11 Task Theoretical Physics VI - Statistics

11.1 (Distribution functions of ideal quantum gases)

(a)

Definition:

$$n(\varepsilon_i) = \langle \hat{n}_i \rangle = tr(\hat{\rho}\hat{n}_i)$$

with:

$$\begin{aligned}\hat{\rho} &= \frac{1}{Z_G} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} \\ Z_G &= tr\left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right)\end{aligned}$$

This leads to:

$$\langle \hat{n}_i \rangle = \frac{tr\left(\hat{n}_i e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right)}{tr\left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right)}$$

with Fock-states ($\hat{H} = \sum_j \varepsilon_j \hat{n}_j$ meaning $E = \sum_j \varepsilon_j n_j$ and $N = \sum_j n_j$) we get:

$$\begin{aligned}\langle \hat{n}_i \rangle &= \frac{\sum_{N=0}^{\infty} \sum_{\{n_j\}}^{\sum n_j = N} n_i e^{-\beta \sum_j n_j(\varepsilon_j - \mu)}}{\sum_{N=0}^{\infty} \sum_{\{n_j\}} e^{-\beta \sum_j n_j(\varepsilon_j - \mu)}} \\ &= \frac{\sum_{\{n_j\}} n_i e^{-\beta \sum_j n_j(\varepsilon_j - \mu)}}{\sum_{\{n_j\}} e^{-\beta \sum_j n_j(\varepsilon_j - \mu)}} \\ &= \frac{\Pi_{j=0}^{\infty} \sum_{n_j=0}^{\infty} n_i e^{-\beta n_j(\varepsilon_j - \mu)}}{\Pi_{j=0}^{\infty} \sum_{n_j=0}^{\infty} e^{-\beta n_j(\varepsilon_j - \mu)}}\end{aligned}$$

We now see, that all terms with $i \neq j$ will lead to 1, while numerator and denominator are the same then. We then get:

$$\langle \hat{n}_i \rangle = \frac{\sum_{n_i=0}^{\infty} n_i e^{-\beta n_i(\varepsilon_i - \mu)}}{\sum_{n_i=0}^{\infty} e^{-\beta n_i(\varepsilon_i - \mu)}} \tag{1}$$

We now are at a point to distingusih between Bosons and Fermions. Starting with Bosons, where $n_i = 0, 1, 2, \ldots$, this means we have to use the geometric series (with $0 < q = e^{-\beta(\varepsilon_i - \mu)} < 1$)

$$\sum_{n_i=0}^{\infty} a_0 q^{n_i} = a_0 \cdot \frac{1}{1-q}$$

While in the numerator we don't have the geometric form, we have to use a "trick", while we first substitute $x = -\beta\left(\varepsilon_i - \mu\right)$:

$$\begin{aligned}\sum_{n_i=0}^{\infty} n_i e^{-n_i x} &= \sum_{n_i=0}^{\infty} \frac{\partial}{\partial x} e^{n_i x} \\ &= \frac{\partial}{\partial x} \sum_{n_i=0}^{\infty} e^{n_i x}\end{aligned}$$

while x doesn't depend on n_i we can interchange the derivative and the sum. This now got the form of a geometric series with $q = e^x$ therefore we get:

$$\begin{aligned}\frac{\partial}{\partial x} \sum_{n_i=0}^{\infty} e^{n_i x} &= \frac{\partial}{\partial x} \frac{1}{1-e^x} \\ &= (-1) \cdot \frac{1}{\left(1-e^x\right)^2} \cdot \left(-e^x\right) \\ &= \frac{e^x}{\left(1-e^x\right)^2}\end{aligned}$$

We can insert this in equation (1)

$$\langle \hat{n}_i \rangle = \frac{\frac{e^x}{(1-e^x)^2}}{\frac{1}{1-e^x}} = \frac{e^x}{1-e^x} = \frac{1}{e^{-x}-1} = \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$

Now starting from equation (1) for Fermions, where $n_i = 0, 1$ we can easily rewrite to:

$$\langle \hat{n}_i \rangle = \frac{0 + e^{-\beta(\varepsilon_i-\mu)}}{1 + e^{-\beta(\varepsilon_i-\mu)}} = \frac{1}{e^{\beta(\varepsilon_i-\mu)}+1}$$

Therefore:

$$\langle \hat{n}_i \rangle = \frac{1}{e^{\beta(\varepsilon_i-\mu)} \mp 1} \tag{2}$$

□

(b)

Figure (1) shows the Bose-Einstein distribution function, which is defined as:

$$\langle \hat{n}_i \rangle^- = \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}$$

with the special case for $T \to 0$:

$$\langle \hat{n}_i \rangle^- \Big|_{T \to 0} = \begin{cases} 0, & \mu < \varepsilon_i \\ \infty, & \mu = \varepsilon_i \\ \text{not defined while negative}, & \mu > \varepsilon_i \end{cases}$$

while for $\mu = \varepsilon_i$ is just a convention.

The graphs will have the same area underneath, meaning $n(\varepsilon_i)$ will get high for low range of energy states. This is especially interesting, since the number of states is getting very high for low temperature, while the range of energy states is very small, this phenomenon for $T \to 0$ is known as Bose-Einstein-Condensation, while the ground state becomes a singularity. The area of $\varepsilon_i < \mu$ isn't accessible, while $n(\varepsilon_i < \mu)$ would be negative there (therefore this part of the plot isn't shown).

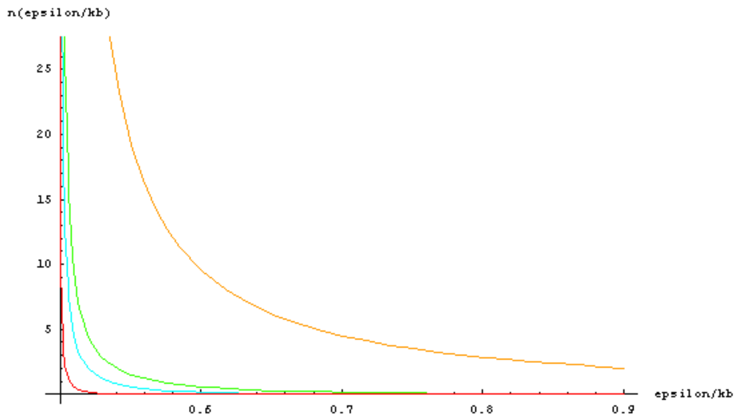

Figure 1: Sketch of the Bose-Einstein distribution

Figure (2) shows the Fermi-Dirac distribution function, which is defined as:

$$\langle \hat{n}_i \rangle^+ = \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}$$

with the special case for $T \to 0$:

$$\langle \hat{n}_i \rangle^+ \Big|_{T \to 0} = \begin{cases} 0, & \mu < \varepsilon_i \\ \frac{1}{2}, & \mu = \varepsilon_i \\ 1, & \mu > \varepsilon_i \end{cases}$$

while for $\mu = \varepsilon_i$ is just a convention.

This distribution describes the behaviour of Fermions, while the Fermi-energy describes the last occupied state, it can be seen in the graph at $\mu = \varepsilon_i$ (best seen for $T \to 0$). The occupation number has always to be between 1 and 0 (pauli principle), the plot shows the probability for energy states to be occupied. For $T \to 0$ the function graph becomes a unit-step-function, therefore occupied states got $n(\varepsilon_i) = 1$ and unoccupied ones got $n(\varepsilon_i) = 0$. As we can see, high energies lead to a much broader probability of occupation across all the energy states. This seems likely, while for higher energy, more Fermions can occupy higher (and different high without having a direct neighbor state) energy levels, while for $T = 0$ Fermions will always occupy the lowest possible state building the Fermi-sea. This again is justified with the Fermi-energy and the graph, which shows it at the jump from 1 to 0.

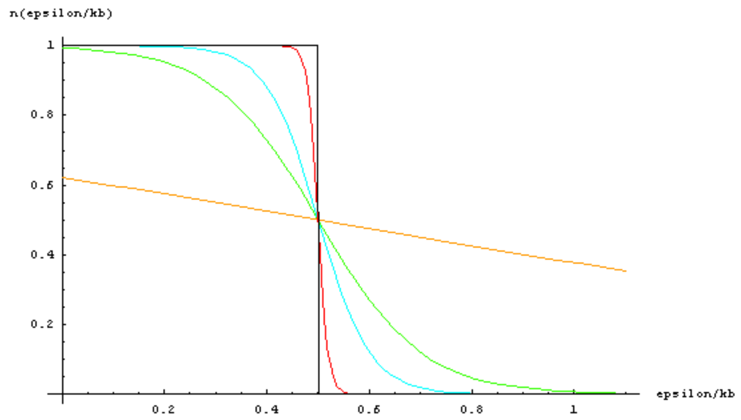

Figure 2: Sketch of the Fermi-Dirac distribution

Figure (3) shows the Boltzmann distribution function.

The Boltzmann distribution is the classical limes of both the forgoing distributions, while $\beta(\varepsilon_i - \mu) \gg 1$ (high ε_i), therefore the ∓ 1 factor can be neglected and we get:

$$\langle \hat{n}_i \rangle \quad = \quad e^{-\beta(\varepsilon_i - \mu)}$$

We therefore get an exponential decaying behaviour. While the higher temperatures lead to very small values compared to the lowest temperature (illustrated in red) you can only see the lightblue colour which is the highest of the three higher temperatures.

11.2 (Fluctuations in ideal quantum gases)

At first a try with creation and destruction-operator-formalism, which didn't succeed.

Definition of single-particle occupation number:

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i = \begin{cases} \hat{a}_i \hat{a}_i^\dagger - 1, & \text{for Bosons} \\ -\left(\hat{a}_i \hat{a}_i^\dagger - 1\right), & \text{for Fermions} \end{cases}$$

with

$$\left[\hat{a}_i, \hat{a}_i^\dagger\right]_- = \hat{a}_i \hat{a}_i^\dagger - \hat{a}_i^\dagger \hat{a}_i = 1 \Leftrightarrow \hat{a}_i^\dagger \hat{a}_i = \hat{a}_i \hat{a}_i^\dagger - 1$$

for Bosons and

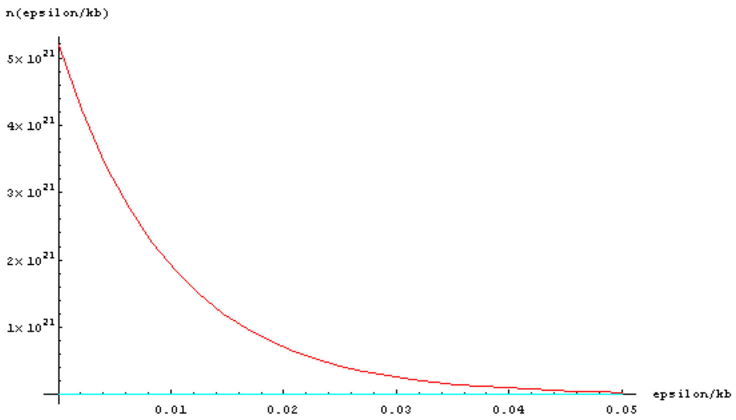

Figure 3: Sketch of the Boltzmann-Distribution

$$\left[\hat{a}_i, \hat{a}_i^\dagger\right]_+ = \hat{a}_i\hat{a}_i^\dagger + \hat{a}_i^\dagger\hat{a}_i = 1 \Leftrightarrow \hat{a}_i^\dagger\hat{a}_i = 1 - \hat{a}_i\hat{a}_i^\dagger$$

for Fermions.
Calculation:

$$(\Delta n_i)^2 = \frac{\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2}{\langle \hat{n}_i \rangle^2}$$

with

$$\hat{n}_i^2 = \hat{a}_i^\dagger\hat{a}_i\hat{a}_i^\dagger\hat{a}_i$$

We can calculate the components:

$$\begin{aligned}
\langle \hat{n}_i \rangle &= \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i^\dagger \hat{a}_i | \varphi_1 \dots \varphi_N \right\rangle \\
&= \pm \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i \hat{a}_i^\dagger - 1 | \varphi_1 \dots \varphi_N \right\rangle \\
&= \pm \left\langle \varphi_i \varphi_1 \dots \varphi_N | \sqrt{N+1}\sqrt{N+1} | \varphi_i \varphi_1 \dots \varphi_N \right\rangle \mp 1 \\
&= \pm (N+1) \mp 1 \\
&= \pm N
\end{aligned}$$

therefore this component will be the same for Bosons and Fermions with:

$$\langle \hat{n}_i \rangle^2 = N^2$$

now for $\langle \hat{n}_i^2 \rangle$

$$
\begin{aligned}
\left\langle \hat{n}_i^2 \right\rangle &= \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{a}_i | \varphi_1 \dots \varphi_N \right\rangle \\
&= \left\langle \varphi_1 \dots \varphi_N | \left(\hat{a}_i \hat{a}_i^\dagger - 1 \right) \left(\hat{a}_i \hat{a}_i^\dagger - 1 \right) | \varphi_1 \dots \varphi_N \right\rangle \\
&= \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger - 2 \hat{a}_i \hat{a}_i^\dagger + 1 | \varphi_1 \dots \varphi_N \right\rangle \\
&= \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger | \varphi_1 \dots \varphi_N \right\rangle - 2 \left\langle \hat{n}_i \right\rangle + 1 \\
&= \pm \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i \left(\hat{a}_i \hat{a}_i^\dagger - 1 \right) \hat{a}_i^\dagger | \varphi_1 \dots \varphi_N \right\rangle - 2 \left\langle \hat{n}_i \right\rangle + 1 \\
&= \pm \left\langle \varphi_1 \dots \varphi_N | \hat{a}_i \hat{a}_i \hat{a}_i^\dagger \hat{a}_i^\dagger | \varphi_1 \dots \varphi_N \right\rangle \mp \left\langle \hat{n}_i \right\rangle - 2 \left\langle \hat{n}_i \right\rangle + 1 \\
&= \pm \left\langle \varphi_i \varphi_i \varphi_1 \dots \varphi_N \right| (N+2)(N+1) \left| \varphi_i \varphi_i \varphi_1 \dots \varphi_N \right\rangle \mp \left\langle \hat{n}_i \right\rangle - 2 \left\langle \hat{n}_i \right\rangle + 1 \\
&= \pm \left(N^2 + 3N + 2 \right) \mp \left\langle \hat{n}_i \right\rangle - 2 \left\langle \hat{n}_i \right\rangle + 1
\end{aligned}
$$

This means for Bosons and Fermions:

$$
\begin{aligned}
\left\langle \hat{n}_i^2 \right\rangle_B &= N^2 + 3 \\
\left\langle \hat{n}_i^2 \right\rangle_F &= -N^2 - 2N - 1
\end{aligned}
$$

Inserting this leads to:

$$
\begin{aligned}
(\Delta n_i)_B^2 &= \frac{N^2 + 3 - N^2}{N^2} = \frac{3}{N^2} \\
(\Delta n_i)_F^2 &= \frac{-N^2 - 2N - 1 - N^2}{N^2} = \frac{-2N^2 - 2N - 1}{N^2} = -\left(2 + \frac{2}{N} + \frac{1}{N^2} \right)
\end{aligned}
$$

This doesn't seem likely, while we got a negative result for Fermions it doesn't even seem to make sense.

Now the classic way (brute force):

We were able to do some prepatory work in task **11.1** which we now will use. Equation (2) shows $\langle \hat{n}_i \rangle$, from which we can easily derive

$$
\begin{aligned}
\langle \hat{n}_i \rangle^2 &= \frac{1}{\left(e^{\beta(\varepsilon_i - \mu)} \mp 1 \right)^2} \\
&= \frac{1}{\left(1 \mp e^{\beta(\varepsilon_i - \mu)} \right)^2}
\end{aligned}
$$

The second occuring term $\left\langle \hat{n}_i^2 \right\rangle$ needs to be calculated, while we can use our results from **11.1** we can already start at a equation similar to equation (1):

$$
\left\langle \hat{n}_i^2 \right\rangle = \frac{\sum_{n_i=0}^{\infty} n_i^2 e^{-\beta n_i (\varepsilon_i - \mu)}}{\sum_{n_i=0}^{\infty} e^{-\beta n_i (\varepsilon_i - \mu)}} \tag{3}
$$

First for Bosons, we again want the geometric series form, therefore we can use the equivalent derivative trick, already used in **11.1** again, while we first substitute $x = -\beta (\varepsilon_i - \mu)$:

$$\sum_{n_i=0}^{\infty} n_i^2 e^{-n_i x} = \frac{\partial^2}{\partial x^2} \sum_{n_i=0}^{\infty} e^{n_i x}$$

this is:

$$\begin{aligned}
\sum_{n_i=0}^{\infty} n_i^2 e^{-n_i x} &= \frac{\partial^2}{\partial x^2} \frac{1}{1-e^x} \\
&= \frac{\partial}{\partial x} \frac{e^x}{(1-e^x)^2} \\
&= \frac{e^x}{(1-e^x)^2} + \frac{2e^{2x}}{(1-e^x)^3} \\
&= \frac{e^x + e^{2x}}{(1-e^x)^3}
\end{aligned}$$

this means:

$$\left\langle \hat{n}_i^2 \right\rangle^+ = \frac{\frac{e^x+e^{2x}}{(1-e^x)^3}}{\frac{1}{(1-e^x)}} = \frac{e^x + e^{2x}}{(1-e^x)^2} = \frac{e^{-x}+1}{(1-e^{-x})^2}$$

For Fermions we get the same result for $\left\langle \hat{n}_i^2 \right\rangle$ and $\langle \hat{n}_i \rangle$ while $n_i = 0, 1$:

$$\left\langle \hat{n}_i^2 \right\rangle^+ = \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}$$

Inserting in the definition of the root-mean-square deviation of the single-particle occupation numbers leads to (first Bosons):

$$\begin{aligned}
(\Delta n_i)^{2\,+} &= \frac{\left\langle \hat{n}_i^2 \right\rangle - \langle \hat{n}_i \rangle^2}{\langle \hat{n}_i \rangle^2} \\
&= \frac{\frac{e^{-x}+1}{(1-e^{-x})^2}}{\frac{1}{(1-e^{-x})^2}} - 1 \\
&= e^{-x} + 1 - 1 \\
&= e^{\beta(\varepsilon_i - \mu)}
\end{aligned}$$

and for Fermions:

$$\begin{aligned}
(\Delta n_i)^{2\,-} &= \frac{\left\langle \hat{n}_i^2 \right\rangle - \langle \hat{n}_i \rangle^2}{\langle \hat{n}_i \rangle^2} \\
&= \frac{\langle \hat{n}_i \rangle}{\langle \hat{n}_i \rangle} \left(\frac{1 - \langle \hat{n}_i \rangle}{\langle \hat{n}_i \rangle} \right) \\
&= \frac{1}{\langle \hat{n}_i \rangle} - 1 \\
&= e^{\beta(\varepsilon_i - \mu)} + 1 - 1 \\
&= e^{\beta(\varepsilon_i - \mu)}
\end{aligned}$$

This means that we get the same result for Fermions and Bosons for the root-mean-square deviation of the single-particle occupation numbers.

11.3 (Trapped ideal Fermi gas)

Given single-particle energy levels:

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega \text{ with } n = 0, 1, 2, \ldots$$

the Hamiltonian is:

$$H = \sum_{n=0}^{\infty}\left(n + \frac{1}{2}\right)\hbar\omega\hat{n}_n$$

(a)

Definition:

$$Z_G = tr\left[e^{-\beta(H-\mu N)}\right]$$

this leads to:

$$\begin{aligned}
Z_G &= \sum_{N=0}^{\infty}\sum_{\{n_n\},\sum n_n=N} e^{-\beta(\epsilon_n n_n - \mu n_n)} \\
&= \sum_{\{n_n\}} e^{-\beta n_n\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)} \\
&= \sum_{\{n_n\}} e^{-\beta\sum_n n_n\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)} \\
&= \Pi_n \sum_{n_n} e^{-\beta n_n\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}
\end{aligned}$$

Now we have to use the condition, that we use fermions, which are limited to $n_n = 0, 1$ this leads to:

$$\begin{aligned}
Z_G &= \Pi_n\left(1 + e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right) && (4) \\
&= \Pi_n\left(1 + e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\cdot e^{-\beta\hbar\omega\cdot n}\right) \\
&= \left(1 + e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\right)\cdot\left(1 + e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\cdot e^{-\beta\hbar\omega}\right)\cdot\ldots\left(1 + e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\cdot e^{-\beta\hbar\omega N}\right) && (5)
\end{aligned}$$

but while this doesn't really simplify the situation we are going to use the form of equation (4). definition grand potential:

$$\begin{aligned}
\Phi &= -\frac{1}{\beta}\ln Z_G \\
&= -\frac{1}{\beta}\ln\Pi_n\left(1 + e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right)
\end{aligned}$$

now the form of equation (5) becomes useful, while we can write:

$$\begin{aligned}\ln \Pi_n \left(1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right) &= \ln\left[\left(1+e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\right)\cdot\ldots\left(1+e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\cdot e^{-\beta\hbar\omega N}\right)\right] \\ &= \ln\left(1+e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\right)+\cdots+\ln\left(1+e^{-\beta\left(\frac{1}{2}\hbar\omega-\mu\right)}\cdot e^{-\beta\hbar\omega N}\right) \\ &= \sum_n \ln\left(1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right)\end{aligned}$$

this leads to

$$\Phi = -\frac{1}{\beta}\sum_n \ln\left(1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right)$$

(b)

definition of $\langle N\rangle$:

$$\begin{aligned}\langle N\rangle &= -\frac{\partial\Phi}{\partial\mu} \\ &= \frac{1}{\beta}\frac{\partial}{\partial\mu}\sum_n \ln\left(1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right) \\ &= \frac{1}{\beta}\sum_n \frac{\partial}{\partial\mu}\ln\left(1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\right) \\ &= \frac{1}{\beta}\sum_n \frac{1}{1+e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}} e^{-\beta\left(\left(n+\frac{1}{2}\right)\hbar\omega-\mu\right)}\left(-\beta\right)\left(-1\right) \\ &= \sum_n \frac{1}{e^{\beta(\epsilon_n-\mu)}+1} \\ &= \sum_n n\left(\epsilon_n\right)\end{aligned}$$

We found, that the number of particles $\langle N\rangle$ can be rewritten in the sum of the average single-particle-occupation numbers.

(c)

Starting from $\beta\hbar\omega \ll 1$ we can rewrite the discrete sum into an integral, while the energy levels become quasi-continous. With the expression:

$$\sum_{n=0}^{\infty} \to \int_0^\infty dn \to \int_0^\infty \frac{dn}{d\epsilon_n}d\epsilon_n$$

while $D\left(\epsilon_n\right) = \frac{dn}{d\epsilon_n}$ is the density of energy states, which can be calculated using:

$$D\left(\epsilon_n\right) = \frac{1}{\frac{d\epsilon_n}{dn}} = \frac{1}{\frac{d}{dn}\left(n+\frac{1}{2}\right)\hbar\omega} = \frac{1}{\hbar\omega}$$

Therefore we can rewrite our sum for $\langle N\rangle$ to:

$$\langle N \rangle = \frac{1}{\hbar\omega} \int_0^\infty d\epsilon_n \frac{1}{e^{\beta(\epsilon_n - \mu)} + 1}$$

While we want the form given in the hint:

$$\int \frac{dx}{e^x + 1} = -\ln\left(1 + e^{-x}\right) \Leftrightarrow -\frac{\partial}{\partial x} \ln\left(1 + e^{-x}\right) = -\frac{(-1)\, e^{-x}}{1 + e^{-x}} = \frac{1}{e^x + 1}$$

we have to substitute $\beta\left(\epsilon_n - \mu\right) = x$ which leads to $\frac{dx}{\beta} = d\epsilon_n$ with the borders $x_1 \rightarrow -\beta\mu$ and $x_2 \rightarrow \infty$, therefore:

$$\begin{aligned} \langle N \rangle &= \frac{1}{\beta\hbar\omega} \int_{\beta\mu}^\infty dx \frac{1}{e^x + 1} \\ &= \frac{1}{\beta\hbar\omega} \left[-\ln\left(1 + e^{-x}\right)\right]_{-\beta\mu}^\infty \\ &= \frac{1}{\beta\hbar\omega} \left[0 + \ln\left(1 + e^{\beta\mu}\right)\right] \\ &= \frac{\ln\left(1 + e^{\beta\mu}\right)}{\beta\hbar\omega} \end{aligned}$$

We only have to rearrange this result now, to find an expression for the chemical potential $\mu\left(\beta, \hbar\omega, \langle N \rangle\right)$:

$$\mu = \frac{1}{\beta} \ln\left(e^{\langle N \rangle \beta\hbar\omega} - 1\right)$$

For the special case $T \rightarrow 0$ meaning $\beta \rightarrow \infty$, the -1 can be neglected and we get:

$$\mu = \langle N \rangle \frac{\hbar\omega}{k_B T}$$

the special case for high temperatures $T \rightarrow \infty$ on the other hand leads to a neglectable exponential term, and then we get:

$$\mu = \lim_{T \rightarrow \infty} k_B \underbrace{T}_{\rightarrow \infty} \cdot \underbrace{\ln(1)}_{=0} = 0$$

11.4 (Ideal Fermi gas in a magnetic field)

We got an ideal gas of spin-$\frac{1}{2}$ fermions in the presence of a magnetic field. All fermions should have a magnetic moment, μ_e. We are meant to compute the magnetization for this gas, which can be defined as ($N_{\uparrow,\downarrow}$ number of occupied states with spin $\uparrow, \downarrow$)

$$m = \mu_e \sum_i n_{\alpha_i} = \frac{\mu_e}{V} \left(N_\downarrow - N_\uparrow\right) \tag{6}$$

while for spin-$\frac{1}{2}$ fermions there are two further possible states (e.g. $\uparrow, \downarrow$, $+1, -1$), beneath being unoccupied/occupied, for each energy state.

We are looking at a one dimensional system, where the magnetization is directed in the z-direction, forced by the external B_z-Field, therefore the two occupied states can be defined as $+1$ and -1.

We now have to get a hamiltonian for this problem, starting with the standard hamiltonian (Fock-states):

$$\hat{H}_0 = \sum_i \varepsilon_i \hat{n}_i$$

but while there is a magnetic field now, we have to add a magnetic field hamiltonian for the total hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{mag}$$

While we already treated the Ising model and it's hamiltonian in task **10.1** we can simplify it from a lattice to a gas, where we will neglect the nearest neighbor term and therefore the magnetic hamiltonian is defined with:

$$\hat{H}_{mag} = -\sum_{i=0}^{N} \vec{\mu}_e \vec{B} = \mu_e B \sum_{i=1}^{N} \hat{S}_i^z = \sum_{i=1}^{N} \sum_{\sigma} s_\sigma \mu_e B \hat{n}_i$$

while N is the total number of particles in the gas, $\hat{S}_i$ can be either $+\frac{1}{2}$ or $-\frac{1}{2}$ and B is the external electric field (coordinate system chosen in z-direction). This leads to the total Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \sum_{s_\sigma = \uparrow, \downarrow} \left(\varepsilon_i + s_\sigma \mu_e B\right) \hat{n}_i$$

with $s_\uparrow = +1$ and $s_\downarrow = -1$. We know, that for a non existent external field the magnetization will be 0, this means, that $N_\uparrow = N_\downarrow$. The external field will direct some of the momenta, therefore $N_\uparrow < N_\downarrow$ for $B \neq 0$. We now only need to calculate $N_\uparrow$ and $N_\downarrow$ to determine M. Therefore we define the density of states for the electrons as:

$$D(E) = D_\uparrow(E) + D_\downarrow(E)$$

while for $B = 0$ we have $N_\uparrow = N_\downarrow$, meaning, that the densities will be equal:

$$\frac{1}{2} D(E) = D_\uparrow(E) = D_\downarrow(E)$$

but for $B \neq 0$ it is $N_\uparrow \neq N_\downarrow$ and therefore $D_\uparrow(E) \neq D_\downarrow(E)$. While $D_\sigma(E)$ will change in dependence of the strength of the magnetic field, while $D(E)$ is constant, we can write:

$$D_\sigma(E) = \frac{1}{2} D(E - s_\sigma \mu_e B) \tag{7}$$

this is clear, if you have a look at the single-particle energy levels, which turn from ε_i to $\varepsilon_i + s_\sigma \mu_e B$. Now we want to determine $D(E - s_\sigma \mu_e B)$, which we can using (from lecture notes)

$$D(\epsilon) = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon} \tag{8}$$

with $\epsilon = E - s_\sigma \mu_e B$ we get:

$$D_\sigma(E) = \frac{1}{2}\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - s_\sigma\mu_e B} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - s_\sigma\mu_e B}$$

while we use electrons, the g-factor is known to be $g = 2$. Finally we got everything prepared to finally get N_σ (formula from the lecture notes):

$$N_\sigma = \int_{-\infty}^{\infty} d\epsilon\, D_\sigma(\epsilon)\, n(\epsilon)$$

we can insert equation (7), while all energy values lower then $\epsilon - s_\sigma\mu_e B$ have a density of zero:

$$N_\sigma = \frac{1}{2}\int_{s_\sigma\mu_0 B}^{\infty} d\epsilon\, D(\epsilon - s_\sigma\mu_e B)\, n(\epsilon)$$

while we want to use the Sommerfeld-expansion later in this task, we have to substitute, to get the border to 0. This means $x = \epsilon - s_\sigma\mu_e B \Leftrightarrow \epsilon = x + s_\sigma\mu_e B$ leading to:

$$N_\sigma = \frac{1}{2}\int_{0}^{\infty} dx\, D(x)\, n(x + s_\sigma\mu_e B)$$

While in laboratories nowadays magnetic fields of 1 T are common and the highest fields you can get are about 40 T it seems likely that $x \gg s_\sigma\mu_e B$, while (using e.g. $\mu_0 = \mu_B = 10^{-4}\,\frac{\mathrm{eV}}{\mathrm{T}}$) we get terms of the order 10^{-3} for $s_\sigma\mu_e B$. Because of that fact we can Taylor-expand $n(x + s_\sigma\mu_e B)$ around $n(x)$ in first order resulting in

$$N_\sigma = \frac{1}{2}\int_{0}^{\infty} dx\, D(x)\left(n(x) + s_\sigma\mu_e B\frac{\partial n}{\partial x}\right)$$

While we want to calculate the magnetization we can insert N_σ in equation (6)

$$\begin{aligned} M &= \frac{\mu_e}{V}(N_\downarrow - N_\uparrow) \\ &= -\frac{\mu_e^2 B}{V}\frac{2}{2}\int_0^\infty dx\, D(x)\frac{\partial n}{\partial x} \end{aligned}$$

partial integration yields the form for the Sommerfeld-expansion:

$$
\begin{aligned}
M &= -\frac{\mu_e^2 B}{V}\left(\left[\frac{\partial n}{\partial x}\frac{\partial D(x)}{\partial x}\right]_0^\infty - \int_0^\infty dx\,\frac{\partial D(x)}{\partial x} n(x)\right)\\
&= \frac{\mu_e^2 B}{V}\int_0^\infty dx\,\frac{\partial D(x)}{\partial x} n(x)
\end{aligned}
$$

border terms can be neglected. We finally reached the Sommerfeld-expansion form with $f(x) = \frac{\partial D(x)}{\partial x}$ and

$$
\begin{aligned}
I &= \int_0^\infty dx\, f(x)\, n(x)\\
&= \int_0^\mu dx\, f(x) + \frac{\pi^2}{6}\frac{1}{\beta^2}\frac{\partial f(\mu)}{\partial \mu} + \frac{7\pi^4}{360}\frac{1}{\beta^4}\frac{\partial^3 f(\mu)}{\partial \mu^3} + \mathcal{O}\left(\frac{1}{\beta^6}\right)
\end{aligned}
$$

we get for the magnetization:

$$
M = \frac{\mu_e^2 B}{V}\int_0^\mu dx\,\frac{\partial D(x)}{\partial x} + \frac{\pi^2}{6}\frac{1}{\beta^2}\frac{\partial^2 D(\mu)}{\partial \mu^2} + \frac{7\pi^4}{360}\frac{1}{\beta^4}\frac{\partial^4 D(\mu)}{\partial \mu^4} + \mathcal{O}\left(\frac{1}{\beta^6}\right)
$$

With equation (8) we therefore get (second order):

$$
\begin{aligned}
M &= \frac{\mu_e^2 B}{V}\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\left(\int_0^\mu dx\,\frac{\partial}{\partial x}\sqrt{x} + \frac{\pi^2}{6}\frac{1}{\beta^2}\frac{\partial^2}{\partial \mu^2}\sqrt{\mu}\right)\\
&= \frac{\mu_e^2 B}{V}\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\left(\sqrt{\mu} - \frac{\pi^2}{24}\frac{\mu^{-\frac{3}{2}}}{\beta^2}\right)\\
&= \frac{\mu_e^2 B g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\left(\sqrt{\mu} - \frac{\pi^2}{24}\frac{\mu^{-\frac{3}{2}}}{\beta^2}\right)
\end{aligned}
$$

Now we want to have a look at the special of $T \to 0$, therefore $\frac{1}{\beta} \to 0$ and all higher order terms will disappear. We therefore get using $\mu = \epsilon_F$ for $T \to 0$ and non degenerate ground state:

$$
M = \frac{\mu_e^2 B g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon_F}
$$

this can be rewritten in an elegant form using $\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} = \frac{3N}{2\epsilon_F^{\frac{3}{2}}}$:

$$
M = \frac{3}{2}\frac{\mu_e^2 B N}{V\epsilon_F}
$$