a constant ϕ , $E(e^{i\phi} \psi) = E(\psi)$, while the ground state and, as a result, anomalous correlators are not. For example,

$$\langle (e^{i\phi} \psi)(e^{i\phi} \psi) \rangle = e^{2i\phi} \langle \psi \psi \rangle \neq \langle \psi \psi \rangle \neq 0. \quad (3.318)$$

Since we have

$$\varepsilon_p \xrightarrow{p \rightarrow 0} 0 \quad (3.319)$$

the choice of a phase breaks the symmetry. So if we consider now a phase which varies slowly in space and time, i.e. the gap is of the form

$$\Delta_0 \rightarrow \Delta_0 e^{2i\phi(\vec{r},t)} \quad (3.320)$$

we describe collective modes. To calculate Δ we have to redo the previous calculation except for the fact that Δ is no longer real. The HAMILTONIAN is now

$$\begin{aligned} \hat{H} = \sum_j \int d^3r \hat{\psi}_j \left\{ -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) - \mu \right\} \psi_j \\ - \int d^3r \left\{ \Delta^* \hat{\psi}_- \hat{\psi}_+ + \Delta \hat{\psi}_+^\dagger \hat{\psi}_-^\dagger \right\} \end{aligned} \quad (3.321)$$

Here the first addend will be called \hat{H}_0 .

Once more we use a time dependent BOGOLYUBOV-DE GENNES equation (i.e. a canonical transformation):

$$\hat{\psi}_j(\vec{r},t) = \sum_{\nu} \left\{ u_{\nu}(\vec{r},t) \tilde{a}_{\nu j} + \text{sign}(j) v_j^*(\vec{r},t) \tilde{a}_{\nu-j}^\dagger \right\} \quad (3.322)$$

The calculation is similar to the BOSE case and it is therefore not repeated here. It can be found in the literature. The results are

$$i\hbar \frac{\partial u_{\nu}}{\partial t} = (\hat{H}_0 - \mu) u_{\nu} + \Delta v_{\nu} \quad (3.323)$$

$$i\hbar \frac{\partial v_{\nu}}{\partial t} = -(\hat{H}_0 - \mu) v_{\nu} + \Delta^* u_{\nu} \quad (3.324)$$

We assume that the phase is switched on adiabatically, i.e.

$$\Delta(\vec{r},t) \xrightarrow{t \rightarrow -\infty} \Delta_0 \quad (3.325)$$

This way, the solutions take the form

$$u_{\nu}(\vec{r},t \rightarrow -\infty) = u_{\nu}^0 e^{-i\varepsilon_{\nu} t} \quad (3.326)$$

$$v_{\nu}(\vec{r},t \rightarrow -\infty) = v_{\nu}^0 e^{-i\varepsilon_{\nu} t} \quad (3.327)$$

Using this (3.323) and (3.324) read

$$\varepsilon_{\nu} u_{\nu}^{(0)} = (\hat{H}_0 - \mu) u_{\nu}^{(0)} + \Delta_0 v_{\nu}^{(0)} \quad (3.328)$$

$$\varepsilon_{\nu} v_{\nu}^{(0)} = (\hat{H}_0 - \mu) v_{\nu}^{(0)} + \Delta_0 u_{\nu}^{(0)} \quad (3.329)$$

Thus v is clear at $t = -\infty$. Now we have to solve self-consistently

$$\Delta(\vec{r}, t) = |V_0| \langle \hat{\psi}_-(\vec{r}, t) \hat{\psi}_+(\vec{r}, t) \rangle \quad (3.330)$$

$$= |V_0| \sum_{\mathbf{v}} u_{\mathbf{v}}(\vec{r}, t) u_{\mathbf{v}}^*(\vec{r}, t) \tanh\left(\frac{\epsilon_{\mathbf{v}}}{2T}\right) \quad (3.331)$$

where we took only the leading term in the fluctuations.

The probability current at $T = 0$ reads now

$$\vec{j} = -\frac{i\hbar}{2m} \sum_j \langle \hat{\psi}_j^\dagger \nabla \hat{\psi}_j - \nabla \hat{\psi}_j^\dagger \hat{\psi}_j \rangle \quad (3.332)$$

$$= -\frac{i\hbar}{2m} \sum_j \sum_{v_1 v_2} (v_{v_1} \nabla_{v_2}^* - \nabla_{v_1} v_{v_2}^*) \underbrace{\langle \tilde{\alpha}_{v_1-j} \tilde{\alpha}_{v_2-j}^\dagger \rangle}_{\delta_{v_1 v_2}} \quad (3.333)$$

$$= -\frac{i\hbar}{2m} \sum_j \sum_{\mathbf{v}} (v_{\mathbf{v}} \nabla_{\mathbf{v}}^* - \nabla_{\mathbf{v}} v_{\mathbf{v}}^*) \quad (3.334)$$

The same way we calculate

$$n = \sum_j \sum_{\mathbf{v}} |v_{\mathbf{v}}|^2 \quad (3.335)$$

If we define new functions

$$u_{\mathbf{v}} = e^{i\phi} \bar{u}_{\mathbf{v}} \quad v_{\mathbf{v}} = e^{-i\phi} \bar{v}_{\mathbf{v}} \quad (3.336)$$

which obey the same initial conditions (because ϕ vanishes at $t = -\infty$) (3.323) and (3.324) simplify

$$\left(i\hbar \frac{\partial}{\partial t} - \hbar \dot{\phi} \right) \bar{u}_{\mathbf{v}} = \left(-\frac{\hbar^2}{2m} (\nabla + i\nabla\phi)^2 - \mu \right) \bar{u}_{\mathbf{v}} + \Delta_0 \bar{v}_{\mathbf{v}} \quad (3.337)$$

$$\left(i\hbar \frac{\partial}{\partial t} + \hbar \dot{\phi} \right) \bar{v}_{\mathbf{v}} = - \left(-\frac{\hbar^2}{2m} (\nabla - i\nabla\phi)^2 - \mu \right) \bar{v}_{\mathbf{v}} + \Delta_0 \bar{u}_{\mathbf{v}} \quad (3.338)$$

We have now

$$\begin{aligned} i\hbar \frac{\partial \bar{u}}{\partial t} &= \left(-\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \bar{u}_{\mathbf{v}} + \Delta_0 \bar{v}_{\mathbf{v}} \\ &\quad + \left\{ \hbar \dot{\phi} + \frac{\hbar^2}{2m} (\nabla\phi)^2 - i \frac{\hbar^2}{m} \nabla\phi \nabla - i \frac{\hbar^2}{2m} \nabla^2 \phi \right\} \bar{u}_{\mathbf{v}} \end{aligned} \quad (3.339)$$

$$\begin{aligned} i\hbar \frac{\partial \bar{v}}{\partial t} &= - \left(-\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \bar{v}_{\mathbf{v}} + \Delta_0 \bar{u}_{\mathbf{v}} \\ &\quad + \left\{ -\hbar \dot{\phi} - \frac{\hbar^2}{2m} (\nabla\phi)^2 - i \frac{\hbar^2}{m} \nabla\phi \nabla - i \frac{\hbar^2}{2m} \nabla^2 \phi \right\} \bar{v}_{\mathbf{v}} \end{aligned} \quad (3.340)$$

If we regard $\{\dots\}$ as perturbation we can apply time dependent perturbation theory here. We will not present detailed calculations here, rather make some comments.

When on the basis of the BOGOLYUBOV-DE GENNES equations (...) we consider single-particle excitations, we restrict ourself only to solutions with positive eigenvalues $\varepsilon_v > 0$. But those are only half of all possible solutions. The other half contains solutions with negative eigenvalues $\varepsilon_v < 0$. The latter can easily be constructed from the former. Namely, if $(u_v^{(0)}, v_v^{(0)})$ is a solution with $\varepsilon_v > 0$, then, as can be easily checked, $(v_v^{(0)*}, -u_v^{(0)*})$ is a solution with the negative eigenvalue $\varepsilon_v < 0$. Together they form a complete set of solutions and, therefore, they both have to be used in studying the perturbed BOGOLYUBOV-DE GENNES equations. In this way we get the answer

$$\bar{u}_v = u_v^{(0)} e^{-i\varepsilon_v t} (1 + \text{derivatives of } \phi) \quad (3.341)$$

$$\bar{v}_v = v_v^{(0)} e^{-i\varepsilon_v t} (1 + \text{derivatives of } \phi) \quad (3.342)$$

After some calculations the current can be written as

$$\vec{j} = -\frac{i\hbar}{2m} \sum_v \left\{ 2i\nabla\phi |v_v^{(0)}|^2 + O\left(\frac{\nabla\phi}{\Delta_0}, \frac{\phi}{\Delta_0}\right) \right\} \quad (3.343)$$

$$= \frac{\hbar}{m} \nabla\phi \sum_v |v_v^{(0)}|^2 = n_0 \frac{\hbar}{m} \nabla\phi = n_0 \vec{v}_s \quad (3.344)$$

$$\vec{v}_s = -\frac{\hbar}{m} \nabla\phi \quad (3.345)$$

This result is rather unexpected. It is not obvious that the constant n_0 from the homogeneous case is the coefficient and not e.g. a fraction of n_0 . As can be

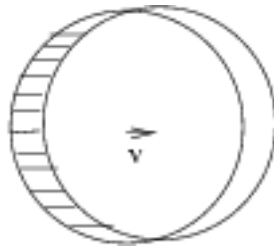


Figure 3.7: Schematic probability flow in BCS

seen in figure (3.7) most particles inside the FERMI sphere are not affected by the probability flow.

Now n and \vec{v}_s have to be solved self-consistently to get an equation for ϕ . Here we want to get the solution more easily:

$$E(\phi, n) = \int d^3r \left\{ \frac{1}{2} mn \vec{v}_s^2 + E(n) - \mu n \right\} \quad (3.346)$$

$$E(n) = E_{0n}(n) + E_{\text{int}} + E_{\text{cooper p.}} \quad (3.347)$$

$$= n \frac{3}{5} \varepsilon_F + O(a) + \underbrace{E_{\text{cooper p.}}}_{\sim e^{-\frac{2}{\lambda}}} \quad (3.348)$$

Here E_{0n} describes free particles in the normal phase. We can estimate the pairing energy as energy gain per pair times number of particles affected, i.e.

$$E_{\text{cooper p.}} \sim (-\Delta) v(\varepsilon_F) \Delta \sim -g \Delta^2 \frac{m p_F}{\hbar^3} = -g \Delta^2 \frac{m}{p_F^2} \frac{p_F^3}{\hbar^3} \quad (3.349)$$

$$\sim -n \frac{\Delta^2}{\varepsilon_F} \sim -n \varepsilon_F \left(\frac{\Delta}{\varepsilon_F} \right)^2 \quad (3.350)$$

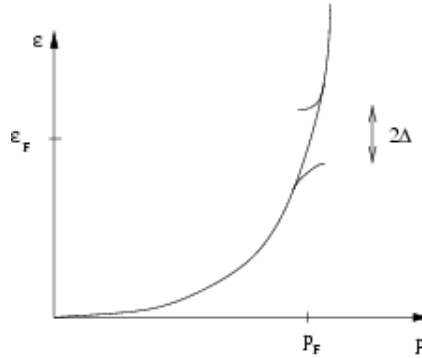


Figure 3.8: BCS gap

Again we note that we consider only slowly varying phase.

If we look at (3.346) with terms up to second order in phase and δn , remembering

$$n_0 : \quad \frac{\partial E}{\partial n} = \mu \quad (3.351)$$

we get

$$E(\phi, n) = \int d^3r \left\{ \frac{1}{2} m n_0 \left(\frac{\hbar}{m} \nabla \phi \right)^2 + E_0(n_0) + \underbrace{\text{linear}}_{=0} + \frac{1}{2} \frac{\partial^2 E}{\partial n^2} \Big|_{n_0} (\delta n)^2 \right\} \quad (3.352)$$

$$= E_0(n_0) \mathcal{V} + \frac{1}{2} \int d^3r \left\{ n_0 \frac{\hbar^2}{m} (\nabla \phi)^2 + \frac{\partial^2 E}{\partial n^2} \Big|_{n_0} \delta n^2 \right\} \quad (3.353)$$

Here we remember that $v \sim \nabla \phi$ and therefore v_s^2 already second order so we can use $n = n_0$.

If we look at this from a quantum mechanical point of view, δn becomes an operator. It has to obey

$$[\phi(\vec{r}), \delta n(\vec{r}')] = -i \delta(\vec{r} - \vec{r}') \quad (3.354)$$

and all other commutators have to vanish.

We have

$$\delta \dot{n} = \frac{i}{\hbar} [\hat{E}, \delta n] = \frac{1}{2} \frac{i}{\hbar} n_0 \frac{\hbar^2}{m} (-2 \nabla^2 \phi) (-i) \quad (3.355)$$

$$= -n_0 \frac{\hbar}{m} \nabla^2 \phi = -\nabla \left(n_0 \frac{\hbar}{m} \nabla \phi \right) = -\nabla \vec{j} \quad (3.356)$$

that corresponds to the continuity equation. On the other hand

$$\dot{\phi} = \frac{i}{\hbar} [\hat{E}, \phi] = \frac{1}{2} \frac{i}{\hbar} \frac{\partial^2 E}{\partial n^2} 2 \delta n i = -\frac{1}{\hbar} \frac{\partial^2 E}{\partial n^2} \delta n, \quad (3.357)$$

therefore,

$$\delta \ddot{n} = -n_0 \frac{\hbar}{m} \nabla^2 \dot{\phi} = \frac{n_0}{m} \frac{\partial^2 E}{\partial n^2} \nabla^2 \delta n \quad \text{and} \quad (3.358)$$

$$\ddot{\phi} = \frac{n_0}{m} \frac{\partial^2 E}{\partial n^2} \nabla^2 \phi. \quad (3.359)$$

Eqn. (3.358) and (3.359) are wave equations with the wave velocity

$$c^2 = \frac{n_0}{m} \frac{\partial^2 E}{\partial n^2} \quad (3.360)$$

Using (3.5) and (3.6) we can calculate the velocity

$$c^2 = \frac{n_0}{m} \frac{\partial^2}{\partial n_0^2} \left(n_0 \frac{3}{5} \frac{1}{2m} \left(\frac{6\pi^2 \hbar^3}{g} n_0 \right)^{\frac{2}{3}} \right) \quad (3.361)$$

$$= \frac{n_0}{m} \frac{1}{2m} \frac{3}{5} \left(\frac{6\pi^2 \hbar^3}{g} \right)^{\frac{2}{3}} \frac{\partial^2}{\partial n_0^2} n_0^{\frac{5}{3}} \quad (3.362)$$

$$= \frac{n_0}{m} \frac{1}{2m} \frac{3}{5} \left(\frac{6\pi^2 \hbar^3}{g} \right)^{\frac{2}{3}} \frac{5 \cdot 2}{3} \frac{1}{n_0^{\frac{1}{3}}} = \frac{1}{3} \frac{p_F^2}{m^2} = \frac{v_F^2}{3} \quad (3.363)$$

$$c = \frac{v_F}{\sqrt{3}} \quad (3.364)$$

This is caused by density fluctuations and differs from zero sound, it is the same as the hydrodynamic sound (BOGOLYUBOV-ANDERSON sound). If the fluctuations couple to density, this GOLDSTONE mode can be excited even if the excitation is less than Δ .

3.6 Andreev reflection

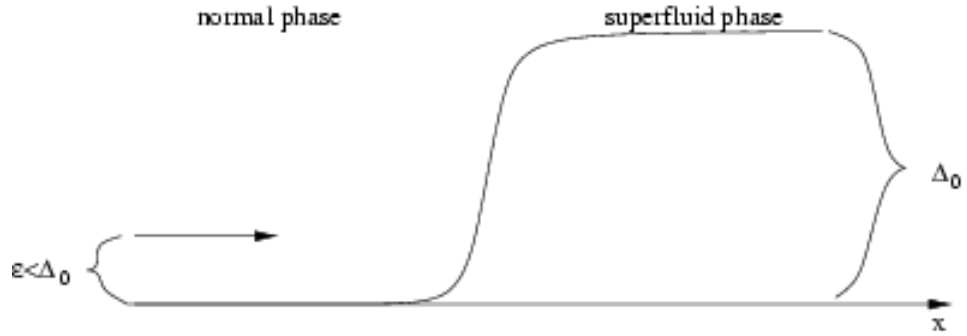


Figure 3.9: Boundary between non superfluid and superfluid region

Suppose we have a situation where the gap Δ is not a constant Δ_0 but depends on the coordinate x in such a way that it is zero for negative x (normal phase), then it increases to its equilibrium value Δ_0 in the transition region of the width ξ at the origin $x = 0$, and is equal to Δ_0 for positive x (superfluid phase), see fig.(3.9) (this situation could be realized if a magnetic field is applied to the part $x < 0$ of the superfluid sample that destroys the COOPER pairing.).

If we now have a particle in the normal part of the sample with the energy $\varepsilon_F + \varepsilon$, where $\varepsilon < \Delta_0$, and momentum $p > p_F$ along the x -axis (a single-particle excitation with the energy ε and momentum p), we would naively expect that it reflects back from the boundary between normal and superfluid parts of the sample because there are no available single-particle states with such energy $\varepsilon < \Delta_0$ in the superfluid region. However, this is not possible because the change of the momentum δp of the particle in the transition region can be estimated as

$$\delta p \sim Ft \quad F \sim \frac{\Delta_0}{\xi} \quad t = \frac{\xi}{v_F} \quad (3.365)$$

$$\sim \frac{\Delta_0}{v_F} \sim p_F \frac{\Delta_0}{\varepsilon_F} \ll p_F \quad (3.366)$$

but an ordinary reflection requires

$$\Delta p|_{\text{reflection}} \sim 2p_F. \quad (3.367)$$

So the particle (excitation) cannot be reflected in a normal way and it cannot penetrate either. What happens instead is that the particle picks another one with an (almost) opposite momentum $p' < p_F$ to form a COOPER pair with total momentum $p - p'$ along the x -axis, and this pair penetrates the superfluid region $x > 0$. As a result, in the normal region $x < 0$ one has a hole in the state with momentum p' moving backwards with the velocity which is a gradient of the energy of the excitation $\varepsilon_{p'} \approx v_F(p_F - p')$ with the respect to its momentum $-\vec{p}'$ (the hole in the state \vec{p}' has momentum $-\vec{p}'$).

$$\vec{v}_{\text{out}} = \nabla_{-p'} \varepsilon_{p'} \approx -\nabla_{p'} (v_F(p_F - p')) \approx v_F \hat{p}' = -v_F \vec{e}_x. \quad (3.368)$$

(For incoming particle one has $v_{\text{in}} \approx \nabla_p (v_F(p - p_F)) \approx v_F \cdot \vec{e}_x$) Therefore, we have a specific form of a reflection (ANDREEV reflection) where an incoming particle reflects as a hole and vice versa. Since the hole has an opposite charge, some interesting effects happen if a magnetic field is applied - the hole travels the path backwards until it hits the boundary again where it becomes a particle that travels the same path forward and so on.

Appendix A

General energy-momentum relation

If we have a non interacting gas of particles we can derive a general energy-momentum relation independent of the statistics involved. We distinguish two types of particles: those with rest mass m and relativistic particles like photons and phonons.

We consider a box with of volume \mathcal{V} with infinite walls. Particles are described by plain waves with momenta

$$p_n = \hbar k_n = \frac{n\pi}{L}i \sim \mathcal{V}^{-\frac{1}{3}} \quad n \in \mathbb{N} \quad (\text{A.1})$$

where L is the length of the box.

For each particle the energy-momentum relation can be stated as

$$\varepsilon_p = \begin{cases} \frac{p^2}{2m} \sim \mathcal{V}^{-\frac{2}{3}} & \text{non relativistic} \\ cp \sim \mathcal{V}^{-\frac{1}{3}} & \text{relativistic} \end{cases} \quad (\text{A.2})$$

The general statistical definition for pressure is

$$\mathbf{p} = -\frac{\partial \langle E \rangle}{\partial \mathcal{V}} = -\sum_{p,j} \frac{\partial \varepsilon_p}{\partial \mathcal{V}} \langle n_p \rangle \quad (\text{A.3})$$

The index j runs over the g values, e.g. spin projections.

Using (A.2) we can now derive the desired relation

$$\mathbf{p} = \begin{cases} \frac{2}{3} \frac{E}{\mathcal{V}} & (\varepsilon_p \sim p^2) \\ \frac{1}{3} \frac{E}{\mathcal{V}} & (\varepsilon_p \sim p) \end{cases} \quad (\text{A.4})$$

This relation is independent of the statistics involved.

This section is based upon [5].

Appendix B

Calculation for section 3.3.1

To derive equation (3.123) we first note, that only excitations with two particles and two holes can be present, i.e. all excited states are of the form

$$|e\rangle = \mathbf{a}_{p_1 j'}^\dagger \mathbf{a}_{p_2 j}^\dagger \mathbf{a}_{p_3 j} \mathbf{a}_{p_4 j'} |g\rangle \quad (\text{B.1})$$

– where $|g\rangle$ is the ground state (filled FERMI sphere) – because otherwise every term in $\langle e | \hat{H}_{\text{int}} | g \rangle$ would be zero.

To better distinguish the summations we rewrite \hat{H}_{int} of (3.111) as

$$\hat{H}_{\text{int}} = \sum_{q_1 q_2 q_3 q_4} ' \sum_{k < k'} \mathbf{a}_{q_4 k'}^\dagger \mathbf{a}_{q_3 k}^\dagger \mathbf{a}_{q_1 k} \mathbf{a}_{q_2 k'} \quad (\text{B.2})$$

If we call the denominator of (3.121) α we have

$$\sum_e |\langle e | \hat{H}_{\text{int}} | g \rangle|^2 = \sum_{p_1 p_2 p_3 p_4} \sum_{j < j'} \alpha \quad (\text{B.3})$$

$$\left| \sum_{q_1 q_2 q_3 q_4} ' \sum_{k < k'} \langle g | \mathbf{a}_{p_4 j'}^\dagger \mathbf{a}_{p_3 j}^\dagger \mathbf{a}_{p_2 j} \underbrace{\mathbf{a}_{p_1 j'}^\dagger \mathbf{a}_{q_4 k'}^\dagger}_{\delta_{j' k'} \delta_{p_1 q_4} (1 - \hat{n}_{p_1})} \mathbf{a}_{q_3 k}^\dagger \mathbf{a}_{q_2 k} \mathbf{a}_{q_1 k'} | g \rangle \right|^2$$

$$= \sum_{p_1 p_2 p_3 p_4} ' \sum_{j < j'} \alpha |\langle g | \hat{n}_{p_4} \hat{n}_{p_3} (1 - \hat{n}_{p_2}) (1 - \hat{n}_{p_1}) | g \rangle|^2 \quad (\text{B.4})$$

$$= \sum_{p_1 p_2 p_3 p_4} ' \sum_{j < j'} \alpha n_{p_4}^2 n_{p_3}^2 (1 - n_{p_2})^2 (1 - n_{p_1})^2 \underbrace{|\langle g | g \rangle|^2}_{=1} \quad (\text{B.5})$$

We can drop the squares now because $n_{p_i} \in \{0, 1\}$ and therefore $(1 - n_{p_i}) \in \{0, 1\}$ and hence $n_{p_i}^2 = n_{p_i}$ and $(1 - n_{p_i})^2 = (1 - n_{p_i})$.

Appendix C

Lifetime and Fermis Golden Rule

In section (3.3.2) FERMIS Golden Rule was used. To derive the formula we start out with the Golden Rule as can be found e.g. in [6]:

$$\Gamma_{if} = \frac{2\pi}{\hbar} \delta(E_f - E_i) |\langle f | U_1 | i \rangle|^2 \quad (\text{C.1})$$

Here Γ_{if} is the transition rate from state $|i\rangle$ to $|f\rangle$ per unit time. The inverse time is the scattering length τ .

Our initial state $|i\rangle$ consists of two particles with momentum \vec{p}_1 (fixed) and \vec{p}_2 and the final state $|f\rangle$ also consists of two particles but now with momenta \vec{p}_1' and \vec{p}_2' . The matrix element has been calculated in (1.81). Since we are interested in the total lifetime (e.g. scattering into any possible state) we have to sum up all probabilities/rates. Using the value for g (1.83) we can now write

$$\frac{1}{\tau}(\vec{p}_1) = \sum_{if} \Gamma_{if} \quad (\text{C.2})$$

$$= \frac{2\pi}{\hbar} \int \frac{d^3 p_2}{(2\pi\hbar)^3} \frac{d^3 p_{1'}}{(2\pi\hbar)^3} \frac{d^3 p_{2'}}{(2\pi\hbar)^3} \delta(\epsilon_1 + \epsilon_2 - \epsilon_{1'} - \epsilon_{2'}) |\langle \vec{p}_{1'} \vec{p}_{2'} | U_1 | \vec{p}_1 \vec{p}_2 \rangle|^2 n(\vec{p}_2) (1 - n(\vec{p}_{1'})) (1 - n(\vec{p}_{2'})) \quad (\text{C.3})$$

$$= \frac{2\pi}{\hbar} \frac{1}{2\pi\hbar} \frac{4\pi\hbar^2}{m} a \int d^3 p_2 d^3 p_{1'} d^3 p_{2'} \delta(\epsilon_1 + \epsilon_2 - \epsilon_{1'} - \epsilon_{2'}) \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_{1'} - \vec{p}_{2'}) n(\vec{p}_2) (1 - n(\vec{p}_{1'})) (1 - n(\vec{p}_{2'})). \quad (\text{C.4})$$

We do not sum (integrate) over \vec{p}_1 because it remains fixed.

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