Appendix A
Second Quantization

An exact description of an interacting many-body system requires the solving of the corresponding many-body Schrödinger equations. The formalism of second quantization leads to a substantial simplification in the description of such a many-body system, but it should be noted that it is only a reformulation of the original Schrödinger equation but not yet a solution. The essential step in the second quantization is the introduction of so-called creation and annihilation operators. By doing this, we eliminate the need for the laborious construction, respectively, of the symmetrized or the anti-symmetrized $N$-particle wavefunctions from the single-particle wavefunctions. The entire statistics is contained in fundamental commutation relations of these operators. Forces and interactions are expressed in terms of these “creation” and “annihilation” operators.

How does one handle an $N$-particle system? In case the particles are distinguishable, that is, if they are enumerable, then the method of description follows directly the general postulates of quantum mechanics:

$\mathcal{H}_1^{(i)}$: Hilbert space of the $i$th particle with the orthonormal basis $\{ |\phi^{(i)}_\alpha \rangle \}$:

$$\langle \phi^{(i)}_\alpha | \phi^{(i)}_\beta \rangle = \delta_{\alpha\beta} \quad (A.1)$$

$\mathcal{H}_N$: Hilbert space of the $N$-particle system

$$\mathcal{H}_N = \mathcal{H}_1^{(1)} \otimes \mathcal{H}_1^{(2)} \otimes \cdots \otimes \mathcal{H}_1^{(N)} \quad (A.2)$$

with the basis $\{ |\phi_N \rangle \}$:

$$|\phi_N \rangle = |\phi^{(1)}_{\alpha_1} \phi^{(2)}_{\alpha_2} \cdots \phi^{(N)}_{\alpha_N} \rangle = |\phi^{(1)}_{\alpha_1} \rangle |\phi^{(2)}_{\alpha_2} \rangle \cdots |\phi^{(N)}_{\alpha_N} \rangle \quad (A.3)$$

An arbitrary $N$-particle state $|\psi_N \rangle$,

$$|\psi_N \rangle = \int \sum_{\alpha_1 \cdots \alpha_N} c(\alpha_1 \cdots \alpha_N) |\phi^{(1)}_{\alpha_1} \phi^{(2)}_{\alpha_2} \cdots \phi^{(N)}_{\alpha_N} \rangle \quad (A.4)$$

underlies the same statistical interpretation as in the case of a 1-particle system. The dynamics of the $N$-particle system results from the formally unchanged Schrödinger equation:

\[ i\hbar \frac{\partial |\psi_N\rangle}{\partial t} = \hat{H} |\psi_N\rangle \]  

(A.5)

The handling of the many-body problem in quantum mechanics, in the case of distinguishable particles, confronts exactly the same difficulties as in the classical physics, simply because of the large number of degrees of freedom. There are no extra, typically quantum mechanical complications.

### A.1 Identical Particles

What are “identical particles”? To avoid misunderstandings let us strictly separate “particle properties” from “measured quantities of particle observables”. “Particle properties” as e.g. mass, spin, charge, magnetic moment, etc. are in principle unchangeable intrinsic characteristics of the particle. The “measured values of particle observables” as e.g. position, momentum, angular momentum, spin projection, etc., on the other hand, can always change with time. We define “identical particles” in the quantum mechanical sense as particles which agree in all their particle properties. Identical particles are therefore particles, which behave exactly in the same manner under the same physical conditions, i.e. no measurement can differentiate one from the other. Identical particles also exist in classical mechanics. However, if the initial conditions are known, the state of the system for all times is determined by the Hamilton’s equations of motion. Thus the particles are always identifiable!

In quantum mechanics, on the contrary, there is the principle of indistinguishability, which says that, identical particles are intrinsically indistinguishable. In quantum mechanics, in some sense, identical particles lose their individuality. This originates from the fact that there do not exist sharp particle trajectories (only “spreading” wave packets!). The regions, where the probability of finding the particle is unequal to zero, overlap for different particles. Any question whose answer requires the observation of one single particle is physically meaningless.

We face now the problem, that, essentially for calculational purposes, we cannot avoid, to number the particles. Then, however, the numbering must be so that all physically relevant statements, that are made, are absolutely invariant under a change of this particle labelling. How to manage this is the subject of the following considerations.

We introduce the permutation operator $\mathcal{P}$, which, in the $N$-particle state, changes the particle indices:

\[ \mathcal{P}|\phi^{(1)}_{a_1} \phi^{(2)}_{a_2} \cdots \phi^{(N)}_{a_N}\rangle = |\phi^{(i_1)}_{a_1} \phi^{(i_2)}_{a_2} \cdots \phi^{(i_N)}_{a_N}\rangle \]  

(A.6)

Every permutation operator can be written as a product of transposition operators $P_{ij}$. On application of $P_{ij}$ to a state of identical particles, results, according to the principle of indistinguishability, in a state, which, at the most, is different from the initial state by an unimportant phase factor $\lambda = \exp(i\eta)$:
A.1 Identical Particles

\[ P_{ij} \ket{\cdots \phi^{(i)}_{\alpha_i} \cdots \phi^{(j)}_{\alpha_j} \cdots} = \ket{\cdots \phi^{(j)}_{\alpha_j} \cdots \phi^{(i)}_{\alpha_i} \cdots} = \lambda \ket{\cdots \phi^{(i)}_{\alpha_i} \cdots \phi^{(j)}_{\alpha_j} \cdots} \] (A.7)

Since \( P_{ij}^2 = 1 \), it is necessary that \( \lambda = \pm 1 \). Therefore, a system of identical particles must be either symmetric or antisymmetric against interchange of particles! This defines two different Hilbert spaces:

\( \mathcal{H}^{(+)}_N \): the space of symmetric states \( \ket{\psi_N}^{(+)} \)

\[ P_{ij} \ket{\psi_N}^{(+)} = \ket{\psi_N}^{(+)} \] (A.8)

\( \mathcal{H}^{(-)}_N \): the space of antisymmetric states \( \ket{\psi_N}^{(-)} \)

\[ P_{ij} \ket{\psi_N}^{(-)} = -\ket{\psi_N}^{(-)} \] (A.9)

In these spaces, \( P_{ij} \) are Hermitian and unitary!

What are the properties the observables must have for a system of identical particles? They must necessarily depend on the coordinates of all the particles

\[ \hat{A} = \hat{A}(1, 2, \ldots, N) \] (A.10)

and must commute with all the transpositions (permutations)

\[ [P_{ij}, \hat{A}]_- = 0 \] (A.11)

This is valid specially for the Hamiltonian \( H \) and therefore also for the time evolution operator

\[ U(t, t_0) = \exp \left( -\frac{i}{\hbar} H(t - t_0) \right) ; \quad (H \neq H(t)) \] (A.12)

\[ [P_{ij}, U]_- = 0 \] (A.13)

That means the symmetry character of an \( N \)-particle state remains unchanged for all times!

Which Hilbert space out of \( \mathcal{H}^{(+)}_N \) and \( \mathcal{H}^{(-)}_N \) is applicable for which type of particles is established in relativistic quantum field theory. We will take over the spin-statistics theorem from there, without any proof.

\( \mathcal{H}^{(+)}_N \): Space of symmetric states of \( N \) identical particles with integral spin. These particles are called Bosons.

\( \mathcal{H}^{(-)}_N \): Space of antisymmetric states of \( N \) identical particles with half-integral spin. These particles are called Fermions.
A.2 Continuous Fock Representation

A.2.1 Symmetrized Many-Particle States

Let $\mathcal{H}_N^{(\varepsilon)}$ be the Hilbert space of a system of $N$ identical particles. Here

$$\varepsilon = \begin{cases} + : \text{Bosons} \\ - : \text{Fermions} \end{cases}$$  \hfill (A.14)

Let $\hat{\phi}$ be a 1-particle observable (or a set of 1-particle observables) with a continuous spectrum, $\phi_\alpha$ being a particular eigenvalue corresponding to the 1-particle eigenstate $|\phi_\alpha\rangle$:

$$\hat{\phi} |\phi_\alpha\rangle = \phi_\alpha |\phi_\alpha\rangle$$  \hfill (A.15)

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta (\phi_\alpha - \phi_\beta) \ (\equiv \delta (\alpha - \beta))$$  \hfill (A.16)

$$\int d\phi_\alpha |\phi_\alpha\rangle \langle \phi_\alpha | = \mathbb{I} \text{ in } \mathcal{H}_1$$  \hfill (A.17)

A basis of $\mathcal{H}_N^{(\varepsilon)}$ is constructed from the following (anti-) symmetrized $N$-particle states:

$$|\phi_{\alpha_1} \cdots \phi_{\alpha_N}\rangle^{(\varepsilon)} = \frac{1}{N!} \sum_{P} \varepsilon^P \mathcal{P} \left\{ |\phi_{\alpha_1}^{(1)}\rangle |\phi_{\alpha_2}^{(2)}\rangle \cdots |\phi_{\alpha_N}^{(N)}\rangle \right\}$$  \hfill (A.18)

$p$ is the number of transpositions in $\mathcal{P}$. The summation runs over all the possible permutations $\mathcal{P}$. The sequence of the 1-particle states in the ket on the left-hand side of (A.18) is called the standard ordering. It is arbitrary, but has to be fixed right at the beginning. Interchange of two 1-particle symbols on the left means only a constant factor $\varepsilon$ on the right.

One can easily prove the following relations for the above introduced $N$-particle states:

**Scalar product:**

$$^{(\varepsilon)}(\phi_{\beta_1} \cdots | \phi_{\alpha_i} \cdots \rangle^{(\varepsilon)} = \frac{1}{N!} \sum_{P} \varepsilon^P \mathcal{P} \left\{ \delta (\phi_{\beta_1} - \phi_{\alpha_1}) \cdots \delta (\phi_{\beta_i} - \phi_{\alpha_i}) \right\}$$  \hfill (A.19)

The index $\alpha$ shall indicate that $\mathcal{P}_\alpha$ permutes only the $\phi_\alpha$’s.

**Completeness relation:**

$$\int \cdots \int d\phi_{\beta_1} \cdots d\phi_{\beta_N} |\phi_{\beta_1} \cdots \rangle^{(\varepsilon)(\varepsilon)} \langle \phi_{\beta_1} \cdots | = \mathbb{I}$$  \hfill (A.20)
This leads to a formal representation of an observable of the N-particle system, which will be used later a few times:

\[
\hat{A} = \int \cdots \int d\phi_{\alpha_1} \cdots d\phi_{\alpha_N} d\phi_{\beta_1} \cdots d\phi_{\beta_N} \ast \\
\ast |\phi_{\alpha_1} \cdots \rangle^{(e)} (\epsilon | \hat{A} | \phi_{\beta_1} \cdots \rangle^{(e)} (\epsilon |
\]

(A.21)

### A.2.2 Construction Operators

We want to build up the basis states of \(H^{(e)}_N\), step by step, from the vacuum state \(|0\rangle (\langle 0|0 \rangle = 1)\) with the help of the operator

\[c_{\phi_\alpha}^\dagger \equiv c_{\alpha}^\dagger\]

These operators are defined by their action on the states:

\[c_{\alpha_1}^\dagger |0\rangle = \sqrt{1}|\phi_{\alpha_1}\rangle^{(e)} \in H^{(e)}_1\]

(A.22)

\[c_{\alpha_2}^\dagger |\phi_{\alpha_1}\rangle^{(e)} = \sqrt{2}|\phi_{\alpha_2} \phi_{\alpha_1}\rangle^{(e)} \in H^{(e)}_2\]

(A.23)

Or, in general

\[c_{\beta}^\dagger |\phi_{\alpha_1} \cdots \phi_{\alpha_N}\rangle^{(e)} = \sqrt{N+1}|\phi_{\beta} \phi_{\alpha_1} \cdots \phi_{\alpha_N}\rangle^{(e)} \in H^{(e)}_{N+1}\]

(A.24)

\(c_{\beta}^\dagger\) is called the creation operator. It creates an extra particle in the N-particle state. The relation (A.24) is obviously reversible:

\[|\phi_{\alpha_1} \phi_{\alpha_2} \phi_{\alpha_3} \cdots \phi_{\alpha_N}\rangle^{(e)} = \frac{1}{\sqrt{N!}} c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger \cdots c_{\alpha_N}^\dagger |0\rangle\]

(A.25)

The N-particle state \(|\phi_{\alpha_1} \cdots \rangle^{(e)}\) can be built up from the vacuum state \(|0\rangle\) by applying a sequence of N creation operators, where the order of the operators is to be strictly obeyed.

For a product of two creation operators, it follows from (A.24)

\[c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger |\phi_{\alpha_1} \cdots \phi_{\alpha_N}\rangle^{(e)} = \sqrt{N(N-1)}|\phi_{\alpha_2} \phi_{\alpha_1} \phi_{\alpha_3} \cdots \phi_{\alpha_N}\rangle^{(e)}\]

(A.26)

If the sequence of the operators is reversed, then we have

\[c_{\alpha_2}^\dagger c_{\alpha_1}^\dagger |\phi_{\alpha_3} \cdots \phi_{\alpha_N}\rangle^{(e)} = \sqrt{N(N-1)}|\phi_{\alpha_2} \phi_{\alpha_1} \phi_{\alpha_3} \cdots \phi_{\alpha_N}\rangle^{(e)}\]

(A.27)
The last step follows because of (A.18). Since the states in (A.26) and (A.27) are basis states, by comparing, we can therefore read off the following operator identity:

$$\left[ c_{\alpha_1}^\dagger, c_{\alpha_2}^\dagger \right]_{\varepsilon} = c_{\alpha_2}^\dagger - \varepsilon c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger = 0 \quad (A.28)$$

The creation operators commute in the case of Bosons ($\varepsilon = +1$) and anticommute ($\varepsilon = -1$) in the case of Fermions.

We now consider the operator $c_{\alpha}$ which is the adjoint of $c_{\alpha}^\dagger$. Because of (A.24) and (A.25), we can write

$$\langle \phi_{\alpha_N} | \cdots | \phi_{\alpha_1} \rangle_{\varepsilon} = \frac{1}{\sqrt{N!}} \langle 0 | c_{\alpha_1} \cdots c_{\alpha_2} \cdots c_{\alpha_N} \rangle_{\varepsilon} \quad (A.29)$$

The meaning of $c_{\gamma}$ is made clear by the following consideration:

$$\langle \phi_{\beta_N} \cdots \phi_{\beta_1} \rangle_{\varepsilon} = \sqrt{N} \langle \phi_{\alpha_N} | \cdots | \phi_{\alpha_1} \rangle_{\varepsilon} = \frac{\varepsilon}{\sqrt{N!}} \sum_{P_\alpha} \varepsilon^{P_\alpha} P_\alpha \left\{ \delta(\phi_{\beta_N} - \phi_{\alpha_N}) \delta(\phi_{\beta_{N-1}} - \phi_{\alpha_{N-1}}) \cdots \delta(\phi_{\beta_2} - \phi_{\alpha_2}) \right\}$$

Here we have used in the first step (A.29) and in the second step (A.19). We can further rewrite the right-hand side

$$\langle \cdots | c_{\gamma} | \cdots \rangle_{\varepsilon} = \frac{1}{\sqrt{N}} \frac{1}{(N - 1)!} \left\{ \delta(\phi_{\gamma} - \phi_{\alpha_1}) \sum_{P_\alpha} \varepsilon^{P_\alpha} P_\alpha \left( \delta(\phi_{\beta_N} - \phi_{\alpha_N}) \delta(\phi_{\beta_{N-1}} - \phi_{\alpha_{N-1}}) \cdots \delta(\phi_{\beta_2} - \phi_{\alpha_2}) \right) \right\}$$

$$+ \varepsilon \delta(\phi_{\gamma} - \phi_{\alpha_2}) \sum_{P_\alpha} \varepsilon^{P_\alpha} P_\alpha \left( \delta(\phi_{\beta_N} - \phi_{\alpha_N}) \delta(\phi_{\beta_{N-1}} - \phi_{\alpha_{N-1}}) \cdots \delta(\phi_{\beta_2} - \phi_{\alpha_2}) \right)$$

$$+ \cdots +$$

$$+ \varepsilon^{N-1} \delta(\phi_{\gamma} - \phi_{\alpha_N}) \sum_{P_\alpha} \varepsilon^{P_\alpha} P_\alpha \left( \delta(\phi_{\beta_N} - \phi_{\alpha_N}) \delta(\phi_{\beta_{N-2}} - \phi_{\alpha_{N-2}}) \cdots \delta(\phi_{\beta_2} - \phi_{\alpha_2}) \right)$$

$$= \frac{1}{\sqrt{N}} \left\{ \delta(\phi_{\gamma} - \phi_{\alpha_1}) \langle \phi_{\beta_2} \cdots \phi_{\beta_N} | \phi_{\alpha_2} \cdots \phi_{\alpha_N} \rangle_{\varepsilon} \right\}$$

$$+ \varepsilon \delta(\phi_{\gamma} - \phi_{\alpha_2}) \langle \phi_{\beta_2} \cdots \phi_{\beta_N} | \phi_{\alpha_1} \phi_{\alpha_2} \cdots \phi_{\alpha_N} \rangle_{\varepsilon}$$

$$+ \cdots +$$

$$+ \varepsilon^{N-1} \delta(\phi_{\gamma} - \phi_{\alpha_N}) \langle \phi_{\beta_2} \cdots \phi_{\beta_N} | \phi_{\alpha_1} \phi_{\alpha_2} \cdots \phi_{\alpha_{N-1}} \rangle_{\varepsilon} \right\}$$
With this, the action of $c_{\gamma}$ is clear, since $^{(e)}\langle \phi_{\beta_2} \cdots \phi_{\beta_N} |$ is an arbitrary $(N - 1)$-particle bra basis-state:

$$
c_{\gamma} | \phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)} = \frac{1}{\sqrt{N}} \sum \delta(\phi_{\gamma} - \phi_{\alpha_i}) | \phi_{\alpha_2} \cdots \phi_{\alpha_N} \rangle^{(e)} + \cdots + e^{N-1} \delta(\phi_{\gamma} - \phi_{\alpha_N}) | \phi_{\alpha_1} \cdots \phi_{\alpha_{N-1}} \rangle^{(e)}
$$

(A.30)

$c_{\gamma}$ annihilates a particle in the state $| \phi_{\gamma} \rangle$ and that is why it is called the annihilation operator. From (A.28), it immediately follows that

$$
[c_{\alpha_1}, c_{\alpha_2}]_{-\varepsilon} = -\varepsilon \left( [c_{\alpha_1}^{\dagger}, c_{\alpha_2}^{\dagger}]_{-\varepsilon} \right) = 0
$$

(A.31)

The annihilation operators commute in the case of Bosons ($\varepsilon = -1$) and anticommutate ($\varepsilon = +1$) in the case of Fermions. From (A.24) and (A.30) one can show that (Problem A.1)

$$(c_{\beta} c_{\gamma}^{\dagger} - \varepsilon c_{\gamma}^{\dagger} c_{\beta}) | \phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)} = \delta(\phi_{\beta} - \phi_{\gamma}) | \phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)}
$$

From this it follows that

$$
[c_{\beta}, c_{\gamma}^{\dagger}]_{-\varepsilon} = \delta(\phi_{\beta} - \phi_{\gamma})
$$

(A.32)

(A.28), (A.31) and (A.32) are the three fundamental commutation rules of the construction operators $a_{\gamma}$ and $a_{\gamma}^{\dagger}$.

### A.2.3 Many-Body Operators

We start with the formal ("spectral") representation of the $N$-particle observable $\hat{A}$ as given in (A.21). Using (A.25) and (A.29), we can write ($d\phi_{\alpha_i} \equiv d\alpha_i$)

$$
\hat{A} = \frac{1}{N!} \int \cdots \int d\alpha_1 \cdots d\alpha_N d\beta_1 \cdots d\beta_N *
$$

$$
* c_{\alpha_1}^{\dagger} \cdots c_{\alpha_N}^{\dagger} |0\rangle^{(e)} \langle \phi_{\alpha_1} \cdots | \hat{A} | \phi_{\beta_1} \cdots \rangle^{(e)} |0\rangle \langle \phi_{\beta_N} \cdots c_{\beta_1}
$$

(A.33)

Normally, such an operator consists of 1-particle and 2-particle parts:

$$
\hat{A} = \sum_{i=1}^{N} \hat{A}_i^{(1)} + \frac{1}{2} \sum_{i,j} \hat{A}_{ij}^{(2)}
$$

(A.34)
Using this, we will calculate the matrix elements in (A.33). We start with the 1-particle part:

\[
\begin{align*}
\langle \phi_{\alpha_1} \cdots | \sum_{i=1}^{N} \hat{A}_i^{(1)} | \phi_{\beta_1} \cdots \rangle^{(e)} &= \frac{1}{(N!)^2} \sum_{P_{\alpha}} \sum_{P_{\beta}} e^{p_{\alpha} + p_{\beta}} * \\
* &\{ \langle \phi_{\alpha_N}^{(N)} | \cdots | \phi_{\alpha_1}^{(1)} \} \left( P_{\alpha}^{\dagger} \sum_{i=1}^{N} \hat{A}_i^{(1)} P_{\beta} \right) \{ | \phi_{\beta_N}^{(N)} \rangle \cdots | \phi_{\beta_1}^{(1)} \} \\
\end{align*}
\]

(A.35)

One can easily see that every summand in the double sum \( \sum_{P_{\alpha}} \sum_{P_{\beta}} \) gives the same contribution, since every permuted ordering of \{ | \phi_{\alpha} \rangle \} or \{ | \phi_{\beta} \rangle \} can be restored to the standard ordering by renumbering the integration variables in (A.33). In order to bring back the creation and annihilation operators, which have been reindexed in the process, into the “correct” sequence, we require, according to (A.28) and (A.31), a factor \( e^{p_{\alpha} + p_{\beta}} \), which along with the corresponding factor in the above equation (A.35) gives a factor +1. Thus for (A.33), we need (A.35) only in the following simplified form:

\[
\begin{align*}
\langle \phi_{\alpha_1} \cdots | \sum_{i=1}^{N} \hat{A}_i^{(1)} | \phi_{\beta_1} \cdots \rangle^{(e)} &\Rightarrow \\
\{ \langle \phi_{\alpha_N}^{(N)} | \cdots | \phi_{\alpha_1}^{(1)} \} \sum_{i=1}^{N} \hat{A}_i^{(1)} \{ | \phi_{\beta_N}^{(N)} \rangle \cdots | \phi_{\beta_1}^{(1)} \} \\
\end{align*}
\]

(A.36)

Substituting this in (A.33), we get

\[
\begin{align*}
\sum_{i=1}^{N} \hat{A}_i^{(1)} &= \frac{1}{N!} \int \cdots \int d\alpha_1 \cdots d\beta_N c^{\dagger}_{\alpha_1} \cdots c^{\dagger}_{\alpha_N} |0\rangle * \\
* &\{ \langle \phi_{\alpha_1}^{(1)} | \hat{A}_1^{(1)} | \phi_{\beta_1}^{(1)} \rangle \langle \phi_{\alpha_2}^{(2)} | \phi_{\beta_2}^{(2)} \rangle \cdots \langle \phi_{\alpha_N}^{(N)} | \phi_{\beta_N}^{(N)} \rangle \\
+ \langle \phi_{\alpha_1}^{(1)} | \phi_{\beta_1}^{(1)} \rangle \langle \phi_{\alpha_2}^{(2)} | \hat{A}_2^{(1)} | \phi_{\beta_2}^{(2)} \rangle \cdots \langle \phi_{\alpha_N}^{(N)} | \phi_{\beta_N}^{(N)} \rangle + \cdots \} * \\
* &\{ 0 | c_{\beta_N} \cdots c_{\beta_1} \\
= \frac{1}{N!} \int \cdots \int d\alpha_1 \cdots d\alpha_N c^{\dagger}_{\alpha_1} \cdots c^{\dagger}_{\alpha_N} |0\rangle * \\
* &\{ \int d\beta_1 \langle \phi_{\alpha_1}^{(1)} | \hat{A}_1^{(1)} | \phi_{\beta_1}^{(1)} \rangle \langle 0 | c_{\alpha_N} \cdots c_{\alpha_2} c_{\beta_1} \\
+ \int d\beta_2 \langle \phi_{\alpha_2}^{(2)} | \hat{A}_2^{(1)} | \phi_{\beta_2}^{(2)} \rangle \langle 0 | c_{\alpha_N} \cdots c_{\alpha_2} c_{\beta_2} c_{\alpha_1} + \cdots \} \\
\end{align*}
\]
A.2 Continuous Fock Representation

\[
\frac{1}{N} \int \int d\alpha_1 d\beta_1 \langle \phi^{(1)}_{\alpha_1} | \hat{A}^{(1)}_{i} | \phi^{(1)}_{\beta_1} \rangle a^\dagger_{\alpha_i} \left\{ \frac{1}{(N-1)!} \right. \\
\int \ldots \int d\alpha_N c^\dagger_{\alpha_2} \ldots c^\dagger_{\alpha_N} |0\rangle \langle c_{\alpha_N} \ldots c_{\alpha_2} \rangle \left. c_{\beta_i} \right. \\
+ \frac{1}{N} \int \int d\alpha_2 d\beta_2 \langle \phi^{(2)}_{\alpha_2} | \hat{A}^{(1)}_{2} | \phi^{(2)}_{\beta_2} \rangle c^\dagger_{\alpha_2} \left\{ \frac{1}{(N-1)!} \right. \\
\int \ldots \int d\alpha_1 d\alpha_3 \ldots d\alpha_N c^\dagger_{\alpha_1} c^\dagger_{\alpha_3} \ldots c^\dagger_{\alpha_N} |0\rangle \\
\langle 0|c_{\alpha_N} \ldots c_{\alpha_3} c_{\alpha_1} \rangle \left. c_{\beta_2} \varepsilon^2 + \ldots \right. \\
(A.37)
\]

The factor \( \varepsilon^2 \) in the last line stems from the (anti)commutation \( c^\dagger_{\alpha_2} \leftrightarrow c^\dagger_{\alpha_1} \) and \( c^\dagger_{\alpha_1} \leftrightarrow c^\dagger_{\beta_2} \). Due to the analogous rearrangements all the other terms get a factor \( \varepsilon^{2m} \) which in any case is equal to +1. The term in each of the curly brackets is the identity for the Hilbert space \( \mathcal{H}_{N-1}^{(\varepsilon)} \) as given in (A.20). Therefore what remains is

\[
\sum_{i=1}^{N} \hat{A}^{(1)}_i = \frac{1}{N} \sum_{i=1}^{N} \int \int d\alpha_i d\beta_i \langle \phi^{(i)}_{\alpha_i} | \hat{A}^{(1)}_{i} | \phi^{(i)}_{\beta_i} \rangle c^\dagger_{\alpha_i} c_{\beta_i} \tag{A.38}
\]

The matrix elements are naturally the same for all the \( N \) identical particles. Therefore, the factor \( 1/N \) and the summation cancel out:

\[
\sum_{i=1}^{N} \hat{A}^{(1)}_i = \int \int d\alpha d\beta \langle \phi_{\alpha} | \hat{A}^{(1)} | \phi_{\beta} \rangle c^\dagger_{\alpha} c_{\beta} \tag{A.39}
\]

The remaining matrix element is in general easy to calculate. On the right-hand side, we do not have the particle number any more. It is of course implicitly present because, in between \( c^\dagger_{\alpha} \) and \( c_{\beta} \), there appears in principle an identity \( \mathbb{I} \), corresponding to the Hilbert space \( \mathcal{H}_{N-1}^{(\varepsilon)} \).

For the two-particle part of the operator \( \hat{A} \), at first, exactly the same considerations are valid which led us from (A.35) to (A.36). Therefore, we can use in (A.33)

\[
\langle \phi_{\alpha_i} \cdots | \varepsilon^{ij} \sum_{i,j} \hat{A}^{(2)}_{ij} | \phi_{\beta_1} \cdots \rangle \Rightarrow \\
\left\{ \langle \phi^{(N)}_{\alpha_N} | \cdots \langle \phi^{(1)}_{\alpha_1} | \varepsilon^{ij} \sum_{i,j} \hat{A}^{(2)}_{ij} \left\{ | \phi^{(1)}_{\beta_1} \cdots | \phi^{(N)}_{\beta_N} \rangle \right\} \right\} \tag{A.40}
\]
Substituting this we are left with

\[ \frac{1}{2} \sum_{i \neq j} A_{ij}^{(2)} = \frac{1}{2 \times N!} \int d\alpha_1 \cdots d\beta_N c_{\alpha_1}^\dagger \cdots c_{\alpha_N}^\dagger |0\rangle \]

* \[ \{ \langle \phi_{\alpha_2}^{(2)} | (\phi_{\alpha_1}^{(1)} | A_{12}^{(2)} | \phi_{\beta_1}^{(1)} | \phi_{\beta_2}^{(2)} ) \langle \phi_{\alpha_3}^{(3)} | \phi_{\beta_3}^{(3)} \rangle \cdots | \phi_{\alpha_N}^{(N)} | \phi_{\beta_N}^{(N)} \rangle \]

\[ = \frac{1}{2 N!} \int \cdots \int d\alpha_1 \cdots d\alpha_N d\beta_1 d\beta_2 c_{\alpha_1} c_{\alpha_2} \cdots c_{\alpha_N} |0\rangle \]

\[ = \frac{1}{2 N(N - 1)} \int \cdots \int d\alpha_1 d\alpha_2 d\beta_1 d\beta_2 \]

* \[ \langle \phi_{\alpha_1}^{(1)} | A_{12}^{(2)} | \phi_{\beta_1}^{(1)} | \phi_{\beta_2}^{(2)} \rangle \langle 0 | c_{\alpha_N} \cdots c_{\alpha_3} \}

\[ = \frac{1}{(N - 2)!} \int \cdots \int d\alpha_3 \cdots d\alpha_N c_{\alpha_3}^\dagger \cdots c_{\alpha_N}^\dagger |0\rangle \]

The curly bracket now gives the identity in the Hilbert space \( \mathcal{H}_{N-2}^{(c)} \), so that we have

\[ \frac{1}{2} \sum_{i \neq j} A_{ij}^{(2)} = \frac{1}{2 N(N - 1)} \sum_{i \neq j} \int \cdots \int d\alpha_i d\alpha_j d\beta_i d\beta_j \times \]

\[ \times \langle \phi_{\alpha_i}^{(i)} | \phi_{\alpha_j}^{(j)} | A_{ij}^{(2)} | \phi_{\beta_i}^{(i)} | \phi_{\beta_j}^{(j)} \rangle c_{\alpha_i}^\dagger c_{\alpha_j}^\dagger c_{\beta_i} c_{\beta_j} \]  \[ (A.41) \]

In a system of identical particles, naturally, all the summands on the right-hand side give identical contributions. Therefore, we have

\[ \frac{1}{2} \sum_{i \neq j} A_{ij}^{(2)} = \frac{1}{2} \int \cdots \int d\alpha_1 d\alpha_2 d\beta_1 d\beta_2 \]

* \[ \langle \phi_{\alpha_1}^{(1)} | A_{12}^{(2)} | \phi_{\beta_1}^{(1)} | \phi_{\beta_2} \rangle c_{\alpha_1}^\dagger c_{\alpha_2}^\dagger c_{\beta_2} c_{\beta_1} \]  \[ (A.42) \]

The remaining matrix element on the right-hand side can be built either with unsymmetrized two-particle states

\[ \langle \phi_{\alpha_1} | \phi_{\alpha_2} \rangle = \langle \phi_{\alpha_1} | | \phi_{\alpha_2} \rangle ; \quad | \phi_{\beta_1} | \phi_{\beta_2} \rangle = | \phi_{\beta_1} \rangle | \phi_{\beta_2} \rangle \]  \[ (A.43) \]
or also with the symmetrized states

$$|\phi_{\beta_1, \beta_2}^{(e)}\rangle = \frac{1}{2!} \left\{ |\phi_{\beta_1}^{(1)}\rangle |\phi_{\beta_2}^{(2)}\rangle + \varepsilon |\phi_{\beta_2}^{(1)}\rangle |\phi_{\beta_1}^{(2)}\rangle \right\}$$

(A.44)

What have we achieved? We have, through (A.25) and (A.29), replaced the laborious building up of symmetrized products from the single-particle states, by the application of products of construction operators to the vacuum state |0⟩. The operation is quite simple, for example,

$$c_\alpha |0\rangle = 0$$

(A.45)

and the whole statistics is taken care by the fundamental commutation relations (A.28), (A.31) and (A.32). The N-particle observables can also be expressed by the construction operators, (A.39) and (A.42) where the remaining matrix elements can be, usually, easily calculated with single-particle states. Note that the choice of the single-particle basis \{|\phi_\alpha\rangle\} is absolutely arbitrary, a great advantage with respect to practical purposes. We will demonstrate this in (A.4) with a few examples.

The theory developed so far is valid for continuous as well as discrete single-particle spectra. Only δ-functions have to be replaced by Kronecker-δs and integrals by summations in the case of discrete spectra.

## A.3 Discrete Fock Representation (Occupation Number Representation)

Let \(\mathcal{H}_N^{(e)}\) be again the Hilbert space of a system of N identical particles. Now, let \(\hat{\phi}\) be a single-particle observable with discrete spectrum. In principle, the same considerations are valid as in (A.2).

### A.3.1 Symmetrized Many-Particle States

We will use the following (anti-) symmetrized N-particle states as the basis of \(\mathcal{H}_N^{(e)}\):

$$|\phi_{\alpha_1} \cdots \phi_{\alpha_N}\rangle^{(e)} = C_\varepsilon \sum_P \varepsilon^P P \left\{ |\phi_{\alpha_1}^{(1)}\rangle \cdots |\phi_{\alpha_N}^{(N)}\rangle \right\}$$

(A.46)

Up to the still to be determined normalization constant \(C_\varepsilon\), this definition agrees with the corresponding definition (A.18) of the continuous case. However, now for the single-particle states, we have

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta_{\alpha\beta} ; \quad \sum_\alpha |\phi_\alpha\rangle \langle \phi_\alpha| = \mathbb{I} \text{ in } \mathcal{H}_1$$

(A.47)
One can see that (A.46) can be written for Fermions ($\varepsilon = -1$), as a determinant

$$\left| \phi^{(1)} \phi^{(2)} \cdots \phi^{(N)} \right|$$

This is known as the *Slater determinant*.

In case two sets of quantum numbers are equal, say, $\alpha_i = \alpha_j$, then, two rows of the Slater determinant are identical, which means, the determinant is equal to zero. Consequently, the probability that such a situation exists for a system of identical Fermions is zero. This is exactly the statement of the *Pauli’s principle*!

We define $n_i$ = *occupation number*, i.e. the frequency with which the state $|\phi^{(i)}\rangle$ appears in the $N$-particle state $|\phi^{(1)} \cdots \phi^{(N)}\rangle$.

Naturally, we have

$$\sum_i n_i = N$$

(A.49)

where the values $n_j$ can be

$$n_i = 0, 1 \quad for \text{Fermions}$$

$$n_i = 0, 1, 2, \cdots \quad for \text{Bosons}$$

(A.50)

First, we want to fix the normalization constant, which we assume to be real:

$$1 = \langle \phi^{(1)} \phi^{(2)} \cdots | \phi^{(1)} \phi^{(2)} \cdots \rangle$$

$$= C^{-2} \sum_{P} \sum_{P'} \varepsilon^{p + p'} \{ \phi^{(N)} \cdots \} P^+ P' \{ \phi^{(1)} \cdots \}$$

(A.51)

In the case of Fermions ($\varepsilon = -1$), every state is occupied only once. Therefore, in the sum, only the terms with $P = P'$ are unequal to zero and due to (A.47), each term is exactly equal to 1. Therefore, we get

$$C_+ = \frac{1}{\sqrt{N!}} \quad (\text{Fermions})$$

(A.52)

In the case of Bosons ($\varepsilon = +1$), the summands are then unequal to zero, when $P$ differs from $P'$ at the most by such transpositions for which only the groups of $n_i$ identical single-particle states $|\phi_i\rangle$ are interchanged among themselves. There are naturally $n_i!$ such possibilities. With this argument, we get for Bosons
A.3 Discrete Fock Representation (Occupation Number Representation)

\[ C_+ = (N! \prod n_i! / N!)^{-1/2} \quad \text{(Bosons)} \]  

(A.53)

Obviously, a symmetrized basis state can be completely specified by giving the occupation numbers. This permits the representation by the Fock states

\[ |N; n_1 n_2 \cdots n_j \cdots \rangle^{(e)} \equiv |\phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)} \]

\[ = C_\varepsilon \sum P \varepsilon^P \left\{ |\phi_{\alpha_1}^{(1)} \rangle |\phi_{\alpha_2}^{(2)} \rangle \cdots |\phi_{\alpha_i}^{(i)} \rangle |\phi_{\alpha_i}^{(i+1)} \rangle \cdots \right\} \]  

(A.54)

One has to give all the occupation numbers, even those with \( n_i = 0 \). Completeness and orthonormality follow from the corresponding relations for the symmetrized states:

\[ \langle N; \cdots n_i \cdots | \tilde{N}; \cdots \tilde{n}_i \cdots \rangle^{(e)} = \delta_{N\tilde{N}} \prod_i \delta_{n_i\tilde{n}_i} \]  

(A.55)

\[ \sum_{n_1} \sum_{n_2} \cdots \sum_{n_i} \cdots |N; \cdots n_i \cdots \rangle^{(e)} \langle N; \cdots n_i \cdots | = 1 \]  

(A.56)

A.3.2 Construction Operators

Up to normalization constants, we define the construction operators exactly in the same manner as we have done for the case of continuous spectrum in (A.2.2):

\[ c_{\alpha_r}^\dagger |\tilde{N}; \cdots \tilde{n}_r \cdots \rangle^{(e)} = c_{\alpha_r}^\dagger |\phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)} \]

\[ = \sqrt{n_r + 1} |\phi_{\alpha_1} \cdots \phi_{\alpha_N} \rangle^{(e)} \]

\[ = \varepsilon^N \sqrt{n_r + 1} |\phi_{\alpha_1} \cdots \phi_{\alpha_r} \cdots \phi_{\alpha_N} \rangle^{(e)} \]

\[ = \varepsilon^N \sqrt{n_r + 1} |N + 1; \cdots n_r + 1 \cdots \rangle^{(e)} \]  

(A.57)

Here, \( N_r \) is the number of transpositions necessary to bring the single-particle state \( |\phi_{\alpha_r} \rangle \) to the “correct” place:

\[ N_r = \sum_{i=1}^{r-1} n_i \]  

(A.58)
Equation (A.57) does not, as yet, contain the Pauli’s principle in a correct way. The operation of the so-called creation operator is precisely defined as follows.

**Bosons**:
\[ c^\dagger_\alpha |N; \cdots n_r \cdots\rangle^{(+)} = \sqrt{n_r + 1} |N + 1; \cdots n_r + 1 \cdots\rangle^{(+)} \]  

(A.59)

**Fermions**:
\[ c^\dagger_\alpha |N; \cdots n_r \cdots\rangle^{(-)} = (-1)^{N_r} \delta_{n_r,0} |N + 1; \cdots n_r + 1 \cdots\rangle^{(-)} \]

Any \(N\)-particle state can be built up by repeated application of the creation operators on the vacuum state \(|0\rangle\):

\[ |N; n_1 n_2 \cdots\rangle^{(e)} = \sum_{n_p=1}^{N} \prod_p \frac{1}{\sqrt{n_p!}} (c^\dagger_\alpha)^{n_p} e^{N_p} |0\rangle \]  

(A.60)

The annihilation operator is again defined as the adjoint of the creation operator:

\[ c_\alpha = (c^\dagger_\alpha)^\dagger \]  

(A.61)

The action of this operator becomes clear from the following:

\[ (e)\langle N; \cdots n_r \cdots | c_\alpha |\bar{N}; \cdots \bar{n}_r \cdots\rangle^{(e)} = e^{N_r} \sqrt{\bar{n}_r + 1} (e)\langle N + 1; \cdots n_r + 1 \cdots | \bar{N}; \cdots \bar{n}_r \cdots\rangle^{(e)} = e^{N_r} \sqrt{\bar{n}_r + 1} \delta_{N+1,\bar{N}} (\delta_{n_1,\bar{n}_1} \cdots \delta_{n_r,\bar{n}_r} \cdots) \]

\[ = e^{N_r} \sqrt{\bar{n}_r} \delta_{N,\bar{N}+1} (\delta_{n_1,\bar{n}_1} \cdots \delta_{n_r,\bar{n}_r-1} \cdots) \]

\[ = e^{N_r} \sqrt{\bar{n}_r} (e)\langle N+1; \cdots n_r \cdots | \bar{N} - 1; \cdots \bar{n}_r - 1 \cdots\rangle^{(e)} \]

\(\bar{N}_r\) is defined as in (A.58). Since \((e)\langle N_1 \cdots N_r \cdots |\) is an arbitrary bra-basis state, we have to conclude

\[ c_\alpha |N; \cdots n_r \cdots\rangle^{(e)} = e^{N_r} \sqrt{\bar{n}_r}|N - 1; \cdots n_r - 1 \cdots\rangle^{(e)} \]  

(A.62)

or, more specifically,

**Bosons**:
\[ c_\alpha |N; \cdots n_r \cdots\rangle^{(+)} = \sqrt{\bar{n}_r}|N - 1; \cdots n_r - 1 \cdots\rangle^{(+)} \]  

(A.63)

**Fermions**:
\[ c_\alpha |N; \cdots n_r \cdots\rangle^{(-)} = \delta_{n_r,1}(-1)^{N_r}|N - 1; \cdots n_r - 1 \cdots\rangle^{(-)} \]

With (A.59) and (A.63), one can easily prove three fundamental commutation rules (Problem A.2):
\[ \left[ c_{\alpha r} , c_{\alpha s} \right]_{-\varepsilon} = \left[ c_{\alpha r}^{\dagger} , c_{\alpha s}^{\dagger} \right]_{-\varepsilon} = 0 \]  
(A.64)

We further introduce two special operators, namely, the \textit{occupation number operator}:

\[ \hat{n}_r = c_{\alpha r}^{\dagger} c_{\alpha r} \]  
(A.65)

and the \textit{particle number operator}:

\[ \hat{N} = \sum_r \hat{n}_r \]  
(A.66)

The Fock states are the eigenstates of \( \hat{n}_r \) as well as of \( \hat{N} \). One can easily show with (A.59) and (A.63) that

\[ \hat{n}_r |N; \cdots n_r \cdots \rangle^{(e)} = n_r |N; \cdots n_r \cdots \rangle^{(e)} \]  
(A.67)

Thus \( \hat{n}_r \) refers to the number of particles occupying the \( r \)th single-particle state. The eigenvalue of \( \hat{N} \) is the total number of particles \( N \):

\[ \hat{N} |N; \cdots n_r \cdots \rangle^{(e)} = \left( \sum_r \hat{n}_r \right) |N; \cdots n_r \cdots \rangle^{(e)} = N |N; \cdots n_r \cdots \rangle^{(e)} \]  
(A.68)

The following relations are valid for both Bosons and Fermions (Problem A.3):

\[ \left[ \hat{n}_r , c^\dagger_s \right] = \delta_{rs} c^\dagger_r \quad ; \quad [\hat{n}_r , c_s ] = -\delta_{rs} c_r \]  
(A.69)

In order to transform a general operator \( \hat{A} \) (A.34) with a discrete spectrum into the formalism of second quantization, we have to follow the same procedure as was done in the case of the continuous spectrum. We only have to replace integrations by summations and delta functions by Kronecker deltas. Thus, we have expressions analogous to (A.39) and (A.42):

\[ \hat{A} \equiv \sum_{r,r'} \langle \phi_{\alpha r} | \hat{A}^{(1)} | \phi_{\alpha r'} \rangle c^\dagger_{\alpha r} c_{\alpha r'} + \frac{1}{2} \sum_{s,s',r,r'} \langle \phi_{\alpha r} | \phi_{\alpha s} | \hat{A}^{(2)} | \phi_{\alpha r'} \phi_{\alpha s'} \rangle c^\dagger_{\alpha s} c^\dagger_{\alpha s'} c_{\alpha s'} c_{\alpha s} c_{\alpha r'} c_{\alpha r} \]  
(A.70)
In contrast to the case of continuous spectrum, here, the matrix elements must be calculated with non-symmetrized two-particle states. The reason for this is the different normalization used here.

### A.4 Examples

In this section, we want to transform a few of the most often used operators from the first to second quantized form.

#### A.4.1 Bloch Electrons

We consider electrons in a rigid ion-lattice. The electrons interact with the lattice potential but do not interact with each other:

$$
H_0 = H_{e,\text{kin}} + H_{ei}^{(0)} = \sum_{i=1}^{N_e} \hbar (i)
$$

(A.71)

$H_{e,\text{kin}}$ is the operator of the kinetic energy

$$
H_{e,\text{kin}} = \sum_{i=1}^{N_e} \frac{p_i^2}{2m}
$$

(A.72)

$N_e$ is the number of electrons which interact with the rigid ion-lattice via $H_{ei}^{(0)}$.

$$
H_{ei}^{(0)} = \sum_{i=1}^{N_e} v(r_i) ; \quad v(r_i) = \sum_{\alpha=1}^{N} V_{ei} (r_i - R_\alpha)
$$

(A.73)

$N$ is the number of lattice atoms, whose equilibrium positions are given by $R_\alpha$. $v(r_i)$ has the same periodicity as the lattice:

$$
v(r_i) = v(r_i + R_\alpha)
$$

(A.74)

$H_0$ is obviously a single-particle operator. The eigenvalue equation for

$$
h_0 = \frac{p^2}{2m} + v(r)
$$

(A.75)

defines the Bloch function $\psi_k(r)$ and the Bloch energy $\varepsilon(k)$:

$$
h_0 \psi_k(r) = \varepsilon(k) \psi_k(r)
$$

(A.76)
For $\psi_k(r)$, we make the usual ansatz

$$\psi_k(r) = u_k(r) e^{i k \cdot r} \quad (A.77)$$

where the amplitude function $u_k(r)$ has the periodicity of the lattice. The Bloch functions build a complete orthonormal set:

$$\int d^3r \, \psi_k^*(r) \psi_k(r) = \delta_{kk'} \quad (A.78)$$

Neither $H_0$ nor $h_0$ contains spin terms. Therefore the complete solutions are

$$|k\sigma\rangle \leftrightarrow \langle r|k\sigma\rangle = \psi_{k\sigma}(r) = \psi_k(r) \chi_\sigma \quad (A.80)$$

$$\chi^\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad \chi^\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (A.81)$$

We define

$c_{k\sigma}^\dagger$ (c_{k\sigma}) - creation (annihilation)

operator of a Bloch electron

Since $H_0$ is a single-particle operator, according to (A.70), we can write

$$H_0 = \sum_{k,\sigma} \langle k\sigma | h_0 | k'\sigma' \rangle c_{k\sigma}^\dagger c_{k'\sigma'} \quad (A.82)$$

The matrix element is given by

$$\langle k\sigma | h_0 | k'\sigma' \rangle = \int d^3r \, \langle k\sigma | r \rangle \langle r | h_0 | k'\sigma' \rangle$$

$$= \varepsilon(k') \int d^3r \, \psi_k^*(r) \psi_{k\sigma'}(r)$$

$$= \varepsilon(k) \delta_{kk'} \delta_{\sigma\sigma'} \quad (A.83)$$

So that we can finally write

$$H_0 = \sum_{k,\sigma} \varepsilon(k) c_{k\sigma}^\dagger c_{k\sigma} \quad (A.84)$$
The Bloch operators satisfy the fundamental commutation relations of Fermion operators:

\[
\begin{align*}
[c_{k\sigma}, c_{k'\sigma'}]_+ &= \left[ c_{k\sigma}^\dagger, c_{k'\sigma'}^\dagger \right]_+ = 0 \\
\left[ c_{k\sigma}, c_{k'\sigma'}^\dagger \right]_+ &= \delta_{kk'} \delta_{\sigma\sigma'}
\end{align*}
\] (A.85)

In the special case, where one can neglect the crystal structure, e.g., as in the Jellium model, the Bloch functions become plane waves

\[
\psi_k(r) \Rightarrow \frac{1}{\sqrt{V}} e^{ik \cdot r}, \quad \varepsilon(k) \Rightarrow \frac{\hbar^2 k^2}{2m} \quad : (\nu(r) \equiv const)
\] (A.86)

A.4.2 Wannier Electrons

The representation using Wannier functions

\[
w_{\sigma}(r - R_i) = \frac{1}{\sqrt{N}} \sum_k \varepsilon^{-i k \cdot R_i} \psi_k^*(r)
\] (A.87)

is a special, frequently used position representation. The typical property of the Wannier function is its strong concentration around the respective lattice site \(R_i\):

\[
\int d^3 r \ w_{\sigma}^*(r - R_i) \ w_{\sigma}(r - R_j) = \delta_{\sigma\sigma'} \delta_{ij}
\] (A.88)

We define

\( c_{i\sigma}^\dagger (c_{i\sigma}) \) - creation (annihilation) operator of an electron with spin \(\sigma\) in a Wannier state at the lattice site \(R_i\).

These construction operators satisfy the following commutation relations:

\[
\begin{align*}
[c_{i\sigma}, c_{j\sigma'}]_+ &= \left[ c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger \right]_+ = 0; \quad \left[ c_{i\sigma}, c_{j\sigma'}^\dagger \right]_+ = \delta_{\sigma\sigma'} \delta_{ij}
\end{align*}
\] (A.89)

In this basis, \(H_0\) looks as follows:

\[
H_0 = \sum_{i,j,\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma'}
\] (A.90)

\[
T_{ij} = \int d^3r \ w_{\sigma}^*(r - R_i) \ h_0 \ w_{\sigma}(r - R_j)
\] (A.91)
$T_{ij}$ is known as the \textit{hopping integral}. In this form, $H_0$ describes, more transparently, the hopping of an electron of spin $\sigma$ from the lattice site $R_j$ to the lattice site $R_i$. The connection with the Bloch representation (A.4.1) is easy to establish by using (A.78) and (A.87):

\[
T_{ij} = \frac{1}{N} \sum_{k}^{1st \ B.Z.} \varepsilon(k) e^{i k \cdot (R_i - R_j)} \tag{A.92}
\]

\[
c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k}^{1st \ B.Z.} e^{i k \cdot R_i} c_{k\sigma} \tag{A.93}
\]

\section*{A.4.3 Density Operator}

The operator for the electron density

\[
\hat{\rho}(r) = \sum_{i=1}^{N_e} \delta(r - \hat{r}_i) \tag{A.94}
\]

is another example for a single-particle operator. It should be noticed that the electron position $\hat{r}_i$ is an operator but not the variable $r$:

\[
\hat{\rho}(r) = \sum_{k\sigma, k'\sigma'} \langle k\sigma | \delta(r - \hat{r}_i) | k'\sigma' \rangle c_{k\sigma}^\dagger c_{k'\sigma'} \tag{A.95}
\]

The matrix element is given by

\[
\langle k\sigma | \delta(r - \hat{r}') | k'\sigma' \rangle = \int d^3 r'' \langle k\sigma | \delta(r - \hat{r}) | r'' \rangle \langle r'' | k'\sigma' \rangle = \delta_{\sigma\sigma'} \int d^3 r'' \delta(r - r'') \langle k\sigma | r'' \rangle \langle r'' | k'\sigma' \rangle = \delta_{\sigma\sigma'} \psi_{k\sigma}(r) \psi_{k'\sigma}(r) \tag{A.96}
\]

If one restricts oneself to plane waves ($v(r) = \text{const.}$), then

\[
\langle k\sigma | \delta(r - \hat{r}') | k + q\sigma' \rangle = \delta_{\sigma\sigma'} \frac{1}{V} e^{i q \cdot r} \tag{A.97}
\]

Using this in (A.95) we get

\[
\hat{\rho}(r) = \frac{1}{V} \sum_{kq\sigma} c_{k\sigma}^\dagger c_{k+q\sigma} e^{i q \cdot r} \tag{A.98}
\]
From the above equation, we therefore find the Fourier component of the density operator:

$$\hat{\rho}_q = \sum_{k \sigma} c^\dagger_{k \sigma} c_{k+q \sigma}$$  \hspace{1cm} (A.99)

### A.4.4 Coulomb Interaction

Now we have to deal with a two-particle operators:

$$H_C = \frac{1}{2} \frac{e^2}{4\pi \varepsilon_0} \sum_{i\neq j} \frac{1}{|\hat{r}_i - \hat{r}_j|}$$  \hspace{1cm} (A.100)

How does this operator look in the formalism of second quantization? We again choose the momentum representation:

$$H_C = \frac{e^2}{8\pi \varepsilon_0} \Psi^* \left( \sum_{k_1 \cdots k_4} \langle (k_1 \sigma_1)(1)(k_2 \sigma_2)(2) | \frac{1}{|\hat{r}_1 - \hat{r}_2|} | (k_3 \sigma_3)(1)(k_4 \sigma_4)(2) \rangle \right) \Psi$$  \hspace{1cm} (A.101)

Since the operator itself is independent of spin, the matrix element is surely nonzero only for $\sigma_1 = \sigma_3$ and $\sigma_2 = \sigma_4$. Therefore, we are left with the following matrix element:

$$v(k_1 \cdots k_4) = \frac{e^2}{4\pi \varepsilon_0} \langle k_1(1) k_2(2) | \frac{1}{|\hat{r}_1 - \hat{r}_2|} | k_3(1) k_4(2) \rangle$$

$$= \frac{e^2}{4\pi \varepsilon_0} \int \int d^3 r_1 d^3 r_2 \langle k_1(1) k_2(2) | \frac{1}{|\hat{r}_1 - \hat{r}_2|} | r_1(1) r_2(2) \rangle \langle r_1(1) r_2(2) | k_3(1) k_4(2) \rangle$$

$$= \frac{e^2}{4\pi \varepsilon_0} \int \int d^3 r_1 d^3 r_2 \frac{1}{|r_1 - r_2|} \psi^*_{k_1}(r_1) \psi^*_{k_2}(r_2) \psi_{k_3}(r_1) \psi_{k_4}(r_2)$$  \hspace{1cm} (A.102)

Translational symmetry demands that we must have

$$k_1 + k_2 = k_3 + k_4$$  \hspace{1cm} (A.103)

Thus we have obtained the following expression for the Coulomb interaction:

$$H_C = \frac{1}{2} \sum_{k \sigma} v(k, p, q) c^\dagger_{k+q \sigma} c^\dagger_{p+q' \sigma'} c_{p \sigma'} c_{k \sigma}$$  \hspace{1cm} (A.104)
with

\[
v(k, p, q) = \frac{e^2}{4\pi \varepsilon_0} \int \int d^3r_1 \, d^3r_2 \, \psi_{k+q}(r_1) \, \psi_{p-q}(r_2) \ast
\]

\[
\ast \frac{1}{|r_1 - r_2|} \psi_k(r_1) \, \psi_p(r_2)
\]

(A.105)

### A.5 Problems

**Problem A.1** Let \( |\varphi_{\alpha_1} \ldots \varphi_{\alpha_N}\rangle^{(e)} \) be an (anti) symmetrized \( N \)-particle basis state for the case of a continuous one-particle spectrum. Then show that

\[
(c_\beta \psi^\dagger_\gamma - \varepsilon c^\dagger_\gamma c_\beta) \, |\varphi_{\alpha_1} \ldots \varphi_{\alpha_N}\rangle^{(e)} = \delta(\varphi_\beta - \varphi_\gamma) \, |\varphi_{\alpha_1} \ldots \varphi_{\alpha_N}\rangle^{(e)}
\]

**Problem A.2** Prove the fundamental commutation relations

\[
[c_{\alpha r}, c_{\alpha s}] = [c^\dagger_{\alpha r}, c^\dagger_{\alpha s}] = 0
\]

\[
[c_{\alpha r}, c^\dagger_{\alpha s}] = \delta_{r,s}
\]

for the creation and annihilation operators for the Bosons and Fermions in the discrete Fock space.

**Problem A.3** \( c_{\varphi_\alpha} \equiv c_\alpha \) und \( c^\dagger_{\varphi_\alpha} \equiv c^\dagger_\alpha \) are the annihilation and creation operators for one-particle states \( |\varphi_\alpha\rangle \) of an observable \( \hat{\Phi} \) with discrete spectrum. With the help of the fundamental commutation relations for Bosons and Fermions, calculate the following commutators:

1. \( \left[ \hat{n}_\alpha, c^\dagger_\beta \right] \)
2. \( \left[ \hat{n}_\alpha, c_\beta \right] \)
3. \( \left[ \hat{N}, c_\alpha \right] \)

Here \( \hat{N} = \sum_\alpha \hat{n}_\alpha = \sum_\alpha c^\dagger_\alpha c_\alpha \) is the particle number operator.

**Problem A.4** Under the same assumptions as in Problem A.3 for Fermions, prove the following relations:

1. \( (c_\alpha)^2 = 0 \); \( (c^\dagger_\alpha)^2 = 0 \)
2. \( \hat{n}_\alpha = n_\alpha \)
3. \( c_\alpha \hat{n}_\alpha = c_\alpha \); \( c^\dagger_\alpha \hat{n}_\alpha = 0 \)
4. \( \hat{n}_\alpha c_\alpha = 0 \); \( \hat{n}_\alpha c^\dagger_\alpha = c^\dagger_\alpha \)

**Problem A.5** Let \( |0\rangle \) be the normalized vacuum state. Let \( c^\dagger_\alpha \) und \( c_\alpha \) be the creation and annihilation operators for a particle in one-particle state \( |\varphi_\alpha\rangle \). Using the fundamental commutation relations derive the relation
\[
\langle 0 | c_{\beta N} \cdots c_{\beta 1} c_{\alpha N}^{\dagger} \cdots c_{\alpha 1}^{\dagger} | 0 \rangle = \sum_{\mathcal{P}} (\pm)^{\alpha} \mathcal{P}_{\alpha} [\delta(\beta_1, \alpha_1)\delta(\beta_2, \alpha_2) \cdots \delta(\beta_N, \alpha_N)]
\]

\(\mathcal{P}_{\alpha}\) is the permutation operator that operates on the indices \(\alpha_i\).

**Problem A.6** For the occupation number density operator calculate the commutators

1) \([\hat{n}_{\alpha}, c_{\beta}^{\dagger}]\); 2) \([\hat{n}_{\alpha}, c_{\beta}]\)

Is there a difference for Bosons and Fermions?

**Problem A.7** The anti-symmetrized basis states \(|\varphi_{\alpha_1} \cdots \varphi_{\alpha_N}^{(\pm)}\rangle\) of \(\mathcal{H}_N^{(\pm)}\) are built from continuous one-particle basis states. They are the eigenstates of the particle number operator \(\hat{N}\). Then show that

1) \(c_{\beta}^{\dagger} |\varphi_{\alpha_1} \cdots \varphi_{\alpha_N}^{(\pm)}\rangle\)
2) \(c_{\beta} |\varphi_{\alpha_1} \cdots \varphi_{\alpha_N}^{(\pm)}\rangle\)

are also eigenstates of \(\hat{N}\) and calculate the corresponding eigenvalues.

**Problem A.8** A system of \(N\) electrons in volume \(V = L^3\) interact among themselves via the Coulomb interaction

\[
V_2 = \frac{1}{2} \sum_{i \neq j} V_2^{(i,j)}, \quad V_2^{(i,j)} = \frac{e^2}{4\pi \varepsilon_0} \frac{1}{|\hat{r}_i - \hat{r}_j|}
\]

\(\hat{r}_i\) und \(\hat{r}_j\) are, respectively, the position operators of the \(i\)th and \(j\)th electron. Formulate the Hamiltonian of the system in second quantization. Use as the one-particle basis plane waves which have discrete wavevectors \(k\) as a consequence of the periodic boundary conditions on \(V = L^3\)

**Problem A.9** Show that the Hamiltonian calculated in Problem A.8 of the interacting \(N\)-electron system

\[
H_N = \sum_{k\sigma} \varepsilon_0(k) c_{k\sigma}^{\dagger} c_{k\sigma} + \frac{1}{2} \sum_{k\sigma q\sigma'} v_0(q) c_{k+q\sigma}^{\dagger} c_{-q\sigma'}^{\dagger} c_{p\sigma'} c_{k\sigma}
\]

commutes with the particle number operator

\[
\hat{N} = \sum_{k\sigma} c_{k\sigma}^{\dagger} c_{k\sigma}
\]

What is the physical meaning of this?
Problem A.10 Two identical particles move in a one-dimensional infinite potential well:

\[ V(x) = \begin{cases} 
0 & \text{for } 0 \leq x \leq a, \\
\infty & \text{for } x < 0 \text{ and } x > a 
\end{cases} \quad (A.106) \]

Calculate the energy eigenfunctions and energy eigenvalues of the two-particle system if they are (a) Bosons and (b) Fermions. What is the ground state energy in the case \( N \gg 1 \) for Bosons and for Fermions?

Problem A.11 There is a system of non-interacting identical Bosons or Fermions described by

\[ H = \sum_{i=1}^{N} H_1^{(i)} \]

The one-particle operator \( H_1^{(i)} \) has a discrete non-degenerate spectrum:

\[ H_1^{(i)} |\varphi_r^{(i)}\rangle = \epsilon_r |\varphi_r^{(i)}\rangle; \quad (\varphi_r^{(i)} |\varphi_s^{(i)}\rangle = \delta_{rs} \]

|\varphi_r^{(i)}\rangle are used to build the Fock states \(|N; n_1, n_2, \ldots\rangle^{(e)}\). The general state of the system is described by the un-normalized density matrix \( \rho \), for which the grand canonical ensemble (variable particle number) holds

\[ \rho = \exp[-\beta(H - \mu \hat{N})] \]

1. How does the Hamiltonian read in second quantization?

2. Show that the grand canonical partition is given by

\[ \Xi(T, V, \mu) = \text{Sp} \rho = \begin{cases} 
\prod_i \{1 - \exp[-\beta(\epsilon_i - \mu)]\}^{-1} & \text{Bosons,} \\
\prod_i \{1 + \exp[-\beta(\epsilon_i - \mu)]\} & \text{Fermions.} 
\end{cases} \]

3. Calculate the expectation value of the particle number:

\[ \langle \hat{N} \rangle = \frac{1}{\Xi} \text{Tr}(\rho \hat{N}) \]

4. Calculate the internal energy:

\[ U = \langle H \rangle = \frac{1}{\Xi} \text{Tr}(\rho H) \]

5. Calculate the average occupation number of the \( i \)th one-particle state
\[ \langle \hat{n}_i \rangle = \frac{1}{\Xi} \text{Tr}(\rho a_i^\dagger a_i) \]

and show that

\[ U = \sum_i \epsilon_i \langle \hat{n}_i \rangle ; \quad \langle \hat{N} \rangle = \sum_i \langle \hat{n}_i \rangle \]

are valid.
Appendix B
The Method of Green’s Functions

B.1 Linear Response Theory

We want to introduce the Green’s functions using a concrete physical context: How does a physical system respond to an external perturbation? The answer is provided by the so-called response functions. Well-known examples are the magnetic or electric susceptibility, the electrical conductivity, the thermal conductivity, etc. These are completely expressed by a special type of Green’s function.

B.1.1 Kubo Formula

Let the Hamiltonian

\[ H = H_0 + V_t \]  \hspace{1cm} (B.1)

consist of two parts. \( V_t \) is the perturbation which is the interaction of the system with a possibly time-dependent external field. \( H_0 \) is the Hamiltonian of the field-free but certainly interacting particle system. Thus \( H_0 \) is already in general not exactly solvable. Let the perturbation be operating through a scalar field \( F_t \) which couples to the observable \( \hat{B} \):

\[ V_t = \hat{B} \cdot F_t \]  \hspace{1cm} (B.2)

The restriction made now to a scalar field can be easily removed later. One should note that \( \hat{B} \) is an operator, whereas \( F_t \) is a \( c \)-number.

Now let \( \hat{A} \) be a not explicitly time-dependent observable. The interesting question is the following:

*How does the measured quantity \( \langle \hat{A} \rangle \) react to the perturbation \( V_t \) ?*

Without the field holds

\[ \langle \hat{A} \rangle_0 = Tr(\rho_0 \hat{A}) \]  \hspace{1cm} (B.3)
\[ \rho_0 = \frac{\exp(-\beta H_0)}{\text{Tr}(\exp(-\beta H_0))} \]  
(B.4)

where \( \rho_0 \) is the statistical operator of the field-free system, at the moment in the canonical ensemble. \( \beta = 1/k_B T \) is as usual the reciprocal temperature.

On the other hand, with field holds:

\[ \langle \hat{A} \rangle_t = \text{Tr}(\rho_t \hat{A}) \]  
(B.5)

\[ \rho_t = \frac{\exp(-\beta H)}{\text{Tr}(\exp(-\beta H))} \]  
(B.6)

where \( \rho_t \) is now the statistical operator of the particle system in the presence of the external field \( F_t \). Thus a measure of the response of the system to the perturbation could be the change in the value of \( \langle \hat{A} \rangle \) under the influence of the external field:

\[ \Delta A_t = \langle \hat{A} \rangle_t - \langle \hat{A} \rangle_0 \]  
(B.7)

To calculate this we need \( \rho_t \). In Schrödinger picture \( \rho_t \) satisfies the equation of motion

\[ i\hbar \dot{\rho}_t = [H_0 + V_t, \rho_t]_- \]  
(B.8)

with the boundary condition that the field for \( t \to -\infty \) is switched off:

\[ \lim_{t \to -\infty} \rho_t = \rho_0 \]  
(B.9)

Because of \( H_0 \), the Schrödinger picture is not convenient for perturbational approaches. More advantageous would be the Dirac picture:

\[ \rho_t^D(t) = e^{\frac{i}{\hbar}H_0 t} \rho_t e^{-\frac{i}{\hbar}H_0 t} \]  
(B.10)

One should note the two different time dependences. The lower index \( t \) denotes the possible explicit time dependence caused by the field. On the contrary, the argument of the statistical operator represents the dynamic time dependence. The equation of motion now is determined solely by the perturbation:

\[ i\hbar \dot{\rho}_t^D(t) = [V_t^D(t), \rho_t^D(t)]_- \]  
(B.11)

The boundary condition follows from (B.9) and (B.10) where \( \rho_0 \) commutes with \( H_0 \):

\[ \lim_{t \to -\infty} \rho_t^D(t) = \rho_0 \]  
(B.12)

We can now formally integrate (B.11):
\begin{equation}
\rho_D^t(t) = \rho_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \left[ V_D^t(t'), \rho_D^t(t') \right]_-	ag{B.13}
\end{equation}

This integral equation can be solved iteratively up to arbitrary accuracy in the perturbation $V_t$. For small perturbations one can restrict oneself to the first non-trivial step (linear response). That means after back-transformation to Schrödinger picture

\begin{equation}
\rho_t \approx \rho_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' e^{-\frac{i}{\hbar}H_0 t} \left[ V_D^t(t'), \rho_0 \right]_- e^{\frac{i}{\hbar}H_0 t} \tag{B.14}
\end{equation}

We now calculate $\langle \hat{A} \rangle_t$ approximately by substituting $\rho_t$ in (B.5):

\begin{align*}
\langle \hat{A} \rangle_t &= \langle \hat{A} \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' Tr \left( e^{-\frac{i}{\hbar}H_0 t} \left[ V_D^t(t'), \rho_0 \right]_- e^{\frac{i}{\hbar}H_0 t} \cdot \hat{A} \right) \\
&= \langle \hat{A} \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \left( V_D^t(t') \rho_0 \hat{A}^D(t) - \rho_0 V_D^t(t') \hat{A}^D(t) \right) \\
&= \langle \hat{A} \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \left( \rho_0 \left[ \hat{A}^D(t), V_D^t(t') \right]_- \right)
\end{align*}

In the reformulation, we many times used the cyclic invariance of trace. We thus obtain the reaction of the system to external perturbation:

\begin{equation}
\Delta A_t = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' F_t \left[ \left[ \hat{A}^D(t), \hat{B}^D(t') \right]_- \right]_0 \tag{B.15}
\end{equation}

As a consequence of linear response, the reaction of the system is determined by an expectation value for the field-free system. One should note that the Dirac representation of the operators $\hat{A}$ and $\hat{B}$ here correspond to the Heisenberg representation without field ($H_0 \rightarrow H$).

One defines: “double-time, retarded Green’s function”

\begin{equation}
G_{AB}^{ret}(t, t') = \langle \langle \hat{A}(t); \hat{B}(t') \rangle \rangle^{ret} = -i \Theta(t - t') \left[ \left[ \hat{A}(t), \hat{B}(t') \right]_- \right] \tag{B.16}
\end{equation}

where $\Theta$ is the Heaviside step function. The operators are in the field-free Heisenberg representation. The properties of the retarded Green’s function will be discussed in more detail in the following. Here, we recognize that it describes the reaction of the system in terms of the observable $\hat{A}$ when the external perturbation couples to the observable $\hat{B}$

\begin{equation}
\Delta A_t = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dt' F_t G_{AB}^{ret}(t, t') \tag{B.17}
\end{equation}

Later we will assume that the (field-free) Hamiltonian $H$ is not explicitly dependent on time. In that case one can show that the Green’s function does not depend
on two times but only on the time difference. Then it is called *homogeneous in time*:

\[ G_{AB}^{\text{rel}}(t, t') \rightarrow G_{AB}^{\text{rel}}(t - t') \]

In such a situation one has the Fourier transformation:

\[
G_{AB}^{\text{rel}}(E) = \langle \hat{A}_i \hat{B}_j \rangle^{\text{rel}}_E = \int_{-\infty}^{+\infty} d(t - t') \ G_{AB}^{\text{rel}}(t - t') e^{\frac{i}{\hbar}E(t-t')} \tag{B.18}
\]

\[
G_{AB}^{\text{rel}}(t - t') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dE \ G_{AB}^{\text{rel}}(E) e^{-\frac{i}{\hbar}E(t-t')} \tag{B.19}
\]

In the following, all the time/energy functions will be transformed in this way. In particular, for the delta function holds:

\[
\delta(E - E') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt \ e^{-\frac{i}{\hbar}(E-E)t} \tag{B.20}
\]

\[
\delta(t - t') = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dE \ e^{\frac{i}{\hbar}E(t-t')} \tag{B.21}
\]

We write the perturbing field as a Fourier integral:

\[
F_t = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dE \ F(E) e^{-\frac{i}{\hbar}(E+i0^+)t} \tag{B.22}
\]

The additional \(i0^+\) takes care of fulfilling the boundary condition (B.9). Substituting this expression now in (B.17) we finally obtain the *Kubo formula*:

\[
\Delta A_t = \frac{1}{2\pi\hbar^2} \int_{-\infty}^{+\infty} dE \ F(E) \ G_{AB}^{\text{rel}}(E + i0^+) e^{-\frac{i}{\hbar}(E+i0^+)t} \tag{B.23}
\]

In the following sections we will present a few applications of this important formula.

### B.1.2 Magnetic Susceptibility

We consider a magnetic induction \( \mathbf{B}_t \) which is homogeneous in space and oscillating in time as *perturbation* which couples to the total magnetic moment \( \mathbf{m} \) of a localized spin system (e.g. Heisenberg model) (Fig. B.1):

\[
\mathbf{m} = \sum_i \mathbf{m}_i \tag{B.24}
\]
i indexes the lattice sites at which the localized moments (spins) are present. The perturbation term then reads

\[ V_t = -\mathbf{m} \cdot \mathbf{B}_t = -\frac{1}{2\pi\hbar} \sum_a \int_{-\infty}^{+\infty} dE \, m^\alpha B^\alpha(E) e^{-\frac{i}{\hbar}(E+i0^+)t} \]  

(B.25)

Interesting here is the reaction of the magnetization of the moment system:

\[ M = \frac{1}{V} \langle \mathbf{m} \rangle = \frac{1}{V} \sum_i \langle \mathbf{m}_i \rangle \]  

(B.26)

It can be approximately calculated with the help of the Kubo formula (B.17):

\[ \Delta M_0^\beta = M_t^\beta - M_0^\beta = -\frac{1}{\mu_0 V \hbar} \int_{-\infty}^{+\infty} dt' \sum_a B^\alpha_{t'} \langle\langle m^\beta(t); m^a(t')\rangle\rangle \]  

(B.27)

Here \( M_0 \) is the field-free magnetization which is unequal zero only for ferromagnets. One defines “magnetic susceptibility tensor”

\[ \chi^\alpha^\beta_{ij}(t, t') = -\frac{\mu_0}{V \hbar} \langle\langle m^\beta_i(t); m^a_j(t')\rangle\rangle \]  

(B.28)

This function, which is so important for magnetism, is thus a retarded Green’s function:

\[ \Delta M_0^\beta = \frac{1}{\mu_0} \sum_{i,j} \sum_a \int_{-\infty}^{+\infty} dt' \chi^\alpha^\beta_{ij}(t, t') B^\alpha_{t'} \]  

(B.29)

If the susceptibility is homogeneous in time, \( \chi^\alpha^\beta_{ij}(t, t') \equiv \chi^\alpha^\beta_{ij}(t-t') \), which we want to assume, then energy representation is meaningful:

\[ \Delta M_0^\beta = \frac{1}{2\pi\hbar \mu_0} \sum_{i,j} \sum_a \int_{-\infty}^{+\infty} dE \, \chi^\alpha^\beta_{ij}(E + i0^+)B^a(E)e^{-\frac{i}{\hbar}(E+i0^+)t} \]  

(B.30)

Of particular interest are

- “longitudinal” susceptibility:

\[ \chi^z^z(E) = -\frac{\mu_0}{V \hbar} \langle\langle m^z_i; m^z_j\rangle\rangle_E \]  

(B.31)
With this function it is possible to make statements about magnetic stability. For example, if one calculates

\[ \chi_{q}^{zz}(E) = \frac{1}{N} \sum_{i,j} \chi_{ij}^{zz}(E)e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \]  

(B.32)

for the paramagnetic moment system, then in the limit \((\mathbf{q}, E) \rightarrow 0\) the singularities

\[ \left[ \lim_{(\mathbf{q}, E) \rightarrow 0} \chi_{q}^{zz}(E) \right]^{-1} \equiv 0 \]

give the instabilities of the paramagnetic state against ferromagnetic ordering. At these points even an infinitesimal, symmetry breaking field produces a finite magnetization. The poles of the function \(\chi_{q}^{zz}(E)\) therefore describe the phase transition para-ferromagnetism.

- “transverse” susceptibility:

\[ \chi_{ij}^{+-}(E) = -\frac{\mu_0}{V\hbar} \langle \langle m_i^+; m_j^- \rangle \rangle_E \]  

(B.33)

Here holds

\[ m_j^\pm = m_j^x \pm im_j^y \]

For this function also the poles are interesting. They represent resonances or eigenoscillations. One obtains from them the energies of spin waves or magnons:

\[ \left( \chi_{q}^{+-}(E) \right)^{-1} \equiv 0 \iff E = \hbar \omega(\mathbf{q}) \]  

(B.34)

Thus the linear response theory is not only an approximate procedure for weak perturbations but also provides valuable information about the unperturbed system.

### B.1.3 Dielectric Function

We want to discuss another application of the linear response theory. Into a system of quasifree conduction electrons (metal), an external charge density is introduced. Because of Coulomb repulsion, the charge carriers react to the perturbation. This leads to changes in the density of metal electrons in such a way that it causes effectively a more or less strong screening of the perturbing charge. This is described by

\[ \varepsilon(\mathbf{q}, E) : \text{dielectric function} \]
We first want to handle the problem classically and undertake the necessary quantization later. For the external charge density we write

$$\rho_{\text{ext}}(r, t) = \frac{1}{2\pi \hbar V} \int_{-\infty}^{+\infty} dE \sum_q \rho_{\text{ext}}(q, E) e^{i q \cdot r} e^{-\frac{i}{\hbar} (E+i0^+) t}$$  \hspace{1cm} (B.35)

A corresponding expression should hold for the conduction electrons:

$$-e \rho(r) = -\frac{e}{V} \sum_q \rho_q e^{i q \cdot r}$$  \hspace{1cm} (B.36)

The interaction of the conduction electrons with the external charge density then reads as

$$V_t = \frac{-e}{4\pi \varepsilon_0} \int \int d^3r d^3r' \frac{\rho(r) \rho_{\text{ext}}(r', t)}{|r - r'|}$$  \hspace{1cm} (B.37)

One shows (Problem 4.3)

$$\int \int d^3r d^3r' \frac{e^{i (q \cdot r + q' \cdot r')}}{|r - r'|} = \frac{4\pi V}{q^2} \delta_{q, -q'}$$  \hspace{1cm} (B.38)

Using this it holds with the Coulomb potential

$$v_0(q) = \frac{1}{V} \frac{e^2}{\varepsilon_0 q^2}$$  \hspace{1cm} (B.39)

after simple reformulation:

$$V_t = \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-\frac{i}{\hbar} (E+i0^+) t} \sum_q v_0(q) \rho_{-q, \text{ext}}(q, E)$$  \hspace{1cm} (B.40)

We assume that without the external perturbation the charge densities of the conduction electrons and the positively charged ions of the solid exactly compensate each other. Then we have for the total charge density

$$\rho_{\text{tot}}(r, t) = \rho_{\text{ext}}(r, t) + \rho_{\text{ind}}(r, t)$$  \hspace{1cm} (B.41)

where $\rho_{\text{ind}}(r, t)$ is the charge density induced by the displacement of charges. With the Fourier transformed Maxwell equations

$$i q \cdot D(q, E) = \rho_{\text{ext}}(q, E)$$  \hspace{1cm} (B.42)

$$i q \cdot F(q, E) = \frac{1}{\varepsilon_0} (\rho_{\text{ext}}(q, E) + \rho_{\text{ind}}(q, E))$$  \hspace{1cm} (B.43)
where $\mathbf{F}$ is the electric field strength and $\mathbf{D}$ is the electric displacement, and the material equation

$$
\mathbf{D}(\mathbf{q}, E) = \varepsilon_0 \varepsilon(\mathbf{q}, E) \mathbf{F}(\mathbf{q}, E) \quad \text{(B.44)}
$$

holds for the induced charge density:

$$
\rho_{\text{ind}}(\mathbf{q}, E) = \left[ \frac{1}{\varepsilon(\mathbf{q}, E)} - 1 \right] \rho_{\text{ext}}(\mathbf{q}, E) \quad \text{(B.45)}
$$

We now translate the formulas obtained classically so far into quantum mechanics. When we do this, the electron density becomes the density operator

$$
\rho_{\mathbf{q}} = \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{q}\sigma} \quad ; \quad \rho_{\mathbf{q}} - \rho_{\mathbf{q}}^\dagger = 0 \quad \text{(B.46)}
$$

Then the interaction energy also becomes an operator. According to (B.40) it holds

$$
V_t = \sum_{\mathbf{q}} \rho_{\mathbf{q}}^\dagger \tilde{F}_t(\mathbf{q}) \quad \text{(B.47)}
$$

The perturbing field

$$
-e \tilde{F}_t(\mathbf{q}) = \frac{v_0(\mathbf{q})}{2\pi \hbar} \int_{-\infty}^{+\infty} dE \rho_{\text{ext}}(\mathbf{q}, E) e^{-\frac{i}{\hbar}(E+i\gamma)t} \quad \text{(B.48)}
$$

however, remains naturally, a $c$-number. How does the induced charge density (operator!) react to the perturbing field produced by the external charge?

$$
\langle \rho_{\text{ind}}(\mathbf{q}, t) \rangle = -e \left\{ \langle \rho_{\mathbf{q}} \rangle_t - \langle \rho_{\mathbf{q}} \rangle_0 \right\} = -e \Delta(\rho_{\mathbf{q}})_t \quad \text{(B.49)}
$$

We now use the Kubo formula (B.17)

$$
\Delta(\rho_{\mathbf{q}})_t = \frac{1}{\hbar} \sum_{\mathbf{q}} \int_{-\infty}^{+\infty} dt' \tilde{F}_t'(\mathbf{q}') \langle\langle \rho_{\mathbf{q}}(t); \rho_{\mathbf{q}}^\dagger(t') \rangle\rangle \quad \text{(B.50)}
$$

We assume a system with translational symmetry so that we can use

$$
\langle\langle \rho_{\mathbf{q}}(t); \rho_{\mathbf{q}}^\dagger(t') \rangle\rangle \rightarrow \delta_{\mathbf{q}, \mathbf{q}'} \langle\langle \rho_{\mathbf{q}}(t); \rho_{\mathbf{q}}^\dagger(t') \rangle\rangle
$$

Then we have

$$
\langle \rho_{\text{ind}}(\mathbf{q}, t) \rangle = \frac{-e}{\hbar} \int_{-\infty}^{+\infty} dt' \tilde{F}_t(\mathbf{q}) \langle\langle \rho_{\mathbf{q}}(t); \rho_{\mathbf{q}}^\dagger(t') \rangle\rangle \quad \text{(B.51)}
$$
or after Fourier transformation

\[ \langle \rho_{\text{ind}}(q, E) \rangle = \frac{v_0(q)}{\hbar} \rho_{\text{ext}}(q, E) \langle \langle \rho_q; \rho_q^\dagger \rangle \rangle_{E+i0^+} \]  

(B.52)

We compare this with the classical result (B.45) and then we can represent the dielectric function by a retarded Green’s function

\[ \frac{1}{\varepsilon(q, E)} = 1 + \frac{1}{\hbar} v_0(q) \langle \langle \rho_q; \rho_q^\dagger \rangle \rangle_{E+i0^+} \]  

(B.53)

The following two limiting cases are interesting:

- \( \varepsilon(q, E) \gg 1 \) : \( \Rightarrow \langle \rho_{\text{ind}}(q, E) \rangle \approx -\rho_{\text{ext}}(q, E) \), almost complete screening of the perturbing charge.
- \( \varepsilon(q, E) \to 0 \) : \( \Rightarrow \) arbitrarily small perturbations produce finite density oscillations \( \Rightarrow \) “resonances”, i.e. collective eigenoscillations of the electron system.

The poles of the Green’s function \( \langle \langle \rho_q; \rho_q^\dagger \rangle \rangle_{E+i0^+} \) are just the energies of the so-called “plasmons”.

## B.2 Spectroscopies and Spectral Densities

An additional important motivation for the study of Green’s functions is their close connection to “elementary excitations” of the system, which are directly observable by appropriate spectroscopies. Thus certain Green’s functions provide a direct access to experiment. This is more directly valid for another fundamental function, namely the so-called “spectral density” which has a close relation to the Green’s functions. Figure B.2 shows in a schematic form, which elementary processes are involved in four well-known spectroscopies for the determination of electronic structure. The photoemission (PES) and the inverse photoemission (IPE) are the so-called one-particle spectroscopies since the system (solid) contains after the excitation process one particle more (less) as compared to before the process. In the photoemission the energy \( \hbar \omega \) of the photon is absorbed by an electron in a (partially) occupied energy band. This gain in energy makes the electron to leave the solid. Analysis of the kinetic energy of the photoelectron leads to conclusions about the occupied states of the concerned energy band. Then the transition operator \( Z_{-1} = c_\alpha \) corresponds to the annihilation operator \( c_\alpha \), if the particle occupies the one-particle state \( |\alpha\rangle \) before the excitation process. In the inverse photoemission, a somewhat reverse process takes place. An electron is shot into the solid and it lands in an unoccupied state \( |\beta\rangle \) of a partially filled energy band. The energy released is emitted as a photon \( \hbar \omega \) which is analysed. Now the system contains one electron more than before the process. This corresponds to the transition operator \( Z_{+1} = c_\beta^\dagger \). PES and IPE are in some ways complementary spectroscopies. The former provides
Fig. B.2 Elementary processes relevant for four different spectroscopies: 1. photoemission (PES),
2. inverse photoemission (IPE), 3. Auger electron spectroscopy (AES), and 4. appearance-potential
spectroscopy (APS). $Z_j$ is the transition operator, where $j$ means the change in the electron
numbers due to the respective excitation.

Auger-electron spectroscopy (AES) and appearance potential spectroscopy (APS)
are two-particle spectroscopies. The starting situation for AES is characterized by
the existence of a hole in a deep lying core state. An electron of the partially filled
band drops down into this core state and transfers the energy to another electron
of the same band so that the latter can leave the solid. The analysis of the kinetic
energy of the emitted electron provides information about the energy structure of the
occupied states (two-particle density of states). The system (energy band) contains
two particles less than before the process: $Z_{-2} = c_\alpha c_\beta$. Almost the reverse process
is exploited in APS. An electron lands in an unoccupied state of an energy band. The energy released is used in exciting a core electron to come up and occupy another unoccupied state of the same energy band. The subsequent de-exciting process can be analyzed to gain information about the unoccupied states of the energy band. In this case then the system (energy band) contains two electrons more after the process as compared to before the process. Therefore the transition operator is $Z_{+2} = c_\beta^\dagger c_\alpha^\dagger$. AES and APS are obviously complementary two-particle spectroscopies.

We now, using simple arguments, want to estimate the associated intensities for the individual processes.

- The system under investigation is described by the Hamiltonian:

$$\mathcal{H} = H - \mu \hat{N} \quad \text{(B.54)}$$

Here $\mu$ is the chemical potential and $\hat{N}$ is the particle number operator. Here we use $\mathcal{H}$ instead of $H$ since in the following we want to perform averages in grand canonical ensemble. This is necessary because the above discussed transition operators change the particle number. However, $H$ and $\hat{N}$ should commute which means they possess a common set of eigenstates:

$$H |E_n(N)\rangle = E_n(N) |E_n(N)\rangle \quad ; \quad \hat{N} |E_n(N)\rangle = N |E_n(N)\rangle$$

Then $\mathcal{H}$ satisfies the eigenvalue equation

$$\mathcal{H} |E_n(N)\rangle = (E_n(N) - \mu N) |E_n(N)\rangle \rightarrow E_n |E_n\rangle \quad \text{(B.55)}$$

In order to save writing effort, in the following, so long as it does not create any confusion, we will write the short forms i.e. for the eigenvalue instead of $(E_n(N) - \mu N)$ write $E_n$ and for the eigenstates instead of $|E_n(N)\rangle$ simply write $|E_n\rangle$. However, the actual dependence of the states and eigenenergies on the particle number should always be kept in mind.

- The system at temperature $T$ finds itself in an eigenstate $|E_n\rangle$ of the Hamiltonian $\mathcal{H}$ with the probability

$$\frac{1}{\Xi} \exp(-\beta E_n)$$

where $\Xi$ is the grand canonical partition function

$$\Xi = Tr (\exp(-\beta \mathcal{H}) \quad \text{(B.56)}$$

- The transition operator $Z_r$ induces transitions between the states $|E_n\rangle$ and $|E_m\rangle$ with the probability

$$|\langle E_m | Z_r | E_n \rangle|^2 \quad r = \pm 1, \pm 2$$
The intensity of the measured elementary process corresponds to the total number of transitions with excitation energies between $E$ and $E + dE$:

$$
I_r(E) = \frac{1}{\Xi} \sum_{m,n} e^{-\beta E_m} \left| \langle E_m | Z_r | E_n \rangle \right|^2 \delta(E - (E_m - E_n))
$$  \hspace{1cm} (B.57)

If the excitation energies are sufficiently dense, as is anyway the case for a solid, then $I_r(E)$ is a continuous function of the energy $E$.

At this point we neglect certain secondary effects, which of course are important for a quantitative analysis of the respective experiments, but are not decisive for the actually interesting processes. This is valid, for example, in PES and AES for the fact that the photoelectron leaving the solid can still couple to the residual system (sudden approximation). In addition, the matrix elements for the transition from band level into vacuum are not taken into account here. However, the bare line forms of the mentioned spectroscopies should be correctly described by (B.57).

One should note that for the transition operator holds

$$
Z_r = Z_{-r}^\dagger
$$  \hspace{1cm} (B.58)

That means complementary spectroscopies are related to each other in some way. This is now investigated in more detail:

$$
I_r(E) = \frac{1}{\Xi} \sum_{m,n} e^{\beta E} e^{-\beta E_m} \left| \langle E_m | Z_r | E_n \rangle \right|^2 \delta(E - (E_m - E_n))
$$

$$
= \frac{1}{\Xi} \sum_{n,m} e^{\beta E} e^{-\beta E_n} \left| \langle E_n | Z_r | E_m \rangle \right|^2 \delta(E - (E_n - E_m))
$$

$$
= e^{\beta E} \sum_{n,m} e^{-\beta E_n} \left| \langle E_m | Z_{-r} | E_n \rangle \right|^2 \delta((-E) - (E_m - E_n))
$$

In the second step only the summation indices $n$ and $m$ are interchanged; the last transition uses (B.58). We then have derived a “symmetry relation” for the complementary spectroscopies:

$$
I_r(E) = e^{\beta E} I_{-r}(-E)
$$  \hspace{1cm} (B.59)

We now define the spectral density which is important for the following:

$$
\frac{1}{\hbar} S_r^{(\pm)}(E) = I_{-r}(E) \mp I_r(-E) = \left( e^{\beta E} \mp 1 \right) I_r(-E)
$$  \hspace{1cm} (B.60)

The freedom in the sign will be explained later. From (B.59) and (B.60) one recognizes that the intensities of the complementary spectroscopies are determined by the
same spectral density in a simple manner:

\[
\hbar I_r(E) = \frac{1}{e^{-\beta E} + 1} S_r^{(\pm)}(-E)
\]  

(B.61)

\[
\hbar I_{-r}(E) = \frac{e^{\beta E}}{e^{-\beta E} + 1} S_r^{(\pm)}(E)
\]  

(B.62)

Thus the just introduced spectral density is closely related to the intensities of spectroscopies. Therefore we want to further investigate this function by performing a Fourier transformation into the time domain:

\[
\frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-i \frac{\hbar}{\pi} E(t-t')} I_{-r}(E)
\]

\[
= \frac{1}{2\pi \hbar} \sum_{m,n} e^{-\beta E_n} e^{-i \frac{\hbar}{\pi} (E_m - E_n)(t-t')} \langle E_m | Z_{-r} | E_n \rangle \langle E_n | Z_r^\dagger | E_m \rangle
\]

\[
= \frac{1}{2\pi \hbar} \sum_{m,n} e^{-\beta E_n} \langle E_m | e^{i \frac{\hbar}{\pi} H(t')} Z_{-r} e^{-i \frac{\hbar}{\pi} H(t')} | E_n \rangle *
\]

\[
* \langle E_n | e^{i \frac{\hbar}{\pi} H(t') Z_r e^{-i \frac{\hbar}{\pi} H(t')} | E_m \rangle
\]

\[
= \frac{1}{2\pi \hbar} \sum_{m,n} e^{-\beta E_n} \langle E_n | Z_{-r} (t) | E_m \rangle \langle E_m | Z_r^\dagger (t') | E_n \rangle
\]

\[
= \frac{1}{2\pi \hbar} \langle Z_{-r} (t) Z_r^\dagger (t') \rangle
\]

Completely analogously one finds

\[
\frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-i \frac{\hbar}{\pi} E(t-t')} I_r(-E) = \frac{1}{2\pi \hbar} \langle Z_r^\dagger (t') Z_r (t) \rangle
\]

That means with (B.60) for the double-time spectral density

\[
S_r^{(\eta)}(t, t') = \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-i \frac{\hbar}{\pi} E(t-t')} S_r^{(\eta)}(E)
\]

\[
= \frac{1}{2\pi} \langle [Z_r(t), Z_r^\dagger(t')]_{-\eta} \rangle
\]  

(B.63)

Here \( \eta = \pm \) is at the moment only an arbitrary sign factor. \([\cdots, \cdots]_{-\eta}\) is either a commutator or an anti-commutator:

\[
[Z_r(t), Z_r^\dagger(t')]_{-\eta} = Z_r(t) Z_r^\dagger(t') - \eta Z_r^\dagger(t') Z_r(t)
\]  

(B.64)
We have shown that spectral density in (B.63) is of central importance for the intensities of spectroscopies. In addition it can also be shown that a generalization of spectral density to arbitrary operators \( \hat{A} \) and \( \hat{B} \) is closely related to the retarded Green’s functions introduced in (B.16). This is also true for the other types of Green’s functions to be defined in the next section. The “spectral density”

\[
S_{AB}^{(\eta)}(t, t') = \frac{1}{2\pi} \left\langle \left[ \hat{A}(t), \hat{B}(t') \right]_{-\eta} \right\rangle
\]

has the same place of importance as the Green’s functions in the many-body theory.

**B.3 Double-Time Green’s Functions**

**B.3.1 Definitions and Equations of Motion**

In order to construct the full Green’s function formalism the retarded Green’s function introduced earlier is not sufficient. One needs two other types:

- **Retarded Green’s function**
  
  \[
  G_{AB}^{ret}(t, t') = \langle \langle A(t); B(t') \rangle \rangle^{ret} = -i \Theta(t - t') \left\langle \left[ A(t), B(t') \right]_{-\eta} \right\rangle
  \]
  \hspace{1cm} (B.66)

- **Advanced Green’s function**
  
  \[
  G_{AB}^{ad}(t, t') = \langle \langle A(t); B(t') \rangle \rangle^{ad} = +i \Theta(t' - t) \left\langle \left[ A(t), B(t') \right]_{-\eta} \right\rangle
  \]
  \hspace{1cm} (B.67)

- **Causal Green’s function**
  
  \[
  G_{AB}^{c}(t, t') = \langle \langle A(t); B(t') \rangle \rangle^{c} = -i \langle T_{\eta} \{ A(t)B(t') \} \rangle
  \]
  \hspace{1cm} (B.68)

The operators here are in their time-dependent Heisenberg picture:

\[
X(t) = e^{\frac{i}{\hbar} \mathcal{H} t} X e^{-\frac{i}{\hbar} \mathcal{H} t}
\]

where, just as in the derivation of the spectral density in the last section, the transformation should be carried out with the grand canonical Hamiltonian \( \mathcal{H} = H - \mu \hat{N} \).

In doing this we assume that \( \mathcal{H} \) is not explicitly dependent on time. The averages are performed in the grand canonical ensemble:

\[
\langle XY \rangle = \frac{1}{\Xi} Tr \left( e^{-\beta \mathcal{H}} XY \right)
\]

\( \Xi \) is the grand canonical partition function (B.56). The choice of the sign \( \eta = \pm \) is arbitrary and appears based on the convenience in a given situation. If \( \hat{A} \) and \( \hat{B} \) are pure Fermi (Bose) operators, then \( \eta = - \) (\( \eta = + \)) is convenient but not necessarily
required. The brackets in (B.66) and (B.67) are anti-commutators in the former case and commutators in the latter case as was fixed in (B.64).

The definition (B.68) of the causal Green’s function contains the Wick’s time ordering operator:

\[ T_\eta \{ A(t)B(t') \} = \Theta(t - t') A(t)B(t') + \eta \Theta(t' - t) B(t')A(t) \] (B.71)

The step function \( \Theta \)

\[ \Theta(t - t') = \begin{cases} 1 & \text{for } t > t' \\ 0 & \text{for } t < t' \end{cases} \] (B.72)

is not defined for equal times. This is reflected in the Green’s functions and so has to be considered later. Because of the averaging in (B.70), the Green’s functions are also temperature dependent. As a result, later, an unusual but convenient relationship between the temperature and time variables will be established.

In addition to the Green’s functions (B.66), (B.67) and (B.68), the spectral density (B.65) is of equal significance.

We now prove “retrospectively” that if \( \mathcal{H} \) is not explicitly dependent on time, then the Green’s functions and the spectral density are homogeneous in time:

\[ \frac{\partial \mathcal{H}}{\partial t} = 0 \quad \Rightarrow \quad G_{AB}^{\text{ret}, \text{ad}, c}(t, t') = G_{AB}^{\text{ret}, \text{ad}, c}(t - t') \] (B.73)

\[ S_{AB}(t, t') = S_{AB}(t - t') \] (B.74)

The proof is complete provided the homogeneity of the “correlation functions”

\[ \langle A(t) B(t') \rangle ; \langle B(t') A(t) \rangle \]

is proved. This is achieved by using the cyclic invariance of trace:

\[
\begin{align*}
\text{Tr} \left( e^{-\beta \mathcal{H}} A(t) B(t') \right) &= \text{Tr} \left( e^{-\beta \mathcal{H}} e^{\frac{i}{\hbar} \mathcal{H} t} e^{\frac{i}{\hbar} \mathcal{H} t'} e^{-\frac{i}{\hbar} \mathcal{H} t'} B e^{-\frac{i}{\hbar} \mathcal{H} t'} e^{\frac{i}{\hbar} \mathcal{H} t'} e^{\frac{i}{\hbar} \mathcal{H} t'} \right) \\
&= \text{Tr} \left( e^{\frac{i}{\hbar} \mathcal{H} t} e^{-\beta \mathcal{H}} e^{\frac{i}{\hbar} \mathcal{H} t} e^{\frac{i}{\hbar} \mathcal{H} t'} e^{-\frac{i}{\hbar} \mathcal{H} t'} e^{\frac{i}{\hbar} \mathcal{H} t'} B \right) \\
&= \text{Tr} \left( e^{-\beta \mathcal{H}} e^{\frac{i}{\hbar} \mathcal{H} t} e^{\frac{i}{\hbar} \mathcal{H} t'} A e^{\frac{i}{\hbar} \mathcal{H} t} e^{\frac{i}{\hbar} \mathcal{H} t'} B \right) \\
&= \text{Tr} \left( e^{-\beta \mathcal{H}} A(t - t') B \right)
\end{align*}
\]

Thus the homogeneity is shown as

\[ \langle A(t) B(t') \rangle = \langle A(t - t') B(0) \rangle \] (B.75)

Analogously one finds

\[ \langle B(t') A(t) \rangle = \langle B(0) A(t - t') \rangle \] (B.76)
For the approximate determination of a Green’s function, one can use the respective equation of motion which is directly derived from the equation of motion of the corresponding time-dependent Heisenberg operators. With

$$\frac{\partial}{\partial t} \Theta(t - t') = \delta(t - t') = -\frac{\partial}{\partial t'} \Theta(t - t')$$  \hspace{1cm} (B.77)

one gets formally the same equation of motion for all the three Green’s functions:

$$i \hbar \frac{\partial}{\partial t} G_{AB}^{ret, ad} (t, t') = \hbar \delta(t - t') \langle [A, B]_{-\eta} \rangle$$

$$+ \langle \langle [A, {\mathcal H}]_- (t); B(t') \rangle \rangle^{ret, ad}$$  \hspace{1cm} (B.78)

The boundary conditions are, however, different:

$$G_{AB}^{ret} (t, t') = 0 \text{ for } t < t'$$  \hspace{1cm} (B.79)
$$G_{AB}^{av} (t, t') = 0 \text{ for } t > t'$$  \hspace{1cm} (B.80)

$$G_{AB}^c (t, t') = \begin{cases} -i \langle A(t - t') B(0) \rangle & \text{for } t > t' \\ -i \eta \langle B(0) A(t - t') \rangle & \text{for } t < t' \end{cases}$$  \hspace{1cm} (B.81)

The boundary conditions for the causal function are quite unmanageable. For that reason this function does not play any role in the equation of motion method. That is why it will not be considered here any more.

On the right-hand side of the equation of motion (B.78) appears a higher Green’s function as \([A, {\mathcal H}]_- (t)\) is itself a time-dependent operator. In some special cases \([A, {\mathcal H}]_- (t) \propto A(t)\) holds. Then an exact solution of the equation of motion is directly possible. However, in general, such a proportionality does not hold. Then the higher Green’s function satisfies its own equation of motion of the form

$$i \hbar \frac{\partial}{\partial t} \langle \langle [A, {\mathcal H}]_- (t); B(t') \rangle \rangle^{ret, ad} =$$

$$= \hbar \delta(t - t') \langle [A, {\mathcal H}]_-, B \rangle_{-\eta} +$$

$$+ \langle \langle [A, {\mathcal H}]_- , {\mathcal H} \rangle_- (t); B(t') \rangle \rangle^{ret, ad}$$  \hspace{1cm} (B.82)

On the right-hand side appears a still higher Green’s function for which again another equation of motion can be written. This leads to an infinite chain of equations of motion which, at some stage, has to be decoupled physically meaningfully.

Going from the time domain into energy domain also does not change anything for this chain of equations. However, with (B.18) and (B.21), one gets a pure algebraic equation which can possibly be of advantage:

$$E \langle \langle A; B \rangle \rangle^\text{ret, ad} = \hbar \langle [A, B]_{-\eta} \rangle + \langle \langle [A, {\mathcal H}]_- ; B \rangle \rangle^\text{ret, ad}$$  \hspace{1cm} (B.83)
The boundary conditions (B.79) and (B.80) manifest themselves as different analytical behaviours of the Green’s functions in the complex $E$-plane. This shall be investigated in detail in the next section.

### B.3.2 Spectral Representations

In order to learn more about the analytical properties of these functions, with the help of the eigenvalues and eigenstates (B.55) of the Hamiltonian $H$, we derive the spectral representations of the retarded and advanced Green’s functions. The eigenstates constitute a complete orthonormal system:

$$\langle E_n | E_m \rangle = \delta_{nm}; \quad \sum_n |E_n\rangle \langle E_n| = \mathbb{1} \quad \text{(B.84)}$$

Using this, we first rewrite the correlation functions $\langle A(t) B(t') \rangle$, $\langle B(t') A(t) \rangle$:

$$\Xi \cdot \langle A(t) B(t') \rangle = \text{Tr} \left\{ e^{-\beta H} A(t) B(t') \right\} = \sum_{n,m} \langle E_n | e^{-\beta H} A(t) B(t') | E_n \rangle \langle E_n | E_m \rangle \langle E_m | B(t') | E_n \rangle$$

$$= \sum_{n,m} e^{-\beta E_n} \langle E_n | A | E_m \rangle \langle E_m | B | E_n \rangle e^{-\frac{i}{\hbar} (E_n - E_m)(t - t')}$$

$$= \sum_{n,m} e^{-\beta E_n} e^{\beta (E_n - E_m)} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle * e^{-\frac{i}{\hbar} (E_n - E_m)(t - t')}$$

In the last step we simply interchanged the summation indices $n$ and $m$. Completely analogously one finds the other correlation function

$$\Xi \cdot \langle B(t') A(t) \rangle = \sum_{n,m} e^{-\beta E_n} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle e^{-\frac{i}{\hbar} (E_n - E_m)(t - t')}$$

Comparing these expressions with the Fourier representation of the spectral density

$$S_{AB}(t, t') = \frac{1}{2\pi} \langle [A(t), B(t')]_{-\eta} \rangle = \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-\frac{i}{\hbar} E(t - t')} S_{AB}(E) \quad \text{(B.85)}$$
we get the important “spectral representation of the spectral density”

$$S_{AB}(E) = \frac{\hbar}{2} \sum_{n,m} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle * e^{-\beta E_n} (e^{\beta E} - \eta) \delta (E - (E_n - E_m)) \quad (B.86)$$

The arguments of the delta functions contain the possible excitation energies! Let us compare this with (B.57), the intensity formula for r-particle spectroscopies and their simple relationships (B.61) and (B.62) with the respective spectral densities.

We now try to express the Green’s functions in terms of spectral density. This is possible with the following representation of the step function:

$$\Theta(t - t') = \frac{i}{2\pi} \int_{-\infty}^{+\infty} dx \frac{e^{-ix(t-t')}}{x + i0^+} \quad (B.87)$$

This is proved using the residue theorem (Problem B.4). Using this we first rewrite the retarded function

$$G_{AB}^{ret}(E) = \int_{-\infty}^{+\infty} d(t - t') e^{\frac{i\hbar}{\pi} E(t-t')} \left(-i \Theta(t - t')\right) (2\pi S_{AB}(t - t'))$$

$$= \int_{-\infty}^{+\infty} d(t - t') e^{\frac{i\hbar}{\pi} E(t-t')} \left(\frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \frac{e^{-ix(t-t')}}{x + i0^+}\right) *$$

$$\left(\frac{1}{\hbar} \int_{-\infty}^{+\infty} dE' S_{AB}(E') e^{\frac{i\hbar}{\pi} E'(t-t')}\right)$$

$$= \int_{-\infty}^{+\infty} dE' S_{AB}(E') \int_{-\infty}^{+\infty} dx \frac{1}{x + i0^+} *$$

$$\left(\frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} d(t - t') e^{\frac{i\hbar}{\pi} (E - E' - \hbar x)(t-t')}\right)$$

$$= \int_{-\infty}^{+\infty} dE' S_{AB}(E') \int_{-\infty}^{+\infty} dx \frac{1}{x + i0^+} \delta(E - E' - \hbar x)$$

$$= \int_{-\infty}^{+\infty} dE' \frac{1}{\hbar} \frac{S_{AB}(E')}{(E - E') + i0^+}$$

This gives the “spectral representation of the retarded Green’s function”:

$$G_{AB}^{ret}(E) = \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{E - E' + i0^+} \quad (B.88)$$
The advanced Green’s function can be treated completely analogously:

\[
G_{AB}^{ad}(E) = \int_{-\infty}^{+\infty} d(t - t') e^{\frac{i}{\hbar} E(t-t')} \left( -\frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \frac{e^{-ix(t-t')}}{x + i0^+} \right) * \left( \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE' S_{AB}(E') e^{-\frac{i}{\hbar} E'(t-t')} \right) \\
= \int_{-\infty}^{+\infty} dE' S_{AB}(E') \int_{-\infty}^{+\infty} dx \frac{-1}{x + i0^+} * \left( \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} d(t - t') e^{\frac{i}{\hbar} (E - E' + \hbar \chi)(t-t')} \right) \\
= \int_{-\infty}^{+\infty} dE' S_{AB}(E') \int_{-\infty}^{+\infty} dx \frac{-1}{x + i0^+} \delta(E - E' + \hbar \chi) \\
= \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{\frac{1}{\hbar}(E - E') - i0^+}
\]

This gives the “spectral representation of the advanced Green’s function”:

\[
G_{AB}^{ad}(E) = \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{E - E' - i0^+} \quad (B.89)
\]

The different sign of \( i0^+ \) in the denominator of the integrand is the only but important difference between the retarded and the advanced functions. The retarded and advanced functions have poles, respectively, in the lower and upper half-planes. This results in different analytical behaviours of the two functions.

\( G_{AB}^{ret}(E) \) in the upper and \( G_{AB}^{av}(E) \) in the lower complex half-plane can be analytically continued!

Finally, we can substitute (B.86) in (B.88) and (B.89):

\[
G_{AB}^{ret}(E) = \frac{\hbar}{\Xi} \sum_{n,m} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle * e^{-\beta E_n} - \eta e^{\beta (E_n - E_m)} - \eta e^{\beta (E_n - E_m)} \pm i0^+ \quad (B.90)
\]

We see that we have meromorphic functions with simple poles at the exact (!) excitation energies of the interacting system. With a suitable choice of the operators \( A \)
and $B$ special poles can be extracted, i.e. $E = E_n - E_m$ appears as a pole only if $\langle E_n | B | E_m \rangle \neq 0$ and $\langle E_m | A | E_n \rangle \neq 0$.

Because of the identical predictive power and the same equation of motion the retarded and advanced functions are considered to be the two branches of a unified Green’s function in the complex plane:

$$G_{AB}(E) = \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{E - E'} = \begin{cases} G_{AB}^{ret}(E), & \text{if } ImE > 0 \\ G_{AB}^{adv}(E), & \text{if } ImE < 0 \end{cases} \quad (B.91)$$

In the following, we want to call this the combined Green’s function. Its poles lie on the real axis.

With the “Dirac identity”,

$$\frac{1}{x - x_0 \pm i0^+} = \mathcal{P} \frac{1}{x - x_0} \mp i\pi \delta(x - x_0) \quad (B.92)$$

where $\mathcal{P}$ represents the Cauchy’s principal value, one finds the following relation between the spectral density and the Green’s functions:

$$S_{AB}(E) = \frac{i}{2\pi} (G_{AB}^{ret}(E) - G_{AB}^{adv}(E)) \quad (B.93)$$

If $S_{AB}(E)$ is real, which it is in many of the important cases (e.g. $B = A^\dagger$), this relation becomes even simpler:

$$S_{AB}(E) = \mp \frac{1}{\pi} ImG_{AB}^{ret}(E) \quad (B.94)$$

Equations (B.88) and (B.89) show that the Green’s functions are completely fixed by the spectral density. On the other hand according to (B.94) only the imaginary part of the Green’s function determines the spectral density. This means there must be relations between the real and the imaginary parts of the Green’s function; they are not independent of each other. These relations are called the Kramers–Kronig relations which we will explicitly derive in Sect. B.3.5.

### B.3.3 Spectral Theorem

The discussion of the last section has shown that the Green’s functions and the spectral density, in addition to their importance in the context of the response functions (Sect. B.1) and intensities of certain spectroscopies, also provide valuable microscopic information. Their singularities correspond to the exact excitation energies of the system. We now want to demonstrate that the whole macroscopic thermodynamics can be determined using suitably defined Green’s functions and spectral densities.
The starting point is the spectral representation of the correlation functions introduced in Sect. B.3.2.

\[ \langle B(t') A(t) \rangle = \frac{1}{\Xi} \sum_{n,m} e^{-\beta E_n} \langle E_n|B|E_m\rangle \langle E_m|A|E_n\rangle e^{-\frac{\eta}{\hbar}(E_n-E_m)(t-t')} \]

Comparing this expression with that for the spectral representation of the spectral density (B.86), we get the fundamental spectral theorem:

\[ \langle B(t') A(t) \rangle = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \frac{S^{(\eta)}_{AB}(E)}{e^{\beta E} - \eta} e^{\frac{\eta}{\hbar} E(t-t')} + \frac{1}{2}(1 + \eta) D \quad \text{(B.95)} \]

Except for the second summand, this result follows directly from the comparison with (B.86). The second term comes into play only for the commutator (\( \eta = +1 \)) spectral density. It disappears for the anti-commutator function (\( \eta = -1 \)). The reason for this is clear from (B.86). For \( E = 0 \), i.e. \( E_n = E_m \), the commutator spectral densities do not contribute the corresponding term because \( (e^{\beta E} - 1) = 0 \), even though they may give a contribution \( \frac{1}{\hbar} D \) unequal zero in the correlation function, where

\[ D = \frac{\hbar}{\Xi} \sum_{n,m} e^{-\beta E_n} \langle E_n|B|E_m\rangle \langle E_m|A|E_n\rangle \quad \text{(B.96)} \]

Experience, however, shows that in fact in many cases \( D = 0 \). But the fact that this is not always necessary is made easily clear from the following example: The operator pairs \( A, B \) and \( \tilde{A} = A - \langle A \rangle I, \tilde{B} = B - \langle B \rangle I \) form identical spectral densities:

\[ S^{(+)}_{AB}(t - t') \equiv S^{(+)}_{\tilde{A}\tilde{B}}(t - t') \quad \text{iff} \quad S^{(+)}_{AB}(E) \equiv S^{(+)}_{\tilde{A}\tilde{B}}(E) \]

On the other hand holds

\[ \langle \tilde{B}(t') \tilde{A}(t) \rangle = \langle B(t') A(t) \rangle - \langle B(t') \rangle \langle A(t) \rangle \]

which would lead to a contradiction without the second term in (B.95) in case \( \langle A(t) \rangle \neq 0 \) and \( \langle B(t') \rangle \neq 0 \). Thus without the extra term \( D \), the spectral theorem would be incomplete for the commutator spectral density.

How does one determine \( D \)? It is possible with the combined Green’s function (B.91) whose spectral representation

\[ G^{(\eta)}_{AB}(E) = \frac{\hbar}{\Xi} \sum_{n,m} \langle E_n|B|E_m\rangle \langle E_m|A|E_n\rangle e^{-\beta E_n} \frac{e^{\beta(E_n-E_m)} - \eta}{E - (E_n - E_m)} \quad \text{(B.97)} \]
leads to the following relation:

\[
\lim_{E \to 0} E \cdot G_{AB}^{(\eta)}(E) = (1 - \eta) D
\]  

(B.98)

The limit must be taken in complex plane. One recognizes the following important consequences:

- Even though \( D \) is needed for the commutator spectral density, the determination succeeds only using the anti-commutator Green’s function.
- The commutator Green’s function \( G_{AB}^{(+)}(E) \) is always regular at \( E = 0 \), i.e. it has no pole there.
- The anti-commutator Green’s function \( G_{AB}^{(-)}(E) \), for \( D \neq 0 \), has a pole of first order with the residue \( 2D \).

**B.3.4 Spectral Moments**

Green’s functions and spectral densities for realistic problems are in general not exactly solvable. Therefore, one must tolerate approximations. These approximations can be checked for correctness by using exactly solvable limiting cases, symmetry relations, sum rules, etc.

In this sense, the moments of spectral density are found to be extraordinarily useful. Let \( n \) and \( p \) be non-negative integers:

\[
n = 0, 1, 2, \cdots \quad ; \quad 0 \leq p \leq n
\]

Then for the time-dependent spectral density holds

\[
\left( i\hbar \frac{\partial}{\partial t} \right)^{n-p} \left( -i\hbar \frac{\partial}{\partial t'} \right)^p (2\pi S_{AB}(t - t')) =
\]

\[
= \left( i\hbar \frac{\partial}{\partial t} \right)^{n-p} \left( -i\hbar \frac{\partial}{\partial t'} \right)^p \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE S_{AB}(E) e^{-\frac{i}{\hbar}E(t-t')}
\]

\[
= \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE E^n S_{AB}(E) e^{-\frac{i}{\hbar}E(t-t')}
\]

\[
= \left( i\hbar \frac{\partial}{\partial t} \right)^{n-p} \left( -i\hbar \frac{\partial}{\partial t'} \right)^p \langle [A(t), B(t')]_{-\eta} \rangle
\]

For \( t = t' \) from the first part of the system of equations one gets the spectral moments

\[
M_{AB}^{(n)} = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE E^n S_{AB}(E)
\]  

(B.99)
An alternative representation results from the last part by using the equation of motion for the time-dependent Heisenberg operators

\[ M_{AB}^{(n)} = \langle \left[ \ldots \left[ A, \mathcal{H}, \ldots, \mathcal{H}, \mathcal{H}, \mathcal{H}, \ldots, \mathcal{H}, \mathcal{H}, B \right] \ldots \right] \rangle^{-(n-p)-\text{fold}}_{-(p-\text{fold})} \]  

(B.100)

With this last relation it is possible in principle to calculate exactly all the moments independently of the respective spectral densities if the Hamiltonian is known. Then one has the possibility to control certain approximate procedures for the spectral density using (B.99).

With the spectral moments, it is possible to formulate a very often useful “high-energy expansion”. For the “combined Green’s function” (B.91) holds

\[ G_{AB}(E) = \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{E' - E} \]

\[ = \frac{1}{E} \int_{-\infty}^{+\infty} dE' \frac{S_{AB}(E')}{1 - \frac{E'}{E}} \]

\[ = \frac{1}{E} \sum_{n=0}^{\infty} \int_{-\infty}^{+\infty} dE' S_{AB}(E') \left( \frac{E}{E'} \right)^n \]

A comparison with (B.99) gives

\[ G_{AB}(E) = \frac{\hbar}{E} \sum_{n=0}^{\infty} \frac{M_{AB}^{(n)}}{E^{n+1}} \]  

(B.101)

For the extreme high-energy behaviour \((E \to \infty)\) this means

\[ G_{AB}(E) \approx \frac{\hbar}{E} M_{AB}^{(0)} = \frac{\hbar}{E} \langle [A, B]_\eta \rangle \]  

(B.102)

The right-hand side is in general easy to calculate and therefore, e.g. the high-energy behaviour of the response functions in Sect. B.1.1 is known.

**B.3.5 Kramer’s–Kronig Relations**

We have already seen that the Green’s function \(G_{AB}^{\text{ret,ad}}(E)\) is completely determined by the spectral density \(S_{AB}(E)\) (B.88) and (B.89). In case it is real, then it can be
The Method of Green’s Functions

538

The Method of Green’s Functions

determined by the imaginary part of the Green’s function alone (B.94). Therefore the real and imaginary parts of the Green’s function cannot be independent of each other. We will now derive the relationship between them.

One calculates the following integral for real $E$

$$I_C(E) = \oint_C d\hat{E} \frac{G_{AB}^{ret}(\hat{E})}{E - \hat{E} - i0^+}$$

Integration is performed over the path $C$ which follows the real axis and is closed in the upper half of the complex plane (Fig. B.3). The integrand has a pole at $\hat{E} = E - i0^+$, i.e. in the lower half-plane. The retarded Green’s function also has a pole only in the lower half-plane so that there is no pole in the region enclosed by $C$. Therefore it holds

$$I_C(E) = 0$$

The semicircle is extended to infinity. The high-energy expansion (B.101) shows that the integrand in (B.103) then goes to zero at least as $1/\hat{E}^2$. As a result, the semicircle does not contribute to the integral (B.103). It remains when the Dirac identity (B.92) is used:

$$0 = \int_{-\infty}^{+\infty} d\hat{E} \frac{G_{AB}^{ret}(\hat{E})}{E - \hat{E} - i0^+} = \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{G_{AB}^{ret}(\hat{E})}{E - \hat{E}} + i\pi G_{AB}^{ret}(E)$$

That means

$$G_{AB}^{ret}(E) = i\pi \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{G_{AB}^{ret}(\hat{E})}{E - \hat{E}}$$

Completely analogous considerations hold for the advanced function $G_{AB}^{ad}(E)$. Now the semicircle will be in the lower half-plane and in the denominator of the integrand (B.103) $-i0^+$ is replaced by $+i0^+$. Then we have

---

**Fig. B.3** Integration path $C$ in the complex $E$-plane for the integral (B.103)
\[ G_{AB}^{ad}(E) = -\frac{i}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{G_{AB}^{ad}(\hat{E})}{E - \hat{E}} \]  (B.106)

Thus it is not at all necessary to know the full Green’s function. The real and imaginary parts account for each other (“Kramers–Kronig relations”)

\[ \text{Re} G_{AB}^{ret}(E) = \mp \frac{i}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{\text{Im} G_{AB}^{ad}(\hat{E})}{E - \hat{E}} \]  (B.107)

\[ \text{Im} G_{AB}^{ret}(E) = \pm \frac{i}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{\text{Re} G_{AB}^{ad}(\hat{E})}{E - \hat{E}} \]  (B.108)

In case the respective spectral density is real the additional relation (B.94) holds. That leads to

\[ \text{Im} G_{AB}^{ret}(E) = -\text{Im} G_{AB}^{ad}(E) = -\pi S_{AB}(E) \]  (B.109)

\[ \text{Re} G_{AB}^{ret}(E) = \text{Re} G_{AB}^{ad}(E) = \mathcal{P} \int_{-\infty}^{+\infty} d\hat{E} \frac{S_{AB}(\hat{E})}{E - \hat{E}} \]  (B.110)

The retarded and advanced Green’s functions are therefore very closely related.

### B.3.6 Simple Applications

We want to apply the above introduced Green’s function formalism to two simple systems.

#### B.3.6.1 Free Band Electrons

As the first example, we discuss a system of electrons in a solid which do not interact with each other, interacting only with a periodic lattice potential. This is described by the following one-particle Hamiltonian:

\[ \hat{H}_0 = H_0 - \mu \hat{N} \quad , \quad H_0 = \sum_{k\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} \]  (B.111)

\[ \hat{N} = \sum_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} \]  (B.112)

All the interesting properties of the electron system can be calculated from the so-called one-electron Green’s function:
\begin{align}
G_{k\sigma}^{ret,ad}(E) &= \langle \langle c_{k\sigma}; c_{k\sigma}^\dagger \rangle \rangle^{ret,ad}_E 
\tag{B.113}
\end{align}

Since we are dealing with a pure Fermi system, the choice of the anti-commutator Green’s function is natural, however, not mandatory.

The first step is setting up the equation of motion (B.83):

\begin{align}
E \ G_{k\sigma}^{ret,ad}(E) &= \hbar \langle [c_{k\sigma}, \ c_{k\sigma}^\dagger]_+ \rangle + \langle \langle [c_{k\sigma}, \ H_0]_-; c_{k\sigma}^\dagger \rangle \rangle^{ret,ad}_E 
\tag{B.114}
\end{align}

With the help of the fundamental commutation relations for Fermions, one easily gets

\begin{align}
[c_{k\sigma}, \ H_0]_- &= (\varepsilon(k) - \mu) \ c_{k\sigma} 
\tag{B.115}
\end{align}

On substituting this leads to a simple equation of motion

\begin{align}
E \ G_{k\sigma}^{ret,ad}(E) &= \hbar + (\varepsilon(k) - \mu) \ G_{k\sigma}^{ret,ad}(E) 
\end{align}

Solving this and introducing \( \pm i0^+ \) in order to satisfy the boundary conditions one gets

\begin{align}
G_{k\sigma}^{ret,ad}(E) &= \frac{\hbar}{E - (\varepsilon(k) - \mu) \pm i0^+} 
\tag{B.116}
\end{align}

The Green’s function is singular at the energy which is required to add an electron of wavevector \( k \) to the non-interacting electron system. That means the singularities of the Green’s function (B.113) correspond to the one-particle excitations of the system. The combined Green’s function is naturally directly given from (B.116) by removing the infinitesimal imaginary term:

\begin{align}
G_{k\sigma}(E) &= \frac{\hbar}{E - (\varepsilon(k) - \mu)} 
\tag{B.117}
\end{align}

The energy \( E \) is thought to be complex here. It is interesting to confirm the result (B.117) by an exact evaluation of high-energy expansion (B.101) (Problem B.7).

Finally the one-electron spectral density is another important quantity, for which with the Dirac identity (B.92) along with (B.94) directly from (B.116) follows:

\begin{align}
S_{k\sigma}(E) &= \hbar \delta (E - \varepsilon(k) + \mu) 
\tag{B.118}
\end{align}

Using the spectral theorem (B.95) one can easily calculate the average occupation number of the \((k, \sigma)\)-level:

\begin{align}
\langle n_{k\sigma} \rangle = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle &= \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \frac{S_{k\sigma}(E)}{\epsilon^\beta E + 1} = \frac{1}{e^{\beta(\varepsilon(k) - \mu)} + 1} 
\tag{B.119}
\end{align}
B.3 Double-Time Green's Functions

This is of course a well-known result of quantum statistics. The average occupation number is given by the Fermi function $f_-(E) = (e^{\beta(E - \mu)} + 1)^{-1}$ at $E = \epsilon(k)$.

From $\langle n_{k\sigma} \rangle$ by summing over all the wavevectors $k$ and the two spin projections $\sigma$ we can fix the total number of electrons $N_e$:

$$N_e = \sum_{k\sigma} \langle n_{k\sigma} \rangle = \sum_{k\sigma} \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \frac{S_{k\sigma}(E)}{e^{\beta E} + 1}$$

$$= \sum_{k\sigma} \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE f_-(E) S_{k\sigma}(E - \mu)$$

We denote by $\rho_\sigma(E)$ the density of states per spin, where self-evidently for the free Fermion system $\rho_\sigma(E) \equiv \rho_{-\sigma}(E)$ holds, so that we can write $N_e$ as

$$N_e = N \sum_\sigma \int_{-\infty}^{+\infty} dE f_-(E) \rho_\sigma(E)$$

Here $N$ is the number of lattice sites with which $\rho_\sigma(E)$ is normalized to 1 since the number of energy band states per each spin direction should be equal to the number of lattice sites. The comparison of the last two equations leads to the important definition of the “quasiparticle density of states”:

$$\rho_\sigma(E) = \frac{1}{N\hbar} \sum_k S_{k\sigma}(E - \mu)$$

(B.120)

In the case of the non-interacting electrons considered here with (B.118)

$$\rho_\sigma(E) = \rho_{-\sigma}(E) \equiv \rho_0(E) = \frac{1}{N} \sum_k \delta(E - \epsilon(k))$$

(B.121)

follows. Without the lattice potential, for the one-particle energies we get the well-known parabolic dispersion $\epsilon(k) = \frac{h^2k^2}{2m}$. One can then easily show that the density of states has a $\sqrt{E}$-dependence.

The considerations for the electron number are correct not only for free electron system but also valid in general. That is why (B.120) will be accepted as the general (!) definition of the quasiparticle density of states for any interacting electron system.

The “internal energy” $U$ as the thermodynamic expectation value of the Hamiltonian is fixed in a simple manner by $\langle n_{k\sigma} \rangle$:
\[ U = \langle H_0 \rangle = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) \langle n_{\mathbf{k}\sigma} \rangle \]
\[ = \frac{1}{\hbar} \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) \int_{-\infty}^{+\infty} dE f_-(E) S_{\mathbf{k}\sigma}(E - \mu) \]
\[ = \frac{1}{2\hbar} \sum_{\mathbf{k}\sigma} \int_{-\infty}^{+\infty} dE \frac{1}{E + \varepsilon(\mathbf{k})} f_-(E) S_{\mathbf{k}\sigma}(E - \mu) \quad (B.122) \]

The bit more complicated representation of the last line will turn out to be the definition of \( U \) which is valid in general for an interacting electron system (see B.4.5).

Finally the time-dependent functions are interesting. For the spectral density (B.118), it is trivial to perform the Fourier transformation:

\[ S_{\mathbf{k}\sigma}(t - t') = \frac{1}{2\pi} \exp \left( -i \frac{\hbar}{i} (\varepsilon(\mathbf{k}) - \mu)(t - t') \right) \quad (B.123) \]

This represents an undamped oscillations with a frequency that corresponds to an exact excitation energy of the system (Fig. B.4). This is typical for non-interacting particle systems. Exactly similarly we find the time-dependent Green’s functions:

\[ G_{\mathbf{k}\sigma}^{ret}(t, t') = -i \Theta(t - t') \exp \left( -i \frac{\hbar}{i} (\varepsilon(\mathbf{k}) - \mu)(t - t') \right) \quad (B.124) \]

\[ G_{\mathbf{k}\sigma}^{av}(t, t') = +i \Theta(t' - t) \exp \left( -i \frac{\hbar}{i} (\varepsilon(\mathbf{k}) - \mu)(t - t') \right) \quad (B.125) \]

![Fig. B.4 Time dependence of the real part of the single-particle spectral density of non-interacting Bloch electrons](image-url)
B.3.6.2 Spin Waves

As another example we consider the (linear) spin waves (magnons) of a ferromagnet. At low temperatures the Heisenberg Hamiltonian (7.1) can be simplified in the Holstein–Primakoff approximation (7.1.1) as follows:

\[ H_{SW} = E_0 + \sum_q \hbar \omega(q) a_q^\dagger a_q \]  

(B.126)

\( a_q^\dagger(a_q) \) are the creation (annihilation) operators for magnons. According to this, the ferromagnet is modelled as a gas of non-interacting magnons with one-particle energies

\[ \hbar \omega(q) = 2 S \hbar^2 (J_0 - J(q)) + g J \mu_B B_0 \]  

(B.127)

\( J(q) \) are the exchange integrals with \( J_0 = J(q = 0) \). The second summand describes the influence of an external magnetic field on the one-particle energies. A precondition for the concept of spin waves is that at \( T = 0 \) the system is ferromagnetic (\( E_0 : \) ground state energy (7.246)). A symmetry breaking field

\[ B_0 \geq 0^+ \]  

(B.128)

has to be present necessarily.

Particle number conservation does not hold for magnons. At a given temperature \( T \), it gives exactly the magnon number for which the free energy is minimum:

\[ \left( \frac{\partial F}{\partial N} \right)_{T,V} = 0 \]  

(B.129)

The differential fraction on the left-hand side is just the definition of the chemical potential \( \mu \). So for magnons holds

\[ \mu = 0 \]  

(B.130)

This means that we can substitute \( \mathcal{H} = H - \mu \hat{N} = H \) in the equation of motion for the Green’s function. We need the commutator

\[ [a_q, H_{SW}]_- = \sum_{q'} \hbar \omega(q') \left[ a_q^\dagger a_q^\dagger a_q \right]_- \]

\[ = \sum_{q'} \hbar \omega(q') \left[ a_q^\dagger a_q^\dagger \right]_- a_q \]

\[ = \hbar \omega(q) a_q \]

Then the equation of motion becomes very simple:

\[ E G^{ret,av}_q(E) = \hbar + \hbar \omega(q) G^{ret,av}_q(E) \]
Solving it along with the boundary conditions then gives

\[ G_{q}^{ret,av}(E) = \frac{\hbar}{E - \hbar \omega(q) \pm i0^+} \]  \hspace{1cm} (B.131)

Here also the pole represents the excitation energy which indicates either a creation or annihilation of a \( q \)-magnon. That is exactly \( \hbar \omega(q) \) in the absence of interaction. With (B.92) and (B.94), the important “one-magnon spectral density” follows:

\[ S_q(E) = \hbar \delta(E - \hbar \omega(q)) \]  \hspace{1cm} (B.132)

One can quickly calculate the time-dependent function and see that it represents as in the case of free Bloch electrons, an undamped oscillation:

\[ S_q(t-t') = \frac{1}{2\pi} \exp(-i\omega(q)(t-t')) \]  \hspace{1cm} (B.133)

The frequency of oscillation again corresponds to an exact excitation energy of the system.

With the help of the spectral theorem (B.95) and the spectral density (B.132) we obtain the “magnon occupation density”:

\[ m_q = \langle a_q^\dagger a_q \rangle = \frac{1}{\exp(\beta \hbar \omega(q)) - 1} + D_q \]  \hspace{1cm} (B.134)

As we started with the commutator Green’s function, we must determine the constant \( D_q \) using the respective anti-commutator Green’s function. The fundamental commutation relation for Bosons give for the inhomogeneity in the equation of motion

\[ \langle [a_q, a_q^\dagger]_+ \rangle = 1 + 2m_q \]

Except for this the anti-commutator Green’s function satisfies the same equation of motion as the commutator Green’s function. One obtains

\[ G_q^{(-)}(E) = \frac{\hbar(1 + 2m_q)}{E - \hbar \omega(q)} \]  \hspace{1cm} (B.135)

In the presence of at least an infinitesimal symmetry breaking external field \( (B_0 \geq 0) \), the magnon energies are always unequal zero and are positive. That according to (B.98) means

\[ 2\hbar D_q = \lim_{E \to 0} E G_q^{(-)}(E) = 0 \]

So that for the occupation density we get

\[ m_q = \frac{1}{\exp(\beta \hbar \omega(q)) - 1} \]  \hspace{1cm} (B.136)
This is the Bose–Einstein distribution function which is a well-known result of elementary quantum statistics for the ideal Bose gas.

B.4 The Quasiparticle Concept

The really interesting many-body problems unfortunately can not be solved exactly. Therefore one must tolerate approximations. For describing the interacting many-particle systems, the concept of “quasiparticles” has proved to be very successful and will be discussed in this section. The basis for this is the following idea:

complex interacting systems of “real” particles
\Rightarrow non- (or weakly-) interacting system of quasiparticles

This replacement is valid only if one assigns certain special properties to the quasiparticles which will be discussed in the following:

- energy renormalization;
- damping, finite lifetimes;
- effective masses;
- spectral weights, etc.

B.4.1 Interacting Electrons

In order to be concrete, we here want to concentrate on a system of electrons in a non-degenerate energy band interacting via Coulomb interaction. For such a system holds in Bloch representation:

\[ H = H - \mu \hat{N} \quad ; \quad \hat{N} = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} \] (B.137)

\[ H = \sum_{k\sigma} \varepsilon(k) c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2} \sum_{kpq\sigma\sigma'} v_{kp}(q) c_{k+q\sigma}^\dagger c_{p-q\sigma'}^\dagger c_{p\sigma'} c_{k\sigma} \] (B.138)

Let the matrix elements be built with Bloch functions \( \psi_k(r) \):

\[ \varepsilon(k) = \int d^3r \psi_k^\ast(r) \left[ -\frac{\hbar^2}{2m} \Delta + V(r) \right] \psi_k(r) \] (B.139)

\[ v_{kp}(q) = \frac{1}{4\pi \varepsilon_0} \int \int d^3r_1 d^3r_2 \frac{\psi_{k+q}^\ast(r_1) \psi_{p-q}^\ast(r_2) \psi_p(r_2) \psi_k(r_1)}{|r_1 - r_2|} \] (B.140)

\[ v_{kp}(q) = v_{pk}(-q) \] (B.141)
Fig. B.5 Diagram of the Coulomb interaction between electrons of a non-degenerate energy band

All the wavevectors $\mathbf{k}$, $\mathbf{p}$, $\mathbf{q}$ stem from the first Brillouin zone. Actually the detailed structure and interpretation of the matrix elements is not important for the following considerations. What is decisive is that the interaction (Fig. B.5) makes the problem definitely unsolvable. In spite of that, is it possible to make a few basic statements?

We will see in the following that also for interacting electrons the one-electron Green’s function can provide a large part of the interesting information:

$$G^{\text{ret,ad}}_{\mathbf{k}\sigma}(E) = \langle \langle c_{\mathbf{k}\sigma}; c_{\mathbf{k}\sigma}^\dagger \rangle \rangle^\text{ret,ad}_E$$ (B.142)

Completely equivalent to this is the one-electron spectral density:

$$S_{\mathbf{k}\sigma}(E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt' e^{-\frac{i}{\hbar} E(t-t')} \langle \left[ c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}^\dagger(t') \right]_+ \rangle$$ (B.143)

We want to determine the spectral density using the equation of motion of the Green’s function, where from now onwards, we consider only the retarded Green’s function and for convenience, drop the index $\text{ret}$. Starting point is the following commutator whose derivation is suggested as an exercise (Problem B.6):

$$[c_{\mathbf{k}\sigma}, \mathcal{H}]_- = (\varepsilon(\mathbf{k}) - \mu) c_{\mathbf{k}\sigma} + \sum_{pq\sigma'} v_{pq\sigma'}(\mathbf{q}) c_{\mathbf{p}+\mathbf{q}\sigma'}^\dagger c_{\mathbf{p}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}$$ (B.144)

With the higher Green’s function

$$\Gamma^{\sigma'\sigma}_{\mathbf{p}\mathbf{k},\mathbf{q}}(E) = \langle \langle c_{\mathbf{p}+\mathbf{q}\sigma'}^\dagger c_{\mathbf{p}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}; c_{\mathbf{k}\sigma}^\dagger \rangle \rangle_E$$ (B.145)

the equation of motion reads as

$$(E - \varepsilon(\mathbf{k}) + \mu) G_{\mathbf{k}\sigma}(E) = \hbar + \sum_{pq\sigma'} v_{pq\sigma}(\mathbf{q}) \Gamma^{\sigma'\sigma}_{\mathbf{p}\mathbf{k},\mathbf{q}}(E)$$ (B.146)

The function $\Gamma$ prevents the exact solution. A formal solution, however, is possible with the following separation
\( \langle \langle [c_{k\sigma}, \mathcal{H} - \mathcal{H}_0]_-; c^\dagger_{k\sigma} \rangle \rangle_E \equiv \Sigma_{k\sigma}(E) \cdot G_{k\sigma}(E) \)  

(B.147)

This equation defines the fundamental “self-energy” which, in general, is a complex function:

\[ \Sigma_{k\sigma}(E) = R_{k\sigma}(E) + i \cdot I_{k\sigma}(E) \]  

(B.148)

With this we can now write the Green’s function as follows:

\[ G_{k\sigma}(E) = \frac{\hbar}{E - (\varepsilon(k) - \mu + \Sigma_{k\sigma}(E))} \]  

(B.149)

One should note that in case the self-energy is real, one has to include the term +i0+ in the denominator. Let it be mentioned as a side remark that because of the Kramers–Kronig relations (B.109) and (B.110), \( (G^{\text{eq}}_{k\sigma}(E))^* = G^{\text{ret}}_{k\sigma}(E) \) follows. Then it must also hold:

\[ (\Sigma_{k\sigma}^* (E))^* = \Sigma_{k\sigma}^{\text{ret}}(E) \]  

(B.150)

We can therefore restrict the discussion to only the retarded self-energy. For simplicity we from now on drop the index \( \text{ret} \).

If we switch off the interaction, then we get the Green’s function for the free system (B.116) which we want to denote by \( G_{k\sigma}^{(0)}(E) \):

\[ G_{k\sigma}^{(0)}(E) = \frac{\hbar}{E - (\varepsilon(k) - \mu) + i0^+} \]  

(B.151)

So the total influence of the interaction is contained in the self-energy, whose knowledge solves the many-body problem. If (B.150) is substituted in (B.149) then we have

\[ \hbar \left( G_{k\sigma}^{(0)}(E) \right)^{-1} G_{k\sigma}(E) = \hbar + \Sigma_{k\sigma}(E) G_{k\sigma}(E) \]

This leads to the “Dyson equation”:

\[ G_{k\sigma}(E) = G_{k\sigma}^{(0)}(E) + G_{k\sigma}^{(0)}(E) \frac{1}{\hbar} \Sigma_{k\sigma}(E) G_{k\sigma}(E) \]  

(B.152)

This equation can be solved by iteration up to any given accuracy by knowing (approximately) the self-energy:

\[ G_{k\sigma}(E) = G_{k\sigma}^{(0)}(E) + G_{k\sigma}^{(0)}(E) \sum_{n=1}^{\infty} \left( \frac{1}{\hbar} \Sigma_{k\sigma}(E) G_{k\sigma}^{(0)}(E) \right)^n \]  

(B.153)
B.4.2 Electronic Self-energy

We want to try to get a picture of the general structure of the fundamental many-body terms such as self-energy, Green’s function and spectral density, without being able to calculate explicitly the influence of the interaction. In doing this we want to restrict to the retarded functions whose relationship with other types is simple because of the Kramers–Kronig relations (see (B.150)). First we rewrite a bit the formal solution for the Green’s function using (B.149):

\[ G_{k\sigma}(E) = \frac{\hbar [E - \varepsilon(k) + \mu - R_{k\sigma}(E)] + i I_{k\sigma}(E)}{[E - \varepsilon(k) + \mu - R_{k\sigma}(E)]^2 + I_{k\sigma}^2(E)} \]

\[ S_{k\sigma}(E) \text{ is real and non-negative as one can easily see from the spectral representation (B.86) for the case } A = c_{k\sigma} \text{ und } B = c_{k\sigma}^\dagger. \text{ Then holds (B.94)} \]

\[ S_{k\sigma}(E) = -\frac{\hbar}{\pi} \frac{I_{k\sigma}(E)}{[E - \varepsilon(k) + \mu - R_{k\sigma}(E)]^2 + I_{k\sigma}^2(E)} \]  \hspace{1cm} (B.154)

Obviously for the imaginary part of the self-energy must hold

\[ I_{k\sigma}(E) \leq 0 \]  \hspace{1cm} (B.155)

In the following we want to analyse spectral density for the argument \( E - \mu \) and we expect prominent maxima at points of resonances given by

\[ E_{n\sigma}(k) - \varepsilon(k) - R_{k\sigma}(E_{n\sigma}(k) - \mu) = 0 \hspace{0.5cm} n = 1, 2, \ldots \]  \hspace{1cm} (B.156)

We must distinguish two cases:

(a) In the immediate \( E \)-neighbourhood of a resonance let

\[ I_{k\sigma}(E - \mu) \equiv 0 \]  \hspace{1cm} (B.157)

Then with \( I_{k\sigma} \rightarrow -0^+ \) and the well-known expression

\[ \delta(E - E_0) = \frac{1}{\pi} \lim_{x \rightarrow 0} \frac{x}{(E - E_0)^2 + x^2} \]  \hspace{1cm} (B.158)

for the delta function, the following representation holds for the spectral density:

\[ S_{k\sigma}(E - \mu) = \hbar \delta \left( E - \varepsilon(k) - R_{k\sigma}(E - \mu) \right) \]  \hspace{1cm} (B.159)

For the case where there lies more than one resonance in the region under consideration (B.157), we use another well-known property of the delta function:
\[ \delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i) \quad ; \quad f(x_i) = 0 \]  

\( x_i \) are the zeros of the function \( f(x) \). With this holds

\[ S_{k\sigma}(E - \mu) = \hbar \sum_{n=1}^{n_0} \alpha_{n\sigma}(k) \delta(E - E_{n\sigma}(k)) \]  

(B.161)

where the coefficients \( \alpha_{n\sigma}(k) \) are known as spectral weights.

\[ \alpha_{n\sigma}(k) = \left| 1 - \frac{\partial}{\partial E} R_{k\sigma}(E - \mu) \right|^{-1} \]  

(B.162)

Summation is over all resonances that lie in the region (B.157). Thus the spectral density appears as a linear combination of positively weighted delta functions in whose arguments the resonance energies appear.

(b) Now let it hold

\[ I_{k\sigma}(E - \mu) \neq 0 \]  

(B.163)

It may still be assumed that, however, in the immediate neighbourhood of a resonance holds:

\[ |I_{k\sigma}(E - \mu)| \ll |\epsilon(k) + R_{k\sigma}(E - \mu)| \]  

(B.164)

Then a more or less prominent maximum is to be expected at \( E = E_{n\sigma}(k) \). We therefore expand the bracket in the denominator of (B.154):

\[ E_{n\sigma}(k) - \epsilon(k) - R_{k\sigma}(E_{n\sigma}(k) - \mu) = 0 + (E - E_{n\sigma}(k)) \left( 1 - \frac{\partial}{\partial E} R_{k\sigma}(E - \mu) \right)_{E=E_{n\sigma}(k)} + \mathcal{O}((E - E_{n\sigma}(k))^2) \]

We substitute this in (B.154) and also further assume that the imaginary part of the self-energy is a well-behaved function of energy, so that we can further simplify in the immediate neighbourhood of the resonance:

\[ I_{k\sigma}(E - \mu) \approx I_{k\sigma}(E_{n\sigma}(k) - \mu) \equiv I_{n\kappa \sigma} \]  

(B.165)

This gives in the surroundings of resonance a Lorentzian structure of the spectral density:

\[ S_{k\sigma}^{(n)}(E - \mu) \approx -\frac{\hbar}{\pi} \frac{\alpha_{n\sigma}^2 I_{n\kappa \sigma}}{(E - E_{n\sigma}(k))^2 + (\alpha_{n\sigma} I_{n\kappa \sigma})^2} \]  

(B.166)
The results (B.161) and (B.166) lead finally to the classical quasiparticle picture. Under the assumptions (B.164) and (B.165) the spectral density is made up of one or more Lorentz curves or delta functions, whose widths and positions are to a large extent determined by the imaginary and the real parts of the self-energy, respectively. However, the assumptions made are not verifiable directly but only after the complete solution of the many-body problem.

We want to physically interpret the general structure of the spectral density as depicted in Fig. B.6. For this, a Fourier transformation into the time domain is very useful:

\[
S_{k\sigma}(t - t') = \frac{1}{2\pi \hbar} \int_{-\infty}^{+\infty} dE e^{-\frac{i}{\hbar}(E - \mu)(t - t')} S_{k\sigma}(E - \mu) \tag{B.167}
\]

This acquires a particularly simple structure for the case (A). With (B.161) follows directly

\[
S_{k\sigma}(t - t') = \frac{1}{2\pi} \sum_{n=1}^{n_0} \alpha_{n\sigma}(k) \exp \left( -\frac{i}{\hbar}(E_{n\sigma}(k) - \mu)(t - t') \right) \tag{B.168}
\]

Thus it is a sum of undamped oscillations with frequencies which correspond to the resonance energies. This is similar to the result (B.123) depicted in Fig. B.4 for the non-interacting electron system.

The transformation of the function of type B is a little more complicated. For simplicity, we will assume that the Lorentz structure (B.166) is valid over the entire energy range for the spectral density \( S_{k\sigma}^{(n)}(E - \mu) \):

\[
S_{k\sigma}^{(n)}(t - t') \approx \frac{1}{4\pi^2 i} \int_{-\infty}^{+\infty} dE e^{-\frac{i}{\hbar}(E - \mu)(t - t')} \alpha_{n\sigma}(k) \star \left[ \frac{1}{E - (E_{n\sigma}(k) - i\alpha_{n\sigma}(k)I_{nk\sigma})} - \frac{1}{E - (E_{n\sigma}(k) + i\alpha_{n\sigma}(k)I_{nk\sigma})} \right] \tag{B.169}
\]

Fig. B.6 Classical quasiparticle picture of the single-electron spectral density
The evaluation is done using the residue theorem noting that $\alpha_{n\sigma}(k) I_{nk\sigma} \leq 0$. Therefore the first summand has a pole in the upper and the second summand in the lower half-plane. For $(t - t') > 0$ the integral in (B.169) is replaced by a contour integral where the path of integration runs along the real axis and closes with an infinite semicircle in the lower half-plane. Only the second summand in (B.169) then has a pole in the region enclosed by the integration path. The semicircle has no contribution because of the exponential function. For $(t - t') < 0$, for the same reason, the semicircle must be in the upper half-plane. In this region only the first summand in (B.169) has a pole. Then finally the residue theorem gives

$$S_{k\sigma}^{(n)}(t - t') \approx \frac{2\pi i}{4\pi^2} \alpha_{n\sigma}(k)e^{-\frac{i}{\hbar}(E_{n\sigma}(k) - \mu)(t - t')} *$$

$$* \left[ \Theta(t - t') e^{\frac{i}{\hbar}\alpha_{n\sigma}(k) I_{nk\sigma}(t - t')} + \Theta(t' - t) e^{-\frac{i}{\hbar}\alpha_{n\sigma}(k) I_{nk\sigma}(t - t')} \right]$$

This can obviously be summarized to

$$S_{k\sigma}^{(n)}(t - t') \approx \frac{1}{2\pi} \alpha_{n\sigma}(k) \exp \left( -\frac{i}{\hbar}(E_{n\sigma}(k) - \mu)(t - t') \right) *$$

$$* \exp \left( -\frac{1}{\hbar} |\alpha_{n\sigma}(k) I_{nk\sigma}(t - t')| \right)$$

(B.170)

It now represents a “damped” oscillation. The frequency corresponds again to a resonance energy. The amount of damping is determined by the imaginary part $I_{nk\sigma}$ of the self-energy. $I_{nk\sigma} \to 0$ reproduces the result (B.108).

The time-dependent spectral density $S_{k\sigma}(t - t')$ for the interacting electron system consists of an overlap of damped and undamped oscillations with frequencies which correspond to the resonances $E_{n\sigma}(k)$. The resulting total time dependence can be naturally quite complicated. In the next section we want to make it clear what these (un)damped oscillations have to do with quasiparticles.

**B.4.3 Quasiparticles**

What does one understand by quasiparticles in many-body theory? It certainly has something to do with the resonance peaks discussed in the last section and shall at least be qualitatively explained here. For that, for simplicity, we consider the special case:

$$T = 0; \quad |k| > k_F; \quad t > t'$$

(B.171)

That means, we assume that there is something like a Fermi edge. In the case of non-interacting electrons it is just the Fermi wavevector, which is the radius of the Fermi sphere. $|k| > k_F$ here means only that at $T = 0$ the one-particle state
with \( |k| \) is unoccupied. Let the system be in the normalized ground state \( |E_0\rangle \). At time \( t' \) a \((k, \sigma)\)-electron is introduced into the \( N \)-particle system. The resulting state

\[
|\varphi_0(t')\rangle = c_k^{\dagger}(t')|E_0\rangle
\]

is not necessarily an eigenstate of the Hamiltonian \( H \). What happens to it in course of time? Because \( |k| > k_F \), we have \( c_k(0)|E_0\rangle = 0 \). Therefore the spectral density simplifies to

\[
2\pi S_{k\sigma}(t-t') = \langle E_0 | [c_{k\sigma}(t), c_{k\sigma}^{\dagger}(t')]_+ |E_0\rangle = \langle \varphi_0(t) | \varphi_0(t') \rangle
\]

The spectral density is therefore the probability amplitude that the state that resulted by introducing of \((k, \sigma)\)-electron at time \( t' \) still exists at time \( t > t' \). That means it describes the “propagation” of an “extra electron” in an \( N \)-electron system. Similarly, for \( |k| < k_F \), the spectral density would describe the propagation of a \textit{hole}.

As typical limiting cases one recognizes

\[
\begin{align*}
\langle \varphi_0(t) | \varphi_0(t') \rangle^2, & \quad \text{"stationary state"} \\
\langle \varphi_0(t) | \varphi_0(t') \rangle^2 \rightarrow \infty, & \quad \text{"state with finite lifetime"}
\end{align*}
\]

First let us consider once again the case of non-interacting (band-)electrons of Sect. B.3.6.1 with the Hamiltonian (B.111) for the special case (B.171). Using the commutator (B.115) we show that \( c_{k\sigma}^{\dagger}|E_0\rangle \) is an eigenstate of \( \mathcal{H}_0 \)

\[
\mathcal{H}_0 \left( c_{k\sigma}^{\dagger}|E_0\rangle \right) = c_{k\sigma}^{\dagger} \mathcal{H}_0 |E_0\rangle + \left[ \mathcal{H}_0, c_{k\sigma}^{\dagger} \right]_+ |E_0\rangle = (E_0 + \varepsilon(k) - \mu) (c_{k\sigma}^{\dagger}|E_0\rangle)
\]

With this we calculate

\[
|\varphi_0(t)\rangle = \exp \left( \frac{i}{\hbar} \mathcal{H}_0 t \right) c_{k\sigma}^{\dagger} \exp \left( -\frac{i}{\hbar} \mathcal{H}_0 t \right) |E_0\rangle
\]

\[
= \exp \left( -\frac{i}{\hbar} E_0 t \right) \exp \left( \frac{i}{\hbar} \mathcal{H}_0 t \right) \left( c_{k\sigma}^{\dagger} |E_0\rangle \right)
\]

\[
= \exp \left( -\frac{i}{\hbar} E_0 t \right) \exp \left( \frac{i}{\hbar} (E_0 + \varepsilon(k) - \mu) t \right) \left( c_{k\sigma}^{\dagger} |E_0\rangle \right)
\]

Then it holds

\[
|\varphi_0(t)\rangle = \exp \left( \frac{i}{\hbar} (\varepsilon(k) - \mu) t \right) |\varphi_0(t = 0)\rangle
\]
Let us consider further the normalization of the state:

\[
\langle \phi_0(t = 0) | \phi_0(t = 0) \rangle = \langle E_0 | c_{k\sigma} \, c_{k\sigma}^\dagger | E_0 \rangle = \langle E_0 | E_0 \rangle - \langle E_0 | c_{k\sigma}^\dagger \, c_{k\sigma} | E_0 \rangle = \langle E_0 | E_0 \rangle = 1
\]

We finally get for the probability amplitude

\[
\langle \phi_0(t) | \phi_0(t') \rangle = \exp\left(-\frac{i}{\hbar} (\varepsilon(k) - \mu)(t - t')\right) = 2\pi S_{k\sigma}^{(0)}(t - t') \quad (B.175)
\]

This naturally agrees exactly with the result (B.123) which we have found in Sect. B.3.6.1 using the equation of motion method for the free band electrons. It gives the undamped harmonic oscillations shown in Fig. B.4. In particular we have

\[
| \langle \phi_0(t) | \phi_0(t') \rangle |^2 = 1 \quad (B.176)
\]

Thus, for the case of free electrons it is a stationary state. This is not surprising because \( |\phi_0 \rangle = c_{k\sigma}^\dagger | E_0 \rangle \) turns out to be an eigenstate of \( \mathcal{H}_0 \). It is, however, no more the case for interacting (band-) electrons.

This one recognizes from the spectral representation of the spectral density. If one carries out the average over the ground state \( |E_0 \rangle \) as is required by definition for \( T = 0 \), and then goes through exactly the same steps as in deriving (B.86), then one gets the spectral density

\[
2\pi S_{k\sigma}(t - t') = \sum_n \left| \langle E_n | c_{k\sigma}^\dagger | E_0 \rangle \right|^2 \exp\left(-\frac{i}{\hbar} (E_n - E_0)(t - t')\right) \quad (B.177)
\]

In the free system, \( c_{k\sigma}^\dagger | E_0 \rangle \) is an eigenstate of \( \mathcal{H}_0 \), so that due to the orthogonality of the eigenstates, only one term in the sum contributes. That does not hold any more for the interacting system. \( c_{k\sigma}^\dagger | E_0 \rangle \) is no more an eigenstate, but can be expanded in terms of the eigenstates:

\[
|\phi_0 \rangle = c_{k\sigma}^\dagger | E_0 \rangle = \sum_n \gamma_n | E_n \rangle
\]

where an arbitrary number, but at least two coefficients \( \gamma_n \) are unequal zero. Every summand in (B.177) represents a harmonic oscillation but with different frequencies. The overlap sees to it that the sum is maximum for \( t = t' \). For increasing \( t - t' \) the phase factors \( \exp\left(-\frac{i}{\hbar} (E_n - E_0)(t - t')\right) \) distribute themselves over the entire unit circle in the complex plane and see to it that, because of the destructive interference, possibly a very complicated and certainly no more harmonic time-dependence results as depicted in Fig. B.7. The state created at \( t' \) is not stationary.
but has to some extent a finite lifetime. One could, however, imagine that the complicated time dependence could be simulated by a few weighted damped oscillations with well-defined frequencies:

$$2\pi S_{k\sigma}(t - t') = \sum_n \alpha_{n\sigma}(k) \exp(-\frac{i}{\hbar}(\eta_{n\sigma}(k) - \mu)(t - t')) \quad (B.178)$$

This expression formally has the same structure as for the free system (B.175) with, however, in general complex one-particle energies:

$$\eta_{n\sigma}(k) = \text{Re} \eta_{n\sigma}(k) + i \text{Im} \eta_{n\sigma}(k) \quad (B.179)$$

In order to realize damping, one must have

$$\text{Im} \eta_{n\sigma}(k) \leq 0 \quad (t - t' > 0) \quad (B.180)$$

The ansatz (B.178) gives the impression as if the extra \((k, \sigma)\)-electron decays into one or more quasiparticles with the following properties:

- Quasiparticle energy \(\Leftrightarrow\) Re \(\eta_{n\sigma}(k)\)
- Quasiparticle lifetime \(\Leftrightarrow\) \(\hbar \cdot |\text{Im} \eta_{n\sigma}(k)|^{-1}\)
- Quasiparticle weight ("spectral") \(\Leftrightarrow\) \(\alpha_{n\sigma}(k)\)

The lifetime is defined here as the time that is required for the respective summand to decrease from its initial value by a fraction \(e\). Because of the particle conservation, for the spectral weights of the quasiparticles

$$\sum_n \alpha_{n\sigma}(k) = 1 \quad (B.181)$$

must still hold. Formally this follows from

$$2\pi S_{k\sigma}(0) = \sum_n \alpha_{n\sigma}(k) = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle_+ = 1$$
We will carry these interpretations now on to the results (B.108) and (B.110) of the last section

- **Quasiparticle energy** ⇔ \( \text{Re} \ E_{n\sigma}(k) \)

\[
E_{n\sigma}(k) = \varepsilon(k) + R_{k\sigma}(E_{n\sigma}(k) - \mu) \tag{B.182}
\]

- **Quasiparticle lifetime** ⇔ \( \tau_{n\sigma}(k) \)

\[
\tau_{n\sigma}(k) = \frac{\hbar}{|\alpha_{n\sigma}(k) I_{k\sigma}(E_{n\sigma}(k) - \mu)|} \tag{B.183}
\]

- **Quasiparticle weight ("spectral")** ⇔ \( \alpha_{n\sigma}(k) \)

\[
\alpha_{n\sigma}(k) = \left| 1 - \frac{\partial}{\partial E} R_{k\sigma}(E - \mu) \right|^{-1}_{E=E_{n\sigma}} \tag{B.184}
\]

The Lorentz-type peaks in the spectral weight are to be assigned to the quasiparticles, whose energies are given by the positions and their lifetimes by the widths of the peaks. The quasiparticle energies are given only by the real part and the lifetimes are given mainly by the imaginary part of the self-energy. Because of \( \alpha_{n\sigma}(k) \), in a limited way, the lifetime is of course influenced by the real part too. \( I_{k\sigma} = 0 \) always means an infinite lifetime. Delta functions in the spectral weight indicate stable, i.e. infinitely long-living quasiparticles.

To conclude, it should be mentioned that these considerations for the classical quasiparticle picture are based on the preconditions (B.164) and (B.165) whose validity can be verified only after the complete solution of the many-body problem.

### B.4.4 Quasiparticle Density of States

While discussing the free electrons as an application of the abstract Green’s function formalism in 3.6., we have learned about the important concept of quasiparticle density of states. Now we want to introduce this quantity for interacting electron system and understand its relation to the one-particle Green’s function and one-particle spectral density.

The starting point is the average occupation number \( \langle n_{k\sigma} \rangle \) of the \((k, \sigma)\)-level, which with the help of the spectral theorem can be expressed by the one-particle spectral density:

\[
\langle n_{k\sigma} \rangle = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \ f_-(E) S_{k\sigma}(E - \mu) \tag{B.185}
\]

Here \( f_-(E) \) is again the Fermi function. A summation over all the wavevectors and both the spin directions gives the total number of electrons \( N_e \).
\[ N_e = \sum_{k\sigma} \langle n_{k\sigma} \rangle \]  \hspace{1cm} (B.186)

Alternatively, the electron number can be expressed in terms of a density of states. \( \hat{\rho}_\sigma(E)dE \) is the number of \( \sigma \)-states in the energy interval \([E, E + dE]\) that can be occupied. Then, \( f_-(E)\hat{\rho}_\sigma(E)dE \) is the density of the occupied states. Therefore

\[ N_e = \sum_{\sigma} \int_{-\infty}^{+\infty} f_-(E)\hat{\rho}_\sigma(E)dE \]  \hspace{1cm} (B.187)

must hold. A non-degenerate energy band (s-band) contains \( 2N \) states, where \( N \) is the number of lattice sites. The factor 2 comes because of the two spin directions. For the completely occupied band \( (f_-(E) \equiv 1) \) therefore

\[ \int_{-\infty}^{+\infty} dE f_-(E)\hat{\rho}_\sigma(E) = N \]

holds. However, the density of states is usually normalized to one: \( \rho_\sigma(E) \equiv \frac{1}{N} \hat{\rho}_\sigma(E) \). A comparison of the two expressions for \( N_e \) then gives the “Quasiparticle density of states”

\[ \rho_\sigma(E) = \frac{1}{N\hbar} \sum_k S_{k\sigma}(E - \mu) \]  \hspace{1cm} (B.188)

All the properties of the spectral density transfer to the quasiparticle density of states. It is in general dependent on temperature and particle number and naturally also depends on lattice structure. We have seen in Sect. B.2 that the one-electron spectral density has a direct relation to \textit{angle resolved} photoemission. In contrast, the quasiparticle density of states is seen directly in \textit{angle averaged} photoemission.

We want to investigate the quasiparticle density of states for an illustrative special case. For that we consider a real, \( k \)-independent self-energy:

\[ R_{k\sigma}(E) \equiv R_\sigma(E) \quad; \quad I_{k\sigma}(E) \equiv 0 \]  \hspace{1cm} (B.189)

This corresponds to the case A of Sect. B.4.2. Therefore (B.159) holds:

\[ S_{k\sigma}(E - \mu) = \hbar \delta (E - R_\sigma(E - \mu) - \varepsilon(k)) \]  \hspace{1cm} (B.190)

For the quasiparticle density of states this means

\[ \rho_\sigma(E) = \frac{1}{N} \sum_k \delta (E - R_\sigma(E - \mu) - \varepsilon(k)) \]  \hspace{1cm} (B.191)

Comparing with the \textit{Bloch density of states} for the non-interacting band electrons (B.121), we get in this special case
\[ \rho_\sigma(E) = \rho_0(E - R_\sigma(E - \mu)) \]  

(B.192)

\( \rho_\sigma(E) \) is unequal zero for such energies for which \( E - R_\sigma(E - \mu) \) lies between the lower and the upper edge of the free Bloch band. If \( R_\sigma(E) \) is only a slowly varying smooth function of \( E \), then \( \rho_\sigma(E) \) will only be slightly deformed from \( \rho_0(E) \) (Fig. B.8). The influence of the particle interaction can possibly be taken into account by a renormalization of certain parameters. On the contrary, new kind of phenomena appear if \( E - R_\sigma(E - \mu) \) is strongly structured, if as in Fig. B.9 the self-energy, e.g. shows a singularity in the interesting region. The result can be a band splitting which cannot be understood from the one-electron picture. At an appropriate band filling, it can happen that in one-electron picture (Bloch picture) the system is metallic, whereas in reality electronic correlations can make it an insulator. Such a system is called a “Mott–Hubbard insulator”.

Fig. B.8 Quasiparticle density of states for a “smooth” real part of the self-energy

Fig. B.9 Quasiparticle density of states of a self-energy with a singularity
B.4.5 Thermodynamics

To conclude we want to show that the one-electron Green’s function (B.142) or the corresponding spectral density (B.143) can provide complete information regarding the macroscopic thermodynamics of the interacting electron system. We start with the “internal energy” which is defined as the expectation value of the Hamiltonian (B.138):

\[
U = \langle H \rangle = \sum_{k_\sigma} \varepsilon(k) \left( c_{k_\sigma}^\dagger c_{k_\sigma} \right) + \\
+ \frac{1}{2} \sum_{k,p,q,\sigma,\sigma'} v_{k,p,q}(q) \left( c_{k+q_\sigma}^\dagger c_{p-q_\sigma'}^\dagger c_{p_\sigma'} c_{k_\sigma} \right)
\]

(B.193)

We substitute \( q \rightarrow -q \) and then \( k \rightarrow k + q \) and use the symmetry relation (B.141). Then \( U \) can also be written as follows:

\[
U = \langle H \rangle = \sum_{k_\sigma} \varepsilon(k) \left( c_{k_\sigma}^\dagger c_{k_\sigma} \right) + \\
+ \frac{1}{2} \sum_{k,p,q,\sigma,\sigma'} v_{p,k+q}(q) \left( c_{k_\sigma}^\dagger c_{p+q_\sigma'}^\dagger c_{p_\sigma'} c_{k_\sigma} \right)
\]

(B.194)

With the help of higher Green’s function (B.145) and the spectral theorem (B.95) it follows that

\[
U = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \frac{dE}{\exp(\beta E) + 1} \left[ \sum_{k_\sigma} \varepsilon(k) \left( -\frac{1}{\pi} \operatorname{Im} G_{k_\sigma}(E) \right) \\
+ \frac{1}{2} \sum_{k,p,q,\sigma,\sigma'} v_{p,k+q}(q) \left( -\frac{1}{\pi} \operatorname{Im} \Gamma_{p,k} \sigma' (E) \right) \right]
\]

(B.195)

From the equation of motion we read off

\[
\frac{1}{2} \sum_{k,p,q,\sigma,\sigma'} v_{p,k+q}(q) \left( -\frac{1}{\pi} \operatorname{Im} \Gamma_{p,k} \sigma' (E) \right) = \\
= \frac{1}{2} \sum_{k_\sigma} \left( -\frac{1}{\pi} \operatorname{Im} \left( (E - \varepsilon(k) + \mu) G_{k_\sigma}(E) - \hbar \right) \right) \\
= \frac{1}{2} \sum_{k_\sigma} (E - \varepsilon(k) + \mu) \left( -\frac{1}{\pi} \operatorname{Im} G_{k_\sigma}(E) \right)
\]
This we substitute in (B.195)

\[ U = \frac{1}{2\hbar} \sum_{k\sigma} \int_{-\infty}^{+\infty} \frac{dE}{\exp(\beta E) + 1} (E + \mu + \varepsilon(k)) \left( -\frac{1}{\pi} \text{Im} G_{k\sigma}(E) \right) \]  \hspace{1cm} (B.196)

Once again substituting \( E \to E - \mu \), we finally obtain

\[ U = \frac{1}{2\hbar} \sum_{k\sigma} \int_{-\infty}^{+\infty} dE \ f_{-}(E) (E + \varepsilon(k)) \ S_{k\sigma}(E - \mu) \] \hspace{1cm} (B.197)

This is a very remarkable result because the contribution of a two-particle Coulomb interaction could be expressed in terms of one-particle spectral density. The result (B.197) was already formally obtained for the case of non-interacting band electrons (B.122).

From \( U \) the “free energy” follows from the generally valid relation

\[ F(T) = U(0) - T \int_{0}^{T} dT' \frac{U(T') - U(0)}{T'} \] \hspace{1cm} (B.198)

which we prove as problem (B.10). Therefore the whole of macroscopic thermodynamics is determined by the one-particle spectral density itself. In this context, for the various energy integrals, particularly the prominent quasiparticle peaks (see Fig. B.6) are important.

**B.5 Problems**

**Problem B.1** Let \( A(t) \) be an arbitrary operator in the Heisenberg picture and \( \rho \) be the statistical operator:

\[ \rho = \frac{\exp(-\beta H)}{Tr(\exp(-\beta H))} \]

Prove the Kubo identity:

\[ \frac{i}{\hbar} [A(t), \rho]_- = \rho \int_{0}^{\beta} d\lambda \ \dot{A}(t - i\lambda \hbar) \]

Assume that the Hamiltonian \( H \) is not explicitly time dependent!

**Problem B.2** With the help of the Kubo identity (Problem B.1) show that the retarded commutator Green’s function can be written as follows:

\[ \langle[A(t); B(t')]_{\text{ret}} = -\hbar \Theta(t - t') \int_{0}^{\beta} d\lambda \ \hat{B}(t' - i\lambda \hbar) A(t) \]
**Problem B.3** For the time-dependent correlation functions, show that

\[ \langle B(0) A(t + i \hbar \beta) \rangle = \langle A(t) B(0) \rangle \]

holds provided the Hamiltonian does not explicitly depend on time.

**Problem B.4** Prove the following representation of the step function:

\[ \Theta(t - t') = \frac{i}{2\pi} \int_{-\infty}^{+\infty} dx \frac{\exp(-ix(t - t'))}{x + i0^+} \]

**Problem B.5** Show that a complex function \( F(E) \) has an analytical continuation in the upper (lower) half-plane, if its Fourier transform \( f(t) \) for \( t < 0 \) \((t > 0)\) vanishes.

**Problem B.6** For an interacting electron system

\[ H = \sum_{k\sigma} \epsilon(k)c_{k\sigma}^+ c_{k\sigma} + \frac{1}{2} \sum_{k,p,q,\sigma,\sigma'} v_{kp}(q)c_{k+q\sigma}^+ c_{p-q\sigma'}^+ c_{p\sigma'} c_{k\sigma} \]

derive the equation of motion for the retarded one-particle Green’s function.

**Problem B.7** For a system of non-interacting electrons

\[ H = \sum_{k\sigma} (\epsilon(k) - \mu) c_{k\sigma}^+ c_{k\sigma} \]

calculate all the spectral moments \( M_{k\sigma}^{(n)} \) and from there the exact spectral density.

**Problem B.8** The BCS theory of superconductivity can be carried out with the simplified Hamiltonian

\[ H = \sum_{k\sigma} (\epsilon(k) - \mu) c_{k\sigma}^+ c_{k\sigma} - \Delta \sum_k \left( b_k + b_k^\dagger \right) + \frac{\Delta^2}{V} \]

Here

\[ b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow} \]

is the “Cooper pair creation operator” and

\[ \Delta = \Delta^* = V \sum_k \langle b_k \rangle = V \sum_k \langle b_k^\dagger \rangle \]
1. Calculate the commutation relations of the operators $b_{k}, b_{k}^\dagger$. Are the Cooper pairs Bosons?
2. Using the one-electron Green’s function (B.142) calculate the excitation spectrum of the superconductor. Show that it has a “gap” $\Delta$.
3. Determine the equation satisfied by $\Delta$!

**Problem B.9** 1. For the superconductivity model in Problem B.8, calculate all the spectral moments of the one-electron spectral density.
2. Choose a two-pole ansatz for the spectral density

$$S_{k\sigma}(E) = \hbar \sum_{i=1}^{2} \alpha_{i\sigma}(k) \delta(E - E_{i\sigma}(k))$$

and determine the spectral weights $\alpha_{i\sigma}(k)$ and the quasiparticle energies $E_{i\sigma}(k)$! By inspecting the spectral moments show that the above ansatz is exact.

**Problem B.10** Prove the following relation between the internal and the free energies:

$$F(T, V) = U(0, V) - T \int_{0}^{T} dT' \frac{U(T', V) - U(0, V)}{T'^{2}}$$

**Problem B.11** Let $|E_{0}\rangle$ be the ground state of the interaction free electron system (Fermi sphere). Calculate the time dependence of the state

$$|\psi_{0}\rangle = c_{k'\sigma}^\dagger c_{k\sigma} |E_{0}\rangle$$

Is it a stationary state?

**Problem B.12** For the one-electron Green’s function of an interacting electron system

$$G_{k\sigma}^{\text{rel}}(E - \mu) = \frac{\hbar}{E - 2\varepsilon(k) + \frac{E^{2}}{v(k)} + i\gamma|E|} \quad (\gamma > 0)$$

may hold.

1. Determine the electronic self-energy $\Sigma_{k\sigma}(E)$.
2. Calculate the energies and lifetimes of the quasiparticles.
3. Under what conditions is the classical quasiparticle concept applicable?
4. Calculate the effective masses of the quasiparticles.

**Problem B.13** For an interacting electron system, let the self-energy

$$\Sigma_{\sigma}(E) = \frac{a_{\sigma}(E + \mu - b_{\sigma})}{E + \mu - c_{\sigma}} \quad (a_{\sigma}, b_{\sigma}, c_{\sigma} \text{ positive, real}; \ c_{\sigma} > b_{\sigma})$$

be calculated. For the density of states of the interaction free system holds
\[ \rho_0(E) = \begin{cases} \frac{1}{W} & \text{for } 0 \leq E \leq W \\ 0 & \text{otherwise} \end{cases} \]

Calculate the quasiparticle density of states. Is there a band splitting?
Appendix C  
Solutions to Problems

Problem 1.1  
Let us take $\mathbf{R}_i = 0$  
With $\nabla \times (\varphi \mathbf{a}) = \varphi \nabla \times \mathbf{a} - \mathbf{a} \times \nabla \varphi$ follows:

\[
\mathbf{j}^{(i)}_{m} = \nabla \times (\mathbf{m}_i f(r)) = f \nabla \times \mathbf{m}_i - \mathbf{m}_i \times \nabla f \\
\nabla \times \mathbf{m}_i = 0, \text{ since } \mathbf{m}_i : \text{ particle property}
\]

Substitute:

\[
\mathbf{m}_i = \frac{1}{2} \int d^3r \ \mathbf{r} \times \mathbf{j}_{m}^{(i)} \\
= \frac{1}{2} \int d^3r \ [\mathbf{r} \times (\nabla f \times \mathbf{m}_i)] \\
= \frac{1}{2} \int d^3r \ [\nabla f(r \cdot \mathbf{m}_i) - \mathbf{m}_i(r \cdot \nabla f)] \\
= \frac{1}{2} \int d^3r \ \nabla f(r \cdot \mathbf{m}_i) - \frac{1}{2} \int d^3r \ \mathbf{m}_i (\text{div}(f \mathbf{r}) - f \text{div} \mathbf{r}) \\
= \frac{1}{2} \int d^3r \ \nabla f(r \cdot \mathbf{m}_i) - \frac{1}{2} \mathbf{m}_i \int d^3r \ \text{div}(f \mathbf{r}) \\
+ \frac{3}{2} \mathbf{m}_i \int \underline{\int d^3r \ f} \\
\equiv 1, \text{ cond.2.} \\
= \frac{1}{2} \int d^3r \ \nabla f(r \cdot \mathbf{m}_i) + \frac{3}{2} \mathbf{m}_i - \frac{1}{2} \mathbf{m}_i \int dS \cdot (f \mathbf{r}) \\
\equiv 0, \text{ cond.1.}
\]

Intermediate result:
\[ \mathbf{m}_i = \frac{1}{2} \int d^3r \nabla f(r \cdot \mathbf{m}_i) + \frac{3}{2} \mathbf{m}_i \]

\[ \iff -\frac{1}{2} \mathbf{m}_i = \frac{1}{2} \int d^3r \left[ \nabla(f(r \cdot \mathbf{m}_i)) - f \nabla(r \cdot \mathbf{m}_i) \right] \]

\[ = \frac{1}{2} \int d^3r \nabla(f(r \cdot \mathbf{m}_i)) - \frac{1}{2} \mathbf{m}_i \int d^3r f \]

\[ \equiv 1, \text{ cond.} 2. \]

\[ \iff 0 = \frac{1}{2} \int d^3r \nabla(f(r \cdot \mathbf{m}_i)) \]

\[ = \frac{1}{2} \oint dS f(r \cdot \mathbf{m}_i) = 0 \quad \text{q.e.d.} \]

**Problem 1.2**

From the definition of the canonical partition function

\[ Z = Tr \left( e^{-\beta \hat{H}} \right) \]

The average magnetic moment is given by

\[ \langle \hat{\mathbf{m}} \rangle = \frac{1}{Z} \frac{1}{Z} \partial \partial B_0 \left( e^{-\beta \hat{H}} \right) \]

\[ = \frac{1}{\beta Z} \frac{1}{\partial B_0} Tr \left( e^{-\beta \hat{H}} \right) \]

\[ = \frac{1}{\beta Z} \partial \partial Z \]

From this follows the susceptibility:

\[ \chi_T = \frac{\mu_0}{V} \left( \frac{\partial}{\partial B_0} \langle \hat{\mathbf{m}} \rangle \right)_T \]

\[ = \frac{\mu_0}{\beta V} \left( -\frac{1}{Z^2} \left( \frac{\partial Z}{\partial B_0} \right)^2 + \frac{1}{Z} \frac{\partial^2 Z}{\partial B_0^2} \right) \]

The first term is clear:

\[ \frac{1}{Z^2} \left( \frac{\partial Z}{\partial B_0} \right)^2 = \beta^2 \langle \hat{\mathbf{m}} \rangle^2 \quad (1.1) \]

The second term is somewhat more complicated:
\[
\frac{1}{Z} \frac{\partial^2 Z}{\partial B_0^2} = \frac{1}{Z} \frac{\partial}{\partial B_0} \left( -\beta Tr \left( \frac{\partial \hat{H}}{\partial B_0} e^{-\beta \hat{H}} \right) \right)
\]

\[
= \frac{-\beta}{Z} Tr \left( \frac{\partial^2 \hat{H}}{\partial B_0^2} e^{-\beta \hat{H}} - \beta \left( \frac{\partial \hat{H}}{\partial B_0} \right)^2 e^{-\beta \hat{H}} \right)
\]

\[
= \frac{\beta^2}{Z} Tr \left( \left( \frac{\partial \hat{H}}{\partial B_0} \right)^2 e^{-\beta \hat{H}} \right)
\]

\[
= \beta^2 \langle \hat{m}^2 \rangle
\]

In the third step we have exploited the condition that we are dealing with a permanent magnetic moment. Therefore for the susceptibility we have

\[
\chi_T = \frac{\mu_0}{V} \beta \left( \langle \hat{m}^2 \rangle - \langle \hat{m} \rangle^2 \right) = \frac{1}{k_B T} \frac{\mu_0}{V} \langle (\hat{m} - \langle \hat{m} \rangle)^2 \rangle
\]

Problem 1.3

In a magnetic field \( B \), the magnetic dipole \( m \) has the potential energy

\[
V = -m \cdot B
\]

It will therefore try to orient itself parallel to the field. If the field is only a homogeneous external field

\[
B_0 = B_0 e_x = \begin{pmatrix} B_0 \\ 0 \\ 0 \end{pmatrix}
\]

then \( m \) will be oriented parallel to x-axis. According to elementary electrodynamics, the current creates an additional azimuthal field of the form

\[
B_I = \mu_0 \frac{I}{2\pi \rho} e_\varphi
\]

It is convenient to use cylindrical coordinates:

\[
x = \rho \cos \varphi, \quad y = \rho \sin \varphi, \quad z = z
\]

\[
\rho = \sqrt{x^2 + y^2}
\]

\[
e_\varphi = \begin{pmatrix} -\sin \varphi \\ \cos \varphi \\ 0 \end{pmatrix} = \frac{1}{\rho} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}
\]

Total field
\[ \mathbf{B} = \mathbf{B}_0 + \mathbf{B}_I = B_0 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \mu_0 \frac{I}{2\pi (x^2 + y^2)} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} \]

Field at the position \( \mathbf{r}_0 = (x_0, 0, 0) \):

\[ \mathbf{B}(\mathbf{r}_0) = B_0 \mathbf{e}_x + \frac{\mu_0 I}{2\pi x_0} \mathbf{e}_y \]

Dipole is oriented parallel to \( \mathbf{B} \), i.e. it makes an angle \( \alpha \) given by

\[ \tan \alpha = \frac{\mu_0 I}{2\pi x_0 B_0} \]

which for small angles gives

\[ \alpha \approx \frac{\mu_0 I}{2\pi x_0 B_0} \]

with the \( x \)-axis.

**Problem 1.4**

For a magnetic system, we use the version (1.80) of the first law. Then the work done is given by

\[ \delta W = V B_0 dM = \mu_0 VH dM \]

\( M \): magnetization; \( V \): constant volume (not a real thermodynamic variable!). From Curie law follows:

\[ (dM)_T = \frac{C}{T} dH \]

\[ \Leftrightarrow (\delta W)_T = \mu_0 \frac{CV}{T} HdH \]

\[ \Leftrightarrow (\Delta W)_{12} = \int_{H_1}^{H_2} (\delta W)_T = \frac{\mu_0 CV}{2T} (H_2^2 - H_1^2) = \mu_0 \frac{VT}{2C} (M_2^2 - M_1^2) \]

**Problem 1.5**

1. \[ c_M = \left( \frac{\partial U}{\partial T} \right)_M \]

follows directly from the first law (1.80). Further holds with \( U = U(T, M) \) and \( N = \text{const.} \):
\[ T \, dS = dU - V B_0 dM \]

\[ = \left( \frac{\partial U}{\partial T} \right)_M \, dT + \left( \frac{\partial U}{\partial M} \right)_T \, dM - V B_0 dM \]

\[ \therefore \, c_H - c_M = \left[ \left( \frac{\partial U}{\partial M} \right)_T - V B_0 \right] \left( \frac{\partial M}{\partial T} \right)_H \]

Curie law:

\[ \left( \frac{\partial M}{\partial T} \right)_H = \frac{-C}{T^2} \, H = -\frac{M^2}{CH} \]

Substitute

\[ c_H = \left( \frac{\partial U}{\partial T} \right)_M + \left( \frac{\partial U}{\partial M} \right)_T \left( \frac{\partial M}{\partial T} \right)_H - V B_0 \left( \frac{\partial M}{\partial T} \right)_H \]

\[ = \left( \frac{\partial U}{\partial T} \right)_M + \left( \frac{\partial U}{\partial M} \right)_T \left( \frac{\partial M}{\partial T} \right)_H + \mu_0 \frac{V}{C} M^2 \]

Since \( U = U(T, M) \) further holds

\[ dU = \left( \frac{\partial U}{\partial T} \right)_M \, dT + \left( \frac{\partial U}{\partial M} \right)_T \, dM \]

\[ \therefore \left( \frac{\partial U}{\partial T} \right)_H = \left( \frac{\partial U}{\partial T} \right)_M + \left( \frac{\partial U}{\partial M} \right)_T \left( \frac{\partial M}{\partial T} \right)_H \]

\[ c_H = \left( \frac{\partial U}{\partial T} \right)_H + \mu_0 \frac{V}{C} M^2 \]

2. It holds

\[ \left( \frac{\partial M}{\partial H} \right)_S = \left( \frac{\partial M}{\partial T} \right)_S \left( \frac{\partial T}{\partial H} \right)_S \]

The two factors are determined separately.

(a) First law (1.80):

\[ dU = T \, dS + V \mu_0 H \, dM \]

adiabatic means \( dS = 0 \). Therefore

\[ dU = \left( \frac{\partial U}{\partial T} \right)_M \, dT + \left( \frac{\partial U}{\partial M} \right)_T \, dM = V \mu_0 H \, dM \]
\begin{align*}
    \sim \left( \left( \frac{\partial U}{\partial T} \right)_M dT \right)_S &= \left( \left( V \mu_0 H - \left( \frac{\partial U}{\partial M} \right)_T \right) dM \right)_S \\
    \sim \left( \frac{\partial M}{\partial T} \right)_S &= \frac{c_M}{V \mu_0 H - \left( \frac{\partial U}{\partial M} \right)_T} \tag{\text{C}}
\end{align*}

(b) Once again the first law for adiabatic changes of state

\[ 0 = dU - V \mu_0 H dM \]

With \( U = U(T, H) \) and \( M = M(T, H) \) follows:

\[ 0 = \left[ \left( \frac{\partial U}{\partial T} \right)_H - V \mu_0 H \left( \frac{\partial M}{\partial T} \right)_H \right] dT + \]

\[ + \left[ \left( \frac{\partial U}{\partial H} \right)_T - V \mu_0 H \left( \frac{\partial M}{\partial H} \right)_T \right] dH \]

According to part 1 the first parenthesis is equal to \( c_H \). Therefore what remains is

\[ c_H dT = \left[ V \mu_0 H \left( \frac{\partial M}{\partial H} \right)_T - \left( \frac{\partial U}{\partial H} \right)_T \right] dH \]

\[ = \left[ V \mu_0 M - \left( \frac{\partial U}{\partial H} \right)_T \right] dH \]

That means

\[ \left( \frac{\partial T}{\partial H} \right)_S = \frac{V \mu_0 M - \left( \frac{\partial U}{\partial H} \right)_T}{c_H} \]

This equation is combined with the final result of part 1:

\[ \left( \frac{\partial M}{\partial H} \right)_S = \frac{c_M}{c_H} \cdot \frac{V \mu_0 M - \left( \frac{\partial U}{\partial H} \right)_T}{V \mu_0 H - \left( \frac{\partial U}{\partial M} \right)_T} \]

That was the original proposition!

**Problem 1.6**

\[ S = S(T, H) \iff dS = \left( \frac{\partial S}{\partial T} \right)_H dT + \left( \frac{\partial S}{\partial H} \right)_T dH = 0 \]
This means
\[
\left( \frac{\partial T}{\partial H} \right)_S = -\left( \frac{\partial S}{\partial H} \right)_T = -\frac{T}{c_H} \left( \frac{\partial S}{\partial H} \right)_T
\]

Free enthalpy \((N = \text{const.})\):
\[
dG = -SdT - MV \mu_0 dH
\]

The corresponding Maxwell’s equation gives
\[
\left( \frac{\partial S}{\partial H} \right)_T = V \mu_0 \left( \frac{\partial M}{\partial T} \right)_H = -V \mu_0 \frac{C}{T^2} H
\]

With this it finally follows:
\[
\left( \frac{\partial T}{\partial H} \right)_S = \mu_0 V \frac{C}{c_H T} H
\]

**Problem 2.1**

- **\(L > S\)**
  \[
  \sum_{J=|L-S|}^{L+S} (2J + 1) = \sum_{J=|L-S|}^{L+S} (2J + 1) = \frac{1}{2}(2S + 1)[2(L + S) + 1 + 2(L - S) + 1] = (2S + 1)(2L + 1)
  \]

- **\(L < S\)**
  \[
  \sum_{J=|L-S|}^{L+S} (2J + 1) = \sum_{J=|S-L|}^{L+S} (2J + 1) = \frac{1}{2}(2L + 1)[2(S + L) + 1 + 2(S - L) + 1] = (2S + 1)(2L + 1)
  \]
Problem 2.2

1. We obviously have

\[
\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I}_2
\]

\[
\sigma_y^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I}_2
\]

\[
\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I}_2
\]

2. Similarly one can easily get

\[
\begin{align*}
[\sigma_x, \sigma_y]_+ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & +i \\ +i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = 0
\end{align*}
\]

\[
\begin{align*}
[\sigma_y, \sigma_z]_+ &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = 0
\end{align*}
\]

\[
\begin{align*}
[\sigma_z, \sigma_x]_+ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} = 0
\end{align*}
\]

3.

\[
\begin{align*}
[\sigma_x, \sigma_z]_- &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \\
&= 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2i \sigma_z
\end{align*}
\]

The other two components are obtained analogously.
\[\sigma_x \sigma_y \sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} = i \mathbb{1}_2\]

**Problem 2.3**

One immediately recognizes \((i, j = x, y, z)\)

\[\hat{\alpha}_i \hat{\alpha}_j = \begin{pmatrix} \sigma_i \sigma_j & 0 \\ 0 & \sigma_i \sigma_j \end{pmatrix}\]

With the commutation relations for the Pauli spin matrices (see Problem 2.1) follows

\[\left[\hat{\alpha}_i, \hat{\alpha}_j\right]_+ = \left[\sigma_i, \sigma_j\right]_+ + 0 = \left[\sigma_i, \sigma_j\right]_+ + 0 = 2 \delta_{ij} \left(\mathbb{1}_2 \ 0 \\ 0 \mathbb{1}_2\right) = 2 \delta_{ij} \mathbb{1}_4\]

One can further calculate

\[\hat{\alpha}_i \hat{\beta} = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix}\]

\[\hat{\beta} \hat{\alpha}_i = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}\]

\[\Rightarrow \left[\hat{\alpha}_i, \hat{\beta}\right]_+ = 0\]

Finally, it remains to be verified

\[\hat{\beta}^2 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & \mathbb{1}_2 \end{pmatrix} = \mathbb{1}_4\]

So that (2.23), (2.24) and (2.25) are proved.

**Problem 2.4**

In solving the problem one uses the commutation relations for the Pauli spin matrices proved in Problem 2.2:
\[ [\hat{s}_i, \hat{s}_j] = \frac{\hbar^2}{4} \left( \begin{bmatrix} \sigma_i, \sigma_j \end{bmatrix} - \begin{bmatrix} 0 \\ \sigma_i, \sigma_j \end{bmatrix} \right) \]

\[ = \frac{\hbar^2}{4} \left( 2i \sum_k \varepsilon_{ijk} \sigma_k - \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) \]

\[ = \frac{i}{2} \hbar \sum_k \varepsilon_{ijk} \left( \sigma_k \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) \]

\[ = i \hbar \sum_k \varepsilon_{ijk} \hat{s}_k \]

**Problem 2.5**

\( H_{(0)}^D \) is defined in (2.38). \( \hat{s} \) commutes with the momentum operator \( \mathbf{p} \). We now have to calculate

\[ \hat{s}_i \hat{\alpha}_j = \frac{\hbar}{2} \begin{bmatrix} \sigma_i, \sigma_j \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 0 & \sigma_i \sigma_j \\ \sigma_i & 0 \end{bmatrix} \]

\[ \hat{\alpha}_j \hat{s}_i = \frac{\hbar}{2} \begin{bmatrix} 0, \sigma_j \\ \sigma_j, 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 0 & \sigma_j \sigma_i \\ \sigma_j & 0 \end{bmatrix} \]

From the result of Problem 2.3 this means

\[ [\hat{s}_i, \hat{\alpha}_j] = \frac{\hbar}{2} \begin{bmatrix} 0 & \sigma_i \sigma_j \\ \sigma_i & 0 \end{bmatrix} \]

\[ = \frac{\hbar}{2} \left( 2i \sum_k \varepsilon_{ijk} \sigma_k - \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) \]

\[ = i \hbar \sum_k \varepsilon_{ijk} \left( \sigma_k \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right) = i \hbar \sum_k \varepsilon_{ijk} \hat{\alpha}_k \]

So that we have

\[ [\hat{s}_i, \mathbf{p} \cdot \hat{\alpha}] = i \hbar \sum_{jk} \varepsilon_{ijk} \mathbf{p}_j \hat{\alpha}_k = i \hbar (\mathbf{p} \times \hat{\alpha}) \]

\[ [\hat{s}, \mathbf{p} \cdot \hat{\alpha}] = i \hbar (\mathbf{p} \times \hat{\alpha}) \]

To this one finds

\[ \hat{s}_i \cdot \hat{\beta} = \frac{\hbar}{2} \begin{bmatrix} \sigma_i, 0 \\ 0 & \sigma_i \end{bmatrix} \left( \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \mathbb{I}_2 \\ 0 & -\mathbb{I}_2 \end{bmatrix} \right) = \frac{\hbar}{2} \begin{bmatrix} \sigma_i & 0 \\ 0 & -\sigma_i \end{bmatrix} = \hat{\beta} \cdot \hat{s}_i \]

So that
\[
\left[ \hat{s}, H_D^{(0)} \right] = i \hbar c (\mathbf{p} \times \hat{\alpha})
\]

For the orbital angular momentum we use the well-known commutation relations with the linear momentum
\[
[l_i, p_j] = i \hbar \sum_k \varepsilon_{ijk} p_k
\]
So that it follows:
\[
[l_i, \hat{\alpha} \cdot \mathbf{p}] = i \hbar \sum_k \varepsilon_{ijk} \hat{\alpha} p_k = i \hbar (\hat{\alpha} \times \mathbf{p})_i
\]
With \([l_i, \hat{\beta}] = 0\) it eventually follows:
\[
\left[ \hat{l}, H_D^{(0)} \right] = i \hbar c (\hat{\alpha} \times \mathbf{p})
\]

**Problem 2.6**
First we use the commutation relations from Problem 2.2:
\[
[\sigma_i, \sigma_j] = 2i \sum_k \varepsilon_{ijk} \sigma_k
\]
\[
[\sigma_i, \sigma_j] = 2 \delta_{ij} \mathbb{1}_2
\]
From this we get the important relation:
\[
\sigma_i \sigma_j = \delta_{ij} \mathbb{1}_2 + i \sum_k \varepsilon_{ijk} \sigma_k
\]
Due to the commutability it holds
\[
(\sigma \cdot \mathbf{a})(\sigma \cdot \mathbf{b}) = \sum_{i,j} a_i b_j \sigma_i \sigma_j = \sum_{i,j} a_i b_j \left( \delta_{ij} + i \sum_k \varepsilon_{ijk} \sigma_k \right)
\]
\[
= \left( \sum_i a_i b_j \right) + i \sum_{ijk} \varepsilon_{ijk} a_i b_j \sigma_k
\]
\[
= (\mathbf{a} \cdot \mathbf{b}) \mathbb{1}_2 + i \mathbf{a} \cdot (\mathbf{b} \times \sigma)
\]
Since \(\sigma\) commutes with \(\mathbf{a}\) and \(\mathbf{b}\), we can cyclically permute the operators in second summand (triple product!).

**Problem 2.7**
\[
H_D = c \mathbf{\hat{\alpha}} \cdot (\mathbf{p} + e \mathbf{A}) + \hat{\beta} m_e c^2 - e \varphi
\]
Heisenberg’s equations of motion:

\[ i \hbar \frac{d}{dt} \mathbf{r} = [\mathbf{r}, H_D] - c [\mathbf{r}, \mathbf{p}] \cdot \mathbf{\hat{a}} = i \hbar \mathbf{\hat{a}} c \]

\[ \therefore \dot{\mathbf{r}}(t) = c \mathbf{\hat{a}} \]

\[ i \hbar \frac{d}{dt} (\mathbf{p} + e \mathbf{A}) \]

\[ = [(\mathbf{p} + e \mathbf{A}), H_D] + i \hbar \frac{d}{dt} (\mathbf{p} + e \mathbf{A}) = \]

\[ = ce [\mathbf{p}, \mathbf{\hat{a}} \cdot \mathbf{A}] - e [\mathbf{p}, \varphi] + ce [\mathbf{A}, \mathbf{\hat{a}} \cdot \mathbf{p}] + ihe \frac{\partial \mathbf{A}}{\partial t} = \]

\[ = ce \frac{\hbar}{i} (\mathbf{\hat{a}} \cdot \nabla \mathbf{A} + \nabla (\mathbf{\hat{a}} \cdot \mathbf{A})) - e \frac{\hbar}{i} \nabla \varphi + ihe \frac{\partial \mathbf{A}}{\partial t} = \]

\[ \therefore \frac{d}{dt} (\mathbf{p} + e \mathbf{A}) = -ec (\mathbf{\hat{a}} \times \mathbf{B}) + e \left( \nabla \varphi + \frac{\partial \mathbf{A}}{\partial t} \right) \]

With

\[ \mathbf{E} = -\nabla \varphi - \frac{\partial \mathbf{A}}{\partial t} \]

finally follows:

\[ \frac{d}{dt} (\mathbf{p} + e \mathbf{A}) = -e (\dot{\mathbf{r}} \times \mathbf{B} + \mathbf{E}). \]

On the right-hand side is the Lorentz force.

**Problem 2.8**

1.

\[ [H_{SB}, L_i] = \sum_{j=1}^{3} \lambda [L_j S_j, L_i] = \sum_{j=1}^{3} \lambda [L_j, L_i] S_j = \]

\[ = \sum_{j=1}^{3} \lambda \sum_k \varepsilon_{jik} L_k S_j i \hbar = i \hbar \lambda \sum_{jk} \varepsilon_{jki} L_k S_j = \]

\[ = i \hbar \lambda (\mathbf{L} \times \mathbf{S})_i \]

\[ \implies [H_{SB}, \mathbf{L}] = i \hbar \lambda (\mathbf{L} \times \mathbf{S}) \]
2. \[
\left[ H_{SB}, S_i \right]_\downarrow = \sum_{j=1}^{3} \lambda \left[ L_j S_j, S_i \right]_\downarrow = \lambda \sum_{j=1}^{3} L_j \left[ S_j, S_i \right]_\downarrow = \\
= \lambda \sum_{j=1}^{3} L_j \hbar \sum_k \varepsilon_{jik} S_k = i \hbar \lambda \sum_{jk} \varepsilon_{kji} S_k L_j = \\
= i \hbar \lambda (S \times L)_i \\
\implies \left[ H_{SB}, S \right]_\downarrow = i \hbar \lambda (S \times L)
\]

3. \[
\left[ H_{SB}, L^2 \right]_\downarrow = \sum_{i=1}^{3} \lambda \left[ L_i S_j, L^2 \right]_\downarrow = \sum_{i=1}^{3} \lambda \left[ L_i, L^2 \right]_\downarrow S_i = 0
\]

4. \[
\left[ H_{SB}, S^2 \right]_\downarrow = \lambda \sum_{i=1}^{3} L_i \left[ S_i, S^2 \right]_\downarrow = 0
\]

5. From 1 and 2 follows:
\[
\left[ H_{SB}, J_i \right]_\downarrow = 0 \text{ for } i = x, y, z \\
\implies \left[ H_{SB}, J^2 \right]_\downarrow = \sum_i \left[ H_{SB}, J_i^2 \right]_\downarrow = 0
\]

**Problem 2.9**

1. According to (2.162) it must hold
\[
R_z(\varepsilon)T_q^{(k)}R_z^{-1}(\varepsilon) = \sum_{q'=-k}^{+k} (R_z(\varepsilon))^{(k)}_{q'q} T_q^{(k)}
\]

Here we have according to (2.145)
\[
R_z(\varepsilon) = 1 - \frac{i}{\hbar} \varepsilon J_z
\]
and according to (2.158)
\[(R_z(\varepsilon))^{(k)}_{q'q} = |kq'\rangle\langle R_z(\varepsilon)|kq\rangle\]
\[
= \langle kq'\rangle(1 - i\frac{\varepsilon}{\hbar}J_z)kq\rangle
\]
\[
= \delta_{q'q} - i\frac{\varepsilon}{\hbar}\hbar q\delta_{q'q}
\]
\[
= (1 - i\varepsilon q)\delta_{q'q}
\]
\[
\sum_{q'=-k}^{k} (R_z(\varepsilon))^{(k)}_{q'q} = (1 - i\varepsilon q)T_q^{(k)}
\]

On the other hand:

\[R_z(\varepsilon)T_q^{(k)}R_z^{-1}(\varepsilon) = (1 - \frac{i}{\hbar}\varepsilon J_z)T_q^{(k)}(1 + \frac{i}{\hbar}\varepsilon J_z)\]
\[
= T_q^{(k)} - \frac{i}{\hbar}\varepsilon [J_z, T_q^{(k)}] + O(\varepsilon^2)
\]

Compare:

\[
[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}
\]

2. According to (2.160) holds

\[(R_x(\varepsilon))^{(k)}_{q'q} = \delta_{q'q} - \frac{1}{2}i\varepsilon \sqrt{k(k+1) - q(q+1)}\delta_{q',q+1}
\]
\[
- \frac{1}{2}i\varepsilon \sqrt{k(k+1) - q(q-1)}\delta_{q',q-1}
\]

So that we have

\[
\sum_{q'=-k}^{+k} (R_x(\varepsilon))^{(k)}_{q'q} T_q^{(k)} = T_q^{(k)} - \frac{1}{2}i\varepsilon \sqrt{k(k+1) - q(q+1)}T_{q+1}^{(k)}
\]
\[
- \frac{1}{2}i\varepsilon \sqrt{k(k+1) - q(q-1)}T_{q-1}^{(k)}
\]

On the other hand we have as in 1.:

\[R_x(\varepsilon)T_q^{(k)}R_x^{-1}(\varepsilon) = T_q^{(k)} - \frac{i}{\hbar}\varepsilon [J_x, T_q^{(k)}] + O(\varepsilon^2)
\]

Then a comparison gives
\[ [J_x, T_q^{(k)}]_- = \frac{\hbar}{2}\sqrt{k(k+1) - q(q+1)}T_{q+1}^{(k)} + \frac{\hbar}{2}\sqrt{k(k+1) - q(q-1)}T_{q-1}^{(k)} \]

Completely analogously one finds

\[ [J_y, T_q^{(k)}]_- = -i\frac{\hbar}{2}\sqrt{k(k+1) - q(q+1)}T_{q+1}^{(k)} + i\frac{\hbar}{2}\sqrt{k(k+1) - q(q-1)}T_{q-1}^{(k)} \]

With \( J_\pm = J_x \pm iJ_y \) follows the final result:

\[ [J_\pm, T_q^{(k)}]_- = \hbar\sqrt{k(k+1) - q(q \pm 1)}T_{q\pm1}^{(k)} \]

**Problem 2.10**

We use (2.150)

\[ [(n \cdot J), (\bar{n} \cdot K)]_- = i\hbar(n \times \bar{n}) \cdot K \quad n, \bar{n} : \text{unit vectors} \]

1. \( n = e_z \)
   If further \( \bar{n} = e_z \) is valid, we have
   \[ n \times \bar{n} = 0 \quad \Rightarrow \quad [J_z, K_z]_- = 0 = \hbar \cdot 0 \cdot K_0^{(1)} \]
   For \( \bar{n} = e_x \) we have
   \[ n \times \bar{n} = e_y \quad \Rightarrow \quad [J_z, K_x]_- = i\hbar K_y \]
   For \( \bar{n} = e_y \) we have
   \[ n \times \bar{n} = -e_x \quad \Rightarrow \quad [J_z, K_y]_- = -i\hbar K_x \]

   \[ K_{\pm1}^{(1)} = \mp \frac{1}{\sqrt{2}}(K_x \pm iK_y) \]

   \[ [J_z, K_{\pm1}^{(1)}]_- = \mp \frac{1}{\sqrt{2}}i\hbar(K_y \mp iK_x) = \hbar \cdot (\pm1) \cdot K_{\pm1}^{(1)} \]
Therefore altogether we have

\[
\left[J_z, K_q^{(1)}\right]_\pm = \hbar q K_q^{(1)}
\]

This is the first part of (2.163).

2. \(\sqrt{k(k+1)} - q(q \pm 1) = \sqrt{2} - q(q \pm 1)\)

(a) \(q = 0\):

\[
K_0^{(1)} = K_z
\]

\[
\left[J_x, K_0^{(1)}\right]_\pm = \left[J_x, K_z\right]_\pm = i\hbar (e_x \times e_z) \cdot \mathbf{K} = -i\hbar K_y
\]

\[
\left[J_y, K_0^{(1)}\right]_\pm = i\hbar (e_y \times e_z) \cdot \mathbf{K} = i\hbar K_x
\]

\[
\left[J_{\mp}, K_0^{(1)}\right]_\pm = i\hbar K_y \pm i(i\hbar K_x)
\]

\[
= \mp \hbar (K_x \pm iK_y)
\]

\[
= \hbar \sqrt{2} K_{\pm 1}^{(1)}
\]

For \(q = 0\) we therefore have

\[
\left[J_{\pm}, K_q^{(1)}\right]_\pm = \hbar \sqrt{2} - q(q \pm 1) K_q^{(1)}_{q \pm 1}
\]

(b) \(q = +1\):

\[
K_{+1}^{(1)} = -\frac{1}{\sqrt{2}} K_+
\]

\[
\left[J_x, K_{+1}^{(1)}\right]_\pm = -\frac{1}{\sqrt{2}} \left[J_x, K_x + iK_y\right]_\pm
\]

\[
= -\frac{i}{\sqrt{2}} \left[J_x, K_y\right]
\]

\[
= \frac{\hbar}{\sqrt{2}} (e_x \times e_y) \cdot \mathbf{K} = \frac{\hbar}{\sqrt{2}} K_z
\]

analogously
\[
\left[ J_y, K^{(1)}_{+1} \right]_\pm = -\frac{1}{\sqrt{2}} \left[ J_y, K_z + iK_y \right]_\pm = -\frac{1}{\sqrt{2}} \left[ J_y, K_z \right]_-
\]
\[
= -\frac{i\hbar}{\sqrt{2}} (e_y \times e_x) \cdot K = i \frac{\hbar}{\sqrt{2}} K_z
\]
\[
\left[ J_+, K^{(1)}_{+1} \right]_\pm = 0
\]
\[
\left[ J_-, K^{(1)}_{+1} \right]_\pm = \hbar \sqrt{2} K_z = \sqrt{2} \hbar K^{(1)}_0
\]

For \( q = +1 \) then holds

\[
\left[ J_\pm, K^{(1)}_q \right]_\pm = \hbar \sqrt{2 - q(q \pm 1)} K^{(1)}_{q \pm 1}
\]

(c) \( q = -1 \):

\[
K^{(1)}_{-1} = \frac{1}{\sqrt{2}} K_- 
\]
\[
\left[ J_x, K^{(1)}_{-1} \right]_\pm = \frac{1}{\sqrt{2}} (-i) \left[ J_x, K_y \right]_\pm = \frac{\hbar}{\sqrt{2}} (e_x \times e_y) \cdot K = \frac{\hbar}{\sqrt{2}} K_z
\]
\[
\left[ J_y, K^{(1)}_{-1} \right]_\pm = \frac{1}{\sqrt{2}} \left[ J_y, K_x \right]_\pm
\]
\[
= \frac{i\hbar}{\sqrt{2}} (e_y \times e_x) \cdot K = -i \frac{\hbar}{\sqrt{2}} K_z
\]
\[
\left[ J_\pm, K^{(1)}_{-1} \right]_\pm = \frac{\hbar}{\sqrt{2}} (K_z \pm K_z)
\]

For \( q = -1 \) we can write the following:

\[
\left[ J_\pm, K^{(1)}_q \right]_\pm = \hbar \sqrt{2 - q(q \pm 1)} K^{(1)}_{q \pm 1}
\]

2a, 2b and 2c together give the second part of (2.163):

\[
\left[ J_\pm, K^{(1)}_q \right]_\pm = \hbar \sqrt{2 - q(q \pm 1)} K^{(1)}_{q \pm 1}
\]

Problem 2.11

1. \([I_\varepsilon, T^{(2)}_q]_\pm = \hbar q T^{(2)}_q\)

One immediately recognizes

\[
\left[ I_\varepsilon, T^{(2)}_0 \right]_\pm = \left[ I_\varepsilon, I^2 - 3I^2_\varepsilon \right]_\pm = 0
\]
On the other hand with a little more effort we have

\[
\begin{align*}
\left[ I_z, T_{\pm 1}^{(2)} \right] &= \pm \frac{1}{2} \sqrt{6} \left\{ [I_z, I_z I_{\pm}]_\pm + [I_z, I_{\pm} I_z]_\pm \right\} \\
&= \pm \frac{1}{2} \sqrt{6} \left\{ I_z [I_z, I_{\pm}]_\pm + [I_z, I_{\pm}]_\pm I_z \right\} \\
&= \frac{1}{2} \hbar \sqrt{6} (I_z I_{\pm} + I_{\pm} I_z) \\
&= \pm \hbar T_{\pm 1}^{(2)}
\end{align*}
\]

\[
\begin{align*}
\left[ I_z, T_{\pm \pm 2}^{(2)} \right] &= -\frac{1}{2} \sqrt{6} [I_z, (I_{\pm})^2]_\pm \\
&= -\frac{1}{2} \sqrt{6} \left\{ I_{\pm} [I_z, I_{\pm}]_\pm + [I_z, I_{\pm}]_\pm I_{\pm} \right\} \\
&= -(\pm \hbar) \sqrt{6} (I_{\pm})^2 \\
&= \pm 2 \hbar T_{\pm \pm 2}^{(2)}
\end{align*}
\]

Thus the first commutation relation is obviously fulfilled

2. \[
\left[ I_{\pm}, T_{q}^{(2)} \right]_\pm \equiv \sqrt{6 - q(q \pm 1)} \hbar q T_{q \pm 1}^{(2)}
\]

\[
\begin{align*}
\left[ I_{\pm}, T_{0}^{(2)} \right]_\pm &= \left[ I_{\pm}, I^2 \right]_\pm - 3 \left[ I_{\pm}, I^2 \right]_\pm \\
&= 0 - 3 I_z [I_{\pm}, I_z]_\pm - 3 [I_{\pm}, I_z]_\pm I_z \\
&= \pm 3 \hbar (I_z I_{\pm} + I_{\pm} I_z) \\
&= \hbar \sqrt{6} \left( \pm \frac{1}{2} \sqrt{6} (I_z I_{\pm} + I_{\pm} I_z) \right) \\
&= \hbar \sqrt{6} T_{\pm 1}^{(2)}
\end{align*}
\]

\[
\begin{align*}
\left[ I_{\mp}, T_{+1}^{(2)} \right]_\pm &= \frac{1}{2} \sqrt{6} \left( [I_{\mp}, I_z I_{\pm}]_\pm + [I_{\mp}, I_{\pm} I_z]_\pm \right) \\
&= \frac{1}{2} \sqrt{6} \left( [I_{\mp}, I_z]_\pm I_{\pm} + I_{\pm} [I_{\mp}, I_z]_\pm \right) \\
&= \frac{1}{2} \sqrt{6} (-2 \hbar (I_{\pm})^2) \\
&= 2 \hbar T_{+2}^{(2)}
\end{align*}
\]
\[
\begin{align*}
\left[ I_+, T_{-1}^{(2)} \right]_- &= -\frac{1}{2} \sqrt{6} \left( [I_+, I_z I_-]_- + [I_+, I_- I_z]_- \right) \\
&= -\frac{1}{2} \sqrt{6} \left( I_z 2h I_z - h I_+ I_- - h I_- I_+ + 2h I_z^2 \right) \\
&= -\frac{1}{2} \sqrt{6} h (4I_z^2 - 2I_z^2 - 2I_z^2) \\
&= -h \sqrt{6} (3I_z^2 - I_z^2) \\
&= h \sqrt{6} T_0^{(2)} \\

\left[ I_-, T_{+1}^{(2)} \right]_- &= -\frac{1}{2} \sqrt{6} \left( [I_-, I_z I_+]_- + [I_-, I_+ I_z]_- \right) \\
&= \frac{1}{2} \sqrt{6} (I_z (-2h I_z) + h I_- I_+ + h I_+ I_- + (-2h I_z) I_z) \\
&= \frac{1}{2} \sqrt{6} h (-4I_z^2 + 2I_z^2 + 2I_z^2) \\
&= h \sqrt{6} (I_z^2 - 2I_z^2) \\
&= h \sqrt{6} T_0^{(2)} \\

\left[ I_-, T_{-1}^{(2)} \right]_- &= -\frac{1}{2} \sqrt{6} \left( [I_-, I_z I_-]_- + [I_-, I_- I_z]_- \right) \\
&= -\frac{1}{2} \sqrt{6} (h I_-)^2 + I_- (+h I_-)) \\
&= 2h T_{-2}^{(2)} \\

\left[ I_+, T_{+2}^{(2)} \right]_- &= -\frac{1}{2} \sqrt{6} \left( [I_+, (I_+)^2]_- \right) = 0 \\

\left[ I_+, T_{-2}^{(2)} \right]_- &= -\frac{1}{2} \sqrt{6} \left( [I_+, (I_-)^2]_- \right) \\
&= -\frac{1}{2} \sqrt{6} (I_- 2h I_z + 2h I_z I_-) \\
&= 2h T_{-1}^{(2)}
\end{align*}
\]
\[
\begin{align*}
\left[I_-, T_{+2}^{(2)}\right]_- &= -\frac{1}{2}\sqrt{6} \left[I_-, (I_+)^2\right]_-
= -\frac{1}{2}\sqrt{6}(-2\hbar I_+ I_z - 2\hbar I_z I_+)
= 2\hbar T_{+1}^{(2)}

\left[I_-, T_{-2}^{(2)}\right]_- &= -\frac{1}{2}\sqrt{6} \left[I_-, (I_-)^2\right]_-
= 0
\end{align*}
\]

**Problem 2.12**

\[
A = \sum_{q=-2}^{+2} t_{q}^{(2)} \cdot (T_{q}^{(2)})^\dagger = \sum_{i=-2}^{+2} A_i
\]

\[
A_0 = (J^2 - 3J_z^2) \left(I^2 - 3I_z^2\right)
\]

\[
\simeq A_0 = J^2 I^2 - 3J_z^2 I^2 - 3I_z^2 J^2 + 9J_z^2 I_z^2
\]

\[
A_{\pm 1} = \frac{3}{2} (J_z J_{\pm} + J_{\pm} J_z) (I_z I_{\mp} + I_{\mp} I_z)
\]

\[
A_{+1} + A_{-1}
= \frac{3}{2} (J_z J_+ I_- + J_z J_+ I_- + J_+ J_z I_+ + J_+ J_z I_+) +
+ J_+ J_- I_+ + J_+ J_- I_+ + J_- J_+ I_+ + J_- J_+ I_+)
= \frac{3}{2} (J_z J_- (J_+ I_- + J_- I_+) + (J_+ I_- + J_- I_+) J_z I_z) +
+ \frac{3}{2} J_z (J_+ I_- + J_- I_+) I_z + \frac{3}{2} (J_+ (J_z I_z) I_+ + J_- (J_z I_z) I_+)
= 3 (J_z I_z (J_+ I_- + J_- I_+) + (J_+ I_- + J_- I_+) J_z I_z) +
+ \frac{3}{2} \hbar (J_+ I_- I_z - J_- I_+ I_z) + \frac{3}{2} \hbar (-J_- I_+ I_z + J_- I_+ I_z)
= 6 (J_z I_z (J_x I_x + J_y I_y) + (J_x I_x + J_y I_y) J_z I_z) +
+ \frac{3}{2} \hbar J_+ [I_-, I_z]_+ + \frac{3}{2} \hbar J_- [I_z, I_+]_-
= 6 (J_z I_x + J_y I_y + J_z I_z)^2 - 6J_z^2 I_z^2 - 6 (J_z I_x + J_y I_y)^2 +
+ \frac{3}{2} \hbar^2 (J_+ I_- + J_- I_+)
\[ A_{+1} + A_{-1} = 6 (J \cdot I)^2 - 6 J_z^2 I_z^2 - \frac{3}{2} (J_+ I_- + J_- I_+)^2 + 3 \hbar^2 (J \cdot I) - 3 \hbar^2 J_z I_z \]

\[ A_{+2} = \frac{3}{2} J_z^2 I_z^2 \]

\[ A_{+2} + A_{-2} = \frac{3}{2} (J_+ I_-^2 + J_- I_+^2) \]

We now sum the terms

\[ A = J^2 I^2 - 3 J_z^2 I_z^2 - 3 I_z^2 J_z^2 + 9 J_z^2 I_z^2 + 6 (J \cdot I)^2 - 6 J_z^2 I_z^2 - \frac{3}{2} (J_+ I_- + J_- I_+)^2 + 3 \hbar^2 (J \cdot I) - 3 \hbar^2 J_z I_z + \frac{3}{2} (J_+ I_-^2 + J_- I_+^2) = 6 (J \cdot I)^2 + 3 \hbar^2 (J \cdot I) - 2 J^2 I^2 + D \]

\[ D = 3 J^2 I^2 - 3 J_z^2 I_z^2 - 3 I_z^2 J_z^2 + 3 J_z^2 I_z^2 - 3 h^2 J_z I_z \frac{3}{2} (J_+ J_- I_+ + J_- J_+ I_-) - 3 (J_x^2 + J_y^2) I_z^2 - 3 (J_x^2 + J_y^2) I_z^2 - 3 \text{Re} (J_+ J_- I_+ I_-) - 3 \hbar^2 J_z I_z = 3 (J_x^2 + J_y^2) (I_x^2 + I_y^2) - 3 \text{Re} \left( \left( J_x^2 + J_y^2 + i [J_y, J_x] \right) \left( I_x^2 + I_y^2 - i [I_y, I_x] \right) \right) - 3 \hbar^2 J_z I_z = -3 \text{Re} ((-i \hbar J_z) (-i \hbar I_z)) - 3 \hbar^2 J_z I_z = 0 \]

Then we have

\[ A = 6 (J \cdot I)^2 + 3 \hbar^2 (J \cdot I) - 2 J^2 I^2 \]

This corresponds to the quadruple term (2.245).
Problem 2.13

1. Build

\[ \text{div}(g f \mathbf{j}) = (g f) \text{div} \mathbf{j} + \mathbf{j} \cdot \text{grad}(g f) = \mathbf{j} \cdot \text{grad}(f g) = f \mathbf{j} \cdot \nabla g + g \mathbf{j} \cdot \nabla f \]

That is exactly the integrand of \( D \). With Gauss theorem we have

\[ D = \int d^3r \text{div}(g f \mathbf{j}) = \int_{s \to \infty} d\mathbf{f} \cdot (g f \mathbf{j}) = 0 \]

since \( \mathbf{j} \) vanishes at infinity.

2. Set \( f = 1, \ g = x, y, z \):

\[ \nabla \cdot 0 = D = \int d^3r \mathbf{j} \cdot \mathbf{e}_{x,y,z} = \int d^3r j_{x,y,z} \]

\[ \nabla \int d^3r \mathbf{j}(\mathbf{r}) = 0 \]

3. Set \( f = x_i, \ g = x_j \) with \( x_{i,j} \in \{x, y, z\} \): Then with 1. we have

\[ 0 = \int d^3r (x_i j_j + x_j j_i) \]

\[ \nabla \int d^3r x_{j} j_i = - \int d^3r x_{i} j_j \]

Now let \( \mathbf{a} \) be an arbitrary vector:

\[ \mathbf{a} \cdot \int d^3r \mathbf{r} j_i(\mathbf{r}) = \sum_j a_j \int d^3r x_{j} j_i(\mathbf{r}) = \frac{1}{2} \sum_j a_j \int d^3r (x_{j} j_i(\mathbf{r}) - x_{i} j_j(\mathbf{r})) = \frac{1}{2} \sum_j a_j \varepsilon_{jik} \int d^3r (\mathbf{r} \times \mathbf{j})_k = -\frac{1}{2} \sum_j \varepsilon_{ijk} a_j \int d^3r (\mathbf{r} \times \mathbf{j})_k = -\frac{1}{2} \left( \mathbf{a} \times \int d^3r (\mathbf{r} \times \mathbf{j}) \right)_i \]
This is valid for all the components $i$:

$$\mathbf{a} \cdot \int d^3r \mathbf{r} \mathbf{j}(\mathbf{r}) = -\frac{1}{2} \left( \mathbf{a} \times \int d^3r (\mathbf{r} \times \mathbf{j}) \right)$$

**Problem 3.1**

Because of the circular motion, every electron has an angular momentum and therefore a magnetic orbital momentum $\mathbf{m}^{(i)}$. In the absence of an external field, the orientations of the electron moments are statistically distributed and hence compensate each other. After the application of a field, the angular momenta precess about the direction of the field while the motion of the electrons in the orbital planes remains unchanged.

Because of the precession there is an extra current:

$$\Delta I = \frac{-e}{\tau} = \frac{-e\omega L}{2\pi}$$

which according to classical electrodynamics induces an additional magnetic moment:

$$\Delta \mathbf{m}^{(i)} = \Delta I \mathbf{F}_i = \frac{-e\omega L}{2\pi} r_{i\perp}^2 \mathbf{e}_z = -\frac{e^2}{4m} (x_i^2 + y_i^2) B_0 \mathbf{e}_z$$

$\mathbf{F}_i$ is the vector area of the circle along which the $i$ th electron moves. Finally the (average) magnetization of the diamagnet ($N$, the number of atoms; $V$, the volume, $N_e$, the number of electrons per atom) is given by

$$\Delta \mathbf{M} = \mathbf{M} = \frac{N}{V} \sum_{i=1}^{N_e} \langle \Delta \mathbf{m}^{(i)} \rangle = -\frac{Ne^2}{6mV} B_0 \sum_{i=1}^{N_e} \langle r_i^2 \rangle$$

In calculating this we have used

$$\sum_{i=1}^{N_e} \langle x_i^2 \rangle = \sum_{i=1}^{N_e} \langle y_i^2 \rangle = \sum_{i=1}^{N_e} \langle z_i^2 \rangle = \frac{1}{3} \sum_{i=1}^{N_e} \langle r_i^2 \rangle$$

Then the diamagnetic susceptibility is given by

$$\chi^{dia} = \mu_0 \left( \frac{\partial \mathbf{M}}{\partial B_0} \right)_T = -\frac{Ne^2 \mu_0}{6mV} \sum_{i=1}^{N_e} \langle r_i^2 \rangle$$

This expression agrees with the quantum mechanically correct expression (3.21). Since the calculation is not strictly classical, there is no contradiction with Bohr–van Leeuwen theorem. The assumption of stationary electron orbits is classically untenable!
Problem 3.2

\( T = 0: \)

\[
\bar{\epsilon} = \frac{1}{N} \left( 2 \sum_{\text{Spin}} \sum_k \epsilon(k) \right) = \frac{2}{N} \frac{1}{\Delta k} \int_{k \leq k_F} \frac{\hbar^2 k^2}{2m}
\]

\( \Delta k = \frac{(2\pi)^3}{V} \) grid volume: Volume per \( k \)-state in \( k \)-space.

\[
\bar{\epsilon} = 2 \frac{V}{N} \frac{4\pi}{8\pi^3} \frac{\hbar^2}{2m} \int_0^{k_F} dk k^4 = \frac{V}{N} \frac{\hbar^2}{2m \pi^2} \frac{1}{5} k_F^5 = \frac{\epsilon_F}{N} \frac{V}{5\pi^2} k_F^3
\]

With \( k_F^3 = 3\pi^2 \frac{N}{V} \) follows:

\( \bar{\epsilon} = \frac{3}{5} \epsilon_F \)

Problem 3.3

\( \hat{H} = \sum_{k\sigma} \epsilon(k) \hat{a}_{k\sigma}^+ \hat{a}_{k\sigma} = \sum_{k\sigma} \epsilon(k) \hat{n}_{k\sigma} \)

1. Statistical operator of the grand canonical ensemble

\( \rho = \exp(-\beta(\hat{H} - \mu \hat{N})) \) (unnormalized)

\( \hat{N} = \sum_{k\sigma} \hat{a}_{k\sigma}^+ \hat{a}_{k\sigma} = \sum_{k\sigma} \hat{n}_{k\sigma} \)

\( \sim [\hat{H}, \hat{N}] = 0 \sim \) combined eigenstates (Fock states)

So that

\[
\text{Tr} \rho = \sum_{N=0}^{\infty} \sum_{\{n_{k\sigma}\}}^{(\sum n_{k\sigma} = N)} \exp(-\beta \sum_{k\sigma} (\epsilon(k) - \mu) n_{k\sigma})
\]

\( = \sum_{N=0}^{\infty} \sum_{\{n_{k\sigma}\}}^{(\sum n_{k\sigma} = N)} \prod_{k\sigma} \exp(-\beta (\epsilon(k) - \mu) n_{k\sigma}), \quad (n_{k\sigma} = 0, 1) \)

\( = \sum_{\{n_{k_1\sigma_1}\}} \sum_{\{n_{k_2\sigma_2}\}} \cdots \prod_{k\sigma} \exp(-\beta (\epsilon(k) - \mu) n_{k\sigma}) \)
\[
\left[ \sum_{n_{k_1 \sigma_1} = 0,1} \exp(-\beta (\varepsilon(k_1) - \mu)n_{k_1 \sigma_1}) \right]^2 \times \left[ \sum_{n_{k_2 \sigma_2} = 0,1} \exp(-\beta (\varepsilon(k_2) - \mu)n_{k_2 \sigma_2}) \right]^2 \ldots \\
= \left[ 1 + \exp(-\beta (\varepsilon(k_1) - \mu)) \right]^2 \left[ 1 + \exp(-\beta (\varepsilon(k_2) - \mu)) \right]^2 \ldots \\
\sim \Xi_\mu(T, V) = \prod_{k_\nu} \left[ 1 + \exp(-\beta (\varepsilon(k_\nu) - \mu)) \right]^2
\]

2. Average occupation number:

\[
\langle \hat{n}_{k_\sigma} \rangle = \frac{1}{\Xi_\mu} \text{Sp} (\rho \hat{n}_{k_\sigma}) \\
= \frac{1}{2} \sum_\sigma \langle \hat{n}_{k_\sigma} \rangle \\
= -\frac{1}{2} \frac{1}{\beta} \frac{\partial}{\partial \varepsilon(k)} \ln \Xi_\mu(T, V) \\
= \frac{\exp(-\beta (\varepsilon(k) - \mu))}{1 + \exp(-\beta (\varepsilon(k) - \mu))} \\
= \frac{1}{\exp(\beta (\varepsilon(k) - \mu)) + 1} = f_-(\varepsilon(k))
\]

3. Entropy:

\[
S = k_B \frac{\partial}{\partial T} (T \ln \Xi_\mu) \\
= k_B \sum_{k_\sigma} \ln \left[ 1 + \exp(-\beta (\varepsilon(k) - \mu)) \right] + \\
+ k_B T \frac{1}{k_B T^2} \sum_{k_\sigma} \frac{\exp(-\beta (\varepsilon(k) - \mu)) (\varepsilon(k) - \mu)}{1 + \exp(-\beta (\varepsilon(k) - \mu))}
\]

\[
\frac{\partial \mu}{\partial T} \approx 0 \sim
\]
\[ S = \sum_{k\sigma} \left\{ k_B \ln \frac{1}{1 - \langle \hat{n}_{k\sigma} \rangle} + k_B \beta (\varepsilon(k) - \mu) \langle \hat{n}_{k\sigma} \rangle \right\} \]

\[ - \beta (\varepsilon(k) - \mu) \]

\[ = \ln \exp(-\beta (\varepsilon(k) - \mu)) \]

\[ = \ln \left\{ \frac{\exp(-\beta (\varepsilon(k) - \mu))}{1 + \exp(-\beta (\varepsilon(k) - \mu))} (1 + \exp(-\beta (\varepsilon(k) - \mu))) \right\} \]

\[ = \ln < \hat{n}_{k\sigma} > - \ln \frac{1}{1 + \exp(-\beta (\varepsilon(k) - \mu))} \]

\[ = \ln < \hat{n}_{k\sigma} > - \ln \{1 - < \hat{n}_{k\sigma} >\} \]

\[ \sim S = -k_B \sum_{k\sigma} \{\ln(1 - < \hat{n}_{k\sigma} >) + < \hat{n}_{k\sigma} > \ln < \hat{n}_{k\sigma} > - \]

\[ - < \hat{n}_{k\sigma} > \ln(1 - < \hat{n}_{k\sigma} >)\} \]

\[ \sim S = -k_B \sum_{k\sigma} \left\{ (1 - < \hat{n}_{k\sigma} >) \ln(1 - < \hat{n}_{k\sigma} >) + \right\} \]

\[ < \hat{n}_{k\sigma} > \ln < \hat{n}_{k\sigma} > \right\} \]

\[ S = 0 \text{ for filled band } (< \hat{n}_{k\sigma} > = 1) \]

3rd law: (Behaviour for \( T \to 0 \))

\[ \varepsilon(k) > \mu: \quad < \hat{n}_{k\sigma} > \xrightarrow{T \to 0} 0 \quad : \quad \ln(1 - < \hat{n}_{k\sigma} >) \xrightarrow{T \to 0} 0 \quad \sim S \xrightarrow{T \to 0} 0 \]

\[ \varepsilon(k) < \mu: \quad < \hat{n}_{k\sigma} > \xrightarrow{T \to 0} 1 \quad : \quad \ln < \hat{n}_{k\sigma} > \xrightarrow{T \to 0} 0 \]

\[ \sim S \xrightarrow{T \to 0} 0 \]

\[ \sim 3rd \text{ law is satisfied!} \]

**Problem 3.4**

Periodic boundary conditions \( \sim \) grid volume

\[ \Delta k^{(1)} = \frac{2\pi}{L}; \quad \Delta k^{(2)} = \frac{(2\pi)^2}{L_x L_y} \]

1. \( d = 1 \) Density of states:

\[ \rho_0^{(1)}(E) = \frac{2}{\Delta k^{(1)}} \frac{d}{dE} \varphi_1(E) \]
Phase volume:

\[ \varphi_1(E) = \int_{\varepsilon(k) \leq E} dk = \int_{-\frac{1}{\hbar}\sqrt{2mE}}^{+\frac{1}{\hbar}\sqrt{2mE}} dk = \frac{2}{\hbar}\sqrt{2mE} \]

\[ \therefore \quad \frac{d}{dE} \varphi_1(E) = \frac{1}{\hbar} \frac{1}{\sqrt{2mE}} 2m = \sqrt{\frac{2m}{E\hbar^2}} \]

\[
\rho_0^{(1)}(E) = \begin{cases} 
    d_1 \cdot \frac{1}{\sqrt{E}}, & \text{if } E > 0 \\
    0, & \text{otherwise}
\end{cases} \quad ; d_1 = \frac{\sqrt{2m}}{\pi \hbar} L
\]

2. \( d = 2 \)

\[ \varphi_2(E) = \int_{\varepsilon(k) \leq E} d^2 k = \pi k^2 |_{\varepsilon(k) \leq E} = \pi \frac{2mE}{\hbar^2} \]

\[ \therefore \quad \frac{d}{dE} \varphi_2(E) = \frac{2m\pi}{\hbar^2} \]

\[
\rho_0^{(2)}(E) = \begin{cases} 
    d_2 > 0, & \text{if } E > 0 \\
    0, & \text{otherwise}
\end{cases} \quad ; d_2 = \frac{L_x L_y}{\pi} \cdot \frac{m}{\hbar^2}
\]

3. \( d \) arbitrary:

\[ \rho_0(E) dE = \frac{2}{\Delta^{(d)}(k)} \int_{E \leq \varepsilon(k) \leq E + dE} d^d k \]

\[ \varepsilon(k) = \frac{\hbar^2 k^2}{2m}; \quad \text{cell volume: } \Delta^{(d)}(k) = \frac{(2\pi)^d}{V_d} \]

Phase volume:

\[ \varphi_d(E) = \Omega_d \int_0^{k_0} dk k^{d-1} = \Omega_d \frac{k_0^d}{d} \quad \overset{k_0 = \left( \frac{\hbar}{2m} \right)^{\frac{1}{d}} E^{\frac{1}{d}}}{=} \frac{\Omega_d}{\frac{d}{\hbar^2}} \left( \frac{2m}{\hbar^2} \right)^{\frac{d}{2}} E^{\frac{d}{2}} \]

\[ \Omega_d: \text{Surface of the } d\text{-dimensional unit sphere} \]

\[ \therefore \quad \text{density of states} \]
\[ \rho_0(E) = 2 \frac{V_d}{(2\pi)^d} \frac{d}{dE} \varphi_d(E) \Theta(E) \]

\[ = V_d \frac{\Omega_d}{(2\pi)^d} \left( \frac{2m}{\hbar^2} \right)^{\frac{d}{2}} E^{\frac{d}{2}-1} \Theta(E) \]

The surface \( \Omega_d \) is still to be determined! Gauss integral in the \( d \)-dimensional space:

\[ g_d = \int d^d r e^{-r^2} = \prod_{i=1}^{d} \int_{-\infty}^{+\infty} dx_i e^{-x_i^2} = (\sqrt{\pi})^d = \pi^{\frac{d}{2}} \]

Spherical coordinates:

\[ g_d = \Omega_d \int_0^{\infty} dx x^{d-1} e^{-x^2} \]

\[ = \Omega_d \frac{1}{2} \int_0^{\infty} dy y^{d-1} e^{-y} \]

\[ = \frac{1}{2} \Omega_d \Gamma\left(\frac{d}{2}\right) \]

(y = \( x^2 \) \( \leadsto \) \( dy = 2x \, dx \) \( \leadsto \) \( dx = \frac{1}{2} \frac{dy}{\sqrt{y}} \) )

by comparing:

\[ \Omega_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \]

\( \leadsto \) Density of states

\[ \rho_0^{(d)}(E) = 2 \frac{V_d \pi^{\frac{d}{2}}}{(2\pi)^d} \cdot \frac{1}{\Gamma\left(\frac{d}{2}\right)} \left( \frac{2m}{\hbar^2} \right)^{\frac{d}{2}} E^{\frac{d}{2}-1} \Theta(E) \]

Check:

1. \( d = 1 \):

\[ \rho_0^{(1)}(E) = d_1 \frac{1}{\sqrt{E}} \Theta(E); \quad d_1 = \frac{L}{\pi} \sqrt{\frac{2m}{\hbar^2}} \]

2. \( d = 2 \):

\[ \rho_0^{(2)}(E) = d_2 \Theta(E); \quad d_2 = \frac{L_x L_y m}{\pi \hbar^2} \]
3. \( d = 3: \)

\[
\rho_0^{(3)}(E) = d_3 \sqrt{E} \Theta(E)
\]

\[
d_3 = \frac{V \pi^{\frac{1}{3}}}{4\pi^3} \cdot \frac{2}{\sqrt{\pi}} \left( \frac{2m}{\hbar^2} \right)^{\frac{1}{2}} = \frac{V}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{1}{2}}
\]

**Problem 3.5**

\[
\varepsilon(k) = \varepsilon(k) = c\hbar k
\]

1. **Density of states:**

\[
\rho(E) = \frac{2V}{(2\pi)^3} \frac{d}{dE} \varphi(E)
\]

\[
\varphi(E) = \int_{\varepsilon(k) \leq E} d^3 k = \frac{4\pi}{3} k^3 \bigg|_{E = \hbar k} = \frac{4\pi}{3\hbar^3 c^3} E^3
\]

\[
\rho(E) = \alpha E^2 \Theta(E) ; \alpha = \frac{V}{\pi^2 c^2 \hbar^3 c^3}
\]

\( \sim \) Fermi energy:

\[
\varepsilon_F = c\hbar k_F = c\hbar \left( 3\pi^2 \frac{N}{V} \right)^{\frac{1}{3}}
\]

where \( k_F \) is derived from the particle number:

\[
N = \frac{2V}{(2\pi)^3} \int_{k \leq k_F} d^3 k = \frac{V}{4\pi^3} \cdot \frac{4\pi}{3} k_F^3
\]

\( \sim \) \( k_F = \left( 3\pi^2 \frac{N}{V} \right)^{\frac{1}{3}} \)

2. **Chemical potential:**

With the help of the particle number:

\[
N = \int_{-\infty}^{\varepsilon_F} dE \rho(E) = \int_{N(T = 0)}^{+\infty} dE \rho_-(E) \rho(E)
\]

\( \sim \) \( \frac{\alpha}{3} \varepsilon_F^3 = \int_{-\infty}^{\mu} dE \rho(E) + \frac{\pi^2}{6} (k_B T)^2 \rho'(\mu) + \ldots \)

(Sommerfeld expansion)
\[ \begin{align*}
\sim & \quad \frac{1}{3} \epsilon_F^3 = \frac{1}{3} \mu^3 + \frac{\pi^2}{3} (k_B T)^2 \mu + \ldots \\
& \approx \frac{1}{3} \mu^3 \left\{ 1 + \pi^2 \left( \frac{k_B T}{\mu} \right)^2 \right\} \\
& \approx \frac{1}{3} \mu^3 \left\{ 1 + \pi^2 \left( \frac{k_B T}{\epsilon_F} \right)^2 \right\}
\end{align*} \]

\[ \sim \mu \approx \epsilon_F \left\{ 1 + \pi^2 \left( \frac{k_B T}{\epsilon_F} \right)^2 \right\}^{\frac{1}{3}} \]

\[ \approx \epsilon_F \left\{ 1 - \frac{\pi^2}{3} \left( \frac{k_B T}{\epsilon_F} \right)^2 \right\} \]

The same structure as in the non-relativistic case, only the numerical factor in front of the correction term is changed from \( \frac{\pi^2}{12} \) to \( \frac{\pi^2}{3} \).

3. Internal energy and heat capacity:

\[ U(T = 0) = \int_{-\infty}^{\mu} dE \, E \cdot \rho(E) = \frac{\alpha}{4} \epsilon_F^4 \]

\[ U(T) = \int_{-\infty}^{\mu} dE \, E \cdot \rho(E) + \frac{\pi^2}{6} (k_B T)^2 (3\alpha \mu^2) + \ldots \]

\[ = \frac{\alpha}{4} \mu^4 + \frac{\pi^2}{6} (k_B T)^2 (3\alpha \mu^2) + \ldots \]

\[ = \frac{\alpha}{4} \epsilon_F^4 \left\{ \left( \frac{\mu}{\epsilon_F} \right)^4 + 2\pi^2 \left( \frac{k_B T}{\epsilon_F} \right)^2 \left( \frac{\mu}{\epsilon_F} \right)^2 \right\} + \ldots \]

\[ \approx U(0) \left\{ 1 - \frac{4}{3} \pi^2 \left( \frac{k_B T}{\epsilon_F} \right)^2 + 2\pi^2 \left( \frac{k_B T}{\epsilon_F} \right)^2 \right\} + \ldots \]

\[ \sim U(T) \approx U(0) \left\{ 1 + \frac{2\pi^2}{3} \left( \frac{k_B T}{\epsilon_F} \right)^2 \right\} \]

\[ N = \frac{\alpha}{3} \epsilon_F^3 \quad \sim \quad \alpha = \frac{3N}{\epsilon_F^3} \quad \sim \quad U(0) = \frac{3}{4} N \epsilon_F \]
**Heat capacity**

\[ c_V = \gamma T; \quad \gamma = U(0) \frac{4\pi^2 k_B^2}{3 \varepsilon_F^2} = N\pi^2 \frac{k_B^2}{\varepsilon_F} \]

Non-relativistic:

\[ \gamma = \frac{1}{2} N\pi^2 \frac{k_B^2}{\varepsilon_F} \]

which means

\[ \frac{\hat{\gamma}}{\gamma} = 2 \frac{\varepsilon_F}{\varepsilon_F} = 2 \frac{\hbar^2 k_F^2}{2mc\hbar k_F} = \frac{\hbar^2}{m} \frac{k_F}{c\hbar} = \frac{\hbar}{mc} \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} \ll 1 \]

**Problem 3.6**

1. Degree of degeneracy of a Landau level (3.117):

\[ 2g_y(B_0) = 2 \frac{eL_xL_y}{2\pi\hbar} B_0 \]

Factor 2 because of the spin degeneracy. \( B_0^{(0)} \) is determined from

\[ N_e = 2g_y \left( B_0^{(0)} \right) \]

Therefore

\[ B_0^{(0)} = N_e \frac{\pi\hbar}{eL_xL_y} \]

2. The degeneracy of the Landau level is independent of the quantum number \( n \). The first \( n_0 \) levels are then exactly fully occupied and the levels \( n > n_0 \) are completely empty if \( B_0 = B_0^{(n_0-1)} \) so that

\[ \frac{N_e}{n_0} = 2g_y \left( B_0^{(n_0-1)} \right) \]

\[ \sim B_0^{(n_0-1)} = \frac{1}{n_0} B_0^{(0)} \]

3. The degree of degeneracy at an arbitrary field \( B_0 \)

\[ 2g_y(B_0) = 2g_y \left( B_0^{(0)} \right) \cdot \frac{B_0}{B_0^{(0)}} = N_e \frac{B_0}{B_0^{(0)}} \]
Now let

\[ B_0^{(n_0-1)} \geq B_0 \geq B_0^{(n_0)} \]

\( \sim \) \( n_0 \) levels are fully occupied and the \((n_0 + 1)\)th level is partially occupied.

The number of electrons in the fully occupied levels:

\[ N^* = n_0 \cdot 2g_y(B_0) = n_0 N_e \frac{B_0}{B_0^{(0)}} \]

The number of electrons in the uppermost level:

\[ N_{n_0} = N_e - N^* = N_e \left( 1 - n_0 \frac{B_0}{B_0^{(0)}} \right) \]

\( \sim \) Energy contribution of the highest level:

\[ E_{n_0} = \hbar \omega_c^* \left( n_0 + \frac{1}{2} \right) \cdot N_{n_0} \]

\[ = N_e \hbar \omega_c^* \left( n_0 + \frac{1}{2} - n_0 \left( n_0 + \frac{1}{2} \right) \frac{B_0}{B_0^{(0)}} \right) \]

\[ = N_e \mu_B^* B_0 \left( 2n_0 + 1 - n_0(2n_0 + 1) \frac{B_0}{B_0^{(0)}} \right) \]

Energy contribution of the fully occupied levels:

\[ E^* = \sum_{n=0}^{n_0-1} \hbar \omega_c^* \left( n + \frac{1}{2} \right) N_e \frac{B_0}{B_0^{(0)}} \]

\[ = \hbar \omega_c^* N_e \frac{B_0}{B_0^{(0)}} \left( n_0 - \frac{1}{2} + \frac{1}{2} \right) \frac{1}{2} n_0 \]

\[ = N_e \mu_B^* B_0 \frac{B_0^{(0)}}{B_0} n_0^2 \]

\( \sim \) Total energy:

\[ E(B_0) = E_{n_0} + E^* = N_e \mu_B^* B_0 \left( 2n_0 + 1 - n_0(n_0 + 1) \frac{B_0}{B_0^{(0)}} \right) \]

This gives the curve of Fig. 3.5.

4. \( B_0 = B_0^{(n_0)} \)

With (2) we have
that is, independent of $n_0$, that means for all critical fields it is the same!

**Problem 3.7**

1. Energy levels (3.112):

$$E_n(k_z) = 2\mu_B B_0 \left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m}$$

Degeneracy (3.117):

$$g_y(B_0) = \frac{eL_x L_y}{2\pi \hbar} B_0$$

Partition function:

$$Z_1 = \frac{1}{2\pi / L_z} \int_{-\infty}^{+\infty} dk_z \sum_{n=0}^{\infty} g_y(B_0) \exp[-\beta E_n(k_z)]$$

$$= eV B_0 \sqrt{\frac{2\pi m}{\beta}} \frac{e^{-\beta \mu_B B_0}}{1 - e^{-2\beta \mu_B B_0}}$$

$$\sim$$

$$Z_1 = V \left(\frac{m}{2\pi \hbar^2 \beta}\right)^{3/2} \frac{\beta \mu_B B_0}{\sinh(\beta \mu_B B_0)} \left(\mu_B = \frac{\hbar}{2m}\right)$$

2. Free energy:

$$dF = -S \, dT - m \, dB_0$$

(to magnetization’s work see Sect. 1.5)
\[ m = -\frac{\partial F}{\partial B_0} = k_B T \frac{\partial}{\partial B_0} \ln Z_N = N k_B T \frac{\partial}{\partial B_0} \ln Z_1 = \]
\[ = N k_B T \frac{\partial}{\partial B_0} \ln \frac{\beta \mu_B B_0}{\sinh(\beta \mu_B B_0)} \]
\[ = -N \mu_B \left( \frac{d}{dx} \ln \frac{\sinh x}{x} \right)_{x=\beta \mu_B B_0} \]

In the bracket is the classical Langevin function (see Problem 4.6):

\[ L(x) = \coth x - \frac{1}{x} \]
\[ m = -N \mu_B L \left( \frac{\mu_B B_0}{k_B T} \right) \]

negative sign

induced magnetic moment is oriented opposite to the field

Diamagnetism

**Problem 3.8**

For \( f(x) \) one can write

\[ f(x) = \delta \left( x - \frac{1}{2} \right) + \delta \left( x + \frac{1}{2} \right) \quad \text{if} \quad -1 \leq x \leq +1 \]

with \( f(x) = f(x + 2) \)

\( f(x) \) is thus periodic with the period 2 and is also symmetric

\[ f(-x) = f(x) \]

Then an ansatz for the Fourier series is possible

\[ f(x) = f_0 + \sum_{m=1}^{\infty} [a_m \cos(m\pi x) + b_m \sin(m\pi x)] \]

\[ f_0 = \frac{1}{2} \int_{-1}^{+1} f(x) \, dx = 1 \]

\[ a_m = \int_{-1}^{+1} f(x) \cos(m\pi x) \, dx \]
\[ = \begin{cases} 
0 & \text{for } m = 2p + 1 \\
2(-1)^p & \text{for } m = 2p 
\end{cases} \]

\[ b_m \equiv 0 \], since \( f(x) \) symmetric

Then it follows:
\[
f(x) = 1 + \sum_{p=1}^{+\infty} 2(-1)^p \cos(2p\pi x)
\]
\[
= 1 + \sum_{p=1}^{+\infty} (-1)^p \left( e^{i2p\pi x} + e^{-i2p\pi x} \right)
\]
\[
= \sum_{p=-\infty}^{+\infty} (-1)^p e^{i2p\pi x}
\]

Problem 4.1

\(q = q'\)

\[
\frac{1}{V} \int_V d^3r \, e^{i(q-q') \cdot r} = \frac{1}{V} \int_V d^3r = 1
\]

\(q \neq q'\)

\[
\frac{1}{V} \int_V d^3r \, e^{i(q-q') \cdot r} = \\
= \frac{1}{V} \int_0^{L_x} dx \int_0^{L_y} dy \int_0^{L_z} dz \exp \left[ 2\pi i \left( \frac{n_x - n'_x}{L_x} x + \frac{n_y - n'_y}{L_y} y + \frac{n_z - n'_z}{L_z} z \right) \right]
\]

Here we must have \((n_x, n_y, n_z) \neq (n'_x, n'_y, n'_z)\). For example, let \(n_x \neq n'_x\). Then the integral over \(x\) gives

\[
\int_0^{L_x} dx \exp \left[ 2\pi i \left( \frac{n_x - n'_x}{L_x} x \right) \right] = \\
\frac{L_x}{2\pi i (n_x - n'_x)} \exp \left[ 2\pi i \left( \frac{n_x - n'_x}{L_x} x \right) \right] \bigg|_0^{L_x}
\]

\[
= 0 \text{ since } n_x - n'_x \in \mathbb{Z}
\]

So that the proposition is proved.

Problem 4.2

1. The solid is a three-dimensional periodic array of primitive unit cells \(V_{UC} (a_1 \cdot (a_2 \times a_3))\) with the total volume

\[
V = N_1 N_2 N_3 (a_1 \cdot (a_2 \times a_3))
\]

Periodic boundary conditions for Bloch functions:
The Bloch functions are

\[ \psi_k(r) = e^{i k \cdot r} u_k(r) \]

where the amplitude functions have the periodicity of the lattice:

\[ u_k(r) = u_k(r + R^n) \]

Periodic boundary conditions therefore demand

\[ e^{i k \cdot (N_1 a_1)} = e^{i k \cdot (N_2 a_2)} = e^{i k \cdot (N_3 a_3)} = 1 \]

This means

\[ k \cdot (N_i a_i) = 2\pi z_i \quad \text{with} \quad z_i \in \mathbb{Z} \]

Then for the allowed wavevectors holds:

\[ k = \frac{z_1}{N_1} b_1 + \frac{z_1}{N_2} b_2 + \frac{z_1}{N_3} b_3 \]

Here \( b_i \) are the primitive translation vectors of the reciprocal lattice, defined by

\[ a_i \cdot b_j = 2\pi \delta_{ij} \iff b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \ldots \]

The first Brillouin zone \( \equiv \) Wigner–Seitz cell of the reciprocal lattice. Therefore for the wavevectors of the first Brillouin zone holds

\[ -\frac{1}{2} N_i < z_i \leq +\frac{1}{2} N_i \]

2. The proposition is valid for \( k = k' \), since

\[ \frac{1}{N} \sum_n 1 = 1 \]

\( k \neq k' \):
According to 1. holds

\[ (k - k') \cdot R^n = 2\pi \sum_{j=1}^{3} \frac{n_j}{N_j} (z_j - z'_j) \]
So that we calculate
\[
\sum_n e^{i(k-k') \cdot R^n} = \sum_{n_1, n_2 \in N_3} \exp \left( 2\pi i \sum_{j=1}^{N_j} \frac{n_j}{N_j} (z_j - z'_j) \right) = \prod_{j=1}^{N_j-1} \sum_{n_j=0}^{N_j-1} \exp \left( 2\pi i \frac{n_j}{N_j} (z_j - z'_j) \right)
\]

\(z_j \neq z'_j\) at least for one \(j\). Then we have
\[
\sum_{n_j=0}^{N_j-1} \left( \exp \left( 2\pi i \frac{z_j - z'_j}{N_j} \right) \right)^{n_j} = \frac{1 - a^{N_j}}{1 - a} = 0
\]

This holds because
\[
a = \exp \left( 2\pi i \frac{z_j - z'_j}{N_j} \right) \neq 1
\]
since \(z_j \neq z'_j\) and in addition \(-N_j < z_j - z'_j < +N_j\). On the other hand
\[
a^{N_j} = \exp \left( 2\pi i (z_j - z'_j) \right) = 1
\]
since \(z_j - z'_j\) is an integer. Thus the proposition is proved.

3. The proposition is trivial for \(R^n = R^m\). Therefore let \(R^n \neq R^m\).

With
\[
k \cdot (R^n - R^m) = 2\pi \sum_{j=1}^{3} \frac{z_j}{N_j} (n_j - m_j)
\]
now holds
\[
\sum_k e^{i k \cdot (R^n - R^m)} = \sum_{z_1, z_2, z_3} \exp \left( 2\pi i \sum_{j=1}^{N_j} \frac{z_j}{N_j} (n_j - m_j) \right) = \prod_{j=1}^{N_j} \sum_{z_j = -1/2N_j+1}^{1/2N_j} \exp \left( 2\pi i z_j \frac{n_j - m_j}{N_j} \right)
\]

\(n_j \neq m_j\) at least for one \(j\). Then we have
\[ \sum_{z_j = -1/2N_j + 1}^{1/2N_j} \exp \left( 2\pi i z_j \frac{n_j - m_j}{N_j} \right) \]

\[ = \sum_{p_j = 0}^{N_j - 1} \exp \left( 2\pi i (p_j - \frac{1}{2}N_j + 1) \frac{n_j - m_j}{N_j} \right) \]

\[ \propto \sum_{p_j = 0}^{N_j - 1} \left( \exp \left( 2\pi i \frac{n_j - m_j}{N_j} \right) \right)^{p_j} \]

\[ = \frac{1 - b^{N_j}}{1 - b} = 0 \]

since

\[ b = \exp \left( 2\pi i \frac{n_j - m_j}{N_j} \right) \neq 1 \]

because \( n_j \neq m_j \) and \(-N_j + 1 \leq n_j - m_j \leq N_j - 1\). On the other hand it holds

\[ b^{N_j} = \exp \left( 2\pi i (n_j - m_j) \right) = 1 \]

because \( n_j - m_j \) is an integer. The proposition is thus proved.

**Problem 4.3**

For both the integrals, it is meaningful (because of \( V \to \infty \)) to introduce relative and centre of mass coordinates:

\[ x = r - r' \quad ; \quad R = \frac{1}{2}(r + r') \]

\[ r = \frac{1}{2}x + R \quad ; \quad r' = -\frac{1}{2}x + R \]

With the help of the Jacobi determinant one can show

\[ d^3r \: d^3r' = d^3R \: d^3x \]

1.

\[ I_1 = \iiint_V d^3r \int_V d^3r' \frac{e^{-\alpha|r - r'|}}{|r - r'|} \]

\[ = \int d^3R \int d^3x \frac{e^{-\alpha x}}{x} = V \cdot 4\pi \int_0^\infty dx \: x e^{-\alpha x} \]

\[ = V \cdot 4\pi \left( -\frac{d}{d\alpha} \right) \int_0^\infty dx \: e^{-\alpha x} \]

\[ = V \cdot 4\pi \left( -\frac{d}{d\alpha} \right) \frac{1}{\alpha} \]
So that we have

\[ I_1 = \frac{4\pi V}{\alpha^2} \]

2. From the result of Problem 4.1 it follows directly:

\[
I_2 = \int_V d^3r \int_V d^3r' \frac{\exp(i(\mathbf{q} \cdot \mathbf{r} + \mathbf{q}' \cdot \mathbf{r}'))}{|\mathbf{r} - \mathbf{r}'|}
\]

\[
= \int \int d^3R d^3x \frac{1}{x} \exp \left(\frac{i}{2}(\mathbf{q} - \mathbf{q}') \cdot \mathbf{x}\right) * \exp \left(i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{R}\right)
\]

\[
= V \delta_{\mathbf{q} - \mathbf{q}'} \cdot \hat{I}
\]

In order to calculate \( \hat{I} \) it is advisable to introduce a factor that ensures convergence:

\[
\hat{I} = \lim_{\alpha \to 0^+} \int d^3x \frac{1}{x} e^{i\mathbf{q} \cdot \mathbf{x}} e^{-\alpha x}
\]

\[
= \lim_{\alpha \to 0^+} 2\pi \int_0^\infty dx x \int_{-1}^{+1} d\cos \vartheta e^{iqx \cos \vartheta} e^{-\alpha x}
\]

\[
= \lim_{\alpha \to 0^+} 2\pi \int_0^\infty dx \frac{x}{iqx} e^{-\alpha x} \left( e^{iqx} - e^{-iqx} \right)
\]

\[
= \lim_{\alpha \to 0^+} \frac{2\pi}{iq} \int_0^\infty dx \left( e^{iqx - \alpha x} - e^{-iqx - \alpha x} \right)
\]

\[
= \lim_{\alpha \to 0^+} \frac{2\pi}{iq} \left\{ \frac{1}{iq - \alpha} e^{iqx - \alpha x} \bigg|_0^\infty - \frac{1}{-iq - \alpha} e^{-iqx - \alpha x} \bigg|_0^\infty \right\}
\]

\[
= \lim_{\alpha \to 0^+} \frac{2\pi}{iq} \left\{ -\frac{1}{iq - \alpha} - \frac{1}{iq + \alpha} \right\}
\]

\[
= \frac{2\pi}{iq} \left( \frac{-2}{iq} \right) = \frac{4\pi}{q^2}
\]

Thus we find

\[ I_2 = \frac{4\pi V}{q^2} \delta_{\mathbf{q} - \mathbf{q}'} \]
Problem 4.4
First we calculate

\[ I_1(\mathbf{r}) = \int_{\mathcal{F}_K} d^3k \, e^{i\mathbf{k}\cdot\mathbf{r}} \]

\[ = 2\pi \int_{-1}^{+1} dx \int_0^{k_F} dk \, k^2 e^{ikr} \]

\[ = \frac{2\pi}{ir} \int_0^{k_F} dk \, k^2 ikr \]

\[ = \frac{4\pi}{r^3} \left[ \frac{1}{r^2} \sin(kr) - \frac{k}{r} \cos(kr) \right]_0^{k_F} \]

\[ = -\frac{4\pi}{r^3} k_F \cos(kr) - \sin(k_Fr) \]

Then we have the intermediate result

\[ I = \int d^3r \frac{I_1^2(\mathbf{r})}{r} \]

\[ = (4\pi)^3 k_F^4 \int_0^{\infty} dx \frac{1}{x^3} (x \cos x - \sin x)^2 \]

To calculate the integral we use integration by parts a number of times.

\[ I_2 = \int_0^{\infty} dx \frac{1}{x^3} (x \cos x - \sin x)^2 \]

\[ = -\frac{1}{4x^4} (x \cos x - \sin x)^2 \bigg|_0^{\infty} + \]

\[ + \frac{1}{4} \int_0^{\infty} \frac{dx}{x^4} 2(x \cos x - \sin x)(-x \sin x) \]

\[ = -\frac{1}{2} \int_0^{\infty} \frac{dx}{x^3} (x \cos x - \sin x) \sin x \]

\[ = \frac{1}{4x^2} (x \cos x - \sin x) \sin x \bigg|_0^{\infty} + \]

\[ + \frac{1}{4} \int_0^{\infty} \frac{dx}{x^2} (x(\sin^2 x - \cos^2 x) + \sin x \cos x) \]

\[ = \frac{1}{4} \int_0^{\infty} \frac{dx}{x^2} (-x \cos 2x + \frac{1}{2} \sin 2x) \]

\[ = \frac{1}{4} \int_0^{\infty} \frac{dy}{y^2} (\sin y - y \cos y) \]
\[= - \frac{1}{4y} (\sin y - y \cos y) \bigg|_0^\infty + \frac{1}{4} \int_0^\infty \frac{dy}{y} y \sin y\]
\[= - \frac{1}{4y} \sin y \bigg|_0^\infty = \frac{1}{4} \lim_{y \to 0} \frac{\sin y}{y}\]
\[= \frac{1}{4}\]

Then we finally have the integral
\[I = 16\pi^3 k_F^4\]

**Problem 4.5**

- \(S\) integer
  
  To show
  \[\sum_{n=-S}^{+S} n^2 = 2\sum_{n=1}^{+S} n^2 = \frac{1}{3} S(S + 1)(2S + 1)\]

  Proof by full induction: The statement is certainly true for \(S = 1\)
  \[2\sum_{n=1}^{+1} n^2 = 2\]

  We assume that it is valid for \(S\) and substitute \(S \leadsto S + 1\)
  \[2\sum_{n=1}^{S+1} n^2 = 2\sum_{n=1}^{S+1} n^2 + 2(S + 1)^2\]
  \[= \frac{1}{3} S(S + 1)(2S + 1) + 2(S + 1)^2\]
  \[= \frac{1}{3} (S + 1)(S(2S + 1) + 6(S + 1))\]
  \[= \frac{1}{3} (S + 1)(2S^2 + 7S + 6)\]
  \[= \frac{1}{3} (S + 1)(S + 2)(2S + 3))\]

  Thus the proposition is proved!

- \(S\) half-integer
\[ \sum_{n=1}^{S+\frac{1}{2}} n^2 = 2 \sum_{n=1}^{S+\frac{1}{2}} \left( n - \frac{1}{2} \right)^2 \]
\[ = 2 \sum_{n=1}^{S+\frac{1}{2}} n^2 - 2 \sum_{n=1}^{S+\frac{1}{2}} n + \frac{1}{2} \sum_{n=1}^{S+\frac{1}{2}} 1 \]
\[ = \frac{1}{3} \left( S + \frac{1}{2} \right) \left( S + \frac{3}{2} \right) (2S + 2) \]
\[ - 2 \frac{1}{2} \left( S + \frac{1}{2} \right) \left( S + \frac{3}{2} \right) + \frac{1}{2} \left( S + \frac{1}{2} \right) \]
\[ = \left( S + \frac{1}{2} \right) \left[ \frac{1}{3} \left( S + \frac{3}{2} \right) (2S + 2) - (S + 1) \right] \]
\[ = \frac{1}{3} (2S + 1)(S + 1) \left[ \left( S + \frac{3}{2} \right) - \frac{3}{2} \right] \]
\[ = \frac{1}{3} S(S + 1)(2S + 1) \]

This is the proposition!

**Problem 4.6**

1. Energy of a magnetic dipole in a magnetic field
\[ E = -\mu \cdot B \]
\[ \leftrightarrow H_1 = -\mu B \sum_{i=1}^{N} \cos \vartheta_i \]

\( \vartheta_i \) is the angle between the magnetic moment of the \( i \)th atom \( \mu_i \) and the field \( B \).

2. Canonical partition function
\[ Z_N(T, B) = \frac{1}{h^{3N} N!} \int \int d^3 q \ d^3 p e^{-\beta H(q, p)} \]
\[ = Z_N(T, 0) \left( \frac{2\pi}{4\pi} \right)^N \int_{-1}^{1} d \cos \vartheta_1 \cdot \cdot \cdot \]
\[ \cdot \cdot \cdot \int_{-1}^{1} d \cos \vartheta_N e^{\beta \mu B \sum_{i=1}^{N} \cos \vartheta_i} \]
\[ = Z_N(T, 0) \left( \frac{1}{2} \int_{-1}^{1} dx e^{\beta \mu B x} \right)^N \]
\[ = Z_N(T, 0) \left( \frac{e^{\beta \mu B} - e^{-\beta \mu B}}{2\beta \mu B} \right)^N \]

\[ = Z_N(T, 0) \left( \frac{\sinh \beta \mu B}{\beta \mu B} \right)^N \]

3.

\[ \mu_i = \mu (\sin \vartheta_i \cos \varphi_i, \sin \vartheta_i \sin \varphi_i, \cos \vartheta_i) \]

Average value:

\[ \mathbf{m} = \frac{\int \int \, d^3N \, q \, d^3N \, p \, (\sum_i \mu_i) \, e^{-\beta H(q, p)}}{\int \int \, d^3N \, q \, d^3N \, p \, e^{-\beta H(q, p)}} \]

The $\varphi_i$-integrations give $m_x = m_y = 0$ and therefore

\[ \mathbf{m} = m \, e_z \quad m = \frac{d}{d(\beta B)} \ln Z_N(T, B) \]

Partition function from 2.

\[ m = N \left( \frac{d}{dx} \ln \sinh \mu x - \ln \mu x \right) (x = \beta B) \]

\[ = N \mu \left( \frac{\cosh \mu x}{\sinh \mu x} - \frac{1}{\mu x} \right) (x = \beta B) \]

\[ \Rightarrow \quad \mathbf{m} = N \mu \, L(\beta \mu B) e_z \]

\[ L(x) = \coth x - \frac{1}{x} \]

$L(x)$ is the Langevin function. This is the classical Langevin paramagnetism.

4. Low temperatures, strong fields: $\beta \mu B \gg 1$

That means

\[ \coth \beta \mu B \to 1 \quad ; \quad \frac{1}{\beta \mu B} \to 0 \]

The system is in saturation:

\[ \mathbf{m} \approx N \mu e_z \]
High temperatures, weak fields: $\beta \mu B \gg 1$

$$\coth x = \frac{1}{x} + \frac{x}{3} + O(x^3)$$

$$\Rightarrow L(x) \approx \frac{x}{3}$$

This result is the Curie law:

$$\mathbf{m} \approx N \mu \frac{\mu B}{3k_B T} \mathbf{e}_z$$

**Problem 4.7**

1. Free energy ($N = \text{const.}$):

$$F = U - TS$$

$$dF = dU - TdS - SdT = -SdT + V B_0 dM$$

$$\Rightarrow \left( \frac{\partial F}{\partial M} \right)_T = \mu_0 V H$$

$$\Rightarrow \left( \frac{\partial^2 F}{\partial M^2} \right)_T = \mu_0 V \left( \frac{\partial H}{\partial M} \right)_T = \frac{\mu_0 V}{\chi_T}$$

From the last equation follows:

$$\left( \frac{\partial F}{\partial M} \right)_T = \mu_0 V \frac{M}{\chi_T} + f(T)$$

since $\chi_T$ is only a function of temperature. The comparison with the above expression requires $f(T) \equiv 0$. Then we have

$$F(T, M) = F(T, 0) + \frac{1}{2} \mu_0 V \frac{M^2}{\chi_T}$$

2. Entropy

$$S(T, M) = -\left( \frac{\partial F}{\partial T} \right)_M = S(T, 0) - \frac{1}{2} \mu_0 V M^2 \left( \frac{d}{dT} \chi_T^{-1} \right)$$

Internal energy
\[ U(T, M) = F(T, M) + TS(T, M) \]
\[ = U(T, 0) + \frac{1}{2}\mu_0 V M^2 \left( \chi_T^{-1} - T \frac{d}{dT} \chi_T^{-1} \right) \]
\[ U(T, 0) = F(T, 0) + TS(T, 0) \]

We assume that the Curie law is valid:
\[ \chi_T = \frac{C}{T} \iff \chi_T^{-1} = \frac{T}{C} \iff T \frac{d}{dT} \chi_T^{-1} = \frac{T}{C} \]

Then we have
\[ U(T, M) = U(T, 0) \]
\[ S(T, M) = S(T, 0) - \frac{1}{2}\mu_0 V M^2 \frac{1}{C} \]
\[ F(T, M) = F(T, 0) + \frac{1}{2}\mu_0 V M^2 \frac{T}{C} \]

3. Third law:
This requires that for \( T \to 0 \) entropy vanishes, independent of the value of the second variable. We therefore must assume in particular
\[ \lim_{T \to 0} S(T, 0) = 0 \]

If we take \( M(T) \neq 0 \) if \( H \neq 0 \), then according to the entropy obtained in 2. it must be concluded that if the Curie law is valid, then the third law is violated. On the contrary, it must further hold
\[ \lim_{T \to 0} \frac{d}{dT} \chi_T^{-1}(T) = \lim_{T \to 0} \frac{1}{\chi_T^2} \frac{d\chi_T}{dT} = 0 \]
with a constant \( c \neq 0 \). \( \chi_T(T) \) therefore should not diverge, specially for \( T \to 0 \).

**Problem 4.8**

1. Internal energy \( U = U(T, M) \) and the equation of state in the form \( M = f(T, H) \) are given. First law (1.80)
\[ dU = \delta Q + \mu_0 V H dM \]
\[ \implies c_M = \left( \frac{\partial U}{\partial T} \right)_M \]

So that it holds
\[ \delta Q = c_M dT + \left[ \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right] dM \]

\[ c_H = \left( \frac{\delta Q}{dT} \right)_H = c_M + \left[ \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right] \left( \frac{\partial M}{\partial T} \right)_H \]

Therefore

\[ c_H - c_M = \left[ \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right] \left( \frac{\partial M}{\partial T} \right)_H \]

2. Ideal paramagnet:

\[ M = \frac{C}{T} H \quad ; \quad \left( \frac{\partial U}{\partial M} \right)_T = 0 \quad C : \text{Curie constant} \]

\[ \left( \frac{\partial M}{\partial T} \right)_H = -\frac{C}{T^2} H \]

\[ c_H - c_M = \frac{\mu_0 V}{C} M^2 \geq 0 \]

3. (a) Maxwell relation obtained from the free energy is

\[ dF = -SdT + \mu_0 V H dM \]

\[ \left( \frac{\partial S}{\partial M} \right)_T = -\mu_0 V \left( \frac{\partial H}{\partial T} \right)_M \]

(b) Maxwell relation of the free enthalpy is

\[ dG = -SdT - \mu_0 V M dH \]

\[ \left( \frac{\partial S}{\partial H} \right)_T = \mu_0 V \left( \frac{\partial M}{\partial T} \right)_H \]

(c) According to 1. from the first law follows:

\[ \delta Q = TdS = c_M dT + \left[ \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right] dM \]

\[ T \left( \frac{\partial S}{\partial M} \right)_T = \left[ \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right] \]
This is the proposition!

4. 

\[ c_H - c_M = 1) \left( \left( \frac{\partial U}{\partial M} \right)_T - \mu_0 V H \right) \left( \frac{\partial M}{\partial T} \right)_H \]

\[ = 3.c) T \left( \frac{\partial S}{\partial M} \right)_T \left( \frac{\partial M}{\partial T} \right)_H \]

\[ = 3.a) -\mu_0 V T \left( \frac{\partial H}{\partial T} \right)_M \left( \frac{\partial M}{\partial T} \right)_H \]

5. 

\[ \left( \frac{\partial H}{\partial T} \right)_M = \frac{M}{C} \Leftrightarrow c_H - c_M = -\mu_0 V T \frac{M}{C} \left( \frac{\partial M}{\partial T} \right)_H \]

Equation of state:

\[ dH = \frac{M}{C} dT + \frac{1}{C} (T - T_C) dM + 3 b M^2 dM \]

\[ \Leftrightarrow \left( \frac{\partial M}{\partial T} \right)_H \left[ \frac{1}{C} (T - T_C) + 3 b M^2 \right] = -\frac{M}{C} \]

So that it follows:

\[ c_H - c_M = \mu_0 V \frac{T M^2}{C (T - T_C) + 3 b C^2 M^2} \]

6. 

\[ \left( \frac{\partial c_M}{\partial M} \right)_T = \left( \frac{\partial}{\partial M} \left( T \left( \frac{\partial S}{\partial M} \right)_M \right) \right)_T \]

\[ = T \left( \frac{\partial}{\partial T} \left( \frac{\partial S}{\partial M} \right)_M \right)_M \]

\[ = 3.a) T(-\mu_0 V) \left( \frac{\partial^2 H}{\partial T^2} \right)_M \]

\[ = 0 \]

7. Because of 6. it holds:
\[
\left( \frac{\partial U}{\partial T} \right)_M = c_M(T)
\]

According to 3. it also holds

\[
\left( \frac{\partial U}{\partial T} \right)_M = T \left( \frac{\partial S}{\partial M} \right)_T + \mu_0 V H
\]

\[= -\mu_0 V T \left( \frac{\partial H}{\partial T} \right)_M + \mu_0 V H\]

\[=-\mu_0 V T \frac{M}{C} + \mu_0 V \frac{1}{C} (T - T_C) M + \mu_0 V b M^3\]

\[= \mu_0 V \left( b M^3 - \frac{T_C}{C} M \right)\]

Integration:

\[
U(T, M) = \mu_0 V \left( \frac{1}{4} b M^4 - \frac{T_C}{2 C} M^2 \right) + f(T)
\]

Then it must be

\[c_M(T) = f'(T)\]

So that we have

\[
U(T, M) = \mu_0 V \left( \frac{1}{4} b M^4 - \frac{T_C}{2 C} M^2 \right) + \int^T c_M(T')dT' + U_0
\]

One gets entropy analogously:

\[\left( \frac{\partial S}{\partial T} \right)_M = \frac{1}{T} c_M(T)\]

\[
\left( \frac{\partial S}{\partial M} \right)_T \overset{3.a.}{=} -\mu_0 V \left( \frac{\partial H}{\partial T} \right)_M = -\mu_0 V \frac{M}{C}
\]

\[
S(T, M) = -\mu_0 V \frac{M^2}{2 C} + \int^T \frac{c_M(T')}{T'}dT' + S_0
\]
That means for the free energy

\[
F = U - TS \\
= F_0 + \frac{1}{4} \mu_0 V b M^4 + \mu_0 V \frac{M^2}{2C} (T - T_C) \\
+ \int_0^T \frac{c_M(T')}{T'} dT' \\
F_0 = U_0 - T S_0
\]

8.

\[
H = \frac{1}{C} (T - T_C) M + b M^3
\]

For \( H \to 0 \) we get the trivial solution \( M = 0 \), but also

\[
M_S = \pm \sqrt{\frac{1}{b C} (T_C - T)}
\]

These solutions are real for \( T \leq T_C \). For the free energy we take the result from 7.:

\[
F(T, M) = f(T) + \frac{\mu_0 V}{2C} (T - T_C) M^2 + \frac{1}{4} \mu_0 V b M^4
\]

We substitute in this expression both the mathematical solutions:

\[
F(T, M = 0) = f(T) \\
F(T; M = \pm M_S) = f(T) + \frac{\mu_0 V}{2C} (T - T_C) \frac{1}{b C} (T_C - T) \\
+ \frac{1}{4} \mu_0 V b \frac{1}{b^2 C^2} (T_C - T)^2 \\
= f(T) - \frac{1}{4} \frac{\mu_0 V}{b C^2} (T_C - T)^2
\]

It obviously holds

\[
F(T, M = \pm M_S) \leq F(T, M = 0)
\]

The equality sign holds for \( T = T_C \). Therefore the ferromagnetic solution is stable. This exists as a real solution only for \( T \leq T_C \).

9. Magnetic susceptibility
\[ \chi_T = \left( \frac{\partial M}{\partial H} \right)_T = \frac{1}{(\partial M/\partial H)_T} = \frac{1}{C(T - T_C) + 3bM^2} \]

\[ \lim_{H \to 0} \chi_T = \frac{1}{C(T - T_C) + 3bM^2} = \frac{C}{2(T_C - T)} \]

\( \chi_T \) diverges for \( T \to T_C \), as required by the general theory of phase transitions. Finally we again use the result from 5.:

\[
\lim_{H \to 0} (c_H - c_M) = \mu_0 V \frac{T M_S^2}{C(T - T_C) + 3bC^2M_S^2} = \mu_0 V \frac{T}{bC^2(T_C - T)}
\]

For \( T \to 0 \) the two heat capacities are therefore equal to zero as demanded by the third law.

**Problem 4.9**

1. According to Problem 4.7 we have

\[ U(T, M) = U(T, 0) \]

Since

\[ c_M = \left( \frac{\partial U}{\partial T} \right)_{M=0} = \gamma T \]

follows:

\[ U(T, M) = U_0 + \frac{1}{2} \gamma T^2 \]

*Isothermal* change of field from 0 to \( H \neq 0 \):

\[ \Delta U = 0 \]

That means

\[ \Delta Q = -\Delta W = -V \mu_0 \int_0^H H' dH' \]

\[ dM' = \frac{C}{T_1} dH' \]

\[ \Delta Q = -V \mu_0 \frac{C}{T_1} \int_0^H H' dH' = -\frac{\mu_0 VC}{2T_1} H^2 < 0 \]
2. *Adiabatic and reversible* means: \( dS = 0 \), therefore

\[
S(T_1, H) \overset{1}{=} S(T_f, 0)
\]

From Problem 4.7 we have

\[
S(T, M) = S(T, 0) - \frac{1}{2} \mu_0 V \frac{1}{C} M^2
\]

\[
S(T, 0) - S_0 = \int_0^T \frac{c_{M=0}(T')}{T'} dT' = \gamma T
\]

\[
\sim S(T, M) = S_0 + \gamma T - \frac{1}{2} \mu_0 V \frac{1}{C} M^2
\]

\[
\sim S(T, H) = S_0 + \gamma T - \frac{1}{2} \mu_0 CV \frac{H^2}{T^2}
\]

Switching off the field

\[
S(T_1, H) = S_0 + \gamma T_1 - \frac{1}{2} \mu_0 CV \frac{H^2}{T_1^2}
\]

\[
\overset{1}{=} S(T_f, 0) = S_0 + \gamma T_f
\]

\[
\sim \text{final temperature:}
\]

\[
T_f = T_1 - \frac{1}{2} \mu_0 CV \frac{H^2}{\gamma T_1^2} < T_1
\]

\[
\sim \text{Cooling effect.}
\]

**Problem 5.1**

*Commutation relations:*

1.

\[
\left[ S_i^+, S_i^- \right] = i \hbar^2 \left[ c_i^{+\uparrow} c_i^{\downarrow}, c_i^{+\downarrow} c_i^{\uparrow} \right] = i \hbar^2 \left( c_i^{+\uparrow} (1 - n_i^{\downarrow}) c_i^{\uparrow} - c_i^{+\downarrow} (1 - n_i^{\uparrow}) c_i^{\downarrow} \right) = i \hbar^2 \left( n_i^{\uparrow} (1 - n_i^{\downarrow}) - n_i^{\downarrow} (1 - n_i^{\uparrow}) \right) = i \hbar^2 \left( n_i^{\uparrow} - n_i^{\downarrow} \right) = 2 \hbar S_i^z
\]
\[ [S^+_i, S^-_i] = \frac{1}{2} \hbar^2 \left( \left[ n_{i\uparrow}, c^+_i c_i \right] - \left[ n_{i\downarrow}, c^+_i c_i \right] \right) \]
\[ = \frac{1}{2} \hbar^2 \left( (n_{i\uparrow} - n_{i\downarrow}) c^+_i c_i \downarrow - c^+_i c_i \downarrow (n_{i\uparrow} - n_{i\downarrow}) \right) \]
\[ = \frac{1}{2} \hbar^2 \left( \frac{n_{i\uparrow} c^+_i c_i \downarrow - c^+_i n_{i\downarrow} c_i \downarrow + c^+_i c_i \downarrow n_{i\downarrow}}{c^+_i \downarrow} \right) \]
\[ = \hbar^2 c^+_i c_i \downarrow \]
\[ = \hbar S^+_i \]

\[ [S^-_i, S^-_i] = \frac{1}{2} \hbar^2 \left( (n_{i\uparrow} - n_{i\downarrow}) c^+_i c_i \uparrow - c^+_i c_i \uparrow (n_{i\uparrow} - n_{i\downarrow}) \right) \]
\[ = \frac{1}{2} \hbar^2 \left( -n_{i\downarrow} c^+_i c_i \uparrow - c^+_i c_i \uparrow n_{i\uparrow} \right) \]
\[ = -\hbar^2 c^+_i c_i \uparrow \]
\[ = -\hbar S^-_i \]

\[ S_i^2 = S^+_i S^-_i + S^+_i S^-_i + S^+_i S^+_i \]
\[ = \frac{1}{2} \left( S^+_i S^-_i + S^-_i S^+_i \right) + S^+_i S^+_i \]
\[ = \frac{\hbar^2}{2} \left( \frac{c^+_i c_i \downarrow + c^+_i c_i \uparrow + c^+_i c_i \uparrow c_i \downarrow}{n_{i\uparrow} + n_{i\downarrow}} \right) + \frac{\hbar^2}{4} \left( n_{i\uparrow} + n_{i\downarrow} - 2n_{i\uparrow} n_{i\downarrow} \right) \]
\[ = \hbar^2 \left( \frac{3}{4} (n_{i\uparrow} + n_{i\downarrow}) - \frac{3}{2} n_{i\uparrow} n_{i\downarrow} \right) \]
\[ = \frac{3}{4} \hbar^2 (n_{i\uparrow} + n_{i\downarrow} - 2n_{i\uparrow} n_{i\downarrow}) \]
\[ = \frac{3}{4} \hbar^2 (n_{i\uparrow} - n_{i\downarrow})^2 \]
\[ = \hbar^2 S(S + 1) \quad \left( S = \frac{1}{2} \right) \]

only if there is exactly one electron per lattice site
2.
\[
\begin{align*}
\left[ c_{q\sigma}, c_{k\sigma}' \right]_+ &= \frac{1}{N} \sum_{i,j} e^{-i(qR_i + i kR_j)} \left[ c_{i\sigma}, c_{j\sigma}' \right]_+ \\
&= \delta_{\sigma\sigma'} \frac{1}{N} \sum_i e^{-i(q-k)R_i} \\
&= \delta_{q,k} \delta_{\sigma\sigma'}
\end{align*}
\]

\[
\left[ c_{q\sigma}, c_{k\sigma} \right]_+ = \left[ c_{q\sigma}', c_{k\sigma}' \right]_+ = 0
\]

**Problem 5.2**

Free energy:

\[
F = U - TS; \quad \quad dF = -SdT + \mu_0 VHdM
\]

Integrability condition:

\[
\left( \frac{\partial S}{\partial M} \right)_T = -\mu_0 V \left( \frac{\partial H}{\partial T} \right)_M
\]

Curie–Weiss law:

\[
M = \frac{C}{T - T_C} H \quad (C : \text{Curie constant})
\]

Heat capacity:

\[
\begin{align*}
\left( \frac{\partial c_M}{\partial M} \right)_T &= T \left( \frac{\partial^2 S}{\partial M \partial T} \right)_M \\
&= T \left[ \frac{\partial}{\partial T} \frac{\partial S}{\partial M} \right] \\
&= -\mu_0 VT \left[ \frac{\partial}{\partial T} \left( \frac{\partial H}{\partial T} \right)_M \right] \\
&= 0
\end{align*}
\]

\[
\therefore c_M(T, M) \equiv c_M(T)
\]

Internal energy:

Equation (1.80): \( dU = TdS + \mu_0 VHdM \)
\begin{align*}
\left( \frac{\partial U}{\partial T} \right)_{M} &= T \left( \frac{\partial S}{\partial T} \right)_{M} = c_M(T) \\
\left( \frac{\partial U}{\partial M} \right)_{T} &= T \left( \frac{\partial S}{\partial M} \right)_{T} + \mu_0 VH \\
&\overset{s.o.}{=} -\mu_0 VT \left( \frac{\partial H}{\partial T} \right)_{M} + \mu_0 VH \\
&= -\mu_0 VT \frac{M}{C} + \mu_0 V \frac{T - T_C}{C} M \\
&= -\mu_0 V \frac{M}{C} T_C
\end{align*}
This means

\[ U(T, M) = -\mu_0 V T_C \frac{M^2}{2C} + f(T) \]
Because of

\[ \left( \frac{\partial U}{\partial T} \right)_{M} = f'(T) = c_M(T) \]
altogether we have

\[ U(T, M) = \int_{0}^{T} c_M(T')dT' - \mu_0 V T_C \frac{M^2}{2C} + U_0 \]

Entropy:

\begin{align*}
\left( \frac{\partial S}{\partial M} \right)_{T} &= \sigma'(M) = -\mu_0 V \left( \frac{\partial H}{\partial T} \right)_{M} = -\mu_0 V \frac{M}{C} \\
\Rightarrow \quad \sigma(M) &= -\mu_0 V \frac{M^2}{2C} + \sigma_0 \\
S(T, M) &= \sigma_0 + \int_{0}^{T} \frac{c_M(T')}{T'}dT' - \mu_0 V \frac{M^2}{2C}
\end{align*}
Free energy:
\[ F(T, M) = U(T, M) - T S(T, M) \]

\[ = F_0(T) + \int_0^T c_M(T') \left( 1 - \frac{T}{T'} \right) dT' + \frac{\mu_0 V}{2C} M^2(T - T_C) \]

\[ F_0(T) = U_0 - T \sigma_0 \]

Check:

\[ S(T, M) = -\left( \frac{\partial F(T, M)}{\partial T} \right)_M \]

Free enthalpy:

\[ G(T, H) = F - \mu_0 V M H \]

\[ = F - \frac{\mu_0 V}{C}(T - T_C)M^2 \]

\[ = F_0(T) + \int_0^T c_M(T') \left( 1 - \frac{T}{T'} \right) dT' - \frac{\mu_0 V}{2C} M^2(T - T_C) \]

\[ G(T, H) \]

\[ = F_0(T) + \int_0^T c_M(T') \left( 1 - \frac{T}{T'} \right) dT' - \frac{1}{2} \frac{\mu_0 VC}{T - T_C} H^2 \]

Problem 5.3

1. 

\[ c_M(T, M = 0) = T \left( \frac{\partial S}{\partial T} \right)_{M=0} \]

\[ S(T, 0) = \int_0^T \frac{c_M(T', M = 0)}{T'}dT' = \gamma T \]

With the result of Problem 5.2

\[ S(T, M) = \gamma T - \mu_0 V \frac{M^2}{2C} + \sigma_0 \]

Because
\[ M = \frac{C}{T - T_C} H \]

directly follows:

\[ S(T, H) = \gamma T - \frac{1}{2} \mu_0 C V \frac{H^2}{(T - T_C)^2} + \sigma_0 \]

For the free energy \( F \) we use

\[ \left( \frac{\partial F}{\partial T} \right)_M = -S(T, M) \]

\[ F(T, M) = F_0(M) - \frac{1}{2} \gamma T^2 + \mu_0 V \frac{M^2}{2C} T - \sigma_0 T \]

According to the considerations of Problem 5.2 we must have

\[ F(T, M) = F_0(T) + \frac{1}{2} \gamma T^2 - \gamma T^2 + \mu_0 V \frac{M^2}{2C} (T - T_C) \]

\[ \Rightarrow F_0(M) = U_0 - \frac{\mu_0 V}{2C} M^2 T_C \]

What remains is only

\[ F(T, M) = U_0 - \frac{1}{2} \gamma T^2 + \frac{\mu_0 V}{2C} M^2 (T - T_C) \]

Internal energy again from Problem 5.2:

\[ U(T, M) = U_0 + \frac{1}{2} \gamma T^2 - \mu_0 VT_C \frac{M^2}{2C} \]

Check:

\[ F(T, M) = U(T, M) - TS(T, M) \]

\[ = U_0 - \frac{1}{2} \gamma T^2 + \frac{\mu_0 V}{2C} M^2 (T - T_C) - \sigma_0 T \]

\[ \Rightarrow \sigma_0 = 0 \]

2. Heat capacities

\[ c_M(T, M) = T \left( \frac{\partial S}{\partial T} \right)_M = \gamma T = c_M(T, M = 0) \]

\[ c_H(T, H) = T \left( \frac{\partial S}{\partial T} \right)_H = \gamma T + \mu_0 CV \frac{TH^2}{(T - T_C)^3} \]
Since $T > T_C$, we have $c_H \geq c_M$.

From elementary thermodynamics

$$\chi_s(T, H) = \chi_T \frac{c_M}{c_H} = \frac{C}{T - T_C + \frac{\mu_0 CV}{\gamma} \frac{H^2}{(T - T_C)^2}}$$

Problem 5.4

1. Spontaneous sub-lattice magnetization $(B_0 = 0)$

$$M_{1S}(T) = -M_{2S}(T)$$

$$\sim B_A^{(i)} = \mu_0 (\lambda - \rho) M_{iS}(T)$$

$$\sim M_{iS}(T) = M_0^* B_J (\beta g_J \mu_B (\lambda - \rho) M_{iS}(T))$$

$T \rightarrow T_c \quad \sim M_{iS}$ will be very small

$$\sim M_{iS} = \frac{J + 1}{3J} (n^* g_J \mu_B) \beta g_J \mu_0 \mu_B (\lambda - \rho) M_{iS}$$

Curie constant: $C = n \frac{\mu_0^2 \mu^2}{3k_B} g_J^2 J (J + 1)$; $n^* = \frac{N}{2V} = \frac{1}{2} n$

$$\sim M_{iS} \approx \frac{1}{2} (\lambda - \rho) C \frac{M_{iS}}{T}$$

Condition for intersection at finite $M_{iS}$:

\[
\frac{d}{dM_{iS}} (M_0 B_j(...)) \bigg|_{M_{iS}=0} \geq 1
\]
1. \[ \frac{1}{2}(\lambda - \rho)CT \geq 1 \]

\[ \implies T_N = \frac{1}{2}(\lambda - \rho)C \]

2. High temperature behaviour:
   No spontaneous sub-lattice magnetization

\[ \beta \mu_B B_0 \ll 1 \]

\[ \sim M_1(T, B_0) \cong \frac{J + \frac{1}{3}n^*g_J J \mu_B}{\mu_0 \mu_B} \beta g_J J \mu_B (B_0 + B_A^{(i)}) \]

\[ = \frac{1}{2} C \frac{1}{T} (B_0 + B_A^{(i)}) \frac{1}{\mu_0} \]

Total magnetization:

\[ M(T, B_0) = M_1(T, B_0) + M_2(T, B_0) \]

\[ = \mu_0 \frac{C}{T} B_0 + \frac{1}{2} \frac{C}{T} \left( B_A^{(1)} + B_A^{(2)} \right) \frac{1}{\mu_0} \frac{1}{\mu_0(\lambda + \rho)(M_1 + M_2)} \]

\[ \sim M(T, B_0) \left( 1 - \frac{1}{2} \frac{C}{T} (\lambda + \rho) \right) = \frac{C}{\mu_0 T} B_0 \]

\[ \sim M(T, B_0) = \frac{C}{T - \frac{1}{2} C(\lambda + \rho)} \frac{1}{\mu_0} B_0 \]

\[ \sim \text{Curie–Weiss law} \]

\[ \chi(T) = \mu_0 \left( \frac{\partial M}{\partial B_0} \right) = \frac{C}{T - \Theta} \]

\[ \Theta = \frac{1}{2} C(\lambda + \rho) \]

paramagnetic Curie temperature

3. necessary: \( \rho < 0 \)

\[ -\frac{\Theta}{T_N} = \frac{\lambda + \rho}{\rho - \lambda} = \frac{|\rho| - \lambda}{|\rho| + \lambda} \]

(a) \( \lambda > 0 \): ferromagnetic coupling within the sub-lattice

\[ -\frac{\Theta}{T_N} < 1 \]

i.a.: \( \Theta < 0 \) \( (\lambda < |\rho|) \)
Example: EuTe: $\Theta = -4.0K$; $T_N = 9.6K$

$(\beta)$ $\lambda < 0$: antiferromagnetic coupling in the sub-lattice in order to have $T_N > 0$:

$|\lambda| < |\rho|$

$$-\frac{\Theta}{T_N} = \frac{|\rho| + |\lambda|}{|\rho| - |\lambda|} \quad \text{always: } \Theta < 0$$

$$-\frac{\Theta}{T_N} > 1$$

Examples:

<table>
<thead>
<tr>
<th>Material</th>
<th>$-\frac{\Theta}{T_N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO</td>
<td>5.3</td>
</tr>
<tr>
<td>NiO</td>
<td>5.7</td>
</tr>
<tr>
<td>MnF$_2$</td>
<td>1.7</td>
</tr>
</tbody>
</table>

Typically: $\Theta < 0$

**Problem 5.5**

According to Problem 4.6 the equation of state of Weiss ferromagnet reads

$$M = M_0 L \left( m \frac{\mu_0 H + \lambda \mu_0 M}{k_B T} \right)$$

1. $m \lambda \mu_0 M = M_0 \frac{N m^2 \lambda \mu_0}{k_B T} = M_0 \frac{3k_B C \lambda}{k_B T}$

Classical Curie constant (Problem 4.6)

$$C = \mu_0 \frac{N m^2}{V 3k_B}$$
Further using (5.13): \(T_C = \lambda C\) and then we have

\[
\hat{M} = L \left( b + 3 \frac{\hat{M}}{\varepsilon + 1} \right)
\]

2. Series expansion of the Langevin function

\[
L(x) = \frac{1}{3}x - \frac{1}{45}x^3 + O(x^5)
\]

\[
B_0 = \mu_0 H = 0 \quad \Rightarrow \quad b = 0
\]

\[
T \rightarrow T_c \quad \Rightarrow \quad \hat{M} \text{ very small}
\]

Then we can write approximately

\[
\hat{M} \approx \frac{\hat{M}}{\varepsilon + 1} - \frac{3}{5} \frac{\hat{M}^3}{(\varepsilon + 1)^3}
\]

For \(\hat{M} \neq 0\) that means

\[
\frac{\varepsilon}{\varepsilon + 1} \approx -\frac{3}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^3} \quad \Rightarrow \quad \hat{M}^2 \approx -\frac{5}{3} \varepsilon(\varepsilon + 1)^2
\]

Since \((\varepsilon + 1)^2 \rightarrow 1\) for \(T \rightarrow T_C\), it follows that

\[
\hat{M} \sim \sqrt[2]{\frac{5}{3}}(-\varepsilon)^{\frac{1}{2}}
\]

The critical exponent \(\beta\) of the order parameter then has the classical value:

\[
\beta = \frac{1}{2}
\]

3. Critical isotherm: \(T = T_c\); \(B_0 \rightarrow 0\)

\[
\Rightarrow \quad \varepsilon = 0 \text{ and } \hat{M} \text{ as well as } b \text{ very small.}
\]

This means
\[
\hat{M} \approx \frac{1}{3} b + \hat{M} - \frac{1}{45} (b + 3\hat{M})^3
\]

\[
\sim 15b \approx (b + 3\hat{M})^3 \quad \leftrightarrow \quad b + 3\hat{M} \approx (15b)^{\frac{1}{3}}
\]

\[
\leftrightarrow 3\hat{M} \approx (15b)^{\frac{1}{3}} - b \approx (15b)^{\frac{1}{3}}, \text{ since } b \to 0
\]

\[
\sim b \sim \frac{9}{5} \hat{M}^3
\]

From this we read off the critical exponent:

\[
\delta = 3
\]

That is also well-known value for classical theories.

4. Susceptibility:

\[
\chi_T = \left( \frac{\partial M}{\partial H} \right)_T = \frac{M_0 \mu_0 m}{k_B T} \left( \frac{\partial \hat{M}}{\partial b} \right)_{T,b=0}
\]

\[
= \frac{\frac{N}{V} m^2 \mu_0}{k_B (\varepsilon + 1) T_c} \left( \frac{\partial \hat{M}}{\partial b} \right)_{T,b=0}
\]

\[
= \frac{3}{\lambda (\varepsilon + 1)} \left( \frac{\partial \hat{M}}{\partial b} \right)_{T,b=0}
\]

In the critical region \( \hat{M} \) is very small. Therefore we can expand

\[
\frac{\partial L}{\partial b} \bigg|_{b=0} = \frac{\partial x}{\partial b} \left( \frac{1}{3} - \frac{1}{15} x^2 \right) \bigg|_{b=0}
\]

\[
\frac{\partial x}{\partial b} = 1 + \frac{3}{\varepsilon + 1} \frac{\partial \hat{M}}{\hat{b}}
\]

\[
\sim \frac{\partial \hat{M}}{\partial b} \bigg|_{b=0} = \left( 1 + \frac{3}{\varepsilon + 1} \frac{\partial \hat{M}}{\partial b} \bigg|_{b=0} \right) \left( \frac{1}{3} - \frac{1}{15} (\varepsilon + 1)^2 \right)
\]

\[
\sim \frac{\partial \hat{M}}{\partial b} \bigg|_{b=0} = \left\{ 1 - \frac{1}{\varepsilon + 1} + \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^3} \right\} = \frac{1}{3} \left( 1 - \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^2} \right)
\]

\[
\sim \frac{\partial \hat{M}}{\partial b} \bigg|_{b=0} = \frac{1}{3} \frac{\varepsilon}{\varepsilon + 1} + \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^2}
\]

\( T \to T_c \) means \( \hat{M} \to 0 \):
\[
\left. \frac{\partial \hat{M}}{\partial b} \right|_{b=0} \approx \frac{1}{3} \left[ \frac{\varepsilon}{\varepsilon + 1} + \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^3} \right] \left( 1 + \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^2} \right)^{-1} \\
\approx \frac{1}{3} \left[ \frac{\varepsilon}{\varepsilon + 1} + \frac{9}{5} \frac{\hat{M}^2}{(\varepsilon + 1)^2} \right]^{-1}
\]

(a) \( T \xrightarrow{>} T_c \):
then \( \hat{M} \equiv 0 \) and \( \varepsilon + 1 \xrightarrow{T \to T_c} 1 \):
\[
\left. \frac{\partial \hat{M}}{\partial b} \right|_{b=0} \approx \frac{1}{3} \varepsilon^{-1} \\
\sim \chi_T \sim \frac{1}{\lambda} \varepsilon^{-1}
\]
\( \sim \) critical exponent:
\[ \gamma = 1 \]

(b) \( T \xleftarrow{<} T_c \):
then according to part 2 we have
\[
\hat{M} \sim \sqrt{\frac{5}{3}} (\varepsilon)^{\frac{1}{2}}
\]
This means
\[
\left. \frac{\partial \hat{M}}{\partial b} \right|_{b=0} \approx \frac{1}{3} \left[ \frac{\varepsilon}{\varepsilon + 1} + 3 \frac{-\varepsilon}{(\varepsilon + 1)^2} \right]^{-1} \\
\xrightarrow{T \to T_c} \frac{1}{3} [-2\varepsilon]^{-1} \\
\sim \chi_T \sim \frac{1}{2\lambda} (\varepsilon)^{-1} \Rightarrow \gamma' = 1
\]
Critical amplitudes:
\[ C \sim \frac{1}{\lambda} ; \quad C' \sim \frac{1}{2\lambda} \sim \frac{C}{C'} = 2 \]
The results obtained for \( \gamma, \gamma' \) and \( \varepsilon_\nu \) are typical for the classical theories of phase transitions. The concluding remark is as follows.
The sign “ \( \sim \)” in the above formulae need not necessarily mean proportionality but should be understood as, “for \( T \to T_c \) behaves like”.
Problem 5.6

1. 

\[ (\sigma^{(1)} \cdot \sigma^{(2)})^2 \]

\[ = (\sigma_x^{(1)} \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_z^{(2)})^2 = \]

\[ = (\sigma_x^{(1)})^2 (\sigma_x^{(2)})^2 + (\sigma_y^{(1)})^2 (\sigma_y^{(2)})^2 + (\sigma_z^{(1)})^2 (\sigma_z^{(2)})^2 + \]

\[ + \sigma_x^{(1)} \sigma_x^{(2)} \sigma_y^{(1)} \sigma_y^{(2)} + \sigma_y^{(1)} \sigma_y^{(2)} \sigma_z^{(1)} \sigma_z^{(2)} + \]

\[ + \sigma_z^{(1)} \sigma_z^{(2)} \sigma_x^{(1)} \sigma_x^{(2)} + \sigma_x^{(1)} \sigma_z^{(2)} \sigma_z^{(1)} \sigma_x^{(2)} + \]

\[ + \sigma_y^{(1)} \sigma_y^{(2)} \sigma_x^{(1)} \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_x^{(2)} \sigma_y^{(1)} \sigma_y^{(2)} = \]

\[ = 3 \mathbb{I}^2 - \sigma_x^{(1)} \sigma_x^{(2)} - \sigma_y^{(1)} \sigma_y^{(2)} - \sigma_z^{(1)} \sigma_z^{(2)} - \]

\[ - \sigma_x^{(1)} \sigma_x^{(2)} - \sigma_y^{(1)} \sigma_y^{(2)} - \sigma_z^{(1)} \sigma_z^{(2)} = \]

\[ = 3 \mathbb{I} - 2 \sigma^{(1)} \cdot \sigma^{(2)} \]

Here the properties (5.81) and (5.82) of the Pauli spin matrices are used many times.

2. Representatively, we calculate the x-component

\[ Q_{12} \sigma_x^{(1)} \]

\[ = \frac{1}{2} (\mathbb{I} + \sigma_x^{(1)} \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_z^{(2)}) \sigma_x^{(1)} = \]

\[ = \frac{1}{2} (\sigma_x^{(1)} + (\sigma_x^{(1)})^2 \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_x^{(1)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_x^{(1)} \sigma_z^{(2)}) \]

\[ = \frac{1}{2} (\sigma_x^{(1)} + \sigma_x^{(2)} - i \sigma_y^{(1)} \sigma_y^{(2)} + i \sigma_y^{(1)} \sigma_z^{(2)}) \]

\[ \sigma_x^{(2)} Q_{12} \]

\[ = \frac{1}{2} \sigma_x^{(2)} (\mathbb{I} + \sigma_x^{(1)} \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_z^{(2)}) = \]

\[ = \frac{1}{2} (\sigma_x^{(2)} + \sigma_x^{(1)} (\sigma_x^{(2)})^2 + \sigma_y^{(1)} \sigma_x^{(2)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_x^{(2)} \sigma_z^{(2)}) \]

\[ = \frac{1}{2} (\sigma_x^{(2)} + \sigma_x^{(1)} + i \sigma_y^{(1)} \sigma_z^{(2)} - i \sigma_z^{(1)} \sigma_y^{(2)}) \]

That means

\[ Q_{12} \sigma_x^{(1)} = \sigma_x^{(2)} Q_{12} \]

so that the proposition for the x-component is proved. Analogously one can prove for the other components.

3. We use
\[ \sigma_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

\[ \sigma_x \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

\[ \sigma_y \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = i \begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

\[ \sigma_y \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

\[ \sigma_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad \sigma_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} \]

So that one immediately recognizes

\[ \sigma^{(1)} \cdot \sigma^{(2)} |\uparrow\uparrow\rangle = |\downarrow\downarrow\rangle + i^2 |\downarrow\uparrow\rangle + |\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle \]

\[ \sigma^{(1)} \cdot \sigma^{(2)} |\downarrow\downarrow\rangle = |\uparrow\uparrow\rangle + (-i)^2 |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle \]

\[ \sigma^{(1)} \cdot \sigma^{(2)} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

\[ = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

\[ = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \]

\[ \sigma^{(1)} \cdot \sigma^{(2)} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \]

\[ = (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle) \]

\[ = 3(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle) \]

The spin states are therefore eigenstates of the operator \( \sigma^{(1)} \cdot \sigma^{(2)} \) with the eigenvalues \((1, 1, 1, -3)\). Therefore they are also the eigenstates of \( Q_{12} \) with the eigenvalues \((1, 1, 1, -1)\).

**Problem 5.7**

\[ R = \int_0^{\infty} dx \ x \frac{\sin x}{x^2 - y^2} = \frac{1}{4i} \int_{-\infty}^{+\infty} dx \ x \frac{\exp(i x) - \exp(-i x)}{x^2 - y^2} \]

We use the residue theorem and for that we choose the integration path parallel to the real axis from \(-\infty + i 0^+\) to \(+\infty + i 0^+\), close it with a semicircle at infinity in the upper half-plane for the first exponential function and in the lower half-plane for the second exponential function. Then the exponentials see to it that the semicircles do not contribute to the integral. The poles at \( x = \pm y \) lie inside the (mathematically
negatively running) integration path $C$ only for the second term. Then from the residue theorem we get

$$R = -\frac{1}{8i} \int_C dx \, e^{-ix} \left( \frac{1}{x+y} + \frac{1}{x-y} \right)$$

$$= \frac{2\pi i}{8i} \left( e^{+iy} + e^{-iy} \right)$$

$$= \frac{\pi}{2} \cos y$$

**Problem 5.8**

1. The diagonal terms $\mu = \nu$ in $\hat{H}_1$ directly give $H_U$:

$$\hat{H}_1(\mu = \nu) = H_U$$

That is why from now on we will consider only the non-diagonal terms $\mu \neq \nu$. For these we have to calculate

$$\hat{H}_1(\mu \neq \nu) = \frac{1}{2} \sum_{\mu \neq \nu} \sum_{i \sigma \sigma'}^{\mu \mu} \left[ U_{\mu \nu} n_{i \mu \sigma} n_{i \nu \sigma'} + J_{\mu \nu} c_{i \mu \sigma}^\dagger c_{i \nu \sigma'}^\dagger c_{i \mu \sigma'} c_{i \nu \sigma} \right]$$

The first summand leads to

$$\hat{H}_{1a}(\mu \neq \nu) = \frac{1}{2} \sum_{i \mu \nu} U_{\mu \nu} n_{i \mu} n_{i \nu}$$

The second summand we somewhat reformulate

$$\hat{H}_{1b}(\mu \neq \nu) = \frac{1}{2} \sum_{i \mu \nu} \sum_{\mu \neq \nu} J_{\mu \nu} \left[ c_{i \mu \uparrow}^\dagger c_{i \nu \uparrow}^\dagger c_{i \mu \uparrow} c_{i \nu \uparrow} + c_{i \mu \uparrow}^\dagger c_{i \nu \downarrow}^\dagger c_{i \mu \downarrow} c_{i \nu \uparrow} +
+ c_{i \mu \downarrow}^\dagger c_{i \nu \uparrow}^\dagger c_{i \mu \uparrow} c_{i \nu \downarrow} + c_{i \mu \downarrow}^\dagger c_{i \nu \downarrow}^\dagger c_{i \mu \downarrow} c_{i \nu \downarrow} \right]$$

$$= \frac{1}{2} \sum_{i \mu \nu} \sum_{\mu \neq \nu} J_{\mu \nu} \left[ -\sigma_{i \mu \uparrow} \sigma_{i \nu \uparrow}^\dagger - \sigma_{i \mu \uparrow}^\dagger \sigma_{i \nu \uparrow} + n_{i \mu \uparrow} n_{i \nu \uparrow} - n_{i \mu \downarrow} n_{i \nu \downarrow} \right]$$

$$= \frac{1}{2} \sum_{i \mu \nu} \sum_{\mu \neq \nu} J_{\mu \nu} \left[ -2\sigma_{i \mu \uparrow}^\dagger \sigma_{i \nu \uparrow} - 2\sigma_{i \mu \downarrow} \sigma_{i \nu \downarrow} + 2\sigma_{i \mu \downarrow}^\dagger \sigma_{i \nu \uparrow} - 2\sigma_{i \mu \uparrow} \sigma_{i \nu \downarrow} \right]$$
We recognize
\[ \hat{H}_1(\mu \neq \nu) = \hat{H}_{1a}(\mu \neq \nu) + \hat{H}_{1b}(\mu \neq \nu) = H_d + H_{ex} \]

Thus the proposition is proved.

2. As an example we consider EuO. This has 5d-conduction bands which are empty and seven half-filled 4f-bands (levels). For the empty (!) conduction bands \( H_U \) does not play any role but for sufficiently large \( U_{\mu\mu} \), it splits each of the f-bands into two sub-bands out of which the lower one is occupied and the upper one is empty. This leads to the localized magnetic 4f-moment. \( H_d \) provides only an unimportant energy shift of the f-levels. \( H_{ex} \) becomes important if \( \mu \) is an index of the conduction band and \( \nu \) is that of an f-band or the converse. Let us assume that the coupling between the conduction band and the f-level is same for all the conduction bands,
\[ J_\mu = \frac{4}{\hbar} J_{\mu\nu} \forall \nu \]
and define as localized spin:
\[ S_{if} = \sum_\nu s_{i\nu} \]
where the \( \nu \)-summation runs exclusively over the f-levels, then, \( H_{ex} \) becomes the interaction operator of the multi-band Kondo lattice model:
\[ H_{df} = -\sum_{i\mu} J_\mu S_{if} \cdot \sigma_{i\mu} \]
The \( \mu \)-summation runs only over the conduction bands.

**Problem 5.9**

1. We use the matrix representation with the basis
\[ | k\sigma\rangle_\alpha = c_{k\sigma\alpha} | 0 \rangle \]
\[ \alpha = A, B \]
Then the “free” matrix reads as
\[ H_{k\sigma}^{(0)} = \sum_{\alpha\beta} \varepsilon_{\alpha\beta}(k)c_{k\sigma\alpha}^\dagger c_{k\sigma\beta} \]
with the elements

\[
(H_{k\sigma}^{(0)})^{\gamma \delta} = \langle 0 | c_{k\sigma \gamma} \sum_{\alpha \beta} \varepsilon_{\alpha \beta}(k) c_{k \sigma \alpha}^\dagger c_{k \sigma \beta} c_{k \sigma \delta}^\dagger | 0 \rangle \\
= \sum_{\alpha \beta} \varepsilon_{\alpha \beta}(k) \delta_{\gamma \alpha} \delta_{\delta \beta} \langle 0 | 0 \rangle = \varepsilon_{\gamma \delta}(k)
\]

Hamilton Matrix:

\[
H_{k\sigma}^{(0)} = \begin{pmatrix}
\varepsilon(k) & t(k) \\
t^*(k) & \varepsilon(k)
\end{pmatrix}
\]

Eigenenergies:

\[
\det \left( E_{0k} - H_{k\sigma}^{(0)} \right) \uparrow = 0
\]

\[
\sim (\varepsilon(k) - E_{0k})^2 - |t(k)|^2 \uparrow = 0
\]

\[
\sim E_{0k}^{(\pm)} = \varepsilon(k) \pm |t(k)|
\]

Eigenstates:

\[
\left( \mp |t(k)| \begin{pmatrix} t(k) \\
t^*(k) \mp |t(k)| \end{pmatrix} \begin{pmatrix} c_A \\
c_B \end{pmatrix} \right) = 0
\]

\[
\sim c_A^{(\pm)} = \pm \gamma c_B^{(\pm)}; \quad \gamma = \frac{t(k)}{|t(k)|}
\]

Normalization \(\sim\)

\[
|E_{0k\sigma}^{(\pm)}\rangle = \frac{1}{\sqrt{2}} \left( \gamma c_{k \sigma A}^\dagger \pm c_{k \sigma B}^\dagger \right) |0\rangle
\]

2. Schrödinger’s first-order perturbation theory:

\[
\langle E_{0k\sigma}^{(\pm)} | H_1 | E_{0k\sigma}^{(\pm)} \rangle
\]

\[
= \frac{1}{2} \left( -\frac{1}{2} Jz_{k\sigma} \right) \sum_\alpha \langle S^z_\alpha \rangle (0) \left( \gamma^* c_{k \sigma A} \pm c_{k \sigma B} \right) \left( \gamma c_{k \sigma A}^\dagger \pm c_{k \sigma B}^\dagger \right) \\
\star \left( \gamma^* c_{k \sigma A} \pm c_{k \sigma B}^\dagger \right) |0\rangle
\]

\[
= -\frac{1}{4} Jz_{k\sigma} \langle S^z \rangle \left( |\gamma|^2 (0|c_{k \sigma A} c_{k \sigma A}^\dagger c_{k \sigma A} c_{k \sigma A}^\dagger |0\rangle) - \langle 0|c_{k \sigma B} c_{k \sigma B}^\dagger c_{k \sigma B} c_{k \sigma B}^\dagger |0\rangle) \right)
\]

\[
= -\frac{1}{4} Jz_{k\sigma} \langle S^z \rangle (|\gamma|^2 - 1) \langle 0|0\rangle
\]
The first order therefore does not contribute

\[ E_{1k\sigma}^{(\pm)} \equiv 0 \]

The energy correction in second order:

We need the following matrix element:

\[
\langle E(\pm) | H_1 | E(\mp) \rangle
\]

\[
= \frac{1}{2} \left( -\frac{1}{2} J z_\sigma \right) \sum_\alpha \langle S^z_\alpha \rangle \langle 0 | (\gamma^* c_{k\sigma A} + c_{k\sigma B}) c_{k\sigma A}^\dagger c_{k\sigma B}^\dagger | 0 \rangle
\]

\[
* (\gamma c_{k\sigma A}^\dagger - c_{k\sigma B}^\dagger) | 0 \rangle
\]

\[
= -\frac{1}{4} J z_\sigma \left( \langle S^z_\sigma \rangle \gamma^2 \langle 0 | c_{k\sigma A} c_{k\sigma A}^\dagger c_{k\sigma A} c_{k\sigma B}^\dagger | 0 \rangle + \langle S^z_\sigma \rangle (-1) \langle 0 | c_{k\sigma B} c_{k\sigma B}^\dagger c_{k\sigma B} c_{k\sigma B}^\dagger | 0 \rangle \right)
\]

\[
= -\frac{1}{4} J z_\sigma \langle S^z \rangle (|\gamma|^2 + 1) | 0 \rangle | 0 \rangle
\]

\[
= -\frac{1}{2} J z_\sigma \langle S^z \rangle
\]

This gives as the energy correction in the second order:

\[
E_{2k\sigma}^{(\pm)} = \frac{\left| \langle E_{0k\sigma}^{(\pm)} | H_1 | E_{0k\sigma}^{(\mp)} \rangle \right|^2}{E_{0k}^{(\pm)} - E_{0k}^{(\mp)}} = \frac{1}{4} J^2 \langle S^z \rangle^2 \pm 2 |t(k)|
\]

Thus the Schrödinger’s second-order perturbation theory leads to the following spin-independent expression:

\[
E_k^{(\pm)} = \varepsilon(k) \pm |t(k)| \pm \frac{1}{8} J^2 \frac{\langle S^z \rangle^2}{|t(k)|}
\]

3. Brillouin–Wigner perturbation theory:

The energy correction in the first order is identical to the Schrödinger’s perturbation theory, i.e. it vanishes in this case also. In the second order, one has to calculate

\[
E_{2k\sigma}^{(\pm)} = \frac{\left| \langle E_{0k\sigma}^{(\pm)} | H_1 | E_{0k\sigma}^{(\mp)} \rangle \right|^2}{E_{0k}^{(\pm)} - E_{0k}^{(\mp)}}
\]

It should be noted that in the denominator the “full” eigenenergy \( E_k^{(\pm)} \) appears.

We have already used the matrix element in part 3 We then have the following determining equation:
This gives a quadratic equation for the energy,

\[
\left( E_{k}^{(\pm)} - \varepsilon(k) \right)^{2} - |t(k)|^{2} = \frac{1}{4} J^{2} \langle S^{z} \rangle^{2}
\]

with the solution:

\[
E_{k}^{(\pm)} = \varepsilon(k) \pm \sqrt{|t(k)|^{2} + \frac{1}{4} J^{2} \langle S^{z} \rangle^{2}}
\]

4. The problem can be easily exactly solved:

\[
H = \sum_{k\sigma\alpha\beta} \left( \varepsilon_{\alpha\beta}(k) - \frac{1}{2} J z_{\sigma} \langle S^{z} \rangle \delta_{\alpha\beta} \right) c_{k\sigma\alpha}^{\dagger} c_{k\sigma\beta} \equiv \sum_{k\sigma} H_{k\sigma}
\]

Matrix representation:

\[
H_{k\sigma} = \begin{pmatrix}
\varepsilon(k) - \frac{1}{2} J z_{\sigma} \langle S^{z} \rangle & t(k) \\
t(k)^{*} & \varepsilon(k) + \frac{1}{2} J z_{\sigma} \langle S^{z} \rangle
\end{pmatrix}
\]

The secular determinant

\[
det \left( E - H_{k\sigma} \right) \equiv 0
\]

is solved by

\[
(E - \varepsilon(k))^{2} - \frac{1}{4} J^{2} \langle S^{z} \rangle^{2} = |t(k)|^{2}
\]

That means

\[
E_{\pm}(k) = \varepsilon(k) \pm \sqrt{|t(k)|^{2} + \frac{1}{4} J^{2} \langle S^{z} \rangle^{2}}
\]

The Brillouin–Wigner perturbation theory gives the exact result already in the second order. If the root is expanded for small \( J \), then the coefficient of the first term in the expansion is the result of Schrödinger’ perturbation theory in the second order.

**Problem 5.10**

1. The total spin \( \hat{S} = S_{1} + S_{2} \) has the quantum numbers \( \hat{S} = 0, 1, 2, \cdots, 2S \) and the z-component \( \hat{S}^{z} = S_{1}^{z} + S_{2}^{z} \) the quantum numbers \( M = -\hat{S}, -\hat{S} + 1, \cdots, +\hat{S} \). Additionally holds
\[(S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 = \hbar^2 \hat{S}(\hat{S}+1) \mathbb{I}\]

\[\sim S_1 \cdot S_2 = \hbar^2 \left( \frac{1}{2} \hat{S}(\hat{S}+1) - S(S+1) \right) \mathbb{I}\]

Possible energy levels:

\[E_{\hat{S}M} = -2J\hbar^2 \left( \frac{1}{2} \hat{S}(\hat{S}+1) - S(S+1) \right) - Mg\mu_B \hat{B}\]

With the abbreviation,

\[b \equiv g\mu_B \hat{B}\]

we have for the canonical partition function:

\[Z_S = Sp \left( e^{-\beta H} \right) = e^{-\beta \hbar^2 J S(S+1)} \sum_{\hat{S}=0}^{\hat{S}} \sum_{M=-\hat{S}}^{\hat{S}} e^{\frac{\beta}{2} \hbar^2 J \hat{S}(\hat{S}+1)} e^{\beta b M}\]

\[M\text{-summation as in (4.94)}:\]

\[\sum_{M=-\hat{S}}^{\hat{S}} e^{\beta b M} = \frac{\sinh(\beta b (\hat{S} + \frac{1}{2}))}{\sinh(\frac{1}{2} \beta b)}\]

Partition function:

\[Z_S = e^{-\beta \hbar^2 J S(S+1)} \sum_{\hat{S}=0}^{\hat{S}} e^{\frac{\beta}{2} \hbar^2 J \hat{S}(\hat{S}+1)} \sinh(\beta b (\hat{S} + \frac{1}{2}))\]

2. Special case \(S_1 = S_2 = \frac{1}{2}\):

\[Z_{1/2} = \frac{e^{-\frac{1}{2} \beta \hbar^2 J}}{\sinh(\frac{1}{2} \beta b)} \left( \sinh(\frac{1}{2} \beta b) + e^{\beta \hbar^2 J} \sinh(\frac{3}{2} \beta b) \right)\]

With

\[\frac{\sinh(\frac{3}{2}x)}{\sinh(\frac{1}{2}x)} = 1 + 2 \cosh(x)\]

we finally get
\[ Z_{1/2} = e^{\frac{1}{2} \beta \hbar^2 J} \left( e^{-\beta \hbar^2 J} + 1 + 2 \cosh(\beta g \mu_B \hat{B}) \right) \]

The magnetization satisfies the following implicit equation:

\[ M = n k_B T \frac{\partial}{\partial B_0} \ln Z_{1/2} \]
\[ = n g \mu_B \frac{2 \sinh(\beta g \mu_B \hat{B})}{e^{-\beta \hbar^2 J} + 1 + 2 \cosh(\beta g \mu_B \hat{B})} \]

For \( J = 0 \), and with \( \tanh x / 2 = \frac{\sinh x}{1 + \cosh x} \) we get the result of the Weiss theory (5.8) for \( S = 1/2 \).

**Problem 6.1**

With the abbreviations \( j = \beta J \); \( b = \beta \mu_B B_0 \); \( \beta = \frac{1}{k_B T} \)

\[ \hat{T} - E \mathbb{1} = \begin{pmatrix} e^{j+b} - E & e^{-j} \\ e^{-j} & e^{j-b} - E \end{pmatrix} \]

The eigenvalues follow from

\[ 0 = \det(\hat{T} - E \mathbb{1}) = (e^{j+b} - E) (e^{j-b} - E) - e^{-2j} \]
\[ = E^2 - E (e^{j+b} + e^{j-b}) + e^{2j} - e^{-2j} \]
\[ = E^2 - E e^j 2 \cosh b + 2 \sinh 2j \]
\[ = (E - e^j \cosh b)^2 - e^{2j} \cosh^2 b + 2 \sinh 2j \]

This gives the eigenvalues

\[ E_{\pm} = e^{\beta J} \left( \cosh \beta \mu_B B_0 \pm \sqrt{\cosh^2 \beta \mu_B B_0 - 2e^{-2\beta J} \sinh 2\beta J} \right) \]

**Problem 6.2**

Partition function (6.35) in thermodynamic limit:

\[ Z_N(T, B_0) = E_+^N \left( 1 + \left( \frac{E_-}{E_+} \right)^N \right) \rightarrow E_+^N \quad \text{for} \quad N \rightarrow \infty \]
$E_+$ as in Problem 6.1.

Free energy per spin:

$$f(T, B_0) = -k_B T \lim_{N \to \infty} \frac{1}{N} \ln T_N(T, B_0) = -k_B T \ln E_+ =$$

$$= -J - k_B T \ln (\cosh \beta \mu_B B_0 \pm \sqrt{r})$$

where

$$\sqrt{r} = \sqrt{\cosh^2 \beta \mu_B B_0 - 2e^{-2\beta J} \sinh 2\beta J}$$

Magnetization:

$$m = -\left( \frac{\partial}{\partial B_0} f(T, B_0) \right)_T =$$

$$\mu_B \sinh b + \frac{\cosh b \sinh b}{\sqrt{r}} \cosh b + \sqrt{r}$$

$$= \mu_B \sinh b \frac{\sqrt{r} + \cosh b}{(\cosh b + \sqrt{r}) \sqrt{r}}$$

$$= \mu_B \sinh b \frac{\sqrt{r}}{\sqrt{\cosh^2 b - 2e^{-2\beta J} \sinh 2\beta J}}$$

That gives

$$m(T, B_0) = \mu_B \frac{\sinh(\beta \mu_B B_0)}{\sqrt{\cosh^2 \beta \mu_B B_0 - 2e^{-2\beta J} \sinh 2\beta J}}$$

Susceptibility:

$$\chi_T(T, B_0) = \mu_0 \left( \frac{\partial m}{\partial B_0} \right)_T =$$

$$\beta \mu_B^2 \left\{ \frac{\cosh b}{\sqrt{\cosh^2 b - 2e^{-2\beta J} \sinh 2\beta J}} \right\}$$

$$- \frac{\sinh^2 b \cosh b}{\left( \sqrt{\cosh^2 b - 2e^{-2\beta J} \sinh 2\beta J} \right)^3}$$
\[
\begin{align*}
&= \beta \mu_B^2 \frac{\cosh b}{\sqrt{\cosh^2 b - 2e^{-2\beta J} \sinh 2\beta J}} \\
&\quad \times \left\{ 1 - \frac{\sinh^2 b}{\cosh^2 b - 2e^{-2\beta J} \sinh 2\beta J} \right\} \\
&= \beta \mu_B^2 \frac{\cosh(\beta \mu_B B_0)(1 - 2e^{-2\beta J} \sinh 2\beta J)}{(\cosh^2(\beta \mu_B B_0) - 2e^{-2\beta J} \sinh 2\beta J)^{3/2}}
\end{align*}
\]

In the limit \( B_0 \to 0 \) this expression simplifies to

\[
\chi_T(T, B_0 \to 0) = \beta \mu_B^2 e^{2\beta J}
\]

**Problem 6.3**

In the classical Ising Model the magnetic moment is given by

\[
m = \mu \sum_i S_i
\]

where \( \mu \) is a positive constant. With the Hamiltonian function

\[
H = -J \sum_{ij} S_i S_j - m B_0
\]

the canonical partition function is given by

\[
Z(T, m) = \sum_{\{S_i\}} \exp \left( -\beta \left( -J \sum_{ij} S_i S_j - m B_0 \right) \right)
\]

Here the summation is over all conceivable spin configurations, where the individual spins can have the values \( \pm 1 \). Therefore the substitution \( S_i \to -S_i \forall i \) cannot affect the partition function. Then in the exponents the first term does not change the sign but for the second term however, \( m \to -m \). That means

\[
Z(T, m) = Z(T, -m)
\]

so that

\[
F(T, m) = -k_B T \ln Z(T, m) = -k_B T \ln Z(T, -m) = F(T, -m)
\]
Problem 6.4

1.

\[ Z_N(T, B_0) = Tr \exp(-\beta H) \]

\[ = Tr(\mathbb{1}) - \beta Tr(H) + \frac{1}{2}\beta^2 Tr(H^2) - \frac{1}{3!}\beta^3 Sp(H^3) + \cdots \]

\[ = \sum_{l=0}^{\infty} \frac{1}{l!} (-\beta)^l Tr(H^l) \]

\[ = Tr(\mathbb{1}) \left[ 1 + \sum_{l=1}^{\infty} \frac{(-\beta)^l}{l!} m_l \right] \]

Each spin has two possible orientations \( S_i = \pm 1 \). That gives a total \( 2^N \) spin configurations. Therefore

\[ Sp(\mathbb{1}) = 2^N \]

2.

\[ c_{B_0} = -T \left( \frac{\partial^2 F_N(T, B_0)}{\partial T^2} \right)_{B_0} \]

\[ = -T \left( \frac{\partial^2}{\partial T^2} (-k_B T \ln Z_N(T, B_0)) \right)_{B_0} \]

\[ = k_B \beta^2 \left( \frac{\partial}{\partial \beta} \ln Z_N(T, B_0) \right)_{B_0} \]

\[ = k_B \beta^2 \left( \frac{1}{Z_N} \frac{\partial^2 Z_N}{\partial \beta^2} - \frac{1}{Z_N^2} \left( \frac{\partial Z_N}{\partial \beta} \right)^2 \right) \]

\[ = k_B \beta^2 \left[ \frac{Tr(\mathbb{1})}{Z_N} \sum_{l=1}^{\infty} \frac{l(l-1)}{l!} (-\beta)^l m_l \right. \]

\[ - \left. \left( \frac{Tr(\mathbb{1})}{Z_N} \sum_{l=1}^{\infty} \frac{l(l-1)}{l!} (-\beta)^l m_l \right)^2 \right] \]

\[ = k_B \beta^2 \left( \frac{2}{2!} m_2 - m_1^2 + O(\beta) \right) \]

\[ = \frac{1}{k_B T^2} (m_2 - m_1^2) + \cdots \]
In the last step we have restricted ourselves to the lowest term in $1/T$. One should notice that the moments are temperature independent. This result for the high-temperature behaviour of the heat capacity is of course valid not only for the Ising spins but also for all magnetic systems (!).

**Problem 6.5**

1. According to Problem 1.2:

$$\chi_T = \frac{1}{k_B T} \frac{\mu_0}{V} \langle (\hat{m} - \langle \hat{m} \rangle)^2 \rangle$$

This means

$$\chi_T = \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 \sum_{ij} \langle (S_i - \langle S_i \rangle) (S_j - \langle S_j \rangle) \rangle$$

So that we directly get

$$\chi_T = \frac{1}{k_B T} \frac{\mu_0}{V} \left( g^2 \mu_B^2 \sum_{ij} \langle S_i S_j \rangle - \langle \hat{m} \rangle^2 \right)$$

2. The spin chain shows no spontaneous magnetization. When an external field is switched off, then, $\langle \hat{m} \rangle \equiv 0$. According to (6.19) for the spin correlation of a one-dimensional chain we have

$$\langle S_i S_j \rangle = v^{|i-j|}$$

One can easily see that, in the double summation, $N$ terms with $|i - j| = 0$ give the contribution $v^0 = 1$; $2(N - 1)$ terms with $|i - j| = 1$ give the contribution $v^1$; $2(N - 2)$ terms with $|i - j| = 2$ give the contribution $v^2$; ..., and finally two terms with $|i - j| = N - 1$ give the contribution $v^{N-1}$. Then all of them together give

$$\chi_T(T, B_0) = \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 \left( N + 2 \sum_{k=1}^{N-1} (N - k)v^k \right)$$

One calculates
\[
2 \sum_{k=1}^{N-1} N v^k = 2N \frac{1 - v^N}{1 - v} - 2N
\]
\[
-2 \sum_{k=1}^{N-1} k v^k = -2 \sum_{k=0}^{N-1} k v^k = 2v \frac{d}{dv} \frac{1 - v^N}{1 - v}
= 2v \frac{(1 - v)(-Nv^{N-1}) + (1 - v^N)}{(1 - v)^2}
\]
\[
\sum_{k=1}^{N-1} (N - k) v^k = 2N \frac{v}{1 - v} - 2v \frac{1 - v^N}{(1 - v)^2}
\]

From this it follows:
\[
\chi_T(T, B_0 = 0) = \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 \left( N \left( 1 + \frac{2v}{1 - v} \right) - 2v \frac{1 - v^N}{(1 - v)^2} \right)
\]

3. For \( N \to \infty \) the expression for susceptibility can be simplified:
\[
\frac{1}{N} \chi_T(T, B_0 = 0) = \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 \left( 1 + \tanh(\beta J) \right)
= \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 \left( e^{\beta J} + e^{-\beta J} + e^{\beta J} - e^{-\beta J} \right)
= \frac{1}{k_B T} \frac{\mu_0}{V} g^2 \mu_B^2 e^{2\beta J}
\]

This agrees with the result (6.46) for the Ising ring in the thermodynamic limit.

**Problem 6.6**

1. The partition function
\[
Z_N(T) = \sum_{S_1} \sum_{S_2} \cdots \sum_{S_N} \exp \left( \sum_{i=1}^{N-1} j_i S_i S_{i+1} \right)
\]
where \( j_i = \beta J_i \) is valid, we have already calculated with (6.14):
Four-spin correlation function $i \neq j$:

\[
\langle S_i S_{i+1} S_j S_{j+1} \rangle = \frac{1}{Z_N} \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} S_i S_{i+1} S_j S_{j+1} \exp \left( \sum_{i=1}^{N-1} j_i S_i S_{i+1} \right)
\]

\[
= \frac{1}{Z_N} \frac{\partial^2 Z_N}{\partial j_i \partial j_j}
\]

\[
= \frac{\cosh j_1 \cdots \sinh j_i \cdots \sinh j_{j-1} \cdots \cosh j_{N-1}}{\cosh j_1 \cdots \cosh_{N-1}}
\]

\[
= \tanh j_i \tanh j_j
\]

For $i = j$ the four-spin correlation function is equal to 1. Let us now set $j_i = j \ \forall i$, then we have

\[
\langle S_i S_{i+1} S_j S_{j+1} \rangle = \begin{cases} 
1 & \text{falls } i = j \\
\tanh^2 j & \text{falls } i \neq j
\end{cases}
\]

2. From Problem 6.4 we have

\[
c_{B_0} = k_B \beta^2 \left( \frac{1}{Z_N} \frac{\partial^2 Z_N}{\partial \beta^2} - \frac{1}{Z_N^2} \left( \frac{\partial Z_N}{\partial \beta} \right)^2 \right)
\]

\[
= k_B \beta^2 \left( \langle H^2 \rangle - \langle H \rangle^2 \right)
\]

With

\[
\langle H^2 \rangle = J^2 \sum_{i,j} \langle S_i S_{i+1} S_j S_{j+1} \rangle
\]

follows:
\[ c_{B_0=0} = k_B \beta^2 J^2 \sum_{i,j=1}^{N-1} \left( \langle S_i S_{i+1} S_j S_{j+1} \rangle - \langle S_i S_{i+1} \rangle \langle S_j S_{j+1} \rangle \right) \]

\[ = k_B \beta^2 J^2 \sum_{i,j=1}^{N-1} (\delta_{ij} + (1 - \delta_{ij}) \tanh^2 j - \tanh^2 j) \]

\[ = k_B \beta^2 J^2 \sum_{i,j=1}^{N-1} \delta_{ij} (1 - \tanh^2 j) \]

\[ c_{B_0=0} = (N - 1) k_B \beta^2 J^2 \frac{1}{\cosh^2 \beta J} \]

Compare this result with (6.45).

**Problem 7.1**

1.

\[ \left[ S_i^x, \ S_j^y \right]_{-} = i \hbar S_i^z \delta_{ij} \text{ and cyclic} \]

\[ \left[ S_i^z, S_j^\pm \right]_{-} = \left[ S_i^z, S_j^y \right]_{-} \pm i \left[ S_i^z, S_j^x \right]_{-} \]

\[ = i \hbar S_i^y \delta_{ij} \mp \hbar (-S_i^x) \delta_{ij} \]

\[ = \pm \hbar (S_i^z \pm i S_i^y) \delta_{ij} \]

\[ = \pm \hbar S_i^\pm \delta_{ij} \]

2.

\[ \left[ S_i^+, S_j^- \right]_{-} = \left[ S_i^x, S_j^y \right]_{-} + \left[ S_i^y, S_j^x \right]_{-} + i \left[ S_i^y, S_j^y \right]_{-} - i \left[ S_i^x, S_j^x \right]_{-} \]

\[ = i(-i \hbar S_i^x) \delta_{ij} - i(i \hbar S_i^y) \delta_{ij} \]

\[ = 2 \hbar S_i^x \delta_{ij} \]

3.

\[ S_i^\pm S_i^\mp = (S_i^x \pm i S_i^y)(S_i^x \mp i S_i^y) \]

\[ = (S_i^x)^2 + (S_i^y)^2 \pm i \left[ S_i^y, S_i^x \right]_{-} \]

\[ = S_i^2 - (S_i^x)^2 \pm \hbar S_i^z \]

(where \( S_i^2 = \hbar^2 S(S + 1) \mathbb{I} \) in the space of the spin states)
4. 
\[
\frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) = \frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ + i S_i^y S_j^x + i S_i^x S_j^y \right) \\
= S_i^z S_j^+ + S_j^z S_i^- \\
\Leftrightarrow S_i \cdot S_j = \frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z
\]

5. 
\[
H = - \sum_{i,j} J_{ij} S_i \cdot S_j \\
= - \frac{1}{2} \sum_{i,j} (S_i^+ S_j^- + S_i^- S_j^+) J_{ij} - \sum_{i,j} J_{ij} S_i^z S_j^z \\
= - \frac{1}{2} \sum_{i,j} J_{ij} S_i^+ S_j^- - \frac{1}{2} \sum_{i,j} J_{ij} S_j^+ S_i^- - \sum_{i,j} J_{ij} S_i^z S_j^z \\
= - \sum_{i,j} J_{ij} \left( S_i^+ S_j^- + S_j^+ S_i^- \right)
\]

Problem 7.2

1. \[
\left[ (S_i^-)^n, S_i^z \right] = n \hbar (S_i^-)^n; \ n = 1, 2, \ldots
\]
   Complete induction:
   \[
n = 1:
   \left[ S_i^-, S_i^z \right] = \hbar S_i^-
   \]
   \[
n \rightarrow n + 1:
   \left[ (S_i^-)^{n+1}, S_i^z \right] = \left[ (S_i^-)^n, S_i^z \right] S_i^- + (S_i^-)^n \left[ S_i^-, S_i^z \right] \\
= n \hbar (S_i^-)^n S_i^- + (S_i^-)^n \hbar S_i^- \\
= (n + 1) \hbar (S_i^-)^{n+1} \quad \text{q.e.d.}
\]

2. \[
\left[ (S_i^-)^n, (S_i^z)^2 \right] = n^2 \hbar^2 (S_i^-)^n + 2 n \hbar S_i^z (S_i^-)^n; \ n = 1, 2, \ldots
\]
   \[
   \left[ (S_i^-)^n, (S_i^z)^2 \right] = S_i^z \left[ (S_i^-)^n, S_i^z \right] + \left[ (S_i^-)^n, S_i^z \right] S_i^z \\
\overset{1)}{=} S_i^z n \hbar (S_i^-)^n + n \hbar (S_i^-)^n S_i^z \\
\overset{1)}{=} 2 n \hbar S_i^z (S_i^-)^n + n^2 \hbar^2 (S_i^-)^n \quad \text{q.e.d.}
\]
3. \[ [S_i^+, (S_i^-)^n] = (2n\hbar S_i^z + \hbar^2 n(n-1)) (S_i^-)^{n-1}; \ n = 1, 2, \ldots \]

Complete induction:

\[ n = 1: \]

\[ [S_i^+, S_i^-] = 2\hbar S_i^z \]

\[ n \to n + 1: \]

\[ [S_i^+, (S_i^-)^{n+1}] = [S_i^+, (S_i^-)^n] S_i^- + (S_i^-)^n [S_i^+, S_i^-] \]

\[ = (2n\hbar S_i^z + \hbar^2 n(n-1)) (S_i^-)^{n-1} S_i^- + (S_i^-)^n 2\hbar S_i^z \]

\[ \overset{\text{1)}}{=} (2n\hbar S_i^z + \hbar^2 n(n-1)) (S_i^-)^n + 2n\hbar^2 (S_i^-)^n + \]

\[ + 2\hbar S_i^z (S_i^-)^n \]

\[ = (2\hbar(n+1) S_i^z + \hbar^2 n(n+1)) (S_i^-)^n \quad \text{q.e.d.} \]

**Problem 7.3**

Starting point is the identity (7.485):

\[ \prod_{m=-S}^{+S} (S_i^z - \hbar m_s) = 0 \]

\[ S = \frac{1}{2} \]

\[ 0 = \left( S_i^z + \frac{\hbar}{2} \right) \left( S_i^z - \frac{\hbar}{2} \right) = (S_i^z)^2 - \frac{\hbar^2}{4} \]

\[ \overset{\text{1)}}{=} \langle (S_i^z)^2 \rangle = \frac{\hbar^2}{4} \]

\[ \text{and} \quad \alpha_0 \left( \frac{1}{2} \right) = \frac{\hbar^2}{4}, \quad \alpha_1 \left( \frac{1}{2} \right) = 0 \]

\[ S = 1 \]

\[ 0 = (S_i^z + \hbar) S_i^z (S_i^z - \hbar) \]

\[ \overset{\text{1)}}{=} \langle (S_i^z)^3 \rangle = \hbar^2 \langle S_i^z \rangle \]

\[ \text{and} \quad \alpha_0(1) = 0, \quad \alpha_1(1) = \hbar^2, \quad \alpha_2(1) = 0 \]

\[ S = \frac{3}{2} \]
\[
0 = \left( S_i^z + \frac{3}{2} \hbar \right) \left( S_i^z + \frac{1}{2} \hbar \right) \left( S_i^z - \frac{1}{2} \hbar \right) \left( S_i^z - \frac{3}{2} \hbar \right) \\
= \left( \left( S_i^z \right)^2 - \frac{9}{4} \hbar^2 \right) \left( \left( S_i^z \right)^2 - \frac{1}{4} \hbar^2 \right)
\]

\[
\alpha_0 \left( \frac{3}{2} \right) = -\frac{9}{16} \hbar^4, \quad \alpha_1 \left( \frac{3}{2} \right) = 0, \quad \alpha_2 \left( \frac{3}{2} \right) = \frac{5}{2} \hbar^2.
\]

\[
\alpha_3 \left( \frac{3}{2} \right) = 0
\]

\[S = 2\]

\[
0 = \left( S_i^z + 2 \hbar \right) \left( S_i^z + \hbar \right) \left( S_i^z - \hbar \right) \left( S_i^z - 2 \hbar \right)
\]

\[
= \left( \left( S_i^z \right)^2 - 4 \hbar^2 \right) \left( \left( S_i^z \right)^2 - \hbar^2 \right) S_i^z
\]

\[
\alpha_0(0) = 0, \quad \alpha_1(0) = -4 \hbar^4, \quad \alpha_2(0) = 0, \quad \alpha_3(0) = 5 \hbar^2, \quad \alpha_4(0) = 0
\]

\[S = \frac{7}{2}\]

\[
0 = \left( S_i^z + \frac{7}{2} \hbar \right) \left( S_i^z + \frac{5}{2} \hbar \right) \left( S_i^z + \frac{3}{2} \hbar \right) \left( S_i^z + \frac{1}{2} \hbar \right) \cdot \\
\cdot \left( S_i^z - \frac{1}{2} \hbar \right) \left( S_i^z - \frac{3}{2} \hbar \right) \left( S_i^z - \frac{5}{2} \hbar \right) \left( S_i^z - \frac{7}{2} \hbar \right)
\]

\[
= \left( \left( S_i^z \right)^2 - \frac{49}{4} \hbar^2 \right) \left( \left( S_i^z \right)^2 - \frac{25}{4} \hbar^2 \right) \left( \left( S_i^z \right)^2 - \frac{9}{4} \hbar^2 \right) \cdot
\]

\[
\ast \left( \left( S_i^z \right)^2 - \frac{1}{4} \hbar^2 \right)
\]

\[
\alpha_0 \left( \frac{7}{2} \right) = -\frac{617}{8} \hbar^8, \quad \alpha_1 \left( \frac{7}{2} \right) = 0, \quad \alpha_2 \left( \frac{7}{2} \right) = \frac{3229}{16} \hbar^6,
\]

\[
\alpha_3 \left( \frac{7}{2} \right) = 0, \quad \alpha_4 \left( \frac{7}{2} \right) = -\frac{987}{8} \hbar^4, \quad \alpha_5 \left( \frac{7}{2} \right) = 0,
\]

\[
\alpha_6 \left( \frac{7}{2} \right) = 21 \hbar^2, \quad \alpha_7 \left( \frac{7}{2} \right) = 0
\]
Problem 7.4
Eu$^{2+}$ on f.c.c.-sites

Each atom of a (111)-plane has six nearest neighbours in the same (111)-plane and three each in the two neighbouring planes and six next nearest neighbours, three each in the two neighbouring (111)-planes.

EuSe:

$2.8\text{K} \leq T \leq 4.6\text{K}$ NNSS-Antiferromagnet

$\sim$ 12 nearest neighbours, 9 in the same and 3 in the other sub-lattice.

$$k_B T_N = \frac{2}{3} \hbar^2 S(S + 1) \left\{ \sum_j \epsilon^1 J_{1j} - \sum_j \epsilon^2 J_{1j} \right\}$$

$$= \frac{2}{3} \hbar^2 S(S + 1) \{9J_1 + 3J_2 - 3J_1 - 3J_2\}$$

$$= \frac{2}{3} \hbar^2 S(S + 1) (6J_1)$$

$$k_B \Theta = \frac{2}{3} \hbar^2 S(S + 1) \left\{ \sum_j \epsilon^1 J_{1j} + \sum_j \epsilon^2 J_{1j} \right\}$$

$$= \frac{2}{3} \hbar^2 S(S + 1) \{9J_1 + 3J_2 + 3J_1 + 3J_2\}$$

$$= \frac{2}{3} \hbar^2 S(S + 1) \{12J_1 + 6J_2\}$$

$$J_1 = \frac{k_B}{4\hbar^2 S(S+1)} T_N$$

$$k_B \Theta - 2k_B T_N = 4\hbar^2 S(S + 1) J_2$$

$$J_2 = \frac{k_B}{4\hbar^2 S(S+1)} (\Theta - 2T_N)$$

Problem 7.5

1. It is convenient to first split the matrix as follows:

$$A = bA' + aI$$

Here the reduced matrix $A'$ is given by
\[
A' = \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 \\
1 & 0 & 1 & 0 & \cdots & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & \cdots & 1 & 0
\end{pmatrix}
\]

Eigenvalues of \(A\):

\[\lambda = a + b \lambda' \quad ; \quad \lambda' : \text{Eigenvalue of } A'\]

Now we have to solve

\[0 = \det(A' - \lambda' \mathbb{I}) \equiv D_d(\lambda')\]

One recognizes

\[D_1(\lambda') = -\lambda' \quad ; \quad D_2(\lambda') = \lambda'^2 - 1\]

In general one obtains by expanding after the first row:

\[D_d(\lambda') = -\lambda' D_{d-1}(\lambda') - 1 * \]

\[= -\lambda' D_{d-1}(\lambda') - D_{d-2}(\lambda')\]

In the last step, the remaining determinant is expanded after the first column.

With the ansatz for solution

\[D_d(\lambda') = e^{\pm id\alpha}\]

follows:

\[e^{\pm id\alpha} = \lambda' e^{\pm i(d-1)\alpha} - e^{\pm i(d-2)\alpha}\]

\[\sim e^{\pm i\alpha} = -\lambda' - e^{\mp i\alpha} \sim \lambda' = -2 \cos \alpha \sim \alpha = \arccos\left(\frac{-\lambda'}{2}\right)\]

General solution
\[ D_d(\lambda') = c_1 \cos(d\alpha) + c_2 \sin(d\alpha) \]

c_1, c_2 from the initial conditions:

\[ D_1(\lambda') = -\lambda' = c_1 \cos(\alpha) + c_2 \sin(\alpha) = 2 \cos(\alpha) \]
\[ D_2(\lambda') = \lambda'^2 - 1 = c_1 \cos(2\alpha) + c_2 \sin(2\alpha) = 4 \cos^2(\alpha) - 1 \]

\[ c_1 = 2 - c_2 \tan \alpha \]

\[ 4 \cos^2 \alpha - 1 = c_1 (2 \cos^2 \alpha - 1) + c_2 2 \sin \alpha \cos \alpha \]
\[ = 4 \cos^2 \alpha - 2 - 2c_2 \sin \alpha \cos \alpha + c_2 \tan \alpha + 2c_2 \sin \alpha \cos \alpha \]

\[ c_2 = \cot \alpha \quad c_1 = 1 \]

Intermediate result:

\[ D_d(\lambda') = \cos(d\alpha) + \frac{\cos \alpha}{\sin \alpha} \sin(d\alpha) \]
\[ = \frac{1}{\sin \alpha} \left( \sin \alpha \cos(d\alpha) + \cos \alpha \sin(d\alpha) \right) \]
\[ = \frac{\sin((d + 1)\alpha)}{\sin \alpha} \]

Requirement:

\[ D_d(\lambda') \neq 0 \quad \Rightarrow \alpha = \frac{r \pi}{d + 1} ; \ r = 1, \ldots, d \]
\[ \Rightarrow \lambda'_r = -2 \cos \frac{r \pi}{d + 1} \]

With this we have the *Eigenvalues of the tridiagonal matrix A*:

\[ \lambda_r = a - 2b \cos \frac{r \pi}{d + 1} \quad , \ r = 1, \ldots, d \]

2. Heisenberg model for films:
Hamiltonian in molecular field approximation (7.124):

\[ H_{MFA} = -2 \sum_{i,j} J_{ij} \langle S_j^z \rangle S_i^z \]
That means we have an effective paramagnet in the molecular field \(2 \sum_{ij} J_{ij} \langle S_j^z \rangle / g_J \mu_B\). Due to the film structure, translational symmetry is applicable only in the plane of the film and not in three dimensions. Let \(B_S\) be the Brillouin function in the following. Then according to (7.134) holds

\[
\langle S_i^z \rangle = \hbar S B_S \left( 2 \hbar \beta \sum_j J_{ij} \langle S_j^z \rangle \right)
\]

Exchange only between the nearest neighbours:

\[
\sum_j J_{ij} \langle S_j^z \rangle = qJ \langle S_\alpha^z \rangle + pJ \langle S_{\alpha+1}^z \rangle + pJ \langle S_{\alpha-1}^z \rangle
\]

\(\langle S_\alpha^z \rangle\): layer magnetization, where \(\alpha\) numbers the layers; \(q(p)\): coordination number (the number of nearest neighbours) within the layer (between the layers). \(q + 2p = z\): volume coordination number. Examples:

- \(sc\ (100)\): \(q = 4, p = 1\)
- \(sc\ (110)\): \(q = 2, p = 2\)
- \(sc\ (111)\): \(q = 0, p = 3\)

For \(T \rightarrow T_C\) linearization of Brillouin function: \(B_S(x) \approx \frac{S+1}{3S} x\):

\[
\langle S_\alpha^z \rangle = \frac{2}{3} \hbar^2 (S + 1) S \beta \left( qJ \langle S_\alpha^z \rangle + pJ \langle S_{\alpha+1}^z \rangle + pJ \langle S_{\alpha-1}^z \rangle \right)
\]

This gives a system of homogeneous equations:

\[
0 = \sum_\gamma M_{\alpha\gamma} \langle S_\gamma^z \rangle
\]

Here the matrix \(\hat{M}\) is given by

\[
\hat{M} = \begin{pmatrix}
qJ - x & pJ & 0 & 0 & 0 & \cdots & 0 \\
pJ & qJ - x & pJ & 0 & 0 & \cdots & 0 \\
0 & pJ & qJ - x & pJ & 0 & \cdots & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & pJ & qJ - x \\
\end{pmatrix}
\]

\[
x = \frac{1}{\frac{2}{3} \hbar^2 S(S + 1) \beta}
\]
We thus have a tridiagonal matrix. There exist non-trivial solutions \((\langle S^z \rangle \to 0)\) only for

\[
\det \hat{M} = 0 = \prod_{r=1}^{d} \lambda_r
\]

\(\lambda_r\) is the \(r\)th eigenvalue of \(\hat{M}\). According to part 1, for the eigenvalues we have

\[
\lambda_r = qJ - x - 2pJ \cos \frac{r\pi}{d+1}
\]

At least one of these eigenvalues must be equal to zero. This gives the following equation for \(T_C\):

\[
k_B T_C^{(r)} = \frac{2}{3} \hbar^2 S(S+1)J \left\{ q - 2p \cos \frac{r\pi}{d+1} \right\}
\]

The physical solution must satisfy the well-known limiting cases

\[
k_B T_C(d = 1) = \frac{2}{3} \hbar^2 S(S+1)Jq
\]

\[
k_B T_C(d = \infty) = \frac{2}{3} \hbar^2 S(S+1)J(q + 2p)
\]

Fig. C.1  Relative change of the Curie temperature of a film with its thickness. \(d\): number of monolayers

That is possible only for \(r = d\) (Fig. C.1):

\[
k_B T_C = \frac{2}{3} \hbar^2 S(S+1)J \left\{ q - 2p \cos \frac{d\pi}{d+1} \right\}
\]
It is instructive to compare the critical temperature of the film with that of the bulk material:

\[
\frac{T_C(\infty) - T_C(d)}{T_C(\infty)} = 2 \frac{z - z_S}{z} \left( 1 + \cos \frac{d\pi}{d + 1} \right)
\]

Here \( z = q + 2p \) is the coordination number of the bulk and \( z_S = q + p \) that of the surface.

**Problem 7.6**

We use the Heisenberg Hamiltonian in the wavenumber representation (7.105):

\[
H = -\frac{1}{N} \sum_k J(k) \left\{ S^+(k)S^-(-k) + S^z(k)S^z(-k) \right\} - \frac{g_J \mu_B B_0 S^z(0)}{\hbar}
\]

For the spin operators (7.106) and (7.107) hold

\[
S^z(k) |0\rangle = \hbar NS |0\rangle \delta_{k,0} \quad ; \quad S^+(k) |0\rangle = 0
\]

With this we calculate

\[
-\frac{1}{N} \sum_k J(k) S^+(k)S^-(-k) |0\rangle =
\]

\[
= -\frac{1}{N} \sum_k J(k) \left\{ 2\hbar S^z(0) + S^-(-k)S^+(k) \right\} |0\rangle
\]

\[
= (2\hbar^2 NS |0\rangle) \left( -\frac{1}{N} \sum_k J(k) \right)
\]

\[
= -(2\hbar^2 NS |0\rangle) J_{ii}
\]

\[ (7.12) \]

\[
0
\]

\[
-\frac{1}{N} \sum_k J(k)S^z(k)S^z(-k) |0\rangle = -\hbar S \sum_k J(k)S^z(k)\delta_{-k,0} |0\rangle
\]

\[
= -\hbar S J(0)S^z(0) |0\rangle
\]

\[
= -N\hbar^2 S^2 J_0 |0\rangle \quad (J(0) \equiv J_0)
\]

\[
-\frac{1}{\hbar} g_J \mu_B B_0 S^z(0) |0\rangle = -Ng_J S\mu_B B_0 |0\rangle
\]
With this it is shown that $|0\rangle$ is the eigenstate with the eigenvalue

$$E_0(B_0) = -N\hbar^2 S^2 J_0 - N g J \mu_B B_0 S$$

Problem 7.7

\[
\langle k | S^z_i | k \rangle = \frac{1}{2SN \hbar^2} \langle 0 | S^+(k) S^z_i S^-(k) | 0 \rangle = \frac{1}{2SN^2 \hbar^2} \sum_q e^{iq \cdot R_i} \langle 0 | S^+(k) S^z(q) S^-(k) | 0 \rangle = \frac{1}{2SN^2 \hbar^2} \sum_q e^{iq \cdot R_i} \langle 0 | S^+(k) \left( (S^-(k) S^z(q) - \hbar S^-(k + q) \right) | 0 \rangle = \frac{1}{2N \hbar} \langle 0 | (2\hbar S^z(0) + S^-(k) S^+(k)) | 0 \rangle - \frac{1}{2SN^2 \hbar} \sum_q e^{iq \cdot R_i} \langle 0 | (2\hbar S^z(q) + S^-(k + q) S^+(k)) | 0 \rangle = \frac{1}{2N \hbar} 2\hbar \cdot Nh S - \frac{1}{2SN^2 \hbar} 2\hbar \cdot Nh S = h S - \frac{1}{N} \hbar = \hbar \left( S - \frac{1}{N} \right) \quad \text{q.e.d.}
\]

Problem 7.8

Holstein–Primakoff transformation:

\[
S^+_i = \hbar \sqrt{2S} \varphi(n_i) a_i \quad \text{; } \varphi(n_i) = \sqrt{1 - \frac{n_i}{2S}} \\
S^-_i = \hbar \sqrt{2S} a_i^+ \varphi(n_i) \\
S^z_i = h(S - n_i) \quad \text{; } n_i = a_i^+ a_i
\]

$a_i$, $a_i^+$: Bose operators

\[
[a_i, a_j^+] = \delta_{ij}; \quad [a_i, a_j] = [a_i^+, a_j^+] = 0 \\
\sim [n_i, a_j] = -a_i \delta_{ij}; \quad [n_i, a_j^+] = a_i^+ \delta_{ij}
\]
1. Commutation relations:

\[
\left[ S^+_i, S^-_j \right] = 2\hbar^2 \delta_{ij} \left[ \varphi(n_i) a_i, a_i^+ \varphi(n_i) \right] = 2\hbar^2 \delta_{ij} \left( \varphi(n_i)(1 + n_i)\varphi(n_i) - a_i^+ \left( 1 - \frac{n_i}{2S} \right) a_i \right)
\]

\[
= 2\hbar^2 \delta_{ij} \left( (1 + n_i) \left( 1 - \frac{n_i}{2S} \right) - n_i + \frac{1}{2S} a_i^+ n_i a_i \right)
\]

\[
= 2\hbar^2 \delta_{ij} \left( 1 - \frac{n_i}{2S} - \frac{n_i^2}{2S} - \frac{1}{2S} n_i + \frac{1}{2S} n_i^2 \right)
\]

\[
= 2\hbar \delta_{ij} \hbar (S - n_i)
\]

\[
= 2\hbar \delta_{ij} S^z_i
\]

\[
\left[ S^z_i, S^+_j \right] = \left[ \hbar (S - n_i), \hbar \sqrt{2S} \varphi(n_j) a_j \right] = -\hbar^2 \sqrt{2S} \left[ n_i, \varphi(n_i) a_i \right] \delta_{ij} = -\hbar^2 \sqrt{2S} \varphi(n_i) [n_i, a_i] \delta_{ij}
\]

\[
= \hbar^2 \sqrt{2S} \varphi(n_i) a_i \delta_{ij} = +\hbar \delta_{ij} S^z_i
\]

\[
\left[ S^z_i, S^-_j \right] = -\hbar^2 \sqrt{2S} \left[ n_i, a_i^+ \varphi(n_i) \right] \delta_{ij} = -\hbar^2 \sqrt{2S} \left[ n_i, a_i^+ \right] \varphi(n_i) \delta_{ij}
\]

\[
= -\hbar \left( \hbar \sqrt{2S} a_i^+ \varphi(n_i) \right) \delta_{ij} = -\hbar \delta_{ij} S^z_i
\]

2. \( S^2_i \):

\[
S^2_i = \frac{1}{2} \left( S^+_i S^-_i + S^-_i S^+_i \right) + \left( S^z_i \right)^2
\]

\[
= \frac{1}{2} 2\hbar^2 \left( \varphi(n_i) a_i a_i^+ \varphi(n_i) + \right.
\]

\[
+ a_i^+ \left( 1 - \frac{n_i}{2S} \right) a_i \Big) + \hbar^2 (S - n_i)^2
\]
\[
\begin{align*}
\hbar^2 S & \left(1 - \frac{n_i}{2S}\right) + n_i \left(1 - \frac{n_i}{2S}\right) + n_i - \frac{1}{2S} a_i^+ a_i + \frac{1}{2S} a_i^+ n_i a_i \right) \\
& \quad + \hbar^2 (S^2 - 2Sn_i + n_i^2) \\
& = \hbar^2 (S + 2n_i S - n_i^2 + S^2 - 2Sn_i + n_i^2) \\
& = \hbar^2 S (S + 1)
\end{align*}
\]

**Problem 7.9**

Dyson–Maléev transformation:

\[
\begin{align*}
S_i^+ &= \hbar \sqrt{2S} \alpha_i \\
S_i^- &= \hbar \sqrt{2S} \alpha_i^+ \left(1 - \frac{n_i}{2S}\right) \\
S_i^z &= \hbar (S - n_i) \\
& \quad ; n_i = \alpha_i^+ \alpha_i
\end{align*}
\]

\(\alpha_i, \alpha_i^+\): Bose operators

1. Commutation relations:

\[
\begin{align*}
\left[ S_i^+, S_j^- \right] & = 2S \hbar^2 \left[ \alpha_i, \alpha_j^+ \left(1 - \frac{n_j}{2S}\right) \right] \\
& = 2S \hbar^2 \delta_{ij} - \hbar^2 \delta_{ij} \left[ \alpha_i, \alpha_j^+ n_i \right] \\
& = 2S \hbar^2 \delta_{ij} - \hbar^2 \delta_{ij} n_i - \hbar^2 \delta_{ij} \alpha_i^+ \left[ \alpha_i, n_i \right] \\
& = 2 \hbar^2 \delta_{ij} (S - n_i) \\
& = 2 \hbar \delta_{ij} S_i^z
\end{align*}
\]

\[
\begin{align*}
\left[ S_i^z, S_j^- \right] & = \hbar^2 \sqrt{2S} \left[ S - n_i, \alpha_j \right] \\
& = -\hbar^2 \sqrt{2S} \delta_{ij} \left[ n_i, \alpha_i \right] \\
& = \hbar^2 \sqrt{2S} \alpha_i \delta_{ij} \\
& = \hbar \delta_{ij} S_i^z
\end{align*}
\]

\[
\begin{align*}
\left[ S_i^z, S_j^+ \right] & = \hbar^2 \sqrt{2S} \left[ S - n_i, \alpha_j^+ \left(1 - \frac{n_j}{2S}\right) \right] \\
& = -\hbar^2 \sqrt{2S} \delta_{ij} \left[ n_i, \alpha_i^+ \left(1 - \frac{n_i}{2S}\right) \right] \\
& = -\hbar^2 \sqrt{2S} \delta_{ij} \left[ n_i, \alpha_i^+ \right] \left(1 - \frac{n_i}{2S}\right)
\end{align*}
\]
\[\begin{align*}
\psi &= -\hbar^2 \sqrt{2S} \delta_{ij} \alpha_i^+ \left( 1 - \frac{n_i}{2S} \right) \\
&= -\hbar \delta_{ij} S_i^-
\end{align*}\]

2. \( S_i^2 \):

\[
S_i^2 = \frac{1}{2} (S_i^+ S_i^- + S_i^- S_i^+) + (S_i^z)^2
\]

\[\begin{align*}
&= S \hbar^2 \left( \alpha_i \alpha_i^+ \left( 1 - \frac{n_i}{2S} \right) + \alpha_i^+ \left( 1 - \frac{n_i}{2S} \right) \alpha_i \right) + \\
&\quad + \hbar^2 (S^2 - 2Sn_i + n_i^2)
\end{align*}\]

\[S_i^2 = \hbar^2 \left( S(1 + n_i) - \frac{1}{2}(n_i + n_i^2) + Sn_i - \frac{1}{2} \alpha_i^+ n_i \alpha_i + S^2 - 2Sn_i + n_i^2 \right)
\]

\[S_i^2 = \hbar^2 \left( S(S + 1) - \frac{1}{2} n_i + \frac{1}{2} n_i^2 + \frac{1}{2} n_i - \frac{1}{2} n_i^2 \right)
\]

\[S_i^2 = \hbar^2 S(S + 1)\]

Problem 7.10

\[S_i^+ \approx \hbar \sqrt{2S} a_i ; \quad S_i^- \approx \hbar \sqrt{2S} a_i^+ ; \quad S_i^z = \hbar(S - n_i)\]

Fourier transformation:

\[
S^+(\mathbf{k}) = \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} S_i^+
\]

\[\approx \hbar \sqrt{2S} \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} a_i \underbrace{\sqrt{N}}_{\sqrt{N}}
\]

\[= \hbar \sqrt{2SN} a_k\]

\[
S^-(\mathbf{k}) = \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} S_i^-
\]

\[\approx \hbar \sqrt{2S} \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} a_i^+ \underbrace{\sqrt{N}}_{\sqrt{N}}
\]

\[= \hbar \sqrt{2SN} a_{-k}^+\]
\[ S^z(\mathbf{k}) = \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} (\hbar S - \hbar a_i^+ a_i) \]
\[ = \hbar SN \delta_{k,0} - \hbar \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} \frac{1}{N} \sum_{k',q} a_{q}^+ a_{k'} e^{i(k' - q) \cdot \mathbf{R}_i} \]
\[ = \hbar SN \delta_{k,0} - \hbar \sum_{k',q} a_{q}^+ a_{k'} \delta_{k',k+q} \]
\[ = \hbar SN \delta_{k,0} - \hbar \sum_q a_{q}^+ a_{k+q} \]

Verification of commutation relations:

1.
\[ \left[ S^+(\mathbf{k}), \ S^-(\mathbf{q}) \right] = \hbar^2 2SN \left[ a_{k'}^+, \ a_{-q}^+ \right] \]
\[ = 2SN \hbar^2 \delta_{k+q} \]
\[ \approx 2\hbar S^z(\mathbf{k} + \mathbf{q}) \]

2.
\[ \left[ S^z(\mathbf{k}), \ S^+(\mathbf{q}) \right] = -\hbar \sum_{q'} \left[ a_{q'}^+ a_{k+q'}, \ a_{q} \right] h\sqrt{2SN} \]
\[ = -\hbar^2 \sqrt{2SN} \sum_{q'} \left[ a_{q'}^+, \ a_{q} \right] \frac{a_{k+q'}}{-\delta_{q'}} \]
\[ = \hbar^2 \sqrt{2SN} a_{k+q} \]
\[ = \hbar S^+(\mathbf{k} + \mathbf{q}) \]

3.
\[ \left[ S^z(\mathbf{k}), \ S^-(\mathbf{q}) \right] = -\hbar^2 \sqrt{2SN} \sum_{q'} \left[ a_{q'}^+ a_{k+q'}, \ a_{-q}^+ \right] \]
\[ = -\hbar^2 \sqrt{2SN} \sum_{q'} a_{q'}^+ \left[ a_{k+q'}, \ a_{-q}^+ \right] \]
\[ = -\hbar^2 \sqrt{2SN} a_{-q-k}^+ \]
\[ = -\hbar S^-(\mathbf{k} + \mathbf{q}) \]
Problem 7.11

\[ \alpha_q = \frac{1}{\sqrt{N}} \sum_i e^{-i q \cdot R_i} \alpha_i \]
\[ \alpha_i = \frac{1}{\sqrt{N}} \sum_q e^{i q \cdot R_i} \alpha_q \]
\[ J(q) = \frac{1}{N} \sum_{i,j} J_{ij} e^{i(q(R_i - R_j))} \]

Dyson–Maléev:
\[ S_i^+ = \hbar \sqrt{2} S \alpha_i \]
\[ S_i^- = \hbar \sqrt{2} \alpha_i^+ \left( 1 - \frac{\hat{n}_i}{2S} \right) \]
\[ S_i^z = \hbar (S - \hat{n}_i) \]

Heisenberg model:
\[ H = E_0 + H_2 + H_4 \]
\[ H_2 = 2 \hbar^2 J_0 \sum_i \hat{n}_i - 2 S \hbar^2 \sum_{i,j} J_{ij} \alpha_i^+ \alpha_j \]

\[ \sum_i \hat{n}_i = \frac{1}{N} \sum_{q,q'} e^{-i(q-q') \cdot R} \alpha_q^+ \alpha_{q'} \]
\[ = \sum_{q,q'} \alpha_q^+ \alpha_{q'} \delta_{qq'} \]
\[ = \sum_q \alpha_q^+ \alpha_q \]

\[ \sum_{i,j} J_{ij} \alpha_i^+ \alpha_j = \]
\[ = \frac{1}{N^2} \sum_{i,j} \sum_{q,q',q''} J(q) \alpha_q^+ \alpha_{q''} e^{i(q(R_i - R_j))} e^{-i q' \cdot R_i} e^{i q'' \cdot R_j} \]
\[ = \sum_{q,q',q''} J(q) \alpha_q^+ \alpha_{q''} \delta_{q,q'} \delta_{q,q''} \]
\[ = \sum_q J(q) \alpha_q^+ \alpha_q \]
\[ \hbar \omega(\mathbf{q}) = 2\hbar \hbar^2 (J_0 - J(\mathbf{q})) \]

\[ \sim H_2 = \sum_{\mathbf{q}} \hbar \omega(\mathbf{q}) \alpha^+_\mathbf{q} \alpha^+_{\mathbf{q}} \]

\[ H_4 = -\hbar^2 \sum_{i,j} J_{ij} \hat{n}_i \hat{n}_j + \hbar^2 \sum_{i,j} J_{ij} \alpha^+_i \hat{n}_i \alpha^+_j \]

\[ \sum_{i,j} J_{ij} \hat{n}_i \hat{n}_j = \]

\[ = \frac{1}{N^3} \sum_{i,j} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \mathbf{J}(\mathbf{q}) \]

\[ \ast \left( e^{-i\mathbf{q}_1 \mathbf{R}_i - \mathbf{R}_j} \right) e^i(\mathbf{q}_1 \mathbf{R}_i - \mathbf{q}_3 \mathbf{R}_j + \mathbf{q}_2 \mathbf{R}_i - \mathbf{q}_4 \mathbf{R}_j) \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \mathbf{J}(\mathbf{q}) \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_4 - \mathbf{q}_2} \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_4} \mathbf{J}(\mathbf{q}_4 - \mathbf{q}_2) \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_4} \mathbf{J}(\mathbf{q}_4 - \mathbf{q}_2) \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \]

\[ + \frac{1}{N} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \mathbf{J}(\mathbf{q}_4 - \mathbf{q}_2) \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_4} \mathbf{J}(\mathbf{q}_4 - \mathbf{q}_2) \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \]

\[ \sum_{i,j} J_{ij} \alpha^+_i \hat{n}_i \alpha^+_j = \]

\[ = \frac{1}{N^3} \sum_{i,j} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \mathbf{J}(\mathbf{q}) \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 e^{-i\mathbf{q}_1 \mathbf{R}_i - \mathbf{R}_j} \ast \]

\[ \ast \left( e^{i\mathbf{q}_1 \mathbf{R}_j + \mathbf{q}_2 \mathbf{R}_i - \mathbf{q}_3 \mathbf{R}_j + \mathbf{q}_4 \mathbf{R}_j} \right) \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \mathbf{J}(\mathbf{q}) \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \delta_{\mathbf{q}_4 - \mathbf{q}_2} \]

\[ = \frac{1}{N} \sum_{\mathbf{q}_1 \ldots \mathbf{q}_4} \mathbf{J}(\mathbf{q}_4) \delta_{\mathbf{q}_1 - \mathbf{q}_3} \delta_{\mathbf{q}_2 - \mathbf{q}_4} \delta_{\mathbf{q}_4 - \mathbf{q}_2} \alpha^+_\mathbf{q}_1 \alpha^+_\mathbf{q}_2 \alpha^+_\mathbf{q}_3 \alpha^+_\mathbf{q}_4 \]
In the first term $q_1$ and $q_2$ commute:

$$\sim H_4 = \frac{\hbar^2}{N} \sum_{q_1 \ldots q_4} (J(q_4) - J(q_4 - q_1)) * \delta_{q_1+q_2+q_3+q_4} \alpha_{q_1}^+ \alpha_{q_2}^+ \alpha_{q_3} \alpha_{q_4}$$

Here we exploit

$$\frac{1}{N} \sum_{q_2} J(q_1 - q_2) = \frac{1}{N^2} \sum_{q_2} \sum_{i,j} J_{ij} e^{i(q_1 - q_2)(R_i - R_j)}$$

$$= \frac{1}{N} \sum_{i,j} J_{ij} e^{i(q_1(R_i - R_j))} \delta_{ij}$$

$$= \frac{1}{N} \sum_i J_{ii} = 0$$

Problem 7.12

$$E_0^0 = E_0(B_0 = 0) = -N J_0 \hbar^2 S^2$$

$$U = < H_{SW} > = E_0^0 + \sum_q \hbar \omega(q) < \hat{n}_q >$$

$$\hbar \omega(q) = 2 \hbar (J_0 - J(q)) \approx D q^2 \text{ for small } |q|$$

Low temperatures $\rightarrow$ only a few magnons are excited:
\[ U \approx E_0^0 + D \sum q^2 e^{-\beta D q^2} - 1 \]
\[ = E_0^0 + D \frac{V}{(2\pi)^3} \int_{BZ} d^3 q \, q^2 e^{-\beta D q^2} \sum_{n=0}^{\infty} e^{-n\beta D q^2} \]
\[ \approx E_0^0 + \frac{DV}{2\pi^2} \sum_{n=1}^{\infty} \int_0^{\infty} dq \, q^4 e^{-n\beta D q^2} \]

Substitution
\[ t = n\beta D q^2 \quad dt = 2n\beta D dq = 2\sqrt{t} \frac{n \beta D}{\sqrt{n \beta D}} dq \]
\[ dq = \frac{1}{2\sqrt{n \beta D}} \frac{dt}{\sqrt{t}} \]

\[ \therefore U \approx E_0^0 + \frac{DV}{4\pi^2} \sum_{n=1}^{\infty} (n\beta D)^{-\frac{5}{2}} \int_0^{\infty} dt \, t^{\frac{3}{2}} e^{-t} \]
\[ \Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2} \Gamma(\frac{1}{2}) \]
\[ U \approx E_0^0 + \frac{3DV}{16\pi^2} \zeta\left(\frac{5}{2}\right) \left( \frac{k_B}{D} \right)^{\frac{3}{2}} T^{\frac{5}{2}} = E_0^0 + \eta T^{\frac{5}{2}} \]

\[ C_{B_0=0} = \left( \frac{\partial U}{\partial T} \right)_{B_0=0} = \frac{5}{2} \eta T^{\frac{1}{2}} \]

is experimentally uniquely confirmed.
Measurement of \( C_{B_0=0} \rightarrow \eta \rightarrow D \rightarrow J_0 = z_1 J_1 \).

Problem 7.13

1. Proof by complete induction:
\[ p = 0; \text{ trivial.} \]
\[ p = 1 \]
\[ \left[ \hat{a}_q, a_q^\dagger \right] = a_q^\dagger \left[ a_q, a_q^\dagger \right] + \left[ a_q^\dagger, a_q^\dagger \right] a_q \]
\[ = a_q^\dagger \]
\[ p \sim p + 1 \]
\[ \left[ \hat{n}_q, (a_q^\dagger)^{p+1} \right] = \]
\[ = (a_q^\dagger)^p \left[ \hat{n}_q, a_q^\dagger \right] + \left[ \hat{n}_q, (a_q^\dagger)^p \right] a_q^\dagger \]
\[ = (a_q^\dagger)^p a_q^\dagger + p(a_q^\dagger)^p a_q^\dagger \]
\[ = (p + 1)(a_q^\dagger)^{p+1} \quad \text{q.e.d.} \]

2.
\[ \hat{n}_k \left( \prod_q (a_q^\dagger)^{n_q} \right) |0\rangle = \]
\[ = \hat{n}_k (a_k^\dagger)^{n_k} \prod_{q \neq k} (a_q^\dagger)^{n_q} |0\rangle \]
\[ = \prod_q (a_q^\dagger)^{n_q} \left( (a_k^\dagger)^{n_k} \hat{n}_k + n_k (a_k^\dagger)^{n_k} \right) |0\rangle \]
\[ = 0 + n_k \prod_{q \neq k} (a_q^\dagger)^{n_q} (a_k^\dagger)^{n_k} |0\rangle \]
\[ = n_k \prod_q (a_q^\dagger)^{n_q} |0\rangle \]
\[ = n_k |\psi\rangle \]

$|\psi\rangle$ is therefore an eigenstate of $\hat{n}_k$ with the eigenvalue $n_k$. Thus $|\psi\rangle$ is also eigenstate of $H$:

\[ H |\psi\rangle = \left( E_0(B_0) + \sum_k \hbar \omega(k) n_k \right) |\psi\rangle \]

**Problem 7.14**

\[ U = <H_{SW}> = \hat{E}_a + \sum_q \left\{ E_\alpha(q) <a_q^\dagger a_q> + E_\beta(q) <\beta_q^\dagger \beta_q> \right\} \]

$B_0 = 0; B_A = 0$:

\[ E_\alpha(q) = E_\beta(q) \approx D \cdot q = \epsilon(q) \]
\[ \sim U = \hat{E}_a + 2D \sum_q \frac{q}{e^{\beta \epsilon(q)} - 1} \]
\[ U \approx \hat{E}_a + \frac{DV}{\pi^2} \sum_{n=1}^{\infty} \int_0^{\infty} dq \ q^3 e^{-\beta D q n} \]
\[ = \hat{E}_a + \frac{DV}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^4} \int_0^{\infty} dy \ y^3 e^{-y} \]

Abbreviation:

\[ C_4 = \frac{6DV}{\pi^2(k_B D)^4} \zeta(4) \]

Heat capacity:

\[ C_{B_0=0} = \left( \frac{\partial U}{\partial T} \right)_{B_0=0} = 4C_4 \cdot T^3 \]

**Problem 7.15**

Sub-lattice magnetization of an antiferromagnet (Eq. (7.304)):

\[ M_A(T) = \frac{1}{V} g_J \mu_B \left\{ \frac{N}{2} S - \sum_q \sinh^2 \eta_q - \sum_q \left( \frac{\cosh^2 \eta_q}{e^\beta E_\alpha(q)} - 1 + \frac{\sinh^2 \eta_q}{e^\beta E_\beta(q) - 1} \right) \right\} \]

\[ B_0 = 0; \ B_A = 0: \]

(7.356) \hspace{1cm} \sim \tanh 2\eta_q \approx -\frac{J(q)}{J(0)} = -\gamma_q \hspace{1cm} (T \text{ independent})

\[ M_A(0) = \frac{1}{V} g_J \mu_B \left[ \frac{N}{2} S - \sum_q \sinh^2 q \right] \]

\[ E_\alpha(q) \equiv E_\beta(q) = 2\hbar^2 \sqrt{(J_0 + J(q))(J_0 - J(q))} \]

\[ \approx \frac{2\hbar^2 |J_0|d|J_0q^2|}{\sqrt{2d}} q \equiv \epsilon(q) \]
\begin{equation}
\sim M_A(T) - M_A(0) = -\frac{1}{V} g_J \mu_B \sum_q \frac{1 + 2 \sinh^2 \eta_q}{e^{\beta \varepsilon(q)} - 1}
\end{equation}

\[ T \to 0; \beta \to \infty: \]

\[ \sum_q \frac{1}{e^{\beta \varepsilon(q)} - 1} = \]

\[ = \frac{V}{(2\pi)^3 \int_{BZ} d^3 q} \frac{e^{-\beta \varepsilon(q)}}{1 - e^{-\beta \varepsilon(q)}} \quad \text{(without correction term)} \]

\[ = \frac{V}{(2\pi)^3 \int_{BZ} d^3 q} \sum_{n=1}^{\infty} e^{-n \beta \varepsilon(q)} \]

\[ \approx \frac{V}{2\pi^2} \sum_{n=1}^{\infty} \int_0^{\infty} dq \ q^2 e^{-n \beta D q} \quad \text{(justification as for ferromagnets!)} \]

\[ = \frac{V}{2\pi^2 (\beta D)^3} \sum_{n=1}^{\infty} \frac{1}{n^3} \int_0^{\infty} dy \ y^2 e^{-y} \underbrace{\int_{\Gamma(3) = 2! = 2}} \]

\[ = \left( \frac{V}{\pi^2 (k_B^{-1} D)^3} \zeta(3) \right) T^3 \]

Abbreviation: \( C_3 = \frac{g_J \mu_B}{\pi^2 (k_B^{-1} D)^3} \zeta(3) \)

\[ \sim \boxed{M_A(T) - M(0) = C_3 \cdot T^3} \quad \text{if without correction term} \]

With correction term:

\[ 1 + 2 \sinh^2 \eta_q = \frac{1}{\sqrt{1 - \tanh^2 2\eta_q}} = \frac{1}{\sqrt{1 - \gamma_q^2}} \]

Consider
\[ \gamma_q \approx 1 - dq^2 \]

\[ \frac{1 \sqrt{1 - \gamma_q^2}}{\sqrt{2dq^2 - d^2q^4}} = \frac{1}{\sqrt{2d}} \cdot \frac{1}{q} \cdot \frac{1}{\sqrt{1 - \frac{1}{2}dq^2}} \approx 1 - \gamma_q^2 \approx 2dq^2 \]

(only small \( q \) play a role in the spin wave approximation)

\[ \sum_q \frac{1 + 2 \sinh^2 \eta_q}{e^{\beta\eta(q)} - 1} \approx \frac{1}{\sqrt{2d}} \sum_q \frac{1}{q} \frac{1}{e^{\beta\eta(q)} - 1} \]

\[ = \frac{1}{\sqrt{2d}} \frac{V}{2\pi^2} \frac{1}{(\beta D)^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \int_0^\infty dy ye^{-y} = 1 \]

Abbreviation: \( C_2 = \frac{g^2 \mu_B}{\sqrt{2\pi^2(k_B D)^2}} \xi(2) \)

\[ M_A(T) - M(0) = C_2 \cdot T^2 \]

Problem 7.16

\[ H = E_a + b_A \sum_q a_q^+ a_q + b_B \sum_q b_q^+ b_q + \sum_q c(q) \{ a_q b_q + a_q^+ b_q^+ \} \]

\( \sim \) in the new operators:

\[ H \sim E_a + b_A \sum_q \left( \cosh \eta \cdot \alpha_q^+ + \sinh \eta \cdot \beta_q \right) \]

\[ \sim \left( \cosh \eta \cdot \alpha_q + \sinh \eta \cdot \beta_q^+ \right) + \]

\[ + b_B \sum_q \left( \sinh \eta \cdot \alpha_q + \cosh \eta \cdot \beta_q^+ \right) \]

\[ \sim \left( \sinh \eta \cdot \alpha_q^+ + \cosh \eta \cdot \beta_q \right) + \]

\[ + \sum_q c(q) \left( \cosh \eta \cdot \alpha_q + \sinh \eta \cdot \beta_q^+ \right) \]

\[ \sim \left( \sinh \eta \cdot \alpha_q^+ + \cosh \eta \cdot \beta_q \right) + \]
\[ + (\cosh \eta \cdot \alpha_q^+ + \sinh \eta \cdot \beta_q) \ast \]
\[ \ast (\sinh \eta \cdot \alpha_q + \cosh \eta \cdot \beta_q^+) \} \]
\[ = E_a + \sum_q \left[ b_A (\cosh^2 \eta \cdot \alpha_q^+ \alpha_q + \sinh^2 \eta \cdot \beta_q \beta_q^+) \right. \]
\[ + \sinh \eta \cdot \cosh \eta \left( \alpha_q^+ \beta_q^+ + \beta_q \alpha_q \right) \]
\[ + b_B \left( \sinh^2 \eta \cdot \alpha_q \alpha_q^+ + \cosh^2 \eta \cdot \beta_q \beta_q^+ + \sinh \eta \cdot \cosh \eta (\alpha_q \beta_q + \beta_q^+ \alpha_q) \right) + \]
\[ + c(q) \left( \cosh^2 \eta (\alpha_q \beta_q + \alpha_q^+ \beta_q^+) + \right. \]
\[ \left. + \sinh^2 \eta (\beta_q^+ \alpha_q + \beta_q \alpha_q) + \right. \]
\[ \left. + \cosh \eta \cdot \sinh \eta \left( \alpha_q \alpha_q^+ + \beta_q \beta_q^+ + \right. \right. \]
\[ \left. \left. \alpha_q^+ \alpha_q + \beta_q \beta_q^+ \right) \right] \]

Use

\[ \sinh \eta \cdot \cosh \eta = \frac{1}{2} \sinh 2\eta \]
\[ \cosh^2 \eta = \frac{1}{2} (\cosh 2\eta + 1) \]
\[ \sinh^2 \eta = \frac{1}{2} (\cosh 2\eta - 1) \]

\[ \sim H = E_a + \frac{1}{2} \sum_q \left[ b_A (\alpha_q^+ \alpha_q - \beta_q \beta_q^+) + b_B (-\alpha_q \alpha_q^+ + \beta_q^+ \beta_q) + \right. \]
\[ + c(q) \left( \alpha_q \beta_q + \alpha_q^+ \beta_q^+ - \beta_q^+ \alpha_q - \beta_q \alpha_q \right) \]
\[ + \frac{1}{2} \sum_q \sinh(2\eta) \left[ b_A (\alpha_q^+ \beta_q^+ + \beta_q \alpha_q) + b_B (\alpha_q \beta_q + \beta_q^+ \alpha_q^+) + \right. \]
\[ \left. + c(q) \left( \alpha_q \alpha_q^+ + \beta_q^+ \beta_q + \alpha_q^+ \alpha_q + \beta_q \beta_q^+ \right) \right] \]
\[ + \frac{1}{2} \sum_q \cosh(2\eta) \left[ b_A (\alpha_q^+ \alpha_q + \beta_q \beta_q^+) + b_B (\alpha_q \alpha_q^+ + \beta_q \beta_q^+) + \right. \]
\[ \left. + c(q) \left( 2\alpha_q \beta_q + 2 \alpha_q^+ \beta_q^+ \right) \right] \]
\[ = E_a + \frac{1}{2} \sum_q ((b_A - b_B) \alpha_q^+ \alpha_q + (b_B - b_A) \beta_q^+ \beta_q - (b_A + b_B)) \]
\[ + \frac{1}{2} \sum_q \sinh(2\eta) ((b_a + b_B) (\alpha_q \beta_q + \alpha_q^+ \beta_q^+) + \right. \]
\[ \left. + c(q) \left( 2\alpha_q^+ \alpha_q + 2 \beta_q^+ \beta_q + 2 \right) \right) \]
\[
+ \frac{1}{2} \sum_{q} \cosh(2\eta) \left[ (b_a + b_B)(\alpha_q^+ \alpha_q + \beta_q^+ \beta_q) + (b_A + b_B) + 2c(q)(\alpha_q \beta_q + \alpha_q^+ \beta_q^+) \right] \\
= E_a - \frac{N}{4}(b_A + b_B) + \frac{1}{2} \sum_{q} ((b_A + b_B) \cosh 2\eta + \frac{1}{2}(b_A + b_B) \cosh 2\eta) + 2c(q) \sinh 2\eta + 2\sinh^2(\eta) \\
= c(q) \sinh 2\eta + \frac{1}{2}(b_A + b_B) \cosh 2\eta = \\
= c(q) \frac{\tanh 2\eta}{\sqrt{1 - \tanh^2 2\eta}} + \frac{1}{2}(b_A + b_B) \frac{1}{\sqrt{1 - \tanh^2 2\eta}} \\
= c(q) \frac{-2c(q)}{b_A + b_B} + \frac{1}{2}(b_A + b_B) \frac{1}{\sqrt{1 - \frac{4c^2}{(b_A + b_B)^2}}} \\
= -\frac{4c^2(q)}{2\sqrt{(b_A + b_B)^2 - 4c^2}} + \frac{1}{2} \frac{(b_A + b_B)^2}{\sqrt{(b_A + b_B)^2 - 4c^2}} \\
= \frac{1}{2} \left( b_A + b_B \right)^2 - 4c^2 \\
= E_{\alpha}(q) - \frac{1}{2}(b_A - b_B) \\
= E_{\beta}(q) + \frac{1}{2}(b_A - b_B)
\]

\[\hat{E}_a = E_a - \frac{N}{4}(b_A + b_B) + \frac{1}{2} \sum_{q} \sqrt{(b_A + b_B)^2 - 4c^2(q)}\]

\[H = \hat{E}_a + \sum_{q} \left( E_{\alpha}(q)\alpha_q^+ \alpha_q + E_{\beta}(q)\beta_q^+ \beta_q \right)\]
Problem 7.17

$$\gamma_q = \frac{1}{z_1} \sum_{\Delta_1} e^{i q \cdot R_{\Delta_1}}$$

$z_1$: number of nearest neighbours

$R_{\Delta_1}$: lattice vector from the origin to a nearest neighbouring site

$$\sum_{q_1} \gamma_{q-q_1} \langle \hat{n}_{q_1} \rangle =$$

$$= \frac{1}{z_1} \sum_{q_1} \sum_{\Delta_1} e^{i (q-q_1) \cdot R_{\Delta_1}} \frac{1}{N} \sum_{i,j} \langle a_i^\dagger a_j \rangle e^{i q_1 \cdot (R_i - R_j)}$$

$$= \frac{1}{z_1} \sum_{i,j} \sum_{\Delta_1} \langle a_i^\dagger a_j \rangle e^{i q R_{\Delta_1}} \delta_{i-j,\Delta_1}$$

$$= \frac{1}{z_1} \sum_{\Delta_1} e^{i q R_{\Delta_1}} \sum_i \langle a_i^\dagger a_{i-\Delta_1} \rangle$$

Due to translational symmetry, the expectation value is the same for all nearest neighbours. That is, independent of any particular $\Delta_1$:

$$\sum_{q_1} \gamma_{q-q_1} \langle \hat{n}_{q_1} \rangle$$

$$= \left( \frac{1}{z_1} \sum_{i,\Delta_1} \langle a_i^\dagger a_{i-\Delta_1} \rangle \right) \frac{1}{z_1} \sum_{\Delta_1} e^{i q R_{\Delta_1}}$$

$$= \gamma_q \frac{1}{z_1} \sum_{i,\Delta_1} \langle a_i^\dagger a_{i-\Delta_1} \rangle$$

$$= \gamma_q \frac{1}{z_1} \sum_{i,\Delta_1} \frac{1}{N} \sum_{q_1, q_2} e^{-i q_1 \cdot R} e^{i q_2 \cdot (R_i - R_{\Delta_1})} \langle a_{q_1}^\dagger a_{q_2} \rangle$$

$$= \gamma_q \frac{1}{z_1} \sum_{\Delta_1} \sum_{q_1, q_2} e^{-i q_2 \cdot R_{\Delta_1}} \delta_{q_1, q_2} \langle a_{q_1}^\dagger a_{q_2} \rangle$$

$$= \gamma_q \sum_{q_1} \left( \frac{1}{z_1} \sum_{\Delta_1} e^{-i q_1 \cdot R_{\Delta_1}} \right) \langle a_{q_1}^\dagger a_{q_1} \rangle$$

$$= \gamma_q \sum_{q_1} \gamma_{q_1} \langle \hat{n}_{q_1} \rangle$$
Problem 7.18

\[ \gamma_q = \frac{1}{z_1} \sum_{\Delta_i} e^{i q \cdot R_{\Delta_i}} \]

\[ R_{\Delta_i} \in \{ a(\pm 1, 0, 0), a(0, \pm 1, 0), a(0, 0, \pm 1) \} \]

\[ c_1 = \frac{1}{N} \sum_q (1 - \gamma_q) : \]

\[ \frac{1}{N} \sum_q 1 = 1 \]

\[ \frac{1}{N} \sum_q \gamma_q = \frac{1}{N} \sum_q \frac{1}{z_1} \sum_{\Delta_i} e^{i q \cdot R_{\Delta_i}} \]

\[ = \frac{1}{z_1} \sum_{\Delta_i} \delta_{\Delta_i, 0} = 0 \]

since \( R_0 = (0, 0, 0) \) is not a nearest neighbour.

\[ \Rightarrow c_1 = 1 \]

\[ c_2 = \frac{1}{N} \sum_q (1 - \gamma_q)^2 : \]

\[ c_2 = \frac{1}{N} \sum_q \left( 1 - 2\gamma_q + \gamma_q^2 \right) \]

\[ \frac{1}{N} \sum_q \gamma_q^2 = \frac{1}{N} \sum_q \frac{1}{z_1^2} \sum_{\Delta_i} \sum_{\Delta'_i} e^{i q \cdot (R_{\Delta_i} + R_{\Delta'_i})} \]

\[ = \frac{1}{z_1^2} \sum_{\Delta_i} \sum_{\Delta'_i} \delta_{\Delta_i, -\Delta'_i} \]

\[ = \frac{1}{z_1^2} \sum_{\Delta_i} 1 \]

\[ = \frac{1}{z_1} \]

\[ \Rightarrow c_2 = 1 + \frac{1}{z_1} \]

\[ c_3 = \frac{1}{N} \sum_q (1 - \gamma_q)^3 : \]
\[ c_3 = \frac{1}{N} \sum_q \left( 1 - 3\gamma q + 3\gamma^2 q^2 - \gamma^3 q^3 \right) \]

\[ \frac{1}{N} \sum_q \gamma^3 q^3 = \frac{1}{N} \sum_q \frac{1}{z_1^3} \sum_{\Delta_1} \sum_{\Delta'_1} \sum_{\Delta''_1} e^{i q \left( \mathbf{R}_{\Delta_1} + \mathbf{R}_{\Delta'_1} + \mathbf{R}_{\Delta''_1} \right)} \]

\[ = \frac{1}{z_1^3} \sum_{\Delta_1} \sum_{\Delta'_1} \sum_{\Delta''_1} \delta_{\Delta''_1, -\Delta_1 - \Delta'_1} \]

\[ = 0 \]

since \((-\mathbf{R}_{\Delta_1} - \mathbf{R}_{\Delta'_1})\) for s.c. lattice cannot be a nearest neighbour.

**Problem 7.19**

Calculation of the anisotropy contribution of the dipole interaction

\[ H_a = -3 \sum_{i,j} D_{ij} \left( \mathbf{S}_i \cdot \mathbf{e}_{ij} \right) \left( \mathbf{S}_j \cdot \mathbf{e}_{ij} \right) \]

in spin wave approximation:

\[ S_i^+ = \hbar \sqrt{2S} a_i \]

\[ S_i^- = \hbar \sqrt{2S} a_i^\dagger \]

\[ S_i^z = \hbar \left( S - a_i^\dagger a_i \right) \]

This gives

\[ H_a = -3 \sum_{i,j} D_{ij} \left( \mathbf{S}_i \cdot \mathbf{e}_{ij} \right) \left( \mathbf{S}_j \cdot \mathbf{e}_{ij} \right) \]

\[ = -3 \sum_{i,j} D_{ij} \left\{ \left( S_i^x x_{ij} + S_i^y y_{ij} + S_i^z z_{ij} \right) * \left( S_j^x y_{ij} + S_j^y y_{ij} + S_j^z z_{ij} \right) \right\} \]

\[ = -3 \sum_{i,j} D_{ij} \left\{ x_{ij} S_i^x S_j^x + y_{ij} S_i^y S_j^y + z_{ij} S_i^z S_j^z + x_{ij} y_{ij} \left( S_i^x S_j^y + S_i^y S_j^x \right) + x_{ij} z_{ij} \left( S_i^x S_j^z + S_i^z S_j^x \right) + y_{ij} z_{ij} \left( S_i^y S_j^z + S_i^z S_j^y \right) \right\} \]

\[ = -3 \hbar^2 \sum_{i,j} D_{ij} \left\{ x_{ij} \frac{2S}{4} \left( a_i + a_i^\dagger \right) \left( a_j + a_j^\dagger \right) + \right\} \]
\[ + \frac{1}{4} \chi_{ij}^2 \left[ 2S - 2 \left( n_i + n_j \right) + n_i n_j \right] + \\
+ \chi_{ij} y_{ij} \frac{2S}{4i} \left( \left( a_i + a_i^\dagger \right) \left( a_j - a_j^\dagger \right) + \\
\quad + \left( a_i - a_i^\dagger \right) \left( a_j + a_j^\dagger \right) \right) + \\
+ x_{ij} z_{ij} \frac{\sqrt{2S}}{2} \left( \left( a_i + a_i^\dagger \right) \left( S - n_j \right) + \\
\quad + \left( S - n_i \right) \left( a_j + a_j^\dagger \right) \right) + \\
+ y_{ij} z_{ij} \frac{\sqrt{2S}}{2i} \left( \left( a_i - a_i^\dagger \right) \left( S - n_j \right) + \\
\quad + \left( S - n_i \right) \left( a_j - a_j^\dagger \right) \right) \right]} \\
= -3\hbar^2 \sum_{i,j} D_{ij} \left\{ \chi_{ij}^2 \left( a_i a_j + a_i a_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger \right) - \\
- \frac{1}{2} \chi_{ij}^2 \chi_{ij} y_{ij} \left( a_i a_j - a_j a_i \right) + \\
+ \frac{1}{2} \chi_{ij}^2 \chi_{ij} y_{ij} \left( a_i a_j - a_j a_i \right) + \\
+ \left( a_i a_j^\dagger + a_i^\dagger a_j \right) \chi_{ij}^2 \chi_{ij} y_{ij} \left( a_i a_j^\dagger + a_i^\dagger a_j \right) \right\} \\
= -3\hbar^2 \chi_{ij}^2 \left( S - 2n_i \right) - \\
-3\hbar^2 \chi_{ij}^2 \sum_{i,j} D_{ij} \left\{ \chi_{ij}^2 \left( a_i a_j^\dagger \frac{1}{2} \chi_{ij}^2 - \frac{1}{2} \chi_{ij} y_{ij} \right) + \\
+ a_i a_j \left( \frac{1}{2} \chi_{ij}^2 - \frac{1}{2} \chi_{ij} y_{ij} \right) + \\
+ \left( a_i a_j^\dagger + a_i^\dagger a_j \right) \left( \frac{1}{2} \chi_{ij}^2 + \frac{1}{2} \chi_{ij} y_{ij} \right) + \\
+ S \sqrt{2S} x_{ij} z_{ij} \left( a_i + a_i^\dagger \right) - S \sqrt{2S} y_{ij} z_{ij} \left( a_i + a_i^\dagger \right) \right\} \}

The mixed terms vanish. In order to see that, hold \( z_{ij} \) fixed. All \( \mathbf{R}_i \) and \( \mathbf{R}_j \) with \( z_{ij} = \text{const} \) define an \( x, y \)-plane. In this for each \( \mathbf{R}_j \) there is a \( \mathbf{R}'_j \) with \( x_{ij} = -x'_{ij} \).
and \( y_{ij} = -y'_{ij} \) and \( |R_{ij}| = |R'_{ij}| \), i.e. \( D_{ij} = D'_{ij} \). That means \( \sum_j D_{ij} x_{ij} z_{ij} = 0 \) in the plane and therefore in the entire space. Analogously: \( \sum_i D_{ij} y_{ij} z_{ij} = 0 \). Therefore what remains is (Fig. C.2)

\[
H_a = -3\hbar^2 S \sum_{i,j} D_{ij} z_{ij}^2 (S - 2n_i) - 3\hbar^2 \sum_{i,j} D_{ij} \left\{ a_i^\dagger a_j^\dagger \frac{1}{2} (x_{ij} + iy_{ij})^2 + a_i a_j \frac{1}{2} (x_{ij} - iy_{ij})^2 + a_i^\dagger a_j (x_{ij}^2 + y_{ij}^2) \right\}
\]

**Fig. C.2** Graphical illustration for the evaluation of the “mixed” terms in \( H_a \) (see text)

Problem 7.20
First derivative

\[
\frac{d\omega}{da} = \hbar x \omega - \frac{e^{\hbar a x} h(1 + \varphi) e^{\hbar a}}{(1 + \varphi) e^{\hbar a} - \varphi} = \hbar \omega (x - \alpha)
\]

with

\[
\alpha = \frac{(1 + \varphi) e^{\hbar a}}{(1 + \varphi) e^{\hbar a} - \varphi} = 1 + \frac{\varphi}{(1 + \varphi) e^{\hbar a} - \varphi}
\]

Second derivative:
\[
\frac{d^2 \omega}{da^2} = \hbar^2 \omega (x - \alpha)^2 + \hbar \omega \frac{\hbar \varphi (1 + \varphi) e^{\hbar a}}{(1 + \varphi e^{\hbar a} - \varphi)^2}
\]

\[
= \hbar^2 \omega (x - \alpha)^2 + \hbar^2 \omega \alpha \frac{\varphi}{(1 + \varphi) e^{\hbar a} - \varphi}
\]

\[
= \hbar^2 \omega \left( (x - \alpha)^2 + \alpha (\alpha - 1) \right)
\]

Coefficient of the second term in the differential equation:

\[
\frac{(1 + \varphi) + \varphi e^{-\hbar a}}{1 + \varphi - \varphi e^{-\hbar a}} = \alpha + \frac{\varphi}{(1 + \varphi) e^{\hbar a} - \varphi} = \alpha + \alpha - 1
\]

Thus what remains is

\[
\hbar^2 \omega \left( (x - \alpha)^2 + \alpha (\alpha - 1) \right) +
\]

\[
\hbar^2 \omega (x - \alpha) (2\alpha - 1) - \hbar^2 S (S + 1) \omega = 0
\]

\[
\Leftrightarrow x^2 - 2\alpha x + \alpha^2 + \alpha^2 - \alpha + 2x\alpha -
\]

\[
x - 2\alpha^2 + \alpha - S (S + 1) = 0
\]

\[
\Leftrightarrow x^2 - x - S (S + 1) = 0
\]

\[
\Leftrightarrow x_1 = -S; \ x_2 = S + 1
\]

General solution:

\[
\Omega(a) = c_1 \omega (-S, a) + c_2 \omega (S + 1, a)
\]

**Problem 8.1**

For the Hamiltonian

\[
H_0 = \sum_{ij} \sum_{\mu \nu} T_{ij}^{\mu \nu} c_{i \mu \sigma}^+ c_{j \nu \sigma}
\]

holds after substituting the Fourier integrals:
\[
H_0 = \sum_{ij\sigma} \sum_{\mu,\nu} \frac{1}{N_i} \sum_{k} T_{k}^{ij\mu\nu} e^{i k \cdot (\mathbf{R}_i - \mathbf{R}_j)} 
\]
\[
* \frac{1}{N_i} \sum_{q,p,m,m'} e^{-i q \cdot \mathbf{R}_i - p \cdot \mathbf{R}_j} c_{q\mu\sigma} c_{m'\nu\sigma} U_{q\sigma}^{m\mu} \left( U_{p\sigma}^{m'\nu} \right)^* 
\]
\[
= \sum_{k,q,p} \sum_{m,m',\sigma,v,\mu} T_{k}^{\mu\nu} U_{q\sigma}^{m\mu} \left( U_{p\sigma}^{m'\nu} \right)^* \delta_{k,q} \delta_{k,p} c_{q\mu\sigma} c_{m'\nu\sigma} 
\]
\[
= \sum_{k} \sum_{m,m',\sigma,v,\mu} T_{k}^{\mu\nu} \left( U_{k\sigma}^{m'\nu} \right)^* \delta_{k,m} \delta_{k,m'} c_{k\mu\sigma} c_{k\nu\sigma} 
\]
\[
= \sum_{k,m,m',\sigma} \epsilon_{m'}(k) \left( U_{k\sigma}^{m'\nu} \right)^* \epsilon_{m}(k) c_{k\nu\sigma} c_{k\mu\sigma} 
\]
\[
= \sum_{k,m,\sigma} \epsilon_{m}(k) c_{k\mu\sigma} c_{k\sigma} 
\]

\textbf{Problem 8.2}

Wannier representation:

\[
H = \sum_{ij\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} 
\]

Hopping integrals:

\[
T_{ij} = \frac{1}{N} \sum_{k} \epsilon(k) e^{i k \cdot (\mathbf{R}_i - \mathbf{R}_j)} 
\]

Construction operators:

\[
c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k} c_{k\sigma} e^{i k \cdot \mathbf{R}_i} 
\]

One-particle part:
\[ H_0 = \sum_{i,j} T_{ij} c^\dagger_i c_j \]
\[ = \frac{1}{N^2} \sum_{k,p,q,\sigma} \varepsilon(k) c^\dagger_{p\sigma} c_{q\sigma} \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} e^{-ip \cdot \mathbf{R}_i} e^{iq \cdot \mathbf{R}_j} \]
\[ = \sum_{k,p,q,\sigma} \varepsilon(k) c^\dagger_{p\sigma} c_{q\sigma} \delta_{k,p} \delta_{k,q} \]
\[ = \sum_{k\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma} \]

Interaction part:
\[ H_1 = \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \]
\[ = \frac{1}{2} U \frac{1}{N^2} \sum_{k_1 \ldots k_4,\sigma} c^\dagger_{k_1\sigma} c_{k_2\sigma} c^\dagger_{k_3-\sigma} c_{k_4-\sigma} * \]
\[ * \sum_{i} e^{i(-k_1+k_3) \cdot \mathbf{R}_i} e^{i(-k_1+k_4) \cdot \mathbf{R}_i} \]
\[ = \frac{1}{2} U \sum_{k_1 \ldots k_4,\sigma} \delta_{k_1+k_3,k_2+k_4} c^\dagger_{k_1\sigma} c_{k_2\sigma} c^\dagger_{k_3-\sigma} c_{k_4-\sigma} \]
\[ \implies H_1 = \frac{1}{2} U \sum_{k,p,q,\sigma} c^\dagger_{k+q\sigma} c^\dagger_{p-q-\sigma} c_{p-\sigma} c_{k\sigma} \]

Total:
\[ H = \sum_{k\sigma} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2} U \sum_{k,p,q,\sigma} c^\dagger_{k+q\sigma} c^\dagger_{p-q-\sigma} c_{p-\sigma} c_{k\sigma} \]

Problem 8.3
Band limit:
\[ G^{U\rightarrow 0}_{k\sigma}(E) = \frac{\hbar}{E - \varepsilon(k) + \mu} \]

Zero bandwidth limit (\(W = 0\)):
\[ G^{W=0}_{\sigma} = \frac{\hbar(1 - n_{-\sigma})}{E - T_0 + \mu} + \frac{\hbar n_{-\sigma}}{E - T_0 - U + \mu} \]

Stoner approximation:
\[ G_{k\sigma}^{(\text{Stoner})}(E) = \frac{\hbar}{E - \varepsilon(k) - U n_{-\sigma} + \mu} \]

obviously satisfies the band limit but not the limit of infinitely narrow band.

**Problem 8.4**

\[ H = \sum_{\kappa\sigma, \alpha, \beta} \varepsilon^{\alpha\beta}_{\sigma}(k) c_{\kappa\alpha\sigma}^{\dagger} c_{k\beta\sigma}, \quad \alpha, \beta \in \{A, B\} \]

\[ \varepsilon^{AA}_{\sigma}(k) = \varepsilon(k) + \frac{1}{2} U n - \frac{1}{2} z_{\sigma} U m - \mu \]

\[ \varepsilon^{BB}_{\sigma}(k) = \varepsilon(k) + \frac{1}{2} U n + \frac{1}{2} z_{\sigma} U m - \mu \]

\[ \varepsilon^{AB}_{\sigma}(k) = t(k) = \varepsilon^{BA}_{\sigma}(k) \]

Here we have used

\[ < n^{AA}_{\sigma} > = - < n^{BB}_{\sigma} > = n_{\sigma} \]

\[ m = n_{\uparrow} - n_{\downarrow}; \quad m_{A} = - m_{B} = m \]

Green’s functions:

\[ G^{\alpha\beta}_{k\sigma}(E) = < c_{k\sigma}\sigma; c_{k\beta\sigma}^{\dagger} > \]

1. Quasiparticle energies:

\[ [c_{kA\sigma}, H]_-= \sum_{\beta} \varepsilon^{AB}_{\sigma}(k) c_{k\beta\sigma} \]

\[ = \varepsilon^{AA}_{\sigma}(k) c_{kA\sigma} + \varepsilon^{AB}_{\sigma}(k) c_{kB\sigma} \]

Equation of motion:

\[ (E - \varepsilon^{AA}_{\sigma}(k)) G^{AA}_{k\sigma}(E) = \hbar + \varepsilon^{AB}_{\sigma}(k) G^{BA}_{k\sigma}(E) \]

With

\[ [c_{kB\sigma}, H]_-= \varepsilon^{BA}_{\sigma}(k) c_{kA\sigma} + \varepsilon^{BB}_{\sigma}(k) c_{kB\sigma} \]

also follows:
\[(E - \varepsilon_{\sigma}^{BB}(k))G_{k\sigma}^{AA}(E) = \varepsilon_{\sigma}^{BA}(k)G_{k\sigma}^{AA}(E)\]
\[\therefore G_{k\sigma}^{BA}(E) = \frac{\varepsilon_{\sigma}^{BA}(k)}{E - \varepsilon_{\sigma}^{BB}(k)} G_{k\sigma}^{AA}(E)\]

Substituting in the equation of motion for \(G_{k\sigma}^{AA}(E)\):

\[(E - \varepsilon_{\sigma}^{AA}(k))G_{k\sigma}^{AA}(E) = \hbar + \frac{|\varepsilon_{\sigma}^{AB}(k)|^2}{E - \varepsilon_{\sigma}^{BB}(k)} G_{k\sigma}^{AA}(E)\]
\[\therefore G_{k\sigma}^{AA}(E) = \hbar \frac{E - \varepsilon_{\sigma}^{BB}(k)}{(E - \varepsilon_{\sigma}^{AA}(k))(E - \varepsilon_{\sigma}^{BB}(k)) - |\varepsilon_{\sigma}^{AB}(k)|^2}\]

Poles:

\[(E_{\pm} - \varepsilon_{\sigma}^{AA}(k))(E - \varepsilon_{\sigma}^{BB}(k)) - |\varepsilon_{\sigma}^{AB}(k)|^2 = 0\]
\[\therefore E_{\pm}(k) = \frac{1}{2}(\varepsilon_{\sigma}^{AA}(k) + \varepsilon_{\sigma}^{BB}(k)) \pm \sqrt{\frac{1}{4} (\varepsilon_{\sigma}^{AA}(k) - \varepsilon_{\sigma}^{BB}(k))^2 + |\varepsilon_{\sigma}^{AB}(k)|^2}\]

That means the spin-independent quasiparticle energies:

\[E_{\pm}(k) = \varepsilon(k) + \frac{1}{2} Un \pm \sqrt{\frac{1}{4} U^2 m^2 + |t(k)|^2 - \mu}\]

2. Spectral weights:

\[G_{k\sigma}^{AA}(E) = \frac{E - \varepsilon_{\sigma}^{BB}(k)}{(E - E_{+}(k))(E - E_{-}(k))}\]
\[\hbar \alpha_{\sigma}^{(\pm)}(k) = \lim_{E \to E_{\pm}(k)} G_{k\sigma}^{AA}(E)(E - E_{\pm}(k))\]
\[\alpha_{\sigma}^{(\pm)}(k) = \frac{E_{\pm}(k) - \varepsilon_{\sigma}^{BB}(k)}{E_{\pm}(k) - E_{\mp}(k)}\]
\[\leftrightarrow \alpha_{\sigma}^{(\pm)}(k) = \frac{1}{2} \left( 1 \mp z_{\sigma} \frac{Um}{\sqrt{U^2 m^2 + 4|t(k)|^2}} \right)\]

Spectral weights are obviously spin dependent
Spectral density:

\[S_{k\sigma}^{(\pm)}(E) = \hbar \alpha_{\sigma}^{(\pm)}(k) \delta(E - E_{+}(k)) + \hbar \alpha_{\sigma}^{(-)}(k) \delta(E - E_{-}(k))\]
Quasiparticle density of states:

\[
\rho_{\sigma}^{(\pm)}(E) = \frac{1}{\hbar N} \sum_{k} \left\{ \alpha_{\sigma}^{(\pm)}(k) \delta(E - \mu - E_{\pm}(k)) + \alpha_{\sigma}^{(-)}(k) \delta(E - \mu - E_{-}(k)) \right\}
\]

\(k\): wavevector of the first Brillouin zone of the sub-lattice.

**Problem 8.5**

Let \(x \neq 0\):

\[
\frac{1}{2} \lim_{\beta \to \infty} \frac{\beta}{1 + \cosh(\beta x)} = \lim_{\beta \to \infty} \beta e^{-\beta |x|} = 0
\]

The expression diverges for \(x = 0\). In addition it holds

\[
\int_{-\infty}^{+\infty} dx \frac{1}{2} \lim_{\beta \to \infty} \frac{\beta}{1 + \cosh(\beta x)} = \lim_{\beta \to \infty} \int_{0}^{\infty} dx \frac{\beta}{1 + \cosh(\beta x)},
\]

\[
\int_{0}^{\infty} dx \frac{\beta}{1 + \cosh(\beta x)} = \int_{0}^{\infty} dy \frac{1}{1 + \cosh(y)} = \int_{0}^{\infty} dy \frac{1}{2 \cosh^{2} \frac{y}{2}}
\]

\[
= \int_{0}^{\infty} dz \frac{1}{\cosh^{2} z} = \tanh \left| \frac{z}{0} \right|
\]

\[
= 1 - 0 = 1.
\]

Thus we have the defining properties of the \(\delta\)-function satisfied!

**Problem 8.6**

According to (8.97) the Hubbard Hamiltonian can be written as follows:

\[
H = \sum_{k\sigma} \varepsilon(k)c_{k\sigma}^{\dagger}c_{k\sigma} - \frac{2U}{3N} \sum_{k} \sigma(k) \cdot \sigma(-k) + \frac{1}{2} U N - 2\mu_{B} B_{0}\sigma^{2}(\mathbf{0})
\]

1. We calculate the commutator termwise:
\[
\left[ \sigma^+(\mathbf{k}), \sum_{m,n,\sigma} T_{mn} \sigma^+_{m\sigma} \sigma_{n\sigma} \right]_-
\]
\[
= \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} \sum_{m,n,\sigma} T_{mn} \left[ \sigma^+_{i\uparrow} \sigma_{i\downarrow}, \sigma^+_{m\sigma} \sigma_{n\sigma} \right]_-
\]
\[
= \sum_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} \sum_{m,n,\sigma} T_{mn} \left( \delta_{im} \delta_{\sigma\downarrow} \sigma^+_{i\uparrow} \sigma_{n\sigma} - \delta_{in} \delta_{\sigma\uparrow} \sigma^+_{m\sigma} \sigma_{i\downarrow} \right)
\]
\[
= \sum_{m,n} T_{mn} \left( \sigma^+_{m\uparrow} \sigma_{n\downarrow} e^{-i\mathbf{k} \cdot \mathbf{R}_n} - \sigma^+_{m\uparrow} \sigma_{n\downarrow} e^{-i\mathbf{k} \cdot \mathbf{R}_m} \right)
\]
\[
= \sum_{m,n} T_{mn} \left( e^{-i\mathbf{k} \cdot \mathbf{R}_n} - e^{-i\mathbf{k} \cdot \mathbf{R}_m} \right) \sigma^+_{m\uparrow} \sigma_{n\downarrow}
\]

We further calculate

\[
\left[ \sigma^+(\mathbf{k}), \sum_{\mathbf{p}} \sigma(\mathbf{p}) \sigma(-\mathbf{p}) \right]_-
\]
\[
= \sum_{\mathbf{p}} \left[ \sigma^+(\mathbf{k}), \sigma^\dagger(\mathbf{p}) \sigma(-\mathbf{p}) \frac{1}{2} \sigma^+(\mathbf{p}) \sigma(-\mathbf{p}) \right]_-
\]
\[
= \sum_{\mathbf{p}} \left\{ \sigma^\dagger(\mathbf{p}) \left[ \sigma^+(\mathbf{k}), \sigma^\dagger(-\mathbf{p}) \right]_+ + \left[ \sigma^+(\mathbf{k}), \sigma^\dagger(\mathbf{p}) \right]_+ \right\}
\]
\[
= \sum_{\mathbf{p}} \left\{ -\sigma^\dagger(\mathbf{p}) \sigma^+(\mathbf{k} - \mathbf{p}) - \sigma^+(\mathbf{k} + \mathbf{p}) \sigma^\dagger(-\mathbf{p}) + \sigma^+(\mathbf{p}) \sigma^\dagger(-\mathbf{k} + \mathbf{p}) + \sigma^\dagger(\mathbf{k} + \mathbf{p}) \sigma^+(\mathbf{p}) \right\}
\]
\[
= 0
\]

One recognizes this when one replaces \(\mathbf{p}\) by \(\mathbf{p} + \mathbf{k}\) in the term before the last and \(\mathbf{p}\) by \(\mathbf{p} - \mathbf{k}\) in the last term:
\[
[\sigma^+(\mathbf{k}), \hat{N}]_- = \sum_{i,m,\sigma} e^{-i\mathbf{k} \cdot \mathbf{R}_i} \left[ c^+_{i \uparrow} c_{i \downarrow}, c^+_{m \sigma} c_{m \sigma} \right]_-
\]
\[
= \sum_{i,m,\sigma} e^{-i\mathbf{k} \cdot \mathbf{R}_i} \left\{ \delta_{\sigma \downarrow} \delta_{im} c^+_{i \uparrow} c_{m \sigma} - \delta_{im} \delta_{\sigma \uparrow} c^+_{m \sigma} c_{i \downarrow} \right\}
\]
\[
= \sum_{i} e^{-i\mathbf{k} \cdot \mathbf{R}_i} \left[ c^+_{i \uparrow} c_{i \downarrow} - c^+_{i \downarrow} c_{i \uparrow} \right]
\]
\[
= 0
\]
\[
[\sigma^+(\mathbf{k}), \sigma^-(\mathbf{0})]_- = -\sigma^+(\mathbf{k})
\]

Therefore what remains is
\[
[\sigma^+(\mathbf{k}), H]_- = 2\mu_B B_0 \sigma^+(\mathbf{k}) + \sum_{m,n} T_{mn} \left( e^{-i\mathbf{k} \cdot \mathbf{R}_m} - e^{-i\mathbf{k} \cdot \mathbf{R}_n} \right) c^+_{m \uparrow} c_{n \downarrow}
\]

This corresponds to (8.106).

2. For the double commutator we need the results of 1.:
\[
\sum_{m,n} T_{mn} \left( e^{-i\mathbf{k} \cdot \mathbf{R}_m} - e^{-i\mathbf{k} \cdot \mathbf{R}_n} \right) \sum_{i} e^{i\mathbf{k} \cdot \mathbf{R}_i} \left[ c^+_{m \uparrow} c_{n \downarrow}, c^+_{i \uparrow} c_{i \downarrow} \right]_-
\]
\[
= \sum_{m,n} T_{mn} \left( e^{-i\mathbf{k} \cdot \mathbf{R}_m} - e^{-i\mathbf{k} \cdot \mathbf{R}_n} \right) \star
\]
\[
\star \sum_{i} e^{i\mathbf{k} \cdot \mathbf{R}_i} \left\{ \delta_{ni} c^+_{m \uparrow} c_{i \downarrow} - \delta_{mi} c^+_{i \uparrow} c_{n \downarrow} \right\}
\]
\[
= \sum_{m,n} T_{mn} \left\{ \left( e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} - 1 \right) c^+_{m \uparrow} c_{n \uparrow} - \left( 1 - e^{i\mathbf{k} \cdot (\mathbf{R}_m - \mathbf{R}_n)} \right) \delta_{mi} c^+_{m \downarrow} c_{n \downarrow} \right\}
\]

So that it follows:
\[
[\sigma^+(\mathbf{k}), H]_-, \sigma^-(\mathbf{-k})_- = 4\mu_B B_0 \sigma^-(\mathbf{0}) + \sum_{m,n,\sigma} T_{mn} \left( e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)} - 1 \right) c^+_{m \sigma} c_{n \sigma}
\]

This is exactly (8.107).

**Problem 8.7**

We use (8.137) and (8.138) and then have the following determining equation for the chemical potential \( \mu \):
\[ n = n_\sigma + n_{-\sigma} = \frac{2 f_-(T_0)}{1 + f_-(T_0) - f_-(T_0 + U)} \]

That is the same thing as

\[ f_-(T_0) = 1 - f_-(T_0 + U) \]

\[ \frac{1}{e^{\beta(T_0 - \mu)} + 1} = 1 - \frac{1}{e^{\beta(T_0 + U - \mu)} + 1} = \frac{e^{\beta(T_0 + U - \mu)}}{e^{\beta(T_0 + U - \mu)} + 1} \]

\[ e^{\beta(T_0 - \mu)} + 1 = 1 + e^{-\beta(T_0 + U - \mu)} \]

\[ T_0 - \mu = -(T_0 + U - \mu) \]

\[ 2T_0 + U = 2\mu \]

\[ \mu = T_0 + \frac{U}{2} \]

**Problem 8.8**

Substituting the spectral density (8.139) for

\[ n_\sigma = n_{-\sigma} = \frac{1}{2} \]

in (8.77), it directly follows:

\[ Z_{W=0} = -\frac{1}{2} \left( f_-'(T_0) + f_-(T_0 + U) \right) \]

On the other hand substituting in (8.78) gives

\[ N_{W=0} = -f_-(T_0) + f_-(T_0 + U) \]

For the susceptibility holds (8.79)

\[ \bar{\chi}_{W=0} = 2\mu B \frac{Z_{W=0}}{1 + N_{W=0}} \]

The chemical potential for half-filling is known from Problem 8.7:

\[ \mu(n = 1) = T_0 + \frac{U}{2} \]

So that we calculate
\[(f_-(T_0 + U) - f_-(T_0)) = \left(\frac{1}{e^{\beta(T_0 + U - \mu)}} + 1\right) - \left(\frac{1}{e^{\beta T_0 - \mu}} + 1\right)\]
\[= \left(\frac{1}{e^{\beta U}} + 1\right) - \left(\frac{1}{e^{-\beta U}} + 1\right)\]
\[= e^{-\beta U} - e^{\beta U}\]
\[= e^{\beta U} + e^{-\beta U}\]
\[\therefore N_{W=0} = - \tanh(\beta \frac{W}{4})\]

For \(Z_{W=0}\) we need the derivative of the Fermi function:

\[f'_-(E) = -\beta \frac{e^{\beta(E - \mu)}}{(e^{\beta(E - \mu)} + 1)^2}\]
\[= -\beta \frac{1}{\left(e^{\frac{1}{2}\beta(E - \mu)} + e^{-\frac{1}{2}\beta(E - \mu)}\right)^2}\]

Then it follows:

\[-\frac{1}{2} \left(f'_-(T_0) + f'_-(T_0 + U)\right) = \frac{\beta}{2} \left(\frac{1}{(e^{-\beta U} + e^{\beta U})^2} + \frac{1}{(e^{\beta U} + e^{-\beta U})^2}\right)\]
\[= \frac{\beta}{2} \cdot 2 \cdot \frac{1}{4} \cdot \frac{1}{\cosh^2(\beta \frac{U}{4})}\]
\[\therefore Z_{W=0} = \frac{1}{4} \beta \frac{1}{\cosh^2(\beta \frac{U}{4})}\]

Susceptibility:

\[\bar{\chi} = \frac{1}{2} \beta \mu B \frac{1}{\cosh^2(\beta \frac{U}{4}) - 1 - \tanh(\beta \frac{U}{4})}\]
\[= \frac{1}{2} \beta \mu B \frac{1 + \tanh(\beta \frac{U}{4})}{\cosh^2(\beta \frac{U}{4})(1 - \tanh^2(\beta \frac{U}{4}))}\]
\[= \frac{1}{2} \beta \mu B \frac{1 + \tanh(\beta \frac{U}{4})}{\cosh^2(\beta \frac{U}{4}) - \sinh^2(\beta \frac{U}{4})}\]

Then we finally have
\[ \tilde{\chi}_{W=0} = \frac{1}{2} \beta \mu_B \left( 1 + \tanh \left( \frac{\beta U}{4} \right) \right) \]

**Problem 8.9**

Complete basis:

\[
\begin{align*}
|E_1^{(1)}\rangle &= c_{1\sigma}^+ |0\rangle \\
|E_2^{(1)}\rangle &= c_{2\sigma}^+ |0\rangle 
\end{align*}
\]

Hamiltonian matrix:

\[
H^{(1)} = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix}
\]

Diagonalization:

\[
\begin{align*}
\text{Det} \left( H^{(1)} - E \right) &\neq 0 \\
\text{Det} \left| -E & t \\ t & -E \right| &= E^2 - t^2 \\
\iff E_1^{(1)} &= -t ; \quad E_2^{(1)} = +t
\end{align*}
\]

For \( E_1^{(1)} \):

\[
\begin{pmatrix} t & t \\ t & t \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = 0
\]

\[ \iff t (\alpha_1 + \alpha_2) = 0 \iff \alpha_2 = -\alpha_1 \]

Normalization:

\[
|E_1^{(1)}\rangle = \frac{1}{\sqrt{2}} \left( c_{1\sigma}^+ |0\rangle - c_{2\sigma}^+ |0\rangle \right)
\]

For \( E_2^{(1)} \):

\[
\begin{pmatrix} -t & t \\ t & -t \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = 0
\]

\[ \iff t (-\beta_1 + \beta_2) = 0 \iff \beta_1 = \beta_2 \]

Normalization:

\[
|E_2^{(1)}\rangle = \frac{1}{\sqrt{2}} \left( c_{1\sigma}^+ |0\rangle + c_{2\sigma}^+ |0\rangle \right)
\]
Problem 8.10
1. We use

\[
\begin{align*}
[c_{i\sigma}, c_{j\sigma}^+] & = \delta_{ij}\delta_{\sigma\sigma'} \\
[c_{i\sigma}, c_{j\sigma'}^+] & = 0 \\
\langle c_{i\sigma} | 0 \rangle & = 0 \quad ; \quad \langle 0 | c_{j\sigma}^+ \rangle = 0 \\
\langle \epsilon^{(2)}_1 | \epsilon^{(2)}_1 \rangle & = \langle 0 | c_{2-\sigma} c_{1\sigma} c_{1\sigma}^+ c_{2-\sigma}^+ | 0 \rangle \\
& = \langle 0 | c_{2-\sigma} c_{2-\sigma}^+ | 0 \rangle = (0 | 0) = 1
\end{align*}
\]

analogously:

\[
\begin{align*}
\langle \epsilon^{(2)}_i | \epsilon^{(2)}_j \rangle & = 1 \quad i = 2, \cdots, 4 \\
\langle \epsilon^{(2)}_1 | \epsilon^{(2)}_2 \rangle & = \langle 0 | c_{2-\sigma} c_{1\sigma} c_{1\sigma}^+ c_{1\sigma}^+ | 0 \rangle \\
& = \langle 0 | c_{2-\sigma} c_{2\sigma}^+ c_{1\sigma}^+ c_{1\sigma} | 0 \rangle \\
& = 0 \\
\langle \epsilon^{(2)}_1 | \epsilon^{(2)}_3 \rangle & = \langle 0 | c_{2-\sigma} c_{1\sigma} c_{1\sigma}^+ c_{1\sigma}^+ | 0 \rangle = 0 \\
\langle \epsilon^{(2)}_1 | \epsilon^{(2)}_4 \rangle & = \langle 0 | c_{2-\sigma} c_{1\sigma} c_{2\sigma}^+ c_{2\sigma}^+ | 0 \rangle = 0 \\
\langle \epsilon^{(2)}_2 | \epsilon^{(2)}_3 \rangle & = \langle 0 | c_{1-\sigma} c_{2\sigma} c_{1\sigma}^+ c_{1\sigma}^+ | 0 \rangle = 0 \\
\langle \epsilon^{(2)}_2 | \epsilon^{(2)}_4 \rangle & = \langle 0 | c_{1-\sigma} c_{2\sigma} c_{2\sigma}^+ c_{2\sigma}^+ | 0 \rangle = 0 \\
\langle \epsilon^{(2)}_3 | \epsilon^{(2)}_4 \rangle & = \langle 0 | c_{1-\sigma} c_{1\sigma} c_{2\sigma}^+ c_{2\sigma}^+ | 0 \rangle = 0
\end{align*}
\]

Therefore it holds

\[
\langle \epsilon^{(2)}_i | \epsilon^{(2)}_j \rangle = \delta_{ij}; \quad i, j = 1 \ldots 4
\]
2.

\[ H \left| \varepsilon_1^{(2)} \right\rangle = t \sum_{\sigma'} \left( c_{1\sigma'}^\dagger c_{2\sigma'} + c_{2\sigma'}^\dagger c_{1\sigma'} \right) c_{1\sigma}^\dagger c_{2-\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \frac{1}{2} U \sum_{i\sigma'} n_{i\sigma'} n_{i-\sigma'} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t c_{1-\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle + t c_{2\sigma}^\dagger c_{2-\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \frac{1}{2} U \sum_{\sigma'} n_{1\sigma'} n_{1-\sigma'} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \frac{1}{2} U \sum_{\sigma'} n_{2\sigma'} n_{2-\sigma'} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t \left( \left| \varepsilon_3^{(2)} \right\rangle + \left| \varepsilon_4^{(2)} \right\rangle \right) + \frac{1}{2} U \left( n_{1\sigma'} c_{1\sigma}^\dagger c_{2\sigma}^\dagger \left| 0 \right\rangle + \right. \]

\[ + c_{1\sigma} n_{1-\sigma'} c_{1\sigma}^\dagger c_{2-\sigma}^\dagger \left| 0 \right\rangle + c_{1\sigma} n_{2\sigma} c_{2\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \left. c_{1\sigma} c_{2-\sigma} n_{2\sigma} \right\rangle \right) \]

\[ = t \left( \left| \varepsilon_3^{(2)} \right\rangle + \left| \varepsilon_4^{(2)} \right\rangle \right) \]

\[ H \left| \varepsilon_2^{(2)} \right\rangle = t \sum_{\sigma'} \left( c_{1\sigma'}^\dagger c_{2\sigma'} + c_{2\sigma'}^\dagger c_{1\sigma'} \right) c_{2\sigma}^\dagger c_{1-\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \frac{1}{2} U \sum_{i\sigma'} n_{i\sigma'} n_{i-\sigma'} c_{2\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle - t c_{2\sigma}^\dagger c_{2\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t \left( \left| \varepsilon_3^{(2)} \right\rangle + \left| \varepsilon_4^{(2)} \right\rangle \right) \]

\[ H \left| \varepsilon_3^{(2)} \right\rangle = t \sum_{\sigma'} \left( c_{1\sigma'}^\dagger c_{2\sigma'} + c_{2\sigma'}^\dagger c_{1\sigma'} \right) c_{1\sigma}^\dagger c_{1-\sigma}^\dagger \left| 0 \right\rangle + \]

\[ + \frac{1}{2} U \sum_{\sigma'} n_{1\sigma'} n_{1-\sigma'} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t \sum_{\sigma'} c_{1\sigma}^\dagger c_{2\sigma} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle + U n_{1\sigma'} n_{1-\sigma'} c_{1\sigma}^\dagger c_{1\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t c_{1\sigma}^\dagger c_{1-\sigma}^\dagger - t c_{2\sigma}^\dagger c_{2-\sigma}^\dagger \left| 0 \right\rangle + U c_{1\sigma}^\dagger c_{1-\sigma}^\dagger \left| 0 \right\rangle \]

\[ = t \left( \left| \varepsilon_1^{(2)} \right\rangle + \left| \varepsilon_2^{(2)} \right\rangle \right) + U \left| \varepsilon_3^{(2)} \right\rangle \]
\[ H \left| \varepsilon_i^{(2)} \right\rangle = t \sum_{\sigma'} \left( c_{1\sigma}^\dagger c_{2\sigma'} + c_{2\sigma}^\dagger c_{1\sigma'} \right) e_{2\sigma}^\dagger e_{2-\sigma} \left| 0 \right\rangle + \]
\[ + \frac{1}{2} U \sum_{i\sigma'} n_{i\sigma} n_{i-\sigma} c_{1\sigma}^\dagger c_{2\sigma}^\dagger \left| 0 \right\rangle \]
\[ = t \left( c_{2\sigma}^\dagger c_{2-\sigma} \left| 0 \right\rangle - c_{1-\sigma}^\dagger c_{2\sigma} \left| 0 \right\rangle \right) + \]
\[ + U n_{2\sigma} n_{2-\sigma} c_{2\sigma}^\dagger c_{2-\sigma} \left| 0 \right\rangle \]
\[ = t \left( c_{2\sigma}^\dagger c_{2-\sigma} \left| 0 \right\rangle + c_{2-\sigma}^\dagger c_{1\sigma} \left| 0 \right\rangle \right) + U c_{2\sigma}^\dagger c_{2-\sigma} \left| 0 \right\rangle \]
\[ = t \left( \left| \varepsilon_1^{(2)} \right\rangle + \left| \varepsilon_2^{(2)} \right\rangle \right) + U \left| \varepsilon_4^{(2)} \right\rangle \]

So that we get from the matrix elements

\[ \left( \left| \varepsilon_i^{(2)} \right\rangle \left| H \right| \varepsilon_j^{(2)} \right\rangle \right); \quad i, j = 1 \ldots 4 \]

the Hamiltonian matrix:

\[ H^{(2)} = \begin{pmatrix} 0 & 0 & t & t \\ t & 0 & t & t \\ t & t & U - E & 0 \\ t & t & 0 & U - E \end{pmatrix} \]

3. The eigenvalues are determined from the secular determinant:

\[ \det \left( H^{(2)} - E \mathbb{I} \right) \]^0 = 0 \]

\[ \det \begin{pmatrix} -E & 0 & t & t \\ 0 & -E & t & t \\ t & t & U - E & 0 \\ t & t & 0 & U - E \end{pmatrix} \]
\[ = -E \det \begin{pmatrix} -E & t & t \\ t & U - E & 0 \\ t & 0 & U - E \end{pmatrix} + \]
\[ + t \det \begin{pmatrix} 0 & -E & t \\ t & t & 0 \\ t & t & U - E \end{pmatrix} - t \det \begin{pmatrix} 0 & -E & t \\ t & t & U - E \\ t & t & 0 \end{pmatrix} \]
\[ = (-E) \left( (-E)(U - E)^2 - 2t^2(U - E) \right) + \]
\[ + t(t^3 - t^3 + E(U - E)t) - t(-E(U - E)t + t^3 - t^3) \]
\[ = E(U - E)(E(U - E) + 4t^2) \]
It must therefore hold

\[ 0 = E(U - E)(E(U - E) + 4t^2) \]

Eigenvalues

\[
\begin{align*}
E_1^{(2)} &= E_- \\
E_2^{(2)} &= 0 \\
E_3^{(2)} &= U \\
E_4^{(2)} &= E_+ 
\end{align*}
\]

with

\[
E_{\pm} = \frac{1}{2} U \pm \sqrt{\frac{1}{4} U^2 + 4t^2}
\]

Eigenstates:
\[ E_1^{(2)} = E_- \]

\[
\begin{pmatrix}
-E_- & 0 & t & t \\
0 & -E_- & t & t \\
t & t & U - E_- & 0 \\
t & t & 0 & U - E_- \\
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
\end{pmatrix} = 0
\]

\[
\begin{align*}
-E_- x_1 + t(x_3 + x_4) &= 0 \\
-E_- x_2 + t(x_3 + x_4) &= 0 \\
t(x_1 + x_2) + (U - E_-)x_3 &= 0 \\
t(x_1 + x_2) + (U - E_-)x_4 &= 0
\end{align*}
\]

\[
\begin{align*}
\Leftrightarrow \quad x_1 &= x_2; \quad x_3 = x_4; \quad x_3 = \frac{E_-}{2t} x_2 ;
\end{align*}
\]

We define (8.168)

\[
\gamma_{\pm} = \frac{E_{\pm}}{2t}
\]

Normalization:
\[\begin{align*}
x_1^2 + x_2^2 + x_3^2 + x_4^2 &= 1 \\
2x_1^2 + 2x_3^2 &= 1 \\
2x_1^2 + 2\gamma^2 x^2 &= 1 \\
x_1^2 &= \frac{1}{2(1 + \gamma^2)}
\end{align*}\]

\[x_1 = \frac{1}{\sqrt{2(1 + \gamma^2)}} = x_2 \]

\[x_3 = \frac{\gamma^-}{\sqrt{2(1 + \gamma^2)}} = x_4 \]

\[\begin{align*}
\sim & \quad |E_1^{(2)}\rangle = \frac{1}{\sqrt{2(1 + \gamma^2)}} \left( |\varepsilon_1^{(2)}\rangle + |\varepsilon_2^{(2)}\rangle \right) \\
& \quad + \gamma^- \left( |\varepsilon_3^{(2)}\rangle + |\varepsilon_4^{(2)}\rangle \right) \right) ; \quad (8.164)
\end{align*}\]

\[E_2^{(2)} = 0 \]

\[\begin{pmatrix}
0 & 0 & t & t \\
0 & 0 & t & t \\
t & t & 0 & U \\
t & t & 0 & U
\end{pmatrix} \begin{pmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4
\end{pmatrix} \stackrel{\sim}{=} 0 \]

\[t(y_3 + y_4) = 0 \]

\[t(y_3 + y_4) = 0 \]

\[t(y_1 + y_2) + U y_3 = 0 \]

\[t(y_1 + y_2) + U y_4 = 0 \]

\[y_3 = -y_4; \quad y_3 = +y_4; \quad y_3 = y_4 = 0; \quad y_1 = -y_2;\]

Normalization:

\[y_1 = \frac{1}{\sqrt{2}} = -y_2 \]

\[\begin{align*}
\sim & \quad |E_2^{(2)}\rangle = \frac{1}{\sqrt{2}} \left( |\varepsilon_1^{(2)}\rangle - |\varepsilon_2^{(2)}\rangle \right) ; \quad (8.165)
\end{align*}\]

\[E_3^{(2)} = U \]
\[
\begin{pmatrix}
-U & 0 & t & t \\
0 & -U & t & t \\
t & t & 0 & 0 \\
t & t & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
z_1 \\
z_2 \\
z_3 \\
z_4 \\
\end{pmatrix}
\overset{!}{=} 0
\]
\[
\begin{align*}
-Uz_1 + t(z_3 + z_4) &= 0 \\
-Uz_2 + t(z_3 + z_4) &= 0 \\
t(z_1 + z_2) &= 0 \\
t(z_1 + z_2) &= 0
\end{align*}
\]
\[
\begin{align*}
z_1 &= z_2; & z_1 &= -z_2; & z_1 &= z_2 = 0; & z_3 &= -z_4;
\end{align*}
\]
Normalization:
\[
z_3 = \frac{1}{\sqrt{2}} = -z_4
\]
\[
\begin{align*}
\begin{pmatrix}
E_3^{(2)} \end{pmatrix} &= \frac{1}{\sqrt{2}} \left( |\varepsilon_3^{(2)} \rangle - |\varepsilon_4^{(2)} \rangle \right); & \quad \text{(8.166)}
\end{align*}
\]
\[
E_4^{(2)} = E_+ 
\]
\[
\begin{pmatrix}
-E_+ & 0 & t & t \\
0 & -E_+ & t & t \\
t & t & U - E_+ & 0 \\
t & t & 0 & U - E_+ \\
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2 \\
w_3 \\
w_4 \\
\end{pmatrix}
\overset{!}{=} 0
\]
Formally as for \(E_1^{(2)} = E_-\), only \(\gamma_-\) is replaced by \(\gamma_+\):
\[
\begin{align*}
\begin{pmatrix}
E_4^{(2)} \end{pmatrix} &= \frac{1}{\sqrt{2(1 + \gamma_+^2)}} \left( |\varepsilon_1^{(2)} \rangle + |\varepsilon_2^{(2)} \rangle + \\
&\quad + \gamma_+ \left( |\varepsilon_3^{(2)} \rangle + |\varepsilon_4^{(2)} \rangle \right) \right); & \quad \text{(8.167)}
\end{align*}
\]
4.
(i)
\[
\begin{align*}
\langle E_1^{(2)} | c_{1\sigma}^\dagger | E_1^{(1)} \rangle &= \frac{1}{\sqrt{2}} \langle E_1^{(2)} | c_{1\sigma}^\dagger (c_{1-\sigma}^\dagger - c_{2-\sigma}^\dagger) | 0 \rangle \\
&= \frac{1}{\sqrt{2}} \langle E_1^{(2)} | \xi_3^{(2)} \rangle - \frac{1}{\sqrt{2}} \langle E_1^{(2)} | \xi_1^{(2)} \rangle \\
&= \frac{1}{\sqrt{2}} \gamma_- - 1 \frac{1}{\sqrt{2}} \\
&= \frac{1}{2} \frac{\gamma_- - 1}{\sqrt{1 + \gamma_-^2}} ;
\end{align*}
\]

\[
E_1^{(2)} - E_1^{(1)} = E_- + t
\]

(ii)

\[
\begin{align*}
\langle E_2^{(2)} | c_{1\sigma}^\dagger | E_1^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_2^{(2)} | \xi_3^{(2)} \rangle - \langle E_2^{(2)} | \xi_1^{(2)} \rangle \right) \\
&= \frac{1}{2} ;
\end{align*}
\]

\[
E_2^{(2)} - E_1^{(1)} = +t
\]

(iii)

\[
\begin{align*}
\langle E_3^{(2)} | c_{1\sigma}^\dagger | E_1^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_3^{(2)} | \xi_3^{(2)} \rangle - \langle E_3^{(2)} | \xi_1^{(2)} \rangle \right) \\
&= \frac{1}{2} ;
\end{align*}
\]

\[
E_3^{(2)} - E_1^{(1)} = U + t
\]

(iv)

\[
\begin{align*}
\langle E_4^{(2)} | c_{1\sigma}^\dagger | E_1^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_4^{(2)} | \xi_3^{(2)} \rangle - \langle E_4^{(2)} | \xi_1^{(2)} \rangle \right) \\
&= \frac{1}{2} \frac{1}{\sqrt{1 + \gamma_+^2}} (\gamma_+ - 1) ;
\end{align*}
\]

\[
E_4^{(2)} - E_1^{(1)} = E_+ + t
\]

(v)
\[
\begin{align*}
\langle E_1^{(2)} | c^\dagger_1 | E_2^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_1^{(2)} | \varepsilon_3^{(2)} \rangle + \langle E_1^{(2)} | \varepsilon_1^{(2)} \rangle \right) \\
&= \frac{1}{2} \frac{1}{\sqrt{1 + \gamma_-^2}} (1 + \gamma_-) \\
E_1^{(2)} - E_1^{(1)} &= E_- + t \\

(vi) \\

\langle E_2^{(2)} | c^\dagger_1 | E_2^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_2^{(2)} | \varepsilon_3^{(2)} \rangle + \langle E_2^{(2)} | \varepsilon_1^{(2)} \rangle \right) \\
&= \frac{1}{2} \\
E_2^{(2)} - E_2^{(1)} &= -t \\

(vii) \\

\langle E_3^{(2)} | c^\dagger_1 | E_2^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_3^{(2)} | \varepsilon_3^{(2)} \rangle + \langle E_3^{(2)} | \varepsilon_1^{(2)} \rangle \right) \\
&= \frac{1}{2} \\
E_3^{(2)} - E_2^{(1)} &= U - t \\

(viii) \\

\langle E_4^{(2)} | c^\dagger_1 | E_2^{(1)} \rangle &= \frac{1}{\sqrt{2}} \left( \langle E_4^{(2)} | \varepsilon_3^{(2)} \rangle + \langle E_4^{(2)} | \varepsilon_1^{(2)} \rangle \right) \\
&= \frac{1}{2} \frac{1}{\sqrt{1 + \gamma_+^2}} (\gamma_+ + 1) \\
E_4^{(2)} - E_2^{(1)} &= E_+ - t
\end{align*}
\]

For the partition function of the one-particle system holds

\[
Z = e^{+\beta t} + e^{-\beta t};
\]

and therefore

\[
\begin{align*}
\frac{e^{-\beta E_1^{(1)}}}{Z} &= \frac{e^{\beta t}}{e^{\beta t} + e^{-\beta t}} = \frac{1}{1 + e^{-2\beta t}} \\
\frac{e^{-\beta E_2^{(1)}}}{Z} &= \frac{e^{\beta t}}{e^{\beta t} + e^{-\beta t}} = \frac{e^{-2\beta t}}{1 + e^{-2\beta t}}
\end{align*}
\]
Then with (8.147) the density of states is given by

\[
\rho_\sigma^{(-\sigma)}(E) = \rho_{\sigma\sigma}^{(-\sigma)}(E) + \rho_{\sigma\sigma}^{(-\sigma)}(E)
\]

\[
\rho_{\sigma\sigma}(E) = \frac{1}{4(1 + e^{-2\beta t})} *
\]

\[
\left\{ \frac{(1 - \gamma_\sigma)}{1 + \gamma_\sigma^2} \delta(E - (E_\sigma + t)) + \delta(E - t) + \frac{(1 + \gamma_\sigma)}{1 + \gamma_\sigma^2} e^{-2\beta t} \delta(E - (E_\sigma + t)) + e^{-2\beta t} \delta(E + t) \right\}
\]

\[
\rho_{\sigma\sigma}(E) = \frac{1}{4(1 + e^{-2\beta t})} *
\]

\[
\left\{ \frac{(1 - \gamma_\sigma)}{1 + \gamma_\sigma^2} \delta(E - (E_\sigma + t)) + \delta(E - (U + t)) + \frac{(1 + \gamma_\sigma)}{1 + \gamma_\sigma^2} e^{-2\beta t} \delta(E - (E_\sigma + t)) + e^{-2\beta t} \delta(E - (U - t)) \right\}
\]

**Problem 8.11**

1. We demonstrate the correctness of the eigenstates by substituting of \( |E^{(3)}_{1,2}\rangle \) in the corresponding eigenvalue equation:

\[
H_0 |E^{(3)}_{1,2}\rangle = \frac{1}{\sqrt{2}} \sum_{\sigma'} t \left( c_{1\sigma'}^\dagger c_{2\sigma} + c_{2\sigma'}^\dagger c_{1\sigma} \right) * \left( c_{1\sigma} - c_{2\sigma} \right) |0\rangle
\]

\[
= \frac{t}{\sqrt{2}} \left( c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right) * \left( c_{1\sigma} - c_{2\sigma} \right) |0\rangle
\]

\[
= \frac{t}{\sqrt{2}} \left( -c_{1\sigma}^\dagger (1 - c_{2\sigma}^\dagger c_{2\sigma}) + c_{2\sigma}^\dagger (1 - c_{1\sigma}^\dagger c_{1\sigma}) \right) |0\rangle
\]

\[
= \frac{t}{\sqrt{2}} \left( -c_{2\sigma}^\dagger (1 - c_{1\sigma}^\dagger c_{1\sigma}) + c_{1\sigma}^\dagger (1 - c_{2\sigma}^\dagger c_{2\sigma}) \right) |0\rangle
\]

\[
= \mp t |E^{(3)}_{1,2}\rangle
\]
\[ H_1 \left| E_{1,2}^{(3)} \right\rangle = \frac{1}{\sqrt{2}} \cdot \frac{1}{2} U \sum_{\sigma'} (n_{1\sigma'} n_{1-\sigma'} + n_{2\sigma'} n_{2-\sigma'}) \star \left( c_{1-\sigma}^\dagger \mp c_{2-\sigma}^\dagger \right) c_{1\sigma}^\dagger c_{2\sigma}^\dagger |0\rangle \]

\[ = \frac{U}{\sqrt{2}} \left( n_{1\sigma} n_{1-\sigma} \mp n_{2\sigma} n_{2-\sigma} \right) \star \left( c_{1-\sigma}^\dagger \mp c_{2-\sigma}^\dagger \right) c_{1\sigma}^\dagger c_{2\sigma}^\dagger |0\rangle \]

\[ = \frac{U}{\sqrt{2}} \left( n_{1\sigma} c_{1-\sigma}^\dagger \mp n_{2\sigma} c_{2-\sigma}^\dagger \right) c_{1\sigma}^\dagger c_{2\sigma}^\dagger |0\rangle \]

\[ = \frac{U}{\sqrt{2}} \left( -c_{1\sigma} c_{1-\sigma}^\dagger \right) c_{2\sigma}^\dagger c_{1\sigma}^\dagger |0\rangle \]

\[ = \frac{U}{\sqrt{2}} \left( c_{1-\sigma} \mp c_{2-\sigma}^\dagger \right) c_{1\sigma}^\dagger c_{2\sigma}^\dagger |0\rangle \]

\[ = U \left| E_{1,2}^{(3)} \right\rangle \]

Therefore they are indeed eigenstates with eigenenergies:

\[ E_1^{(3)} = U - t; \quad E_2^{(3)} = U + t \]

2. Density of states

\[ \rho_{\sigma,-\sigma}(E) = \sum_n \left| \left( E_n^{(3)} \right| c_{1\sigma}^\dagger \left| E_1^{(2)} \right\rangle \right|^2 \delta(E - (E_n^{(3)} - E_-)) + \]

\[ + \sum_m \left| \left( E_m^{(1)} \right| c_{1\sigma}^\dagger \left| E_1^{(2)} \right\rangle \right|^2 \delta(E - (E_- - E_m^{(1)})) \]

At \( T = 0 \), for the averaging in \( \rho_{\sigma,-\sigma}(E) \), the ground state \( \left| E_{1}^{(2)} \right\rangle \) of the two-electron system can be used (see Problem 8.10, Eq. (8.164)) with the ground state energy \( E_1^{(2)} = E_- \) (8.163).

Matrix elements:
\[ \left< E_{1,2}^{(3)} \left| c_{1\sigma}^\dagger \right| E_{1}^{(2)} \right> \]
\[ = \frac{1}{\sqrt{2(1 + \gamma^2)}} \left< E_{1,2}^{(3)} \left| c_{1\sigma}^\dagger \left( c_{1\sigma}^\dagger c_{2\sigma}^\dagger + c_{2\sigma}^\dagger c_{1\sigma}^\dagger \right) + \gamma \sum_{i=1}^{2} c_{i\sigma}^\dagger c_{i\sigma}^\dagger \right| 0 \right> \]
\[ = \frac{1}{\sqrt{2(1 + \gamma^2)}} \left< E_{1,2}^{(3)} \left( c_{1\sigma}^\dagger c_{2\sigma}^\dagger c_{1\sigma}^\dagger + \gamma c_{2\sigma}^\dagger c_{1\sigma}^\dagger c_{2\sigma}^\dagger \right) \right| 0 \right> \]
\[ \mp \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \gamma \left< 0 \left| c_{2\sigma} c_{1\sigma} c_{2\sigma}^\dagger c_{1\sigma}^\dagger \right| 0 \right> \]
\[ = \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \left< 0 \right| 0 \right> \mp \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \gamma \left< 0 \right| 0 \right> \]
\[ = \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \gamma \]

With (8.160) and (8.161) we calculate

\[ \left< E_{1,2}^{(1)} \left| c_{1\sigma} \right| E_{1}^{(2)} \right> = \frac{1}{\sqrt{2}} \left< 0 \left| (c_{1\sigma}^\dagger c_{2\sigma}) c_{1\sigma} \right| E_{1}^{(2)} \right> \]
\[ = \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \left< 0 \left| c_{1\sigma} c_{1\sigma} \gamma c_{1\sigma}^\dagger c_{1\sigma}^\dagger \right| 0 \right> \]
\[ \mp \left< 0 \left| c_{2\sigma} c_{1\sigma} c_{2\sigma}^\dagger c_{1\sigma}^\dagger \right| 0 \right> \]
\[ = \frac{1}{2} \frac{1}{\sqrt{1 + \gamma^2}} \gamma \]

Density of states:
\[ \rho^{(\sigma, -\sigma)}_\sigma(E) = \frac{(1 - \gamma_-)^2}{4(1 + \gamma_-^2)} \{ \delta(E - (U - t - E_-)) + \delta(E - (E_- + t)) \} + \frac{(1 + \gamma_-)^2}{4(1 + \gamma_-^2)} \{ \delta(E - (U + t - E_-)) + \delta(E - (E_- - t)) \} \]

**Problem 8.12**

The expression

\[ \frac{1}{N} \sum_{i \neq j} T_{ij} \left( c_{i-\sigma}^\dagger c_{j-\sigma}^\dagger (2n_{i\sigma} - 1) \right) \]

should be expressed in terms of the one-electron spectral density!

(a) Spectral theorem:

\[ \frac{1}{N} \sum_{i \neq j} T_{ij} \left( c_{i-\sigma}^\dagger c_{j-\sigma}^\dagger \right) = \frac{1}{N} \sum_{i, j} T_{ij} \left( c_{i-\sigma}^\dagger c_{j-\sigma}^\dagger \right) - T_0 \left( c_{i-\sigma}^\dagger c_{i-\sigma} \right) \]

\[ = \frac{1}{N} \sum_{i, j} T_{ij} \int_{-\infty}^{+\infty} dE \left( -\frac{1}{\pi \hbar} \text{Im} G_{ji-\sigma}(E - \mu) \right) f_-(E) - \]

\[ - T_0 \int_{-\infty}^{+\infty} dE \left( -\frac{1}{\pi \hbar} \text{Im} G_{ii-\sigma}(E - \mu) \right) f_-(E) \]

\[ = \frac{1}{N} \sum_{i, j} \frac{1}{N} \sum_{k_1} e^{i k_1 \cdot (R_i - R_j)} \epsilon(k_1) \int_{-\infty}^{+\infty} dE \ f_-(E) \cdot \]

\[ \cdot \frac{1}{N} \sum_{k_2} e^{i k_2 \cdot (R_j - R_i)} \left( -\frac{1}{\pi \hbar} \text{Im} G_{k_2-\sigma}(E - \mu) \right) - \]
\[- T_0 \int_{-\infty}^{+\infty} dE \ f_-(E) \frac{1}{N} \sum_k \left( - \frac{1}{\pi \hbar} \right) \text{Im} G_{k-\sigma}(E - \mu)\]

\[= \frac{1}{N \hbar} \sum_{k_1, k_2}^{+\infty} \int dE \ f_-(E) \delta_{k_1, k_2} \delta_{k_1, k_2} \epsilon(k_1) S_{k_2-\sigma}(E - \mu) - \]

\[- T_0 \frac{1}{N \hbar} \sum_k^{+\infty} \int dE \ f_-(E) S_{k-\sigma}(E - \mu)\]

\[= \frac{1}{N \hbar} \sum_k (\epsilon(k) - T_0) \int_{-\infty}^{+\infty} dE \ f_-(E) S_{k-\sigma}(E - \mu)\]

(b) Real expectation value:

\[\langle c_{i-\sigma}^\dagger c_{j-\sigma} n_{i\sigma} \rangle = \langle n_{i\sigma} c_{j-\sigma}^\dagger c_{i-\sigma} \rangle = \langle c_{j-\sigma}^\dagger n_{i\sigma} c_{i-\sigma} \rangle\]

\[\Leftrightarrow \frac{1}{N} \sum_{i \neq j} T_{ij} \langle c_{i-\sigma}^\dagger c_{j-\sigma} n_{i\sigma} \rangle\]

\[= \frac{1}{N} \sum_{i, j} T_{ij} \langle c_{j-\sigma}^\dagger n_{i\sigma} c_{i-\sigma} \rangle - T_0 \langle c_{j-\sigma}^\dagger n_{i\sigma} c_{i-\sigma} \rangle\]

\[= \frac{1}{N} \sum_{i, j} T_{ij} \left( - \frac{1}{\pi \hbar} \right) \int_{-\infty}^{+\infty} dE \ f_-(E) \text{Im} \Gamma_{iii;j-\sigma}(E - \mu) - \]

\[- T_0 \int_{-\infty}^{+\infty} dE \ f_-(E) \left( - \frac{1}{\pi \hbar} \right) \text{Im} \Gamma_{iii;j-\sigma}(E - \mu)\]

The “higher” Green’s function is defined in (8.124). From (8.125) one reads off

\[\text{Im} \Gamma_{iii;j-\sigma}(E - \mu) = \frac{1}{U} \sum_m (E \delta_{im} - T_{im}) \text{Im} G_{m-\sigma}(E - \mu)\]

Therewith follows:
\[
\frac{1}{N} \sum_{i,j} T_{ij} < c_{i-\sigma}^\dagger c_{j-\sigma} n_{i\sigma} >
\]
\[
= \frac{1}{N} \sum_{i,j} (T_{ij} - T_0 \delta_{ij}) \int_{-\infty}^{+\infty} dE f_-(E) * \frac{1}{U} \sum_k_r (E \delta_{mi} - T_{im}) S_{m-j-\sigma}(E - \mu)
\]
\[
= \frac{1}{N} \sum_{i,j} \frac{1}{N^3} \sum_{k_1,k_2,k_3} e^{i{k_1}(R_i-R_j)}(\epsilon(k_1) - T_0) * \int_{-\infty}^{+\infty} dE f_-(E) \frac{1}{U} \sum_m e^{i{k_2}(R_i-R_m)} e^{i{k_3}(R_m-R_j)} * (E - \epsilon(k_2)) S_{k_2-\sigma}(E - \mu)
\]
\[
= \frac{1}{Nh} \sum_k (\epsilon(k) - T_0) \int_{-\infty}^{+\infty} dE f_-(E) \frac{1}{U} (E - \epsilon(k_2)) * S_{k_2-\sigma}(E - \mu) \delta_{k_1,-k_2} \delta_{k_2,-k_3} \delta_{k_3,-k_1} + \infty
\]
\[
= \frac{1}{Nh} \sum_k (\epsilon(k) - T_0) \int_{-\infty}^{+\infty} dE f_-(E) \frac{1}{U} (E - \epsilon(k)) * S_{k-\sigma}(E - \mu) + \infty
\]

Together with the result of (a) we have found

\[
n_{-\sigma} (1 - n_{-\sigma}) B_{-\sigma}
\]
\[
= \frac{1}{N} \sum_{i,j} T_{ij} \left< c_{i-\sigma}^\dagger c_{j-\sigma} (2n_{i\sigma} - 1) \right>
\]
\[
= \frac{1}{Nh} \sum_k (\epsilon(k) - T_0) \int_{-\infty}^{+\infty} dE f_-(E) \left( \frac{2}{U} (E - \epsilon(k)) - 1 \right) * S_{k-\sigma}(E - \mu) + \infty
\]

This is exactly (8.217)

**Problem 8.13**

0th spectral moment:

\[
M_{ij\sigma}^{(0)} = \left< [c_{i\sigma}, c_{j\sigma}^\dagger]_+ \right> = \delta_{ij} \iff M_{k\sigma}^{(0)} = 1
\]
1st spectral moment:

\[
M^{(1)}_{ij\sigma} = \left\langle \left[ [c_{i\sigma}, H]_-, c^\dagger_{j\sigma} \right]_+ \right\rangle
\]

\[
[c_{i\sigma}, H]_- = \sum_{m,n,\sigma'} (T_{mn} - \mu \delta_{mn}) \left[ c_{i\sigma}, c^\dagger_{m\sigma'} c_{n\sigma'} \right]_- + \\
\frac{1}{2} U \sum_{m,\sigma'} \left[ c_{i\sigma}, n_{m\sigma} n_{m-\sigma'} \right]_- + \\
= \sum_{m,n,\sigma'} (T_{mn} - \mu \delta_{mn}) \delta_{im} \delta_{\sigma\sigma'} c_{n\sigma'} + \\
\frac{1}{2} U \sum_{m,\sigma'} \delta_{im} (\delta_{\sigma\sigma'} c_{m\sigma} n_{m-\sigma'} + \delta_{\sigma-\sigma'} n_{m\sigma} c_{m-\sigma'}) \\
= \sum_n (T_{in} - \mu \delta_{in}) c_{n\sigma} + Un_{i-\sigma} c_{i\sigma}
\]

(c) \( \Rightarrow \left\langle \left[ [c_{i\sigma}, H]_-, c^\dagger_{j\sigma} \right]_+ \right\rangle = (T_{ij} - \mu \delta_{ij}) + Ud_{ij} n_{i-\sigma} \) (d) \( \Rightarrow M^{(1)}_{ij\sigma} = (T_{ij} - \mu \delta_{ij}) + Un_{-\sigma} \delta_{ij} \) (e) \( \Rightarrow M^{(1)}_{k\sigma} = \varepsilon_{(k)} - \mu + Un_{-\sigma} \)

2nd spectral moment:

\[
M_{ij\sigma}^{(2)} = \left\langle \left[ \left[ [c_{i\sigma}, H]_-, H \right]_-, c^\dagger_{j\sigma} \right]_+ \right\rangle 
\]

abbreviation: \( t_{ij} = T_{ij} - \mu \delta_{ij} \)

Then with (b) holds

\[
\left[ [c_{i\sigma}, H]_-, H \right]_- = \sum_n t_{in} [c_{n\sigma}, H]_- + U [n_{i-\sigma} c_{i\sigma}, H]_-
\]
\[
\left[ n_{i-\sigma} c_{i\sigma}, H \right]_-
\]
\[
= \sum_{m,n,\sigma'} t_{mn} \left[ n_{i-\sigma} c_{i\sigma}, c_m^{\dagger} c_{n\sigma'} \right]_+ + \frac{1}{2} U \sum_{m,\sigma'} \left[ n_{i-\sigma} c_{i\sigma}, n_{m\sigma} n_{m-\sigma'} \right]_-
\]
\[
= \sum_{m,n,\sigma'} t_{mn} (\delta_{im} \delta_{\sigma\sigma'} n_{i-\sigma} c_{m\sigma'} + \delta_{im} \delta_{\sigma-\sigma'} c_{i-\sigma}^{\dagger} c_{n\sigma'} c_{i\sigma} - \delta_{in} \delta_{\sigma-\sigma'} c_{i-\sigma}^{\dagger} c_{m\sigma'} c_{i\sigma}) + \frac{1}{2} U \sum_{m\sigma'} (\delta_{im} \delta_{\sigma\sigma'} n_{i-\sigma} c_{m\sigma'} n_{m-\sigma'} + \delta_{im} \delta_{\sigma-\sigma'} n_{i-\sigma} n_{m\sigma'} c_{m-\sigma'})
\]
\[
= \sum_n t_{in} n_{i-\sigma} c_{n\sigma} + \sum_n t_{in} c_{i-\sigma}^{\dagger} c_{n-\sigma} c_{i\sigma} - \sum_m t_{mj} c_{m-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma} + \frac{1}{2} U (n_{i-\sigma} c_{i\sigma} n_{i-\sigma} + n_{i-\sigma} n_{i-\sigma} c_{i\sigma})
\]
\[
= \sum_m t_{im} (n_{i-\sigma} c_{m\sigma} + c_{i-\sigma}^{\dagger} c_{m-\sigma} c_{i\sigma} - c_{m-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}) + U n_{i-\sigma} c_{i\sigma} \quad (g)
\]

Here we have used \( n_{i-\sigma}^2 = n_{i-\sigma} \) which is an identity valid for Fermions. Then what remains is

\[
\left[ [c_{\sigma}, H]_-, H \right]_-
\]
\[
= \sum_n t_{in} [c_{n\sigma}, H]_+ + U \sum_m t_{im} (n_{i-\sigma} c_{m\sigma} + c_{i-\sigma}^{\dagger} c_{m-\sigma} c_{i\sigma} - c_{m-\sigma}^{\dagger} c_{i-\sigma} c_{i\sigma}) + U^2 n_{i-\sigma} c_{i\sigma} \quad (h)
\]

With this follows:

\[
M_{ij\sigma}^{(2)} = \sum_n t_{in} M_{nj\sigma}^{(1)} + U t_{ij} n_{-\sigma} + \delta_{ij} U \sum_m t_{im} \left( c_{i-\sigma}^{\dagger} c_{m-\sigma} \right) - \delta_{ij} U \sum_m t_{im} \left( c_{m-\sigma}^{\dagger} c_{i-\sigma} \right) + U^2 \delta_{ij} n_{-\sigma}
\]
Because of (8.268), the third and the fourth terms cancel each other. Then it remains with (d):

\[
M^{(2)}_{ij\sigma} = \sum_n t_{in} t_{nj} + 2U t_{ij} n_{-\sigma} + U^2 n_{-\sigma} \delta_{ij} \tag{i}
\]

After Fourier transformation follows:

\[
M^{(2)}_{k\sigma} = (\varepsilon(k) - \mu)^2 + 2(\varepsilon(k) - \mu)U n_{-\sigma} + U^2 n_{-\sigma}
\]

3rd spectral moment:

\[
M^{(3)}_{ij\sigma} = \left\langle \left[ \left[ [c_{i\sigma}, H]_-, H \right]_-, H \right]_-, c_{j\sigma}^\dagger \right\rangle
\]

For the triple commutator holds with (h):

\[
\begin{align*}
&\left[ \left[ [c_{i\sigma}, H]_-, H \right]_-, H \right]_-
= \sum_n t_{in} \left[ [c_{n\sigma}, H]_-, H \right]_-
+ U \sum_m t_{im} \left( n_{i-\sigma} c_{m\sigma} + c_{i-\sigma}^\dagger c_{m-\sigma} c_{i\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma} \right) H \right]_-
+ U^2 \left[ n_{i-\sigma} c_{i\sigma}, H \right]_- \\
&= \sum_n t_{in} \left[ [c_{n\sigma}, H]_-, H \right]_- + U \left[ [c_{i\sigma}, H]_-, H \right]_- - U \sum_n t_{in} 
\left[ c_{n\sigma}, H \right]_- + U \sum_m t_{im} \left\{ n_{i-\sigma} c_{m\sigma}, H \right\}_- \\
&\quad + \left[ c_{i-\sigma}^\dagger c_{m-\sigma} c_{i\sigma}, H \right]_- - \left[ c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}, H \right]_-
\end{align*}
\tag{j}
\]

Three commutators remain to be calculated:
\[ (I) = U \sum_m t_{im} \left[ n_{i-\sigma} c_{m\sigma}, H \right]_+ \]
\[ = U \sum_m t_{im} \sum_{s, t, \sigma'} t_{st} \left[ n_{i-\sigma} c_{m\sigma}, c_{s\sigma'}^\dagger c_{t\sigma}^\dagger \right]_+ + \]
\[ + \frac{1}{2} U^2 \sum_m t_{im} \sum_{s, \sigma'} \left[ n_{i-\sigma} c_{m\sigma}, n_{s\sigma'} n_{s-\sigma'} \right]_+ \]
\[ = U \sum_{m, s, t, \sigma'} t_{im} t_{st} \left\{ \delta_{m\sigma} \delta_{s\sigma'} n_{i-\sigma} c_{t\sigma}^\dagger + \right. \]
\[ + \left. \delta_{s\sigma} c_{i-\sigma}^\dagger c_{t\sigma}^\dagger c_{m\sigma} - \delta_{t\sigma} c_{i-\sigma}^\dagger c_{s\sigma'} c_{i-\sigma} c_{m\sigma} \right\} + \]
\[ + \frac{1}{2} U^2 \sum_{m, s, \sigma'} t_{im} \left[ \delta_{ms} \delta_{s\sigma'} n_{i-\sigma} c_{s\sigma'} n_{s-\sigma'} + \right. \]
\[ + \left. \delta_{m\sigma} \delta_{s\sigma'} n_{i-\sigma} n_{s\sigma'} c_{s-\sigma'} \right] \]
\[ = U \sum_{m, t} t_{im} t_{mt} n_{i-\sigma} c_{t\sigma} + U \sum_{m, t} t_{im} t_{it} c_{i-\sigma}^\dagger c_{t\sigma} - \]
\[ - U \sum_{m, s} t_{im} t_{si} c_{s-\sigma}^\dagger c_{i-\sigma} c_{m\sigma} + \frac{1}{2} U^2 \sum_m t_{im} n_{i-\sigma} c_{m\sigma} n_{m-\sigma} + \]
\[ + \frac{1}{2} U^2 \sum_m t_{im} n_{i-\sigma} c_{m\sigma} n_{m-\sigma} \]
\[ = U \sum_{m, t} t_{im} t_{mt} n_{i-\sigma} c_{t\sigma} + U \sum_{m, t} t_{im} t_{it} \left( c_{i-\sigma}^\dagger c_{t-\sigma} c_{m\sigma} - \right. \]
\[ - c_{i-\sigma}^\dagger c_{i-\sigma} c_{m\sigma} \right) + U^2 \sum_m t_{im} n_{i-\sigma} n_{m-\sigma} c_{m\sigma} \]

\[ \overset{\sim}{\left[ (I), c_{j\sigma}^\dagger \right]} = U \sum_m t_{im} t_{mj} n_{i-\sigma} + \]
\[ + U \sum_t t_{it} t_{ij} \left( c_{i-\sigma}^\dagger c_{t-\sigma} - c_{i-\sigma}^\dagger c_{i-\sigma} \right) + \]
\[ + U^2 t_{ij} n_{i-\sigma} n_{j-\sigma} \]

We again use (8.268):

\[ \left[ \left[ (I), c_{j\sigma}^\dagger \right]_+ \right] = U n_{-\sigma} \sum_m t_{im} t_{mj} + U^2 t_{ij} \left\{ n_{i-\sigma} n_{j-\sigma} \right\} \quad (k) \]

In the same manner we calculate
\[ (II) = U \sum_{m} t_{im} \left[ c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}}, H \right]_{\sigma} + \]

\[ = U \sum_{m} t_{im} \sum_{s,t,\sigma'} t_{sl} \left[ c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}}, c_{s_{\sigma'}} c_{t_{\sigma'}} \right]_{\sigma} + \]

\[ + \frac{1}{2} U^{2} \sum_{m} t_{im} \sum_{s,\sigma'} \left[ c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}}, n_{s_{\sigma'}} n_{s_{-\sigma'}} \right]_{\sigma} + \]

\[ = U \sum_{m,s,t,\sigma'} t_{im} t_{sl} \left\{ \delta_{\sigma\sigma'} \delta_{l_{i}} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} + \right. \]

\[ + \delta_{\sigma_{-\sigma'}} \delta_{l_{i} m} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma'}} c_{i_{\sigma}} - \delta_{\sigma_{-\sigma'}} \delta_{l_{i} m} c_{m_{-\sigma}}^{\dagger} c_{m_{-\sigma'}} c_{i_{\sigma}} + \]

\[ + \frac{1}{2} U^{2} \sum_{m,s,\sigma'} t_{im} \left\{ \delta_{l_{i} \sigma_{-\sigma'}} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{\sigma_{-\sigma'}} + \right. \]

\[ + \delta_{l_{i} \sigma_{-\sigma'}} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} n_{s_{\sigma'}} c_{s_{-\sigma'}} + \]

\[ + \delta_{l_{i} s_{\sigma'}} c_{l_{-\sigma}}^{\dagger} c_{s_{\sigma}} c_{s_{-\sigma}} c_{i_{\sigma}} - \]

\[ = \sum_{m,s} t_{im} t_{is} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} + \sum_{m,s} t_{im} t_{mt} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} - \]

\[ - U \sum_{m,s} t_{im} t_{is} c_{s_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} + \]

\[ + \frac{1}{2} U^{2} \sum_{m} t_{im} \left\{ c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} n_{i_{-\sigma}} + c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} n_{i_{-\sigma}} c_{i_{\sigma}} + \right. \]

\[ + c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} n_{m_{\sigma}} c_{i_{\sigma}} + c_{l_{-\sigma}}^{\dagger} n_{m_{\sigma}} c_{m_{-\sigma}} c_{i_{\sigma}} - \]

\[ - c_{l_{-\sigma}}^{\dagger} n_{i_{\sigma}} c_{m_{-\sigma}} c_{i_{\sigma}} - n_{i_{\sigma}} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} c_{i_{\sigma}} \right\} \]

\[ \sim \left[ (II), c_{j_{\sigma}}^{\dagger} \right]_{+} = \sum_{m,s} t_{im} t_{ij} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} + \]

\[ + U \delta_{ij} \sum_{m,t} t_{im} (t_{mt} c_{l_{-\sigma}}^{\dagger} c_{i_{-\sigma}} - t_{ij} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}}) + \]

\[ + U^{2} \sum_{m} t_{im} \left\{ \delta_{ij} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} n_{i_{-\sigma}} + \right. \]

\[ + \delta_{ij} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} n_{m_{\sigma}} - \delta_{ij} c_{m_{-\sigma}} c_{m_{-\sigma}} c_{i_{\sigma}} + \]

\[ - \delta_{ij} c_{i_{-\sigma}} n_{i_{\sigma}} c_{m_{-\sigma}} - \delta_{ij} c_{i_{-\sigma}} c_{i_{-\sigma}} c_{m_{-\sigma}} c_{i_{\sigma}} \right\} \]

\[ = U t_{ij} \sum_{m} t_{im} c_{l_{-\sigma}}^{\dagger} c_{m_{-\sigma}} + \]
\[\begin{align*}
+ U \delta_{ij} \sum_{m,t} t_{im} (t_{mt} c_{i-\sigma}^\dagger c_{l-\sigma}^\dagger - t_{lt} c_{l-\sigma}^\dagger c_{m-\sigma}^\dagger) - \\
- U^2 t_{ij} c_{i-\sigma}^\dagger c_{j\sigma}^\dagger c_{i-\sigma} c_{j-\sigma} + \\
+ U^2 \delta_{ij} \sum_{m} t_{im} \left\{ c_{i-\sigma}^\dagger c_{m-\sigma} n_{i-\sigma} + c_{i-\sigma}^\dagger c_{m-\sigma} n_{m\sigma} \right\}
\end{align*}\]

\[(III) = -U \sum_{m} t_{im} \left[ c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}, H \right]_ - \\
= -U \sum_{m} t_{im} \sum_{s,t,\sigma,\sigma'} t_{st} \left[ c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}, c_{s\sigma'}^\dagger c_{i\sigma} \right] _- \\
- \frac{1}{2} U^2 \sum_{m} t_{im} \sum_{s,\sigma'} \left[ c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}, n_{s\sigma'} n_{s-\sigma} \right] _- \\
= -U \sum_{m} t_{im} \sum_{s,t,\sigma,\sigma'} t_{st} \left\{ \delta_{is} \delta_{\sigma\sigma'} c_{m-\sigma}^\dagger c_{i-\sigma} c_{t\sigma'} + \\
+ \delta_{is} \delta_{\sigma\sigma'} c_{m-\sigma}^\dagger c_{i-\sigma} c_{s\sigma}^\dagger c_{i\sigma} - \\
- \delta_{mt} \delta_{\sigma\sigma'} c_{s\sigma'}^\dagger c_{i-\sigma} c_{i\sigma} \right\} _- \\
- \frac{1}{2} U^2 \sum_{m,s,\sigma,\sigma'} t_{im} \left\{ \delta_{is} \delta_{\sigma\sigma'} c_{m-\sigma}^\dagger c_{i-\sigma} c_{s\sigma}^\dagger n_{s-\sigma'} + \\
+ \delta_{is} \delta_{\sigma\sigma'} c_{m-\sigma}^\dagger c_{i-\sigma} n_{s\sigma'} c_{s-\sigma'} + \\
+ \delta_{is} \delta_{\sigma\sigma'} c_{m-\sigma}^\dagger n_{s\sigma'} c_{s-\sigma'} c_{i\sigma} - \\
- \delta_{ms} \delta_{\sigma\sigma'} c_{s\sigma}^\dagger n_{s-\sigma'} c_{s-\sigma} c_{i\sigma} - \\
- \delta_{ms} \delta_{\sigma\sigma'} n_{s\sigma'} c_{s-\sigma}^\dagger c_{s-\sigma} c_{i\sigma} \right\} _- \\
= -U \sum_{m,t} t_{im} t_{lt} c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma} _- \\
- U \sum_{m,t} t_{im} t_{lt} c_{m-\sigma}^\dagger c_{t-\sigma} c_{i\sigma} _+ \\
+ U \sum_{m,s} t_{im} t_{sm} c_{s-\sigma}^\dagger c_{i-\sigma} c_{i\sigma} _- \\
- \frac{1}{2} U^2 \sum_{m} t_{im} \left\{ c_{m-\sigma}^\dagger c_{i-\sigma} c_{i\sigma} n_{i-\sigma} + \\
+ c_{m-\sigma}^\dagger c_{i-\sigma} n_{i-\sigma} c_{i\sigma} - \\
- c_{m-\sigma} n_{m\sigma} c_{i-\sigma} c_{i\sigma} - \right\} _- 
\]
\[-n_{m\sigma}c_m^{\dagger}c_{i\sigma}c_{i\sigma}\]

\[= -U \sum_{m,t} t_{\text{im}} t_{\text{ij}} (c_{m\sigma}^{\dagger}c_{i\sigma}c_{i\sigma} + c_{m\sigma}^{\dagger}c_{i\sigma}c_{i\sigma}) +
\]

\[+ U \sum_{m,s} t_{\text{im}} t_{\text{sm}} c_{s\sigma}^{\dagger}c_{i\sigma}c_{i\sigma} -
\]

\[- U^2 \sum_{m} t_{\text{im}} \left\{ c_{m\sigma}^{\dagger}c_{i\sigma}n_{i\sigma}c_{i\sigma} - c_{m\sigma}^{\dagger}c_{i\sigma}n_{m\sigma}c_{i\sigma} \right\} \]

\[\sim \left[ (III), c_{j\sigma}^{\dagger} \right] = -U \sum_{m} t_{\text{im}} t_{\text{ij}} c_{m\sigma}^{\dagger}c_{i\sigma} +
\]

\[+ U \delta_{ij} \sum_{m,t} t_{\text{im}} t_{\text{ij}} c_{m\sigma}^{\dagger}c_{t\sigma} -
\]

\[- U \delta_{ij} \sum_{m,t} t_{\text{im}} t_{\text{it}} c_{t\sigma}^{\dagger}c_{i\sigma} -
\]

\[- U^2 \delta_{ij} \sum_{m} t_{\text{im}} c_{m\sigma}^{\dagger}c_{i\sigma}n_{i\sigma} +
\]

\[+ U^2 \delta_{ij} \sum_{m} t_{\text{im}} c_{m\sigma}^{\dagger}c_{i\sigma}n_{m\sigma} -
\]

\[- U^2 t_{\text{ij}} c_{j\sigma}^{\dagger}c_{i\sigma}c_{j\sigma}c_{i\sigma} \]

With this follows:

\[\left\langle \left[ (II) + (III), c_{j\sigma}^{\dagger} \right] \right\rangle
\]

\[= U t_{\text{ij}} \sum_{m} t_{\text{im}} \left[ c_{i\sigma}^{\dagger}c_{m\sigma} - (c_{m\sigma}^{\dagger}c_{i\sigma}) \right] +
\]

\[+ U \delta_{ij} \sum_{m,t} t_{\text{im}} t_{\text{it}} \left[ c_{i\sigma}^{\dagger}c_{t\sigma} - (c_{t\sigma}^{\dagger}c_{i\sigma}) \right] -
\]

\[- U \delta_{ij} \sum_{m,t} t_{\text{im}} t_{\text{it}} \left[ c_{t\sigma}^{\dagger}c_{m\sigma} - (c_{m\sigma}^{\dagger}c_{t\sigma}) \right] +
\]

\[+ U^2 \delta_{ij} \sum_{m} t_{\text{im}} \left[ c_{i\sigma}^{\dagger}c_{m\sigma}n_{i\sigma} - (c_{m\sigma}^{\dagger}c_{i\sigma}n_{i\sigma}) \right] +
\]

\[+ U^2 \delta_{ij} \sum_{m} t_{\text{im}} \left[ c_{i\sigma}^{\dagger}c_{m\sigma}n_{m\sigma} + (c_{m\sigma}^{\dagger}c_{i\sigma}n_{m\sigma}) \right] -
\]

\[- U^2 t_{\text{ij}} \left[ c_{i\sigma}^{\dagger}c_{j\sigma}c_{i\sigma}c_{j\sigma} \right] + U^2 t_{\text{ij}} \left[ c_{j\sigma}^{\dagger}c_{j\sigma}c_{i\sigma}c_{i\sigma} \right] \]

Translational symmetry:
\[
\sum_{m} t_{im} \left( \left( c_{i-\sigma}^\dagger c_{m-\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} \right) \right) \\
= \frac{1}{N} \sum_{i,m} t_{im} \left( \left( c_{i-\sigma}^\dagger c_{m-\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} \right) \right) \\
= \frac{1}{N} \sum_{i,m} (t_{im} - t_{mi}) \left( c_{i-\sigma}^\dagger c_{m-\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} \right) = 0 \\
\sum_{m,t} t_{im} t_{mt} \left( \left( c_{i-\sigma}^\dagger c_{t-\sigma} - c_{t-\sigma}^\dagger c_{i-\sigma} \right) \right) \\
= \frac{1}{N} \sum_{m,t} (t_{im} t_{mt} - t_{im} t_{mi}) \left( c_{i-\sigma}^\dagger c_{t-\sigma} - c_{t-\sigma}^\dagger c_{i-\sigma} \right) = 0 \\
\sum_{m,t} t_{im} t_{it} \left( \left( c_{t-\sigma}^\dagger c_{m-\sigma} - c_{m-\sigma}^\dagger c_{t-\sigma} \right) \right) \\
= \sum_{m,t} (t_{im} t_{it} - t_{ii} t_{im}) \left( c_{t-\sigma}^\dagger c_{m-\sigma} \right) = 0 \\
\sum_{m} t_{im} \left( \left( c_{i-\sigma}^\dagger c_{m-\sigma} n_{i-\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} n_{i-\sigma} \right) \right) \\
= \sum_{m} t_{im} \left( \delta_{im} n_{-\sigma} - c_{m-\sigma}^\dagger c_{i-\sigma} \right) \\
= (T_{0} - \mu)n_{-\sigma} - \sum_{m} t_{im} \left( c_{m-\sigma}^\dagger c_{i-\sigma} \right)
\]

Real expectation values:

\[
\left\langle c_{i-\sigma}^\dagger c_{m-\sigma} n_{m\sigma} \right\rangle = n_{m\sigma} c_{m-\sigma}^\dagger c_{i-\sigma}
\]

Then we finally have

\[
\left\langle \left[ (I) + (II) + (III), c_{j\sigma}^\dagger \right] \right\rangle \\
= U^{2} \delta_{ij} \left( (T_{0} - \mu)n_{-\sigma} - \sum_{m} t_{im} \left( c_{m-\sigma}^\dagger c_{i-\sigma} \right) \right) + \\
+ Un_{-\sigma} \sum_{m} t_{im} t_{mj} + \\
+ U^{2} \delta_{ij} \sum_{m} t_{im} \left( 2 \left( c_{m-\sigma}^\dagger c_{i-\sigma} n_{m\sigma} \right) \right) + \\
+ U^{2} t_{ij} \left\{ n_{i-\sigma} n_{j-\sigma} + \left( c_{j\sigma}^\dagger c_{i\sigma} c_{i-\sigma} c_{j-\sigma} \right) + \left( c_{j\sigma}^\dagger c_{i\sigma} c_{i-\sigma} c_{j-\sigma} \right) \right\}
\]
Fourier transformation:

\[
\frac{1}{N} \sum_{i,j} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} t_{ij} \left\{ \{n_{i-\sigma} n_{j-\sigma}\} + \left\{ c_{j-\sigma}^\dagger c_{j-\sigma}^\dagger c_{i-\sigma} c_{i-\sigma}\right\} + \\
+ \left\{ c_{j-\sigma}^\dagger c_{i-\sigma} c_{i-\sigma} c_{j-\sigma}\right\} \right\} = \\
t_0 \{n_{-\sigma} - 2 \langle n_{i-\sigma} n_{i-\sigma}\rangle\} + \frac{1}{N} \sum_{i,j} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} t_{ij} \{\ldots\} \\
= (T_0 - \mu) (n_{-\sigma} - 2 \langle n_{i-\sigma} n_{i-\sigma}\rangle) + n_{-\sigma}^2 (\epsilon(\mathbf{k}) - T_0) + \\
+ n_{-\sigma} (1 - n_{-\sigma}) F_{k-\sigma}
\]

The second summand is exactly the bandwidth correction of (8.213):

\[
\frac{1}{N} \sum_{i,j} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \delta_{ij} \sum_m t_{im} \left( 2\left\{ c_{m-\sigma}^\dagger c_{i-\sigma} n_m\right\} \\
- \left\{ c_{m-\sigma}^\dagger c_{i-\sigma}\right\} \right) = \\
= \frac{1}{N} \sum_{i,m} t_{im} (\ldots) \\
= \frac{1}{N} \sum_{i,m} t_{im} (\ldots) + t_0 (2 \langle n_{i-\sigma} n_{i-\sigma}\rangle - n_{-\sigma}) \\
= n_{-\sigma} (1 - n_{-\sigma}) B_{-\sigma} + (T_0 - \mu) (2 \langle n_{i-\sigma} n_{i-\sigma}\rangle - n_{-\sigma})
\]

We have used here the definition (8.212) of spin-dependent band shift. Then finally what remains is

\[
\frac{1}{N} \sum_{i,j} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \left\{ \left[ (I) + (III) + (III), c_{j-\sigma}^\dagger \right]_+ \right\} = \\
= Un_{-\sigma} (\epsilon(\mathbf{k}) - \mu)^2 + U^2 n_{-\sigma} (T_0 - \mu) + \\
+ U^2 n_{-\sigma}^2 (\epsilon(\mathbf{k}) - T_0) + U^2 n_{-\sigma} (1 - n_{-\sigma}) B_{k-\sigma} \quad (1)
\]

We substitute (l) in (j) and then have
This is the 3rd spectral moment (8.224).

**Problem 8.14**

Hamiltonian of the Stoner model (8.34):

\[
H_S = \sum_{k\sigma}(\varepsilon(k) + Un_{-\sigma} - \mu)\sigma c^\dagger_{k\sigma} c_{k\sigma}
\]

That means

\[
[c_{k\sigma}, H]_\sim = (\varepsilon(k) + Un_{-\sigma} - \mu)c_{k\sigma}
\]

\[
\underbrace{\cdots [c_{k\sigma}, H]_\sim \cdots, H]_\sim}_{n-fold} = (\varepsilon(k) + Un_{-\sigma} - \mu)^n c_{k\sigma}
\]

\sim Spectral moments:

\[
M_{k\sigma}^{(n)} = (\varepsilon(k) + Un_{-\sigma} - \mu)^n
\]

Then it holds

\[
\Delta_{k\sigma}^{(0)} = M_{k\sigma}^{(0)} = 1
\]

\[
\Delta_{k\sigma}^{(1)} = \begin{pmatrix} M_{k\sigma}^{(0)} & M_{k\sigma}^{(1)} \\ M_{k\sigma}^{(1)} & M_{k\sigma}^{(2)} \end{pmatrix} - M_{k\sigma}^{(0)}M_{k\sigma}^{(2)} - (M_{k\sigma}^{(1)})^2 = 0
\]

\sim Therefore the spectral density is a one-pole function!
Problem 8.15

1. \[ H = T_0 \sum_{i,\sigma} n_{i\sigma} + \frac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} \]

It holds

\[ [c_{i\sigma}, n_{i\sigma'}]_\sigma = \delta_{\sigma\sigma'} c_{i\sigma} \]

With this it directly follows:

\[ [c_{i\sigma}, \mathcal{H}]_\sigma = (T_0 - \mu)c_{i\sigma} + U c_{i\sigma} n_{i-\sigma} \]
\[ [c_{i\sigma} n_{i-\sigma}, \mathcal{H}]_\sigma = [c_{i\sigma}, \mathcal{H}]_\sigma n_{i-\sigma} \]
\[ = (T_0 - \mu + U)c_{i\sigma} n_{i-\sigma} \]

Here we have used once more \( n_{i-\sigma}^2 = n_{i-\sigma} \)

\[ M_{i\sigma}^{(0)} = 1 \]
\[ M_{i\sigma}^{(1)} = (T_0 - \mu) + U n_{-\sigma} \]
\[ = (T_0 - \mu)^1 + [(T_0 + U - \mu)^1 - (T_0 - \mu)^1] n_{-\sigma} \]

Complete induction:

Let the proposition be true for \( n \). That means

\[ \left[ \cdots \left[ [c_{i\sigma}, \mathcal{H}]_\sigma, \mathcal{H}]_\sigma \cdots, \mathcal{H} \right]_\sigma \right] = \]
\[ = (T_0 - \mu)^n c_{i\sigma} + [(T_0 + U - \mu)^n - (T_0 - \mu)^n] c_{i\sigma} n_{i-\sigma} \]
\[ \cap \left[ \cdots \left[ [c_{i\sigma}, \mathcal{H}]_\sigma, \mathcal{H}]_\sigma \cdots, \mathcal{H} \right]_\sigma \right] = \]
\[ \left( T_0 - \mu \right)^n \left[ c_{i\sigma}, \mathcal{H} \right]_\sigma - \]
\[ - \left[ (T_0 + U - \mu)^n - (T_0 - \mu)^n \right] [c_{i\sigma} n_{i-\sigma}, \mathcal{H}]_\sigma - \]
\[ = (T_0 - \mu)^n ((T_0 - \mu)c_{i\sigma} + Un_{i-\sigma} c_{i\sigma}) + \]
\[ + [(T_0 - \mu + U)^n - (T_0 - \mu)^n] (T_0 - \mu + U)c_{i\sigma} n_{i-\sigma} \]
\[ = (T_0 - \mu)^n c_{i\sigma} + U(T_0 - \mu)^n n_{i-\sigma} c_{i\sigma} + \]
\[ + (T_0 - \mu + U)^{n+1} c_{i\sigma} n_{i-\sigma} - \]
\[ - (T_0 - \mu)^n (T_0 - \mu + U)c_{i\sigma} n_{i-\sigma} \]
\[ = (T_0 - \mu)^n c_{i\sigma} + \]
\[ + [(T_0 - \mu + U)^{n+1} - (T_0 - \mu)^{n+1}] c_{i\sigma} n_{i-\sigma} \]
So that it holds
\[
\left[ \cdots \left[ [c_{i\sigma}, \mathcal{H}]_-, \mathcal{H} \right]_- \cdots, \mathcal{H} \right]_- = (T_0 - \mu)^n c_{i\sigma} + \left[ (T_0 - \mu + U)^n - (T_0 - \mu)^n \right] c_{i\sigma} n_{i-\sigma}
\]

Then the spectral moments are
\[
M_{ii\sigma}^{(n)} = (T_0 - \mu)^n + \left[ (T_0 - \mu + U)^n - (T_0 - \mu)^n \right] n_{-\sigma}
\]

2. Lonke theorem [24]
\[
\Delta_{ii\sigma}^{(1)} = \left( \begin{array}{ccc}
M_{ii\sigma}^{(0)} & M_{ii\sigma}^{(1)} & M_{ii\sigma}^{(2)} \\
M_{ii\sigma}^{(1)} & M_{ii\sigma}^{(2)} & M_{ii\sigma}^{(3)} \\
M_{ii\sigma}^{(2)} & M_{ii\sigma}^{(3)} & M_{ii\sigma}^{(4)} 
\end{array} \right)
\]
\[
= M_{ii\sigma}^{(0)} M_{ii\sigma}^{(2)} - (M_{ii\sigma}^{(0)})^2
= (T_0 - \mu)^2 + \left[ (T_0 - \mu + U)^2 - (T_0 - \mu)^2 \right] n_{-\sigma} - \\
- (T_0 - \mu + U n_{-\sigma})^2
= -2U n_{-\sigma}(T_0 - \mu) - U^2 n_{-\sigma}^2 + 2U(T_0 - \mu)n_{-\sigma} + \\
+ U^2 n_{-\sigma}
= U^2 n_{-\sigma}(1 - n_{-\sigma}) \neq 0, \quad \text{if } n_{-\sigma} \neq 0, 1
\]

For empty bands \((n = 0)\), fully occupied bands \((n = 2)\) and fully polarized and half-filled bands \((n_{\sigma} = 1, n_{-\sigma} = 0)\) the spectral density consists of only one (!) \(\delta\)-function. In all other cases
\[
\Delta_{ii\sigma}^{(1)} > 0
\]

We now calculate
\[
\Delta_{ii\sigma}^{(2)} = \left( \begin{array}{ccc}
M_{ii\sigma}^{(0)} & M_{ii\sigma}^{(1)} & M_{ii\sigma}^{(2)} \\
M_{ii\sigma}^{(1)} & M_{ii\sigma}^{(2)} & M_{ii\sigma}^{(3)} \\
M_{ii\sigma}^{(2)} & M_{ii\sigma}^{(3)} & M_{ii\sigma}^{(4)} 
\end{array} \right)
\]
\[
= M_{ii\sigma}^{(0)} M_{ii\sigma}^{(2)} M_{ii\sigma}^{(4)} + 2M_{ii\sigma}^{(1)} M_{ii\sigma}^{(3)} M_{ii\sigma}^{(2)} - \\
- (M_{ii\sigma}^{(2)})^3 - M_{ii\sigma}^{(0)} (M_{ii\sigma}^{(3)})^2 - (M_{ii\sigma}^{(1)})^2 M_{ii\sigma}^{(4)}
\]
\[
= \left\{ M_{ii\sigma}^{(0)} M_{ii\sigma}^{(2)} - (M_{ii\sigma}^{(1)})^2 \right\} M_{ii\sigma}^{(4)} + \\
+ \left\{ M_{ii\sigma}^{(1)} M_{ii\sigma}^{(3)} - (M_{ii\sigma}^{(2)})^2 \right\} M_{ii\sigma}^{(2)} + \\
+ \left\{ M_{ii\sigma}^{(1)} M_{ii\sigma}^{(3)} - M_{ii\sigma}^{(0)} M_{ii\sigma}^{(2)} \right\} M_{ii\sigma}^{(3)}
\]
We calculate the individual terms with the abbreviation:

\[ t_0 = T_0 - \mu \]

\[
\left\{ M^{(0)}_{i\sigma} M^{(2)}_{i\sigma} - (M^{(1)}_{i\sigma})^2 \right\} =
\]
\[
= t_0^2 + ((t_0 + U)^2 - t_0^2)n_{-\sigma} - (t_0 + (t_0 + U - t)n_{-\sigma})^2
\]
\[
= t_0^2 - t_0^2 + n_{-\sigma} \{ 2t_0U + U^2 - 2t_0U \} - n_{-\sigma}^2 U^2
\]
\[
= U^2 n_{-\sigma} (1 - n_{-\sigma})
\]

\[
\left\{ M^{(1)}_{i\sigma} M^{(3)}_{i\sigma} - (M^{(2)}_{i\sigma})^2 \right\} =
\]
\[
= (t_0 + U n_{-\sigma})(t_0^3 + ((t_0 + U)^3 - t_0^3)n_{-\sigma} -
- (t_0^2 + ((t_0 + U)^2 - t_0^2)n_{-\sigma})^2
\]
\[
= (t_0 + U n_{-\sigma})(t_0^3 + n_{-\sigma}(3t_0^2U + 3t_0U^2 + U^3)) -
- (t_0^2 + n_{-\sigma}(2t_0U + U^2))^2
\]
\[
= t_0^4 + n_{-\sigma}(3t_0^2U + 3t_0U^2 + t_0U^3) + U n_{-\sigma} t_0^3 +
+ U n_{-\sigma} (3t_0^2U + 3t_0U^2 + U^3) - t_0^4 -
- n_{-\sigma}^2(2t_0U + U^2)^2 - 2n_{-\sigma} t_0^2(2t_0U + U^2)
\]
\[
= n_{-\sigma}(3t_0^2U + 3t_0U^2 + t_0U^3 + U t_0^3 - 4t_0^2U -
- 2t_0^2U^2) + n_{-\sigma} (3t_0^2U^2 + 3t_0U^3 + U^4 - 4t_0^2U^2 -
- U^4 - 4t_0U^3)
\]
\[
= n_{-\sigma}(t_0^2U^2 + t_0U^3) + n_{-\sigma}^2(-t_0^2U^2 - t_0U^3)
\]
\[
= U^2 n_{-\sigma} (t_0^2 + t_0U) - U^2 n_{-\sigma}^2(t_0^2 + t_0U)
\]
\[
= U^2 n_{-\sigma} (1 - n_{-\sigma})t_0(t_0 + U)
\]

\[
\left\{ M^{(1)}_{i\sigma} M^{(2)}_{i\sigma} - M^{(0)}_{i\sigma} M^{(3)}_{i\sigma} \right\} =
\]
\[
= (t_0 + U n_{-\sigma})(t_0^2 + n_{-\sigma}((t_0 + U)^3 - t_0^3))) -
- (t_0^3 + n_{-\sigma}((t_0 + U)^3 - t_0^3))
\]
\[
= t_0^3 + n_{-\sigma}(2t_0U + t_0U^2) + U n_{-\sigma} (t_0^2 +
+ n_{-\sigma}(2t_0U + U^2)) -
- (t_0^3 + n_{-\sigma}(3t_0^2U + 3t_0U^2 + U^3))
\]
\[
= n_{-\sigma}(2t_0U + t_0U^2 + U t_0^2 -
- 3t_0^2U - 3t_0U^2 - U^3) + n_{-\sigma} (2t_0U^2 + U^3)
\]
\[
= n_{-\sigma}(-2t_0U^2 - U^3) + n_{-\sigma}^2 U^2(2t_0 + U)
\]
\[
= -U^2 n_{-\sigma} (1 - n_{-\sigma})(2t_0 + U)
\]
Intermediate result:

\[
\frac{\Delta_{ii\sigma}^{(2)}}{U^2n_{-\sigma}(1 - n_{-\sigma})} = M_{ii\sigma}^{(4)} + t_0(t_0 + U)M_{ii\sigma}^{(2)} - (2t_0 + U)M_{ii\sigma}^{(3)}
\]

We now finally calculate the right-hand side:

\[
\frac{\Delta_{ii\sigma}^{(2)}}{U^2n_{-\sigma}(1 - n_{-\sigma})} = t_0^4 + ((t_0 + U)^2 - t_0^2)n_{-\sigma} + t_0(t_0 + U)\left[ t_0^2 + ((t_0 + U)^2 - t_0^2)\right]n_{-\sigma} - (2t_0 + U)\left[ t_0^3 + ((t_0 + U)^3 - t_0^3)\right]n_{-\sigma} = (t_0^4 + t_0^3(t_0 + U) - 2t_0^4 - Ut_0^3) + n_{-\sigma}\left\{ (t_0 + U)^2 - t_0^2 \right\}(t_0(t_0 + U) + (t_0 + U)^2 + t_0^2) - (2t_0 + U)((t_0 + U)^3 - t_0^3)) \]

\[
= n_{-\sigma}\left\{ 2(t_0U + U^2)(3t_0^2 + t_0U + 2t_0U + U^2) - (2t_0 + U)(3t_0^2U + 3t_0U^2 + U^3) \right\} = n_{-\sigma}\left\{ 6t_0^2U^2 + 3U^2t_0^2 - 6t_0^2U^2 - 3t_0^2U^2 + 2t_0U^3 + 3t_0U^3 - 2t_0U^3 - 3t_0U^3 \right\} = 0
\]

With this it is proved that the one-electron spectral density in the limit of infinitely narrow band is a two-pole function:

\[
S_\sigma(E) = \alpha_1\sigma\delta(E - E_{1\sigma}) + \alpha_2\sigma\delta(E - E_{2\sigma})
\]

3. Spectral moments:

\[
M_{ii\sigma}^{(n)}(E) = (T_0 - \mu)^n(1 - n_{-\sigma}) + (T_0 + U - \mu)^n n_{-\sigma}
\]

On the other hand it follows from part 2

\[
M_{ii\sigma}^{(n)}(E) = \alpha_1\sigma E_{1\sigma}^n + \alpha_2\sigma E_{2\sigma}^n
\]

Compare:

\[
E_{1\sigma} = T_0 - \mu; \ \alpha_1\sigma = 1 - n_{-\sigma}
\]

\[
E_{2\sigma} = T_0 + U - \mu; \ \alpha_2\sigma = n_{-\sigma}
\]
This agrees with (8.129), (8.130) and (8.131)!

**Problem 8.16**

One can easily calculate

\[ [c_{d\sigma}, H]_- = (\epsilon_d - \mu)c_{d\sigma} + \]
\[ + \sum_k V_{kd} c_{k\sigma} + \left[ c_{d\sigma}, \frac{1}{2} U \sum_{\sigma'} n_{d\sigma'} n_{d-\sigma'} \right]_- \]

With (8.334) follows then the equation of motion:

\[ (E + \mu - \epsilon_d - \Sigma_{d\sigma}(E)) G_{d\sigma}(E) = \hbar + \sum_k V_{kd} \left\langle \left\langle c_{k\sigma} ; c_{d\sigma}^\dagger \right\rangle \right\rangle_E \]

We calculate the “mixed” Green’s function

\[ [c_{k\sigma}, H]_- = (\epsilon(k) - \mu)c_{k\sigma} + V_{kd} c_{d\sigma} \]
\[ \sim (E + \mu - \epsilon(k)) \left\langle \left\langle c_{k\sigma} ; c_{d\sigma}^\dagger \right\rangle \right\rangle_E = V_{kd} \left\langle \left\langle c_{d\sigma} ; c_{d\sigma}^\dagger \right\rangle \right\rangle \]

So that it follows:

\[ \left\langle \left\langle c_{k\sigma} ; c_{d\sigma}^\dagger \right\rangle \right\rangle_E = \frac{V_{kd}}{E + \mu - \epsilon(k)} G_{d\sigma}(E) \]

With the definition of (8.335) of the “hybridization function”, what remains is:

\[ (E + \mu - \epsilon_d - \Sigma_{d\sigma}(E)) G_{d\sigma}(E) = \hbar + \Delta(E) G_{d\sigma}(E) \]

This proves the proposition:

\[ G_{d\sigma}(E) = \frac{\hbar}{E + \mu - \epsilon_d - \Sigma_{d\sigma}(E) - \Delta(E)} \]

**Problem 8.17**

\[ n_{d\sigma}(1 - n_{d\sigma})(B_{d\sigma} - \epsilon_d) = \sum_k V_{kd} \left\langle \left\langle c_{k\sigma}^\dagger c_{d\sigma} (2n_{d-\sigma} - 1) \right\rangle \right\rangle \]

We begin with

\[ \sum_k V_{kd} \left\langle \left\langle c_{k\sigma}^\dagger c_{d\sigma} \right\rangle \right\rangle = \]
\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \sum_k V_{kd} \left\langle \left\langle c_{d\sigma} ; c_{k\sigma}^\dagger \right\rangle \right\rangle_{E-\mu} \quad (1) \]
We have calculated the mixed Green’s function in Problem 8.16:
\[
\left\langle c_{k\sigma}^\dagger c_{d\sigma}^\vphantom{\dagger}\right\rangle = \frac{V_{kd}}{E + \mu - \varepsilon(k)} G_{d\sigma}(E) = \left\langle c_{d\sigma}^\vphantom{\dagger} c_{k\sigma}^\dagger\right\rangle
\]
(2)

Because of the assumption that \(V_{kd}\) is real, the last step can be easily proved:
\[
\sum_k V_{kd} \left\langle c_{k\sigma}^\dagger c_{d\sigma}\right\rangle = -\frac{1}{\pi \hbar} \int dE \, f_-(E)\Delta(E - \mu)G_{d\sigma}(E - \mu)
\]
(3)

\(\Delta\): “hybridization function” (8.335):
\[
\Delta(E) = \sum_k \frac{V_{kd}^2}{E + \mu - \varepsilon(k)}
\]

It holds
\[
[c_{d\sigma}, H]_- = (\varepsilon_d - \mu)c_{d\sigma} + U c_{d\sigma} n_{d-\sigma} + \sum_p V_{pd} c_{p\sigma}
\]

So that
\[
\left\langle c_{k\sigma}^\dagger c_{d\sigma} n_{d-\sigma}\right\rangle = -\frac{1}{U} (\varepsilon_d - \mu) \left\langle c_{k\sigma}^\dagger c_{d\sigma}\right\rangle - \\
- \frac{1}{U} \sum_p V_{pd} \left\langle c_{k\sigma}^\dagger c_{p\sigma}\right\rangle + \frac{1}{U} \left\langle c_{k\sigma}^\dagger [c_{d\sigma}, H]_-\right\rangle
\]

Now for the band shift we still have to calculate
\[
n_{d\sigma} (1 - n_{d\sigma}) (B_{d\sigma} - \varepsilon_d) = \left( -2 \frac{\varepsilon_d - \mu}{U} - 1 \right) \sum_k V_{kd} \left\langle c_{k\sigma}^\dagger c_{d\sigma}\right\rangle - \\
- \frac{2}{U} \sum_{k,p} V_{kd} V_{pd} \left\langle c_{k\sigma}^\dagger c_{p\sigma}\right\rangle + \\
+ \frac{2}{U} \sum_k V_{kd} \left\langle c_{k\sigma}^\dagger [c_{d\sigma}, H]_-\right\rangle
\]
(4)

The first summand is known from (3). For the second summand we need \(\left\langle c_{k\sigma}^\dagger c_{p\sigma}\right\rangle\):
\[ (E + \mu - \varepsilon(p)) \left\langle \left\{ c_{p\sigma} ; c_{k\sigma}^{\dagger} \right\} \right\rangle_E = \hbar \delta_{pk} + V_{pd} \left\langle \left\{ c_{d\sigma} ; c_{k\sigma}^{\dagger} \right\} \right\rangle_E \]

\[ \equiv \hbar \delta_{pk} + \frac{V_{kd} V_{pd}}{E + \mu - \varepsilon(k)} G_{d\sigma}(E) \]

That means

\[ \sum_{k,p} V_{kd} V_{pd} \left\langle c_{k\sigma}^{\dagger} c_{p\sigma} \right\rangle = \]

\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \sum_{k,p} V_{kd} V_{pd} \left\langle \left\{ c_{p\sigma} ; c_{k\sigma}^{\dagger} \right\} \right\rangle_{E-\mu} \]

\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \left\{ \hbar \sum_k \frac{V_{kd}^2}{E - \varepsilon(k)} + \sum_{k,p} \frac{V_{pd}^2 V_{kd}^2}{(E - \varepsilon(k))(E - \varepsilon(p))} G_{d\sigma}(E - \mu) \right\} \]

\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) \Delta(E - \mu) \ast \]

\[ \ast \{ \hbar + \Delta(E - \mu) G_{d\sigma}(E - \mu) \} \] (5)

Finally it still holds

\[ \left\langle \left\{ c_{d\sigma} , \mathcal{H} \right\}_{-} ; c_{k\sigma}^{\dagger} \right\rangle_E = E \left\langle \left\{ c_{d\sigma} ; c_{k\sigma}^{\dagger} \right\} \right\rangle_E - \hbar \left\langle \left\{ c_{d\sigma} , c_{k\sigma}^{\dagger} \right\} \right\rangle_E \]

\[ \equiv \left\langle \left\{ c_{d\sigma} , c_{k\sigma}^{\dagger} \right\} \right\rangle_+ \]

Spectral theorem:

\[ \sum_{k} V_{kd} \left\langle c_{k\sigma}^{\dagger} [c_{d\sigma} , \mathcal{H}]_{-} \right\rangle = \]

\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE f_-(E) (E - \mu) \Delta(E - \mu) G_{d\sigma}(E - \mu) \] (6)

In (4) we need (3), (5) and (6):
\[ I = \left(-2 \frac{\varepsilon_d - \mu}{U} - 1\right) \Delta(E - \mu) G_{d\sigma}(E - \mu) \]
\[ - \frac{2}{U} \Delta(E - \mu) \{ \hbar + \Delta(E - \mu) G_{d\sigma}(E - \mu) \} + \]
\[ + \frac{2}{U} \Delta(E - \mu) (E - \mu) G_{d\sigma}(E - \mu) \]
\[ = -\Delta(E - \mu) \frac{2}{U} \hbar + \Delta(E - \mu) G_{d\sigma}(E - \mu) \]
\[ * \left\{ -1 + \frac{2}{U} (-\varepsilon_d + \mu - \Delta(E - \mu) + E - \mu) \right\} \]

Equation of motion:
\[ (E + \mu - \varepsilon_d - \Sigma_{d\sigma}(E) - \Delta(E)) G_{d\sigma}(E) = \hbar \]
\[ \Leftrightarrow I = -\Delta(E - \mu) \frac{2}{U} \hbar - \Delta(E - \mu) G_{d\sigma}(E - \mu) + \]
\[ + \frac{2}{U} \Delta(E - \mu) (\hbar + \Sigma_{d\sigma}(E - \mu) G_{d\sigma}(E - \mu)) \]
\[ = \Delta(E - \mu) G_{d\sigma}(E - \mu) \left( \frac{2}{U} \Sigma_{d\sigma}(E - \mu) - 1 \right) \]

Then it finally follows:
\[ n_{d\sigma}(1 - n_{d\sigma})(B_{d\sigma} - \varepsilon_d) = \]
\[ = -\frac{1}{\pi \hbar} \text{Im} \int_{-\infty}^{+\infty} dE \ f_-(E) \Delta(E - \mu) G_{d\sigma}(E - \mu) \]
\[ * \left( \frac{2}{U} \Sigma_{d\sigma}(E - \mu) - 1 \right) \]

This is exactly the proposition (8.352).

**Problem A.1**

With (A.24) and (A.30) we first have
\[ c_\beta \left( \sum_{\gamma \alpha_1} \varphi_{\alpha_1} \cdots \varphi_{\alpha_N} \right)^{(e)} = \sqrt{N + 1} a_\beta \varphi_{\gamma \alpha_1} \cdots \varphi_{\alpha_N} \]
\[ = \{ \delta(\varphi_\beta - \varphi_\gamma) \varphi_{\alpha_1} \cdots \varphi_{\alpha_N} \}
\[ + \varepsilon_1 \delta(\varphi_\beta - \varphi_{\alpha_1}) \varphi_{\gamma \varphi_{\alpha_2} \cdots \varphi_{\alpha_N}} \]
\[ + \cdots + \]
\[ + \varepsilon^N \delta(\varphi_\beta - \varphi_{\alpha_N}) \varphi_{\gamma \varphi_{\alpha_1} \cdots \varphi_{\alpha_{N-1}}} \}

On the other hand it is also valid that
\[ c_y \left( c_\beta |\varphi_{\alpha_1} \cdots \varphi_{\alpha_N} \rangle^{(e)} \right) = \delta(\varphi_\beta - \varphi_\alpha) |\varphi_y \varphi_{\alpha_2} \cdots \varphi_{\alpha_N} \rangle^{(e)} + \cdots + \epsilon^{N-1} \delta(\varphi_\beta - \varphi_{\alpha_N}) |\varphi_y \varphi_{\alpha_1} \cdots \varphi_{\alpha_{N-1}} \rangle^{(e)} \]

One multiplies the last equation by \( \epsilon \) and then subtracts one equation from the other to get

\[ (c_\beta c_y^\dagger - \epsilon c_y^\dagger c_\beta) |\varphi_{\alpha_1} \cdots \varphi_{\alpha_N} \rangle^{(e)} = \delta(\varphi_\beta - \varphi_y) |\varphi_{\alpha_1} \cdots \varphi_{\alpha_N} \rangle^{(e)} \]

**Problem A.2**

**Bosons**: \( \cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \rangle^{(\nu)} \): arbitrary Fock state.

\( r \neq s \):

\[ c_{\alpha_r}^\dagger c_{\alpha_s}^\dagger |\cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \rangle^{(\nu)} = \sqrt{n_{\alpha_r} + 1} \sqrt{n_{\alpha_s} + 1} |\cdots n_{\alpha_r} + 1 \cdots n_{\alpha_s} + 1 \cdots \rangle^{(\nu)} = c_{\alpha_r}^\dagger c_{\alpha_s}^\dagger |\cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \rangle^{(\nu)} \Rightarrow [c_{\alpha_r}, c_{\alpha_s}]_- = 0. \]

For \( r = s \) this relation is trivially valid.

Since

\[ [c_{\alpha_r}, c_{\alpha_s}]_- = \left( [c_{\alpha_r}^\dagger, c_{\alpha_s}^\dagger]_- \right)^\dagger \]

directly follows:

\[ [c_{\alpha_r}, c_{\alpha_s}]_- = 0. \]

\( r \neq s \):

\[ c_{\alpha_r} c_{\alpha_s}^\dagger |\cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \rangle^{(\nu)} = \sqrt{n_{\alpha_s}} \sqrt{n_{\alpha_r} + 1} |\cdots n_{\alpha_r} - 1 \cdots n_{\alpha_s} + 1 \cdots \rangle^{(\nu)} = c_{\alpha_s}^\dagger c_{\alpha_r} |\cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \rangle^{(\nu)}. \]

\( r = s \):
Since

\[ N_s' = N_s + 1 \]

\[ \Longrightarrow (c_{\alpha r}^\dagger c_{\alpha s}^\dagger + c_{\alpha s} c_{\alpha r}) | \cdots n_{\alpha r} \cdots n_{\alpha s} \cdots \rangle = 0 \]

\[ \Longrightarrow [c_{\alpha r}, c_{\alpha s}]_+ = 0. \]

Since

\[ [c_{\alpha r}, c_{\alpha s}]_+ = (\{c_{\alpha r}^\dagger, c_{\alpha s}^\dagger \}_+)^\dagger \]

again the second anti-commutator relation follows directly:

\[ [c_{\alpha r}, c_{\alpha s}]_+ = 0 \]

\[ r = s : \]

\[ c_{\alpha r} c_{\alpha r}^\dagger | \cdots n_{\alpha r} \cdots \rangle = c_{\alpha r} (-1)^{N_s} \delta_{n_{\alpha r}, 0} | \cdots n_{\alpha r} + 1 \cdots \rangle = \]

\[ = (-1)^{2N_r} \delta_{n_{\alpha r}, 0} | \cdots n_{\alpha r} \cdots \rangle = \]

\[ = \delta_{n_{\alpha r}, 0} | \cdots n_{\alpha r} \cdots \rangle, \]

\[ c_{\alpha r}^\dagger c_{\alpha r} | \cdots n_{\alpha r} \cdots \rangle = \delta_{n_{\alpha r}, 1} | \cdots n_{\alpha r} \cdots \rangle. \]
Since in every case \( n_{\alpha_r} = 0 \) or \( 1 \), we have

\[
(c_{\alpha_r}c_{\alpha_r}^\dagger + c_{\alpha_s}^\dagger c_{\alpha_r})\cdots n_{\alpha_r} \cdots = \cdots n_{\alpha_r} \cdots .
\]

\( r < s \):

\[
c_{\alpha_r}c_{\alpha_r}^\dagger \cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \langle (-) = \langle \cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots (\cdot) -
\]

\[
c_{\alpha_s}c_{\alpha_r}^\dagger \cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \langle (-) = c_{\alpha_r}(-1)^{N_r} \delta_{n_{\alpha_r}0} \cdots n_{\alpha_r} + 1 \cdots \langle (-)
\]

\[
= (-1)^{N_r + N_s} \delta_{n_{\alpha_r}1} \delta_{n_{\alpha_r}0} \cdots n_{\alpha_r} - 1 \cdots n_{\alpha_s} + 1 \cdots \langle (-)
\]

\[
N_s'' = N_s - 1
\]

\[
\implies (c_{\alpha_r}c_{\alpha_s}^\dagger + c_{\alpha_s}^\dagger c_{\alpha_r})\cdots n_{\alpha_r} \cdots n_{\alpha_s} \cdots \langle (-) = 0.
\]

So altogether we have

\[
[c_{\alpha_r}, c_{\alpha_s}^\dagger]_+ = \delta_{r,s}.
\]

**Problem A.3**

1. Bosons:

\[
\hat{n}_{\alpha} c_{\beta}^\dagger = c_{\alpha}^\dagger c_{\beta} c_{\beta}^\dagger
\]

\[
= c_{\alpha}^\dagger c_{\beta}^\dagger c_{\alpha} + \delta_{\alpha\beta} c_{\alpha}^\dagger
\]

\[
= c_{\beta}^\dagger c_{\alpha}^\dagger c_{\alpha} + \delta_{\alpha\beta} c_{\alpha}^\dagger
\]

\[
= c_{\beta}^\dagger \hat{\pi}_{\alpha} + \delta_{\alpha\beta} c_{\alpha}^\dagger
\]

So that we have

\[
[\hat{\pi}_{\alpha}, c_{\beta}^\dagger] = \delta_{\alpha\beta} c_{\beta}^\dagger
\]

Fermions:
\[ \hat{n}_\alpha \, c_\beta^\dagger = c_\alpha^\dagger c_\beta c_\beta^\dagger \]
\[ = -c_\alpha^\dagger c_\beta c_\alpha + \delta_{\alpha\beta} c_\alpha^\dagger \]
\[ = c_\beta^\dagger c_\alpha c_\alpha + \delta_{\alpha\beta} c_\alpha^\dagger \]
\[ = c_\beta^\dagger \hat{n}_\alpha + \delta_{\alpha\beta} c_\alpha^\dagger \]

So that just as in the case of Bosons we get

\[ \left[ \hat{n}_\alpha, \, c_\beta^\dagger \right]_\_ = \delta_{\alpha\beta} c_\alpha^\dagger \]

2. Bosons :

\[ \hat{n}_\alpha \, c_\beta = c_\alpha^\dagger c_\beta c_\alpha \]
\[ = c_\alpha^\dagger c_\beta c_\alpha = c_\beta c_\alpha^\dagger c_\alpha - \delta_{\alpha\beta} c_\alpha \]
\[ = c_\beta^\dagger \hat{n}_\alpha - \delta_{\alpha\beta} c_\alpha \]

With this follows:

\[ \left[ \hat{n}_\alpha, \, c_\beta \right]_\_ = -\delta_{\alpha\beta} c_\alpha \]

Fermions:

\[ \hat{n}_\alpha \, c_\beta = c_\alpha^\dagger c_\beta c_\alpha \]
\[ = -c_\alpha^\dagger c_\beta c_\alpha = c_\beta c_\alpha^\dagger c_\alpha - \delta_{\alpha\beta} c_\alpha \]
\[ = c_\beta^\dagger \hat{n}_\alpha - \delta_{\alpha\beta} c_\alpha \]

With this, as in the case of Bosons we get

\[ \left[ \hat{n}_\alpha, \, c_\beta \right]_\_ = -\delta_{\alpha\beta} c_\alpha \]

3. For Bosons as well as for Fermions, with part 1

\[ \left[ \hat{N}, \, c_\alpha^\dagger \right]_\_ = \sum_\gamma \left[ \hat{n}_\gamma, \, c_\alpha^\dagger \right]_\_ = \sum_\gamma \delta_{\alpha\gamma} c_\alpha^\dagger = c_\alpha^\dagger \]

is valid.

4. For Bosons as well as Fermions with part 2

\[ \left[ \hat{N}, \, c_\alpha \right]_\_ = \sum_\gamma \left[ \hat{n}_\gamma, \, c_\alpha \right]_\_ = \sum_\gamma (-\delta_{\alpha\gamma} c_\alpha) = -c_\alpha \]

is valid.
Problem A.4

1.
\[
\begin{align*}
[c_\alpha, c_\beta]_+ &= 0 \quad \Leftrightarrow \quad [c_\alpha, c_\alpha]_+ = 2c_\alpha^2 = 0 \quad \Leftrightarrow \quad c_\alpha^2 = 0 \\
[c_\alpha^\dagger, c_\beta^\dagger]_+ &= 0 \quad \Leftrightarrow \quad [c_\alpha^\dagger, c_\alpha^\dagger]_+ = 2(c_\alpha^\dagger)^2 = 0 \\
&\quad \Leftrightarrow \quad (c_\alpha^\dagger)^2 = 0 \quad \text{(Pauli principle)}
\end{align*}
\]

2.
\[
\hat{n}_\alpha^2 = c_\alpha^\dagger c_\alpha c_\alpha^\dagger c_\alpha = c_\alpha^\dagger (1 - c_\alpha^\dagger c_\alpha) c_\alpha \\
= c_\alpha^\dagger c_\alpha - (c_\alpha^\dagger)^2 (c_\alpha)^2 \gg \hat{n}_\alpha \quad \text{(Pauli principle)}
\]

3.
\[
c_\alpha \hat{n}_\alpha = c_\alpha c_\alpha^\dagger c_\alpha = (1 - c_\alpha^\dagger c_\alpha) c_\alpha \gg c_\alpha \\
c_\alpha^\dagger \hat{n}_\alpha = c_\alpha^\dagger c_\alpha^\dagger c_\alpha \gg 0
\]

4.
\[
\hat{n}_\alpha c_\alpha = c_\alpha^\dagger c_\alpha c_\alpha \gg 0 \\
\hat{n}_\alpha c_\alpha^\dagger = c_\alpha^\dagger c_\alpha c_\alpha^\dagger = c_\alpha^\dagger (1 - c_\alpha^\dagger c_\alpha) \gg c_\alpha^\dagger
\]

Problem A.5
Proof by complete induction

\[N = 1:\]
\[
\langle 0 | c_{\beta_1} c_{\alpha_1}^\dagger | 0 \rangle = \delta(\beta_1, \alpha_1) \left[ \delta(\beta_1, \alpha_1) \pm c_{\alpha_1}^\dagger c_{\beta_1} \right] | 0 \rangle = \delta(\beta_1, \alpha_1) \]
\[
\text{because } c_{\beta_1} | 0 \rangle > \gg 0.
\]

\[N - 1 \rightarrow N:\]
\[ \langle 0|c_{\beta_N} \cdots c_{\beta_1}c_{\alpha_1}^\dagger \cdots c_{\alpha_N}^\dagger |0 \rangle \]

taking \( c_{\beta_1} \) to the right

\[ = \delta(\beta_1, \alpha_1) \langle 0| c_{\beta_N} \cdots c_{\beta_2}c_{\alpha_2}^\dagger \cdots c_{\alpha_N}^\dagger |0 \rangle + \]
\[ + (\pm)^1 \delta(\beta_1, \alpha_2) \langle 0| c_{\beta_N} \cdots c_{\beta_2}c_{\alpha_1}^\dagger c_{\alpha_3} \cdots c_{\alpha_N}^\dagger |0 \rangle + \]
\[ + \cdots + \]
\[ + (\pm)^{N-1} \delta(\beta_1, \alpha_N) \langle 0| c_{\beta_N} \cdots c_{\beta_2}c_{\alpha_1}^\dagger \cdots c_{\alpha_N}^\dagger |0 \rangle = \]

condition for induction

\[ = \delta(\beta_1, \alpha_1) \sum_{P_\alpha} (\pm)^{P_\alpha} P_\alpha \left[ \delta(\beta_2, \alpha_2) \cdots \delta(\beta_N, \alpha_N) \right] + \]
\[ (\pm)^1 \delta(\beta_1, \alpha_2) \sum_{P_\alpha} (\pm)^{P_\alpha} P_\alpha \left[ \delta(\beta_2, \alpha_1) \delta(\beta_3, \alpha_3) \cdots \delta(\beta_N, \alpha_N) \right] + \]
\[ + \cdots + \]
\[ + (\pm)^{N-1} \delta(\beta_1, \alpha_N) \sum_{P_\alpha} (\pm)^{P_\alpha} P_\alpha \left[ \delta(\beta_2, \alpha_1) \delta(\beta_3, \alpha_2) \cdots \delta(\beta_N, \alpha_{N-1}) \right] \]
\[ = \sum_{P_\alpha} (\pm)^{P_\alpha} P_\alpha \left[ \delta(\beta_1, \alpha_1) \delta(\beta_2, \alpha_2) \cdots \delta(\beta_N, \alpha_N) \right] \quad \text{q.e.d.} \]

Problem A.6

1. \[
\begin{align*}
\left[ \hat{n}_\alpha, c_\beta^\dagger \right] &= c_\alpha^\dagger c_\beta^\dagger - c_\beta^\dagger c_\alpha^\dagger c_\alpha \\
&= \delta(\alpha - \beta) c_\alpha^\dagger \pm c_\alpha^\dagger c_\beta^\dagger c_\alpha - c_\beta^\dagger c_\alpha^\dagger c_\alpha \\
&= \delta(\alpha - \beta) c_\alpha^\dagger + c_\beta^\dagger c_\alpha^\dagger c_\alpha - c_\beta^\dagger c_\alpha^\dagger c_\alpha \\
&= \delta(\alpha - \beta) c_\alpha^\dagger
\end{align*}
\]

2. \[
\begin{align*}
\left[ \hat{n}_\alpha, c_\beta \right] &= c_\alpha^\dagger c_\alpha c_\beta - c_\beta c_\alpha^\dagger c_\alpha \\
&= c_\alpha^\dagger c_\alpha c_\beta - \delta(\alpha - \beta) c_\alpha \mp c_\alpha^\dagger c_\beta c_\alpha \\
&= c_\alpha^\dagger c_\alpha c_\beta - \delta(\alpha - \beta) c_\alpha - c_\alpha^\dagger c_\alpha^\dagger c_\beta \\
&= -\delta(\alpha - \beta) c_\alpha
\end{align*}
\]

These relations are equally valid for both Bosons and Fermions.

Problem A.7

\[ \hat{N} = \int d\alpha \hat{n}_\alpha. \]
We first calculate the following commutators:

\[
\left[ \hat{N}, c_\beta^\dagger \right] = \int d\alpha \left[ \hat{n}_\alpha, c_\beta^\dagger \right] \quad \text{Problem A.6} \Rightarrow \int d\alpha \, c_\alpha^\dagger \delta(\alpha - \beta) = c_\beta^\dagger, \\
\left[ \hat{N}, c_\beta \right] = \int d\alpha \left[ \hat{n}_\alpha, c_\beta \right] \quad \text{Problem A.6} \Rightarrow \int d\alpha \left[ -\delta(\alpha - \beta) c_\alpha \right] = -c_\alpha.
\]

We therefore have

\[
\hat{N} c_\beta^\dagger = c_\beta^\dagger (\hat{N} + \mathbb{1}) \\
\hat{N} c_\beta = c_\beta (\hat{N} - \mathbb{1}).
\]

1.

\[
\hat{N} \left( c_\beta^\dagger | \varphi_{\alpha_1} \cdots \right)^{(\pm)} = c_\beta^\dagger (\hat{N} + \mathbb{1}) | \varphi_{\alpha_1} \cdots \rangle^{(\pm)} = (N + 1) \left( c_\beta^\dagger | \varphi_{\alpha_1} \cdots \rangle^{(\pm)} \right)
\]

As proposed, it is an eigenstate. The eigenvalue is \(N + 1\). The name creator for \(c_\beta^\dagger\) is therefore appropriate.

2.

\[
\hat{N} \left( c_\beta | \varphi_{\alpha_1} \cdots \right)^{(\pm)} = c_\beta (\hat{N} - \mathbb{1}) | \varphi_{\alpha_1} \cdots \rangle^{(\pm)} = (N - 1) \left( c_\beta | \varphi_{\alpha_1} \cdots \rangle^{(\pm)} \right)
\]

\(c_\beta | \varphi_{\alpha_1} \cdots \rangle^{(\pm)}\) is also an eigenstate of the particle number operator \(\hat{N}\) with the eigenvalue \(N - 1\). The name annihilator for \(c_\beta\) is therefore appropriate.

**Problem A.8**

Plane waves:

\[
\varphi_k(r) = \frac{1}{\sqrt{V}} e^{i k \cdot r} = \langle r | k \rangle
\]

Kinetic energy:

One-particle basis: \(| k \sigma \rangle = | k \rangle | \sigma \rangle\)
\( \langle k \sigma | \frac{p^2}{2m} | k' \sigma' \rangle = \frac{\hbar^2 k'^2}{2m} \delta_{kk'} \delta_{\sigma \sigma'} \)

\( \sim \sum_{i=1}^{N} \frac{p_i^2}{2m} = \sum_{kk' \sigma \sigma'} \langle k \sigma | \frac{p^2}{2m} | k' \sigma' \rangle c_{k \sigma}^\dagger c_{k' \sigma'} \)

= \sum_{k \sigma} \frac{\hbar^2 k'^2}{2m} c_{k \sigma}^\dagger c_{k \sigma}

Interaction:

\( \langle k_1 \sigma_1, k_2 \sigma_2 \mid \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \mid k_3 \sigma_3, k_4 \sigma_4 \rangle \)

= \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4} \langle k_1 k_2 \mid \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \mid k_3 k_4 \rangle

The interaction is spin independent. Therefore the spin parts of the eigenstates can be evaluated directly and they yield the two Kronecker deltas. The two-particle states used are not symmetrized:

\[ \langle k_1 k_2 \mid \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \mid k_3 k_4 \rangle \]

= \int \int d^3r_1 d^3r_2 \langle k_1 k_2 \mid \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \mid r_1 r_2 \rangle \langle r_1 r_2 \mid k_3 k_4 \rangle

= \int \int d^3r_1 d^3r_2 \frac{1}{|r_1 - r_2|} \left\{ k_1^{(1)} \mid r_1^{(1)} \right\} \left\{ k_2^{(2)} \mid r_2^{(2)} \right\} \ast \left\{ r_1^{(1)} \mid k_3^{(1)} \right\} \left\{ r_2^{(2)} \mid k_4^{(2)} \right\}

= \frac{1}{V^2} \int \int d^3r_1 d^3r_2 \frac{1}{|r_1 - r_2|} e^{i(k_1 - k_1) \cdot r_1} e^{i(k_2 - k_2) \cdot r_2}

= \delta_{k_1 + k_2, k_3 + k_4} \frac{1}{V} \int d^3r \frac{1}{r} e^{i(k_1 - k_1) \cdot r}

The last step is obtained by introducing the centre of mass and relative coordinates. We get the Kronecker delta when the centre of mass part is integrated out. The remaining integral is calculated using a convergence ensuring factor \( \alpha \):
Then the interaction matrix element reads as

\[
\left\langle k_1 \sigma_1, k_2 \sigma_2 \left| \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \right| k_3 \sigma_3, k_4 \sigma_4 \right\rangle
= \delta_{\sigma_1 \sigma_3} \delta_{\sigma_2 \sigma_4} \delta_{k_1 + k_2, k_3 + k_4} \frac{4\pi}{V |k_3 - k_1|^2}
\]

Interaction operator in second quantization:

\[
\frac{1}{2} \sum_{i \neq j} \frac{1}{|\hat{r}_i - \hat{r}_j|} =
\]

\[
= \frac{1}{2} \sum_{k_1 \sigma_1, k_2 \sigma_2, k_3 \sigma_3, k_4 \sigma_4} \left\langle k_1 \sigma_1, k_2 \sigma_2 \left| \frac{1}{|\hat{r}(1) - \hat{r}(2)|} \right| k_3 \sigma_3, k_4 \sigma_4 \right\rangle *
\]

\[
* \chi_{k_1 \sigma_1} \chi_{k_2 \sigma_2} \chi_{k_4 \sigma_4} \chi_{k_3 \sigma_3}
\]

\[
= \frac{1}{2} \sum_{k_1 \sigma_1, k_2 \sigma_2, k_3} \frac{4\pi}{V |k_3 - k_1|^2} \chi_{k_1 \sigma_1} \chi_{k_2 \sigma_2} \chi_{k_1 + k_2 - k_3 \sigma_2} \chi_{k_3 \sigma_3}
\]

We further set

\[
k_1 \rightarrow k + q ; \quad k_2 \rightarrow p - q ; \quad k_3 \rightarrow k ; \quad \sigma_1 \rightarrow \sigma ; \quad \sigma_2 \rightarrow \sigma'
\]

and have the Hamiltonian of the \(N\)-electron system in second quantization:

\[
H_N = \sum_{k \sigma} \varepsilon_0(k) \chi_{k \sigma} \chi_{k \sigma} + \frac{1}{2} \sum_{kpq \sigma \sigma'} v_0(q) \chi_{k + q \sigma} \chi_{p - q \sigma} \chi_{p \sigma} \chi_{k \sigma}
\]

\[
\varepsilon_0(k) = \frac{\hbar^2 k^2}{2m} ; \quad v_0(q) = \frac{e^2}{\varepsilon_0 V q^2}
\]
Problem A.9

\[ \hat{n}_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma} \implies [\hat{n}_{k\sigma}, \hat{n}_{k'\sigma'}] = 0 \]

Therefore the kinetic energy commutes in any case with \( \hat{N} \). Therefore we only have to calculate the commutator with the interaction:

\[
\frac{1}{2} \sum_{k,p,q} v_0(q) \left[ c_{k+q\sigma}^\dagger c_{p-q\sigma'}^\dagger c_{p\sigma'} c_{k\sigma}, c_{k'\sigma'} c_{k^\prime\sigma^\prime} \right] -
\]

\[
= \frac{1}{2} \sum_{k,p,q} v_0(q) \left\{ \delta_{kk'} \delta_{\sigma\sigma'} c_{k+q\sigma}^\dagger c_{p-q\sigma'} c_{k\sigma} c_{k'\sigma'} -
\right.
\]

\[
- \delta_{p,k} \delta_{\sigma\sigma'} c_{k+q\sigma} c_{p-q\sigma'} c_{k\sigma} c_{k'\sigma'} +
\]

\[
+ \delta_{p-k} \delta_{\sigma\sigma'} c_{k'\sigma'} c_{k+q\sigma} c_{p\sigma'} c_{k\sigma} -
\]

\[
\delta_{k-k'} \delta_{\sigma\sigma'} c_{k'\sigma'} c_{p-q\sigma'} c_{p\sigma'} c_{k\sigma}
\right\}
\]

\[
= \frac{1}{2} \sum_{k,p,q} v_0(q) \left\{ c_{k+q\sigma}^\dagger c_{p-q\sigma'} c_{p\sigma'} c_{k\sigma} - c_{k+q\sigma}^\dagger c_{p-q\sigma'} c_{k\sigma} c_{p\sigma'} +
\right.
\]

\[
+ c_{p-q\sigma} c_{k+q\sigma} c_{p\sigma'} c_{k\sigma} - c_{k+q\sigma}^\dagger c_{p-q\sigma'} c_{p\sigma'} c_{k\sigma}
\right\} = 0
\]

\[ [H_N, \hat{N}] = 0 \]

\( H_N \) and \( \hat{N} \) have common eigenstates. The particle number is a conserved quantity.

Problem A.10

1. Hamiltonian of the two-particle system:

\[ H = H_1 + H_2 = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) + V(x_1) + V(x_2) \]

Unsymmetrized eigenstate:

\[ |\varphi_{\alpha_1, \alpha_2} \rangle = |\varphi_{\alpha_1}^{(1)} \rangle |\varphi_{\alpha_2}^{(2)} \rangle \]

Position space representation:

\[ \langle x_1 x_2 | \varphi_{\alpha_1, \alpha_2} \rangle = \varphi_n(x_1) \varphi_m(x_2) \chi_S(m_S^{(1)}) \chi_S(m_S^{(2)}) \]

\( \chi_S \): spin function (identical particles have the same spin \( S \))

\( \alpha_1 = (n, m_S); \quad \alpha_2 = (m, m_S') \)
2. Solution of the one-particle problem:

\[
\left( -\frac{\hbar^2}{2m} \Delta + V(x) \right) \varphi(x) = E \varphi(x)
\]

We first have

\[\varphi(x) \equiv 0 \text{ for } x < 0 \text{ and } x > a\]

For \(0 \leq x \leq a\) we have to solve

\[-\frac{\hbar^2}{2m} \Delta \varphi(x) = E \varphi(x)\]

Ansatz for solution:

\[\varphi(x) = c \sin(\gamma_1 x + \gamma_2)\]

Boundary conditions:

\[\varphi(0) = 0 \implies \gamma_2 = 0,\]
\[\varphi(a) = 0 \implies \gamma_1 = n\frac{\pi}{a}; \quad n = 1, 2, 3, \ldots\]

Energy eigenvalues:

\[E = \frac{\hbar^2}{2m} \gamma_1^2 \implies E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2; \quad n = 1, 2, \ldots\]

Eigen functions:

\[\varphi_n(x) = c \sin \left( n\frac{\pi}{a} x \right),\]
\[1 \equiv c^2 \int_0^a \sin^2 \left( n\frac{\pi}{a} x \right) \, dx \implies c = \sqrt{\frac{2}{a}},\]
\[\varphi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \left( n\frac{\pi}{a} x \right) & \text{for } 0 \leq x \leq a, \\ 0 & \text{otherwise} \end{cases}\]

3. Two-particle problem:

\[|\varphi_{q_1} \varphi_{q_2}|^{\pm} \rightarrow \frac{1}{\sqrt{2}} \left\{ \varphi_n(x_1) \varphi_m(x_2) \chi_S(m^{(1)}_S) \chi_S(m^{(2)}_S) \pm \varphi_n(x_2) \varphi_m(x_1) \chi_S(m^{(2)}_S) \chi_S(m^{(1)}_S) \right\}\]
(+) Bosons,
(−): Fermions: \((n, m_s) \neq (m, m_s')\) because of Pauli’s principle.

4. Ground state energy of the \(N\)-particle system:
   Bosons:
   All particles in the \(n = 1\)-state:
   \[
   E_0 = N \frac{\hbar^2 \pi^2}{2ma^2}.
   \]
   Fermions:
   \[
   E_0 = 2 \sum_{n=1}^{N} \frac{\hbar^2 \pi^2}{2ma^2} n^2 \approx \frac{\hbar^2 \pi^2}{2ma^2} \frac{N^3}{24}
   \]
   with
   \[
   \sum_{n=1}^{N} n^2 \approx \int_{1}^{N} n^2 dn = \frac{1}{3} \left( \frac{N^3}{8} - 1 \right) \approx \frac{N^3}{24}
   \]

Problem A.11

1. Non-interacting, identical Bosons or Fermions:
   \[
   H = \sum_{i=1}^{N} H_1^{(i)}
   \]
   Eigenvalue equation:
   \[
   H_1^{(i)} \psi_r^{(i)} = \epsilon_r \psi_r^{(i)}, \quad \langle \psi_r^{(i)} | \psi_r^{(i)} \rangle = \delta_{rs}
   \]
   One-particle operator in second quantization:
   \[
   H = \sum_{r,s} \langle \psi_r | H_1 | \psi_s \rangle a_r^\dagger a_s = \sum_{r,s} \epsilon_r \delta_{rs} a_r^\dagger a_s
   \]
   \[
   \implies H = \sum_{r} \epsilon_r a_r^\dagger a_r = \sum_{r} \epsilon_r \hat{n}_r.
   \]

2. Unnormalized density matrix of the grand canonical ensemble:
   \[
   \rho = \exp[-\beta(H - \mu \hat{N})],
   \]
   \[
   \hat{N} = \sum_{r} \hat{n}_r
   \]
   The normalized Fock states
are the eigenstates of $\hat{n}_r$ and therefore also of $\hat{N}$ und $H$:

$$H |N; n_1 \ldots \rangle^{(e)} = \left( \sum_{r} \epsilon_r n_r \right) |N; n_1 \ldots \rangle^{(e)},$$

$$\hat{N} |N; n_1 \ldots \rangle^{(e)} = N |N; n_1 \ldots \rangle^{(e)}$$

That is why it is convenient to build the trace with these Fock states:

$$\langle N; n_1 n_2 \ldots | \exp \left[ -\beta (H - \mu \hat{N}) \right] | N; n_1 n_2 \ldots \rangle^{(e)} = \exp \left[ -\beta \sum_{r} (\epsilon_r - \mu) n_r \right]$$

with $\sum_{r} n_r = N$

From this follows:

$$\text{Tr} \rho = \sum_{N=0}^{\infty} \left( \sum_{\{n_r\}} \text{exp} \left[ -\beta \sum_{r} (\epsilon_r - \mu) n_r \right] \right)$$

$$= \sum_{N=0}^{\infty} \left( \prod_{r} e^{-\beta(\epsilon_r - \mu)n_r} \right)$$

$$= \left( \sum_{n_1} e^{-\beta n_1(\epsilon_1 - \mu)} \right) \left( \sum_{n_2} e^{-\beta n_2(\epsilon_2 - \mu)} \right) \ldots$$

Grand canonical partition function:

$$\Xi(T, V, \mu) = \text{Tr} \rho = \prod_{r} \left( \sum_{n_r} e^{-\beta n_r(\epsilon_r - \mu)} \right)$$

Bosons ($n_r = 0, 1, 2, \ldots$):

$$\Xi_B(T, V, \mu) = \prod_{r} \frac{1}{1 - e^{-\beta(\epsilon_r - \mu)}}$$

Fermions ($n_r = 0, 1$):

$$\Xi_F(T, V, \mu) = \prod_{r} (1 + e^{-\beta(\epsilon_r - \mu)})$$
3. Expectation value of the particle number:

\[ \langle \hat{N} \rangle = \frac{1}{\Xi} \text{Sp}(\rho \hat{N}) \]

To build the trace Fock states are preferred because they are the eigenstates of \( \hat{N} \):

\[
\langle \hat{N} \rangle = \frac{1}{\Xi} \sum_{N=0}^{\infty} \sum_{\{n_r\}}^\infty N \exp \left[ -\beta \sum_r (\epsilon_r - \mu)n_r \right]
\]

\[ = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \Xi \]

With part 2

\[
\frac{\partial}{\partial \mu} \ln \Xi_B = \frac{\partial}{\partial \mu} \left\{ -\sum_r \ln \left[ 1 - e^{-\beta(\epsilon_r - \mu)} \right] \right\}
\]

\[ = -\sum_r \frac{-\beta e^{-\beta(\epsilon_r - \mu)}}{1 - e^{-\beta(\epsilon_r - \mu)}} \]

\[ = \beta \sum_r \frac{1}{e^{\beta(\epsilon_r - \mu)} - 1} \]

\[
\frac{\partial}{\partial \mu} \ln \Xi_F = \frac{\partial}{\partial \mu} \left\{ \sum_r \ln \left[ 1 + e^{-\beta(\epsilon_r - \mu)} \right] \right\}
\]

\[ = \beta \sum_r \frac{e^{-\beta(\epsilon_r - \mu)}}{1 + e^{-\beta(\epsilon_r - \mu)}} \]

\[ = \beta \sum_r \frac{1}{e^{\beta(\epsilon_r - \mu)} + 1} \]

This means

\[ \langle \hat{N} \rangle = \begin{cases} 
\sum_r \frac{1}{e^{\beta(\epsilon_r - \mu)} - 1} & \text{Bosons} \\
\sum_r \frac{1}{e^{\beta(\epsilon_r - \mu)} + 1} & \text{Fermions}
\end{cases} \]

4. Internal energy:

\[ U = \langle H \rangle = \frac{1}{\Xi} \text{Tr}(\rho H) \]

Fock states are the eigenstates of \( H \) and therefore appropriate for building the trace required here:
\[ U = \frac{1}{\Xi} \sum_{N=0}^{\infty} \sum_{\{n_r\}} \left[ \left( \sum_i \epsilon_i n_i \right) e^{-\beta \sum_r (\epsilon_r - \mu) n_r} \right] \]

\[ = -\frac{\partial}{\partial \beta} \ln \Xi + \mu \langle \hat{N} \rangle \]

\[ -\frac{\partial}{\partial \beta} \ln \Xi_B = \sum_r \frac{(\epsilon_r - \mu)e^{-\beta(\epsilon_r - \mu)}}{1 - e^{-\beta(\epsilon_r - \mu)}} \]

\[ = -\mu \langle \hat{N} \rangle + \sum_r \frac{\epsilon_r}{e^{\beta(\epsilon_r - \mu)} - 1}, \]

\[ -\frac{\partial}{\partial \beta} \ln \Xi_F = -\sum_r \frac{-(\epsilon_r - \mu)e^{-\beta(\epsilon_r - \mu)}}{1 + e^{-\beta(\epsilon_r - \mu)}} \]

\[ = -\mu \langle \hat{N} \rangle + \sum_r \frac{\epsilon_r}{e^{\beta(\epsilon_r - \mu)} + 1} \]

We finally get

\[ U = \begin{cases} \sum_r \frac{\epsilon_r}{e^{\beta(\epsilon_r - \mu)} - 1} & \text{Bosons} \\ \sum_r \frac{\epsilon_r}{e^{\beta(\epsilon_r - \mu)} + 1} & \text{Fermions}. \end{cases} \]

5. Fock states are also eigenstates of the occupation number operator:

\[ \langle \hat{n}_i \rangle = \frac{1}{\Xi} \text{Tr}(\rho \hat{n}_i) \]

\[ = \frac{1}{\Xi} \sum_{N=0}^{\infty} \sum_{\{n_r\}} \left[ n_i e^{-\beta \sum_r (\epsilon_r - \mu) n_r} \right] \]

\[ = -\frac{1}{\beta} \partial_{\epsilon_i} \ln \Xi, \]

\[ -\frac{1}{\beta} \partial_{\epsilon_i} \ln \Xi_B = +\frac{1}{\beta} \sum_r \frac{+\beta e^{-\beta(\epsilon_r - \mu)} \partial \epsilon_r}{1 - e^{-\beta(\epsilon_r - \mu)}} \partial \epsilon_i \]

\[ = \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} \quad \text{(Bose function)}, \]

\[ -\frac{1}{\beta} \partial_{\epsilon_i} \ln \Xi_F = -\frac{1}{\beta} \sum_r \frac{-\beta e^{-\beta(\epsilon_r - \mu)} \partial \epsilon_r}{1 + e^{-\beta(\epsilon_r - \mu)}} \partial \epsilon_i \]

\[ = \frac{1}{e^{\beta(\epsilon_i - \mu)} + 1} \quad \text{(Fermi function)}. \]

It follows:
\[ \langle \hat{n}_i \rangle = \begin{cases} \{ \exp[\beta(\epsilon_i - \mu)] - 1 \}^{-1} & \text{Bosons,} \\ \{ \exp[\beta(\epsilon_i - \mu)] + 1 \}^{-1} & \text{Fermions.} \end{cases} \]

One immediately recognizes by comparison with the earlier problems:

\[ \langle \hat{N} \rangle = \sum_r \langle \hat{n}_r \rangle; \quad U = \sum_r \epsilon_r \langle \hat{n}_r \rangle \]

**Problem B.1**

\[
\rho \int_0^\beta d\lambda \dot{A}(t - i\lambda\hbar) = \rho \int_0^\beta d\lambda \frac{i}{\hbar} \frac{d}{d\lambda} A(t - i\lambda\hbar) = \\
= \frac{i}{\hbar} \rho \left[ A(t - i\hbar\beta) - A(t) \right] = \\
= \frac{i}{\hbar} \rho \left[ e^{\frac{i}{\hbar}(t - i\hbar\beta)\mathcal{H}} A(t) e^{-\frac{i}{\hbar}(t - i\hbar\beta)\mathcal{H}} - A(t) \right] = \\
= \frac{i}{\hbar} \rho \left( e^{\beta\mathcal{H}} A(t) e^{-\beta\mathcal{H}} - A(t) \right) = \\
= \frac{i}{\hbar} \left[ e^{-\beta\mathcal{H}} e^{\beta\mathcal{H}} A(t) e^{-\beta\mathcal{H}} - \rho A(t) \right]_\mathcal{H} = \\
= \frac{i}{\hbar} \rho (A(t) - \rho A(t)) = \frac{i}{\hbar} [A(t), \rho]_\mathcal{H} \quad \text{q.e.d.}
\]

**Problem B.2**

\[
\left[ [A(t), B(t')] \right] = \text{Sp} \left\{ \rho [A(t), B(t')]_\mathcal{H} \right\} = \\
= \text{Sp} \left\{ \rho A(t) B(t') - \rho B(t') A(t) \right\} = \\
= \text{Sp} \left\{ B(t') \rho A(t) - \rho B(t') A(t) \right\} = \\
= \text{Sp} \left\{ [B(t'), \rho]_\mathcal{H} A(t) \right\}
\]

(cyclic invariance of trace).

Substitute Kubo identity:

\[
\langle \langle A(t); B(t') \rangle \rangle^{\text{Kubo}} = -i \Theta(t - t') \left[ [A(t), B(t')] \right] = \\
= -\hbar \Theta(t - t') \int_0^\beta d\lambda \text{Sp} \left\{ \rho \dot{B}(t' - i\lambda\hbar) A(t) \right\} = \\
= -\hbar \Theta(t - t') \int_0^\beta d\lambda \supopt{\dot{B}(t' - i\lambda\hbar) A(t)} \quad \text{q.e.d.}
\]
Problem B.3

\[
\langle B(0)A(t + i\beta) \rangle = \frac{1}{2\pi} \text{Sp} \left\{ e^{-\beta\mathcal{H}} B e^{\frac{i}{\hbar} \mathcal{H}(t + i\beta)} A e^{-\frac{i}{\hbar} \mathcal{H}(t + i\beta)} \right\}
\]

Here the cyclic invariance of trace has been used several times.

Problem B.4

1. \( t - t' > 0 \):
   The integrand has a pole at \( x = x_0 = -i0^+ \). Residue:
   \[
c_{1} = \lim_{x \to x_0} \left( x - x_0 \right) e^{-ix(t-t')} \frac{e^{-ix(t-t')}}{x + i0^+} = \lim_{x \to x_0} e^{-ix(t-t')} = 1
   \]
   Since \( t - t' > 0 \), the semicircle closes in the lower half-plane; then the exponential function sees to it that the contribution from the semicircle vanishes. The contour runs mathematically negatively. Therefore it follows that
   \[
   \Theta(t - t') = \frac{i}{2\pi} (-2\pi i)1 = 1
   \]

2. \( t - t' < 0 \):
   In order that no contribution from the semicircle appears, now it closes in the upper half-plane. Then it follows that
   \[
   \Theta(t - t') = 0
   \]
   as there is no pole in the region of integration.

Problem B.5

\[
f(\omega) = \int_{-\infty}^{+\infty} dt \, \tilde{f}(t)e^{i\omega t}
\]
Let the integral exist for real $\omega$. Set

$$\omega = \omega_1 + i \omega_2$$

$$\implies f(\omega) = \int_{-\infty}^{+\infty} dt \, \bar{f}(t) e^{i\omega_1 t} e^{-\omega_2 t}$$

1. $\bar{f}(t) = 0$ for $t < 0$:

$$\implies f(\omega) = \int_{0}^{\infty} dt \, \bar{f}(t) e^{i\omega_1 t} e^{-\omega_2 t}$$

Converges for all $\omega_2 > 0$, therefore it is possible to analytically continue in the upper half-plane.

2. $\bar{f}(t) = 0$ for $t > 0$:

$$\implies f(\omega) = \int_{-\infty}^{0} dt \, \bar{f}(t) e^{i\omega_1 t} e^{-\omega_2 t}$$

Converges for all $\omega_2 < 0$, therefore it is possible to analytically continue in the lower half-plane.

**Problem B.6**

With

$$\mathcal{H}_0 = \sum_{k\sigma} (\varepsilon(k) - \mu) a_{k\sigma}^\dagger a_{k\sigma}$$

we first calculate

$$[a_{k\sigma}, \mathcal{H}_0]_- = \sum_{k'\sigma'} (\varepsilon(k') - \mu) [a_{k\sigma}, a_{k'\sigma'}^\dagger, a_{k'\sigma'}]_- =$$

$$= \sum_{k'\sigma'} (\varepsilon(k') - \mu) \delta_{kk'} \delta_{\sigma\sigma'} a_{k'\sigma'} = (\varepsilon(k) - \mu) a_{k\sigma}.$$

The interaction term requires more effort:
\[ [a_{k\sigma}, \mathcal{H} - \mathcal{H}_0]_- = \frac{1}{2} \sum_{k'pq} \sigma' \sigma'' v_{k'p}(q) \left[ a_{k\sigma}, a_{k'+q\sigma'}^\dagger a_{p-q\sigma'}^\dagger a_{p\sigma'} a_{k'\sigma''} \right]_- \]

\[ = \frac{1}{2} \sum_{k'pq} \sigma' \sigma'' v_{k'p}(q) \left( \delta_{\sigma\sigma''} \delta_{k,k'} q a_{p-q\sigma'}^\dagger a_{p\sigma'} a_{k'\sigma''} - \delta_{\sigma\sigma'} \delta_{kp-q} a_{k+q\sigma'}^\dagger a_{p\sigma'} a_{k'\sigma''} \right) \]

\[ = \frac{1}{2} \sum_{pq\sigma''} v_{k-pq}(q) a_{p-q\sigma'}^\dagger a_{p\sigma'} a_{k-q\sigma} \]

\[ - \frac{1}{2} \sum_{k'q\sigma''} v_{k'k+q}(q) a_{k'+q\sigma'}^\dagger a_{k+q\sigma} a_{k'\sigma''} \]

In the first summand:

\[ q \rightarrow -q: \quad v_{k+q,p}(-q) = v_{p,k+q}(q) \]

In the second summand:

\[ k' \rightarrow p: \quad \sigma'' \rightarrow \sigma' \]

Then the two summands can be combined:

\[ [a_{k\sigma}, \mathcal{H} - \mathcal{H}_0]_- = \sum_{pq\sigma'} v_{p,k+q}(q) a_{p+q\sigma'}^\dagger a_{p\sigma'} a_{k+q\sigma} \]

Equation of motion:

\[ (E - \varepsilon(k) + \mu) G_{k\sigma}^{\text{ret}}(E) = \hbar + \sum_{pq\sigma'} v_{p,k+q}(q) \langle \langle a_{p+q\sigma'}^\dagger a_{p\sigma'} a_{k+q\sigma} ; a_{k\sigma}^\dagger \rangle \rangle_{E}^{\text{ret}} \]

Problem B.7

\[ \mathcal{H} = \sum_{k\sigma} \varepsilon(k) a_{k\sigma}^\dagger a_{k\sigma} - \mu \hat{N} = \sum_{k\sigma} (\varepsilon(k) - \mu) a_{k\sigma}^\dagger a_{k\sigma} \]

One can easily calculate
\[ [a_{k\sigma}, \mathcal{H}]_{-} = \sum_{k'\sigma'} (\epsilon(k') - \mu)[a_{k\sigma}', a_{k'\sigma'}^\dagger]_{-} \]
\[ = \sum_{k'\sigma'} (\epsilon(k') - \mu)\delta_{kk'}\delta_{\sigma\sigma'}a_{k'\sigma'} \]
\[ = (\epsilon(k) - \mu)a_{k\sigma} \]

From this it further follows that
\[ [[a_{k\sigma}, \mathcal{H}]_{-}, \mathcal{H}]_{-} = (\epsilon(k) - \mu)[a_{k\sigma}, \mathcal{H}]_{-} = (\epsilon(k) - \mu)^2a_{k\sigma} \]

For the spectral moments this means
\[
M_{k\sigma}^{(0)} = \langle [a_{k\sigma}, a_{k\sigma}^\dagger]_+ \rangle = 1
\]
\[
M_{k\sigma}^{(1)} = \langle [[a_{k\sigma}, \mathcal{H}]_{-}, a_{k\sigma}^\dagger]_+ \rangle = (\epsilon(k) - \mu)\langle [a_{k\sigma}, a_{k\sigma}^\dagger]_+ \rangle = (\epsilon(k) - \mu)
\]
\[
M_{k\sigma}^{(2)} = \langle [[[a_{k\sigma}, \mathcal{H}]_{-}, \mathcal{H}]_{-}, a_{k\sigma}^\dagger]_+ \rangle = (\epsilon(k) - \mu)^2\langle [a_{k\sigma}, a_{k\sigma}^\dagger]_+ \rangle = (\epsilon(k) - \mu)^2
\]

Then by complete induction one gets immediately
\[
M_{k\sigma}^{(n)} = (\epsilon(k) - \mu)^n; \quad n = 0, 1, 2, \ldots
\]

The relationship (B.99) with the spectral density,
\[
M_{k\sigma}^{(n)} = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE E^n S_{k\sigma}(E)
\]
then leads to the solution:
\[ S_{k\sigma}(E) = \hbar\delta(E - \epsilon(k) + \mu) \]

**Problem B.8**

1. Creation and annihilation operators for Cooper pairs:
\[ b_k^\dagger = a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger; \quad b_k = a_{-k\downarrow} a_{k\uparrow} \]
Fundamental commutation relations
(a)

\[ [b_k, b_{k'}]_- = [b^\dagger_k, b^\dagger_{k'}]_- = 0 \]

because the creation and annihilation operators of fermions anticommute among themselves. Therefore products of even number of Fermion construction operators then commute.

(b)

\[ \left[ b^\dagger_k, b^\dagger_{k'} \right]_- = \left[ a^\dagger_{-k\downarrow} a_{k\uparrow}, a^\dagger_{k\uparrow} a^\dagger_{-k'\downarrow} \right]_- = \delta_{kk'} (1 - \hat{n}_{-k\downarrow} - \hat{n}_{k\uparrow}) \]

Therefore the Cooper pairs inspite of their total spin being zero are not real Bosons because only two of the three basic commutation relations are satisfied.

(c) Since

\[ [b_k, b_{k'}]_+ = 2b_k b_{k'} \neq 0 \text{ for } k \neq k' \]

they are naturally also not real Fermions, either, even though

\[ (b^\dagger_k)^2 = b^2_k = 0 \]

is valid for them.

2. Equation of motion:

\[ \left[ a_{k\sigma}, H^\ast \right]_- = \sum_{p\sigma'} t(p) \left[ a_{k\sigma}, a^\dagger_{p\sigma}, a_{p\sigma'} \right]_- \]

\[ - \Delta \sum_p \left[ a_{k\sigma}, a_{-p\downarrow} a_{p\uparrow} + a^\dagger_{p\uparrow} a^\dagger_{-p\downarrow} \right]_- \]

\[ = \sum_{p\sigma'} t(p) \delta_{\sigma\sigma'} \delta_{kp} a_{p\sigma'} \]

\[ - \Delta \sum_p \left( \delta_{kp} \delta_{\sigma\uparrow} a^\dagger_{-p\downarrow} - \delta_{k-p} \delta_{\sigma\downarrow} a^\dagger_{p\uparrow} \right) \]

\[ = t(k) a_{k\sigma} - \Delta(\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}) a^\dagger_{-k-\sigma}, \]

\[ z_{\sigma} = \begin{cases} +1, & \text{for } \sigma = \uparrow, \\ -1, & \text{for } \sigma = \downarrow \end{cases} \]

Then the equation of motion reads as
\[(E - t(k))G_{k\sigma}(E) = \hbar - \Delta z_\sigma \langle \langle a_{-k-\sigma}^\dagger; a_{k\sigma}^\dagger \rangle \rangle. \]

The Green’s function on the right-hand side prevents a direct solution. Therefore we set up the corresponding equation of motion for this:

\[\begin{bmatrix} a_{-k-\sigma}^\dagger, H^* \end{bmatrix} = -t(-k)a_{-k-\sigma}^\dagger - \Delta \sum_p \left[ a_{-k-\sigma}^\dagger, a_{-p\uparrow} a_{p\uparrow} \right]_-
\]
\[= -t(k)a_{-k-\sigma}^\dagger - \Delta \sum_p \left( \delta_{kp}\delta_{-\sigma\uparrow} a_{p\uparrow}^\dagger - \delta_{-kp}\delta_{-\sigma\uparrow} a_{-p\uparrow} \right)
\]
\[= -t(k)a_{-k-\sigma}^\dagger - \Delta z_\sigma a_{k\sigma} \]

This gives us the following equation of motion:

\[(E + t(k))\langle \langle a_{-k-\sigma}^\dagger; a_{k\sigma}^\dagger \rangle \rangle = -\Delta z_\sigma G_{k\sigma}(E)
\]
\[\langle \langle a_{-k-\sigma}^\dagger; a_{k\sigma}^\dagger \rangle \rangle = -\frac{z_\sigma \Delta}{E + t(k)} G_{k\sigma}(E) \]

This is substituted in the equation of motion for \(G_{k\sigma}^{\text{ret}}(E)\):

\[\left( E - t(k) - \frac{\Delta^2}{E + t(k)} \right) G_{k\sigma}(E) = \hbar \]

Excitation energies:

\[E(k) = \pm \sqrt{t^2(k) + \Delta^2} \quad \text{as } t \to 0 \quad \Delta \quad \text{(Energy gap)}. \]

Green’s function:

\[G_{k\sigma}(E) = \frac{\hbar(E + t(k))}{E^2 - E^2(k)} \]

Imposing the boundary conditions:

\[G_{k\sigma}^{\text{ret}}(E) = \frac{\hbar}{2E(k)} \left[ \frac{t(k) + E(k)}{E - E(k) + i0^+} - \frac{t(k) - E(k)}{E + E(k) + i0^+} \right] \]

3. For \(\Delta\) we need the expectation value:

\[\langle \langle a_{k\uparrow}^\dagger, a_{-k\uparrow}^\dagger \rangle \rangle \]

Its determination is via spectral theorem and the Green’s function used in part 2.
\begin{align*}
\langle a_{-k}^\dagger; a_{k}^\dagger \rangle &= \frac{-\Delta}{E + i(t(k))} G_{k}^\dagger(E) = \frac{-\hbar \Delta}{E^2 - E^2(k)} \\

\text{Taking into account the boundary conditions we obtain for the corresponding retarded function:} \\
\langle a_{-k}^\dagger; a_{k}^\dagger \rangle_{E}^{\text{ret}} &= \frac{\hbar \Delta}{2E(k)} \left[ \frac{1}{E + E(k) + i0^+} - \frac{1}{E - E(k) + i0^+} \right] \\

\text{The spectral density corresponding to this} \\
S_{-k_\downarrow; k_\uparrow}(E) &= \frac{\hbar \Delta}{2E(k)} [\delta(E + E(k)) - \delta(E - E(k))] \\

\text{Spectral theorem:} \\
\langle a_{k_\uparrow}^\dagger a_{-k_\downarrow}^\dagger \rangle &= \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \frac{S_{-k_\downarrow; k_\uparrow}(E)}{\exp(\beta E) + 1} \\
&= \frac{\Delta}{2E(k)} \left( \frac{1}{\exp(-\beta E(k)) + 1} - \frac{1}{\exp(\beta E(k)) + 1} \right) \\
&= \frac{\Delta}{2E(k)} \tanh \left( \frac{1}{2} \beta E(k) \right) \\

\text{Then we finally get} \\
\Delta &= \frac{1}{2} \Delta V \sum_{k} \frac{\tanh \left( \frac{1}{2} \beta \sqrt{t^2(k) + \Delta^2} \right)}{\sqrt{t^2(k) + \Delta^2}} \\

\Delta = \Delta(T) \Rightarrow \text{Energy gap is } T \text{ dependent. Special case:} \\
T \to 0 \Rightarrow \tanh \left( \frac{1}{2} \beta \sqrt{t^2(k) + \Delta^2} \right) \to 1
\end{align*}
Problem B.9

1. We first show that

\[
\begin{cases}
(t^2(k) + \Delta^2)^{n}, & \text{if } p = 2n \\
(t^2(k) + \Delta^2)^{n}(t(k) a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger), & \text{if } p = 2n + 1
\end{cases}
\]

is valid.

Here \( n = 0, 1, 2, \ldots \). We prove this by complete induction.

Induction’s start \( p = 1, 2 \):

\[
\left[a_{k\sigma}, H^*\right]_\sigma = t(k) a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger \quad \text{(see Problem B.8)}
\]

\[
\left[a_{k\sigma}, H^*\right]_\sigma, H^* \right)_\sigma = t(k) \left( t(k) a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger \right)
- z_\sigma \Delta \left( -t(k) a_{k-\sigma}^\dagger - z_\sigma \Delta a_{k\sigma} \right)
= (t^2(k) + \Delta^2) a_{k\sigma}.
\]

Induction’s end \( p \to p + 1 \):

(a) \( p \) even:

\[
\begin{aligned}
\underbrace{\ldots \left[ a_{k\sigma}, \left[ a_{k\sigma}, H^* \right]_\sigma, H^* \right]_\sigma, \ldots, H^* \right]_\sigma}_{(p+1)-\text{fold commutator}} \\
&= (t^2 + \Delta^2)^{\frac{p}{2}} \left[ a_{k\sigma}, H^* \right]_\sigma \\
&= (t^2 + \Delta^2)^{\frac{p}{2}} \left( t a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger \right)
\end{aligned}
\]

(b) \( p \) odd:

\[
\begin{aligned}
\underbrace{\ldots \left[ a_{k\sigma}, \left[ a_{k\sigma}, H^* \right]_\sigma, H^* \right]_\sigma, \ldots, H^* \right]_\sigma}_{(p+1)-\text{fold commutator}} \\
&= (t^2 + \Delta^2)^{\frac{p-1}{2}} \left[ t a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger, H^* \right]_\sigma \\
&= (t^2 + \Delta^2)^{\frac{p-1}{2}} \left[ t(t a_{k\sigma} - z_\sigma \Delta a_{k-\sigma}^\dagger) \\
&\quad - z_\sigma \Delta (-t a_{k-\sigma}^\dagger - \Delta z_\sigma a_{k\sigma}) \right] \\
&= (t^2 + \Delta^2)^{\frac{p+1}{2}} a_{k\sigma} \quad \text{q.e.d.}
\end{aligned}
\]
For the spectral moments of the one-electron spectral density we directly get

\[ M_{k\sigma}^{(2n)} = (t^2(k) + \Delta^2)^n, \]
\[ M_{k\sigma}^{(2n+1)} = (t^2(k) + \Delta^2)^n t(k). \]

2. We use

\[ M_{k\sigma}^{(n)} = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE E^n S_{k\sigma}(E) \]

Determining equations from the first four spectral moments:

\[ \alpha_{1\sigma} + \alpha_{2\sigma} = \hbar, \]
\[ \alpha_{1\sigma} E_{1\sigma} + \alpha_{2\sigma} E_{2\sigma} = \hbar t, \]
\[ \alpha_{1\sigma} E_{1\sigma}^2 + \alpha_{2\sigma} E_{2\sigma}^2 = \hbar (t^2 + \Delta^2), \]
\[ \alpha_{1\sigma} E_{1\sigma}^3 + \alpha_{2\sigma} E_{2\sigma}^3 = \hbar (t^2 + \Delta^2)t \]

Reformulating them:

\[ \alpha_{2\sigma} (E_{2\sigma} - E_{1\sigma}) = \hbar (t - E_{1\sigma}), \]
\[ \alpha_{2\sigma} E_{2\sigma} (E_{2\sigma} - E_{1\sigma}) = \hbar [t^2 + \Delta^2 - t E_{1\sigma}], \]
\[ \alpha_{2\sigma} E_{2\sigma}^2 (E_{2\sigma} - E_{1\sigma}) = \hbar [(t^2 + \Delta^2)(t - E_{1\sigma})] \]

After division follows:

\[ E_{2\sigma}^2 = t^2 + \Delta^2 \quad \Rightarrow \quad E_{2\sigma}(k) = +\sqrt{t^2(k) + \Delta^2} \equiv E(k) \]

This has the further consequence:

\[ E(k) = \frac{t^2 + \Delta^2 - t E_{1\sigma}}{t - E_{1\sigma}} = t + \frac{\Delta^2}{t - E_{1\sigma}} \]
\[ \Rightarrow \quad (E(k) - t(k))^{-1} \Delta^2 = t(k) - E_{1\sigma}(k) \]
\[ \Rightarrow \quad E_{1\sigma}(k) = t(k) - \frac{\Delta^2}{E(k) - t(k)} = \frac{E(k)t(k) - E^2(k)}{E(k) - t(k)} \]
\[ \Rightarrow \quad E_{1\sigma}(k) = -E(k) = -E_{2\sigma}(k) \]

Spectral weights:
\[
\alpha_2(\mathbf{k})2E(\mathbf{k}) = \hbar(t(\mathbf{k}) + E(\mathbf{k}))
\]
\[
\Rightarrow \quad \alpha_2(\mathbf{k}) = \frac{\hbar(t(\mathbf{k}) + E(\mathbf{k}))}{2E(\mathbf{k})},
\]
\[
\alpha_1(\mathbf{k}) = \hbar - \alpha_2(\mathbf{k}) = \frac{\hbar E(\mathbf{k}) - t(\mathbf{k})}{2E(\mathbf{k})},
\]
\[
\Rightarrow \quad S_{\mathbf{k}^0}(E) = \hbar \left[ \frac{E(\mathbf{k}) - t(\mathbf{k})}{2E(\mathbf{k})} \delta(E + E(\mathbf{k})) + \frac{E(\mathbf{k}) + t(\mathbf{k})}{2E(\mathbf{k})} \delta(E - E(\mathbf{k})) \right]
\]

**Problem B.10**

Free energy:

\[
F(T, V) = U(T, V) - TS(T, V) = U(T, V) + T \left( \frac{\partial F}{\partial T} \right)_V
\]

So that for the internal energy we get

\[
U(T, V) = -T^2 \left\{ \frac{\partial}{\partial T} \left( \frac{1}{T} F(T, V) \right) \right\}_V
\]

\[
F(0, V) \equiv U(0, V)
\]

\[
U(T, V) - U(T, 0) = -T^2 \left\{ \frac{\partial}{\partial T} (F(T, V) - F(0, V)) \right\}
\]

\[
- \int_0^T dT' \frac{U(T', V) - U(0, V)}{T'^2} = \frac{1}{T} (F(T, V) - F(0, V)) - \lim_{T \to 0} \left\{ \frac{1}{T} (F(T, V) - F(0, V)) \right\}
\]

Third law:

\[
\lim_{T \to 0} \left\{ \frac{1}{T} (F(T, V) - F(0, V)) \right\} = \left( \frac{\partial F}{\partial T} \right)_V (T = 0) = -S(T = 0, V) = 0
\]

Then it follows that
\[
F(T, V) = F(0, V) - T \int_{0}^{T} dT' \frac{U(T', V) - U(0, V)}{T'}
\]

**Problem B.11**

\[
\mathcal{H}_{0} = \sum_{\mathbf{k} \sigma} (\epsilon(\mathbf{k}) - \mu) a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k} \sigma}
\]

Then one can easily calculate

\[
[a_{\mathbf{k} \sigma}, \mathcal{H}_{0}]_{-} = (\epsilon(\mathbf{k}) - \mu) a_{\mathbf{k} \sigma},
\]

\[
[a_{\mathbf{k} \sigma}^{\dagger}, \mathcal{H}_{0}]_{-} = - (\epsilon(\mathbf{k}) - \mu) a_{\mathbf{k} \sigma}^{\dagger},
\]

\[
[a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'}, \mathcal{H}_{0}]_{-} = [a_{\mathbf{k} \sigma}^{\dagger}, \mathcal{H}_{0}]_{-} a_{\mathbf{k}' \sigma'} + a_{\mathbf{k} \sigma} [a_{\mathbf{k} \sigma}, \mathcal{H}_{0}]_{-}
\]

\[
= -(\epsilon(\mathbf{k}) - \mu) a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'} + (\epsilon(\mathbf{k}') - \mu) a_{\mathbf{k} \sigma} a_{\mathbf{k}' \sigma'}
\]

\[
= (\epsilon(\mathbf{k}') - \epsilon(\mathbf{k})) a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'}
\]

\(|\psi_{0}\rangle\) is eigenstate of \(\mathcal{H}_{0}\), because

\[
\mathcal{H}_{0}|\psi_{0}\rangle = a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'} \mathcal{H}_{0}|E_{0}\rangle - [a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'}, \mathcal{H}_{0}]_{-}|E_{0}\rangle
\]

\[
= (E_{0} - \epsilon(\mathbf{k}') + \epsilon(\mathbf{k})) |\psi_{0}\rangle
\]

Time dependence:

\[
|\psi_{0}(t)\rangle = a_{\mathbf{k} \sigma}^{\dagger}(t) a_{\mathbf{k}' \sigma'}(t) |E_{0}\rangle
\]

\[
= e^{\frac{i}{\hbar} \mathcal{H}_{0}t} a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'} e^{-\frac{i}{\hbar} \mathcal{H}_{0}t} |E_{0}\rangle
\]

\[
= e^{-\frac{i}{\hbar} E_{0}t} e^{\frac{i}{\hbar} \mathcal{H}_{0}t} |\psi_{0}\rangle
\]

\[
= e^{-\frac{i}{\hbar} E_{0}t} e^{\frac{i}{\hbar} (E_{0} + \epsilon(\mathbf{k}') - \epsilon(\mathbf{k}))t} |\psi_{0}\rangle
\]

\[
\implies |\psi_{0}(t)\rangle = e^{-\frac{i}{\hbar} (\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}))t} |\psi_{0}\rangle
\]

Further with \(\langle E_{0}|E_{0}\rangle = 1\) follows:

\[
\langle \psi_{0}|\psi_{0}\rangle = \langle E_{0}|a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k} \sigma} a_{\mathbf{k}' \sigma'}^{\dagger} a_{\mathbf{k}' \sigma'}|E_{0}\rangle
\]

\[
= \langle E_{0}|a_{\mathbf{k} \sigma}^{\dagger} (1 - n_{\mathbf{k} \sigma}) a_{\mathbf{k}' \sigma'}|E_{0}\rangle
\]

\[
= \langle E_{0}|a_{\mathbf{k} \sigma}^{\dagger} a_{\mathbf{k}' \sigma'}|E_{0}\rangle \quad (k > k_{F})
\]

\[
= \langle E_{0}|(1 - a_{\mathbf{k} \sigma} a_{\mathbf{k}' \sigma'}^{\dagger})|E_{0}\rangle \quad (k < k_{F})
\]

\[
= \langle E_{0}|E_{0}\rangle \quad (k < k_{F})
\]

\[
= 1
\]
 Therewith we finally have

\[
(\psi_0(t)|\psi_0(t')) = \exp\left(-\frac{i}{\hbar}(\epsilon(k') - \epsilon(k))(t - t')\right)
\]

\[
\Rightarrow |\langle \psi_0(t)|\psi_0(t') \rangle|^2 = 1: \text{ stationary state}
\]

**Problem B.12**

\[
G_{k\sigma}^\text{ret} = \hbar(E - \epsilon(k) + \mu - \Sigma_\sigma(k, E))^{-1}
\]

general representation

1. It must hold

\[
E - \epsilon(k) + \mu - \Sigma_\sigma(k, E) \overset{!}{=} E - 2\epsilon(k) + \frac{E^2}{\epsilon(k)} + i\gamma|E|
\]

\[
\Rightarrow \Sigma_\sigma(k, E) = R_\sigma(k, E) + i I_\sigma(k, E)
\]

\[
= \left(\epsilon(k) + \mu - \frac{E^2}{\epsilon(k)}\right) - i\gamma|E|
\]

\[
\Rightarrow R_\sigma(k, E) = \epsilon(k) + \mu - \frac{E^2}{\epsilon(k)}, \quad I_\sigma(k, E) = -\gamma|E|.
\]

2.

\[
E_{i\sigma} \overset{!}{=} \epsilon(k) - \mu + R_\sigma(k, E_{i\sigma}(k)) = 2\epsilon(k) - \frac{E_{i\sigma}^2(k)}{\epsilon(k)}
\]

\[
\Rightarrow E_{i\sigma}^2(k) + \epsilon(k)E_{i\sigma}(k) = 2\epsilon^2(k),
\]

\[
\left(E_{i\sigma}(k) + \frac{1}{2}\epsilon(k)\right)^2 = \frac{9}{4} \epsilon^2(k)
\]

Then we get two quasiparticle energies:

\[
E_{1\sigma}(k) = -2\epsilon(k); \quad E_{2\sigma}(k) = \epsilon(k).
\]

Spectral weights (B.162);
\[ \alpha_{i\sigma}(k) = \left| 1 - \frac{\partial}{\partial E} R_{\sigma}(k, E) \right|_{E=E_{i\sigma}}^{-1} = \left| 1 + 2 \frac{E_{i\sigma}(k)}{\epsilon(k)} \right|^{-1} \]

\[ \Rightarrow \alpha_{1\sigma}(k) = \alpha_{2\sigma}(k) = \frac{1}{3} \]

Lifetimes:

\[ I_\sigma(k, E_{1\sigma}(k)) = -2\gamma |\epsilon(k)| = I_{1\sigma}(k), \]
\[ I_\sigma(k, E_{2\sigma}(k)) = -\gamma |\epsilon(k)| = I_{2\sigma}(k) \]

\[ \Rightarrow \tau_{1\sigma}(k) = \frac{3\hbar}{2\gamma|\epsilon(k)|}; \quad \tau_{2\sigma}(k) = \frac{3\hbar}{\gamma|\epsilon(k)|}. \]

3. Quasi particle concept is applicable provided

\[ |I_\sigma(k, E)| \ll |\epsilon(k) - \mu + R_\sigma(k, E)| \]
\[ \iff |I_\sigma(k, E_{i\sigma})| \ll |E_{i\sigma}(k)| \]
\[ \iff \gamma |E_{i\sigma}(k)| \ll |E_{i\sigma}(k)| \]
\[ \iff \gamma \ll 1 \]

4.

\[ \left( \frac{\partial R_{\sigma}(k, E)}{\partial E} \right)_{\epsilon(k)} = -\frac{2E}{\epsilon(k)} \]
\[ \left( \frac{\partial R_{\sigma}(k, E)}{\partial \epsilon(k)} \right)_{E} = 1 + \frac{E^2}{\epsilon^2(k)} \]

\[ \Rightarrow m_{1\sigma}^*(k) = m \frac{1 - 4}{1 + 5} = -\frac{1}{2} m, \]
\[ m_{2\sigma}^*(k) = m \frac{1 + 2}{1 + 2} = m \]

**Problem B.13**

The self-energy is real and \( k \) independent. Then with (B.192),

\[ \rho_\sigma(E) = \rho_0(E - \Sigma_\sigma(E - \mu)) = \rho_0 \left( E - a_\sigma \frac{E - b_\sigma}{E - c_\sigma} \right) \]

Lower band edges:
\[ 0 = E - a_\sigma \frac{E - b_\sigma}{E - c_\sigma} \]
\[ \iff 0 = E^2 - (a_\sigma + c_\sigma)E + a_\sigma b_\sigma \]
\[ = \left( E - \frac{1}{2}(a_\sigma + c_\sigma) \right)^2 + a_\sigma b_\sigma - \frac{1}{4}(a_\sigma + c_\sigma)^2 \]
\[ \implies E_{1,2\sigma}^{(l)} = \frac{1}{2} \left( a_\sigma + c_\sigma \mp \sqrt{(a_\sigma + c_\sigma)^2 - 4a_\sigma b_\sigma} \right) \]

Upper band edges:
\[ W = E - a_\sigma \frac{E - b_\sigma}{E - c_\sigma} \]
\[ \iff -c_\sigma W = E^2 - (a_\sigma + c_\sigma + W)E + a_\sigma b_\sigma \]
\[ 0 = \left( E - \frac{1}{2}(a_\sigma + c_\sigma + W) \right)^2 + (a_\sigma b_\sigma + c_\sigma W) - \frac{1}{4}(a_\sigma + c_\sigma + W)^2 \]
\[ \implies \]
\[ E_{1,2\sigma}^{(u)} = \frac{1}{2} \left( a_\sigma + c_\sigma + W \mp \sqrt{(a_\sigma + c_\sigma + W)^2 - 4(a_\sigma b_\sigma + c_\sigma W)} \right) \]

Quasi particle density of states:
\[ \rho_\sigma(E) = \begin{cases} \frac{1}{W}, & \text{falls } E_{1\sigma}^{(u)} \leq E \leq E_{1\sigma}^{(o)} \\ \frac{1}{W}, & \text{falls } E_{2\sigma}^{(u)} \leq E \leq E_{2\sigma}^{(o)} \\ 0, & \text{otherwise} \end{cases} \]

Band splitting into two quasi particle sub-bands.
### Index

#### A
- ABAB-structure, 306
- Actinides, 16, 137
- Adiabatic demagnetization, 174
- Advanced Green’s function, 528, 531, 533, 539
- Alkali metals, 120, 121, 387
- Alloy analogy of the Hubbard model, 471
- Angle averaged photoemission, 556
- Angle resolved photoemission, 556
- Anisotropy field, 283, 337, 340, 341
- Annihilation operator, 177, 201, 202, 226, 275, 278, 322, 391, 477, 491, 497, 498, 504, 507, 508, 511, 523, 543, 732, 733
- Anomalous Zeeman effect, 61, 80, 164, 280
- Antiferromagnetism, 18, 87, 175, 431
- Antisymmetric N-particle states, 197
- Antisymmetric singlet state, 187
- Appearance potential spectroscopy, 524
- Atomic-limit self-energy, 418
- Auger-electron spectroscopy (AES), 524, 525, 526
- Average occupation number, 134, 324, 458, 468, 513, 540, 541, 555, 557

#### B
- Band
  - correction, 435, 436, 439, 441, 465, 468, 472
  - ferromagnetic solid, 389
  - magnetism, 12, 176, 387, 389, 395
  - magnets, 12, 176, 184, 194, 233, 387, 388, 389, 391, 393, 395
  - occupation, 394, 451, 457, 460, 461, 464, 466, 467, 468, 473, 481, 483, 485
  - shift, 177, 435, 436, 460, 461, 464, 465, 466, 468, 469, 475, 480, 483, 485, 488, 489, 703, 710
  - structure, 185, 391
- Bandwidth correction, 436, 437, 465, 468, 703
- BCS theory, 560
- Bernoulli number, 355
- Binding energy, 388
- Bloch density of states, 398, 399, 402, 403, 437, 445, 446, 455, 458, 462, 471, 473, 478, 556
- Bloch energy, 506
- Bloch function, 124, 171, 506, 507, 508, 504, 505, 507, 508, 511, 523, 543, 732, 733
- Bohr magneton, 11, 16, 106
- Bohr radius, 89, 151
- Bohr–Sommerfeld condition, 132, 133
- Bose–Einstein distribution function, 324, 343, 545
- Bose operator, 276, 277, 279, 323, 384, 528, 650, 652
- Bound current density, 3
- Bravais lattice, 171
- Brillouin function, 159, 160, 161, 181, 227, 298, 299, 300, 308, 319, 484, 647

#### C
- Callen decoupling, 371
- Callen method, 371–381, 385
- Callen theory, 380

Cauchy’s principal value, 534
Causal Green’s function, 528, 529
Central field approximation, 74, 75, 80
Centre of gravity, 163, 434, 437, 460, 468
Centre of gravity of the energy spectrum, 437
Centre of mass coordinates, 149, 600
Chain of equations of motion, 372, 530
Charge density, 3, 6, 62, 520, 521, 522
Chemical potential, 19, 95, 97, 100–101, 109, 117, 119, 135, 324, 399, 409, 417, 474, 475, 476, 478, 481, 487, 525, 543, 591, 677, 678
Classical Langevin paramagnetism, 173, 605
Classical limit, 133
Classical quasiparticle picture, 550, 555
Classical theories, 405, 623, 624
Closed orbit, 125, 127, 132
Closed paths, 262, 263
Closed polygons, 247
Cluster configuration, 212
Cluster model, 210, 212, 213, 216, 217, 219
CMR system, 217
c-number, 31, 32, 43, 234, 297, 301, 304, 313, 347, 353, 396, 515, 522
Coherent potential approximation (CPA), 471, 472, 473, 471
Collective eigenoscillations, 523
Collective magnetism, 15, 17, 18, 85, 89, 142, 175, 176, 184, 226, 229, 280, 281, 387, 410, 471, 482
Collective phenomena, 87, 175
Colossal magneto-resistance, 217
Combined Green’s function, 534, 535, 537, 540
Commutation relations for the spin operators, 203
Compensation temperature, 317, 318
Completeness relations, 206, 284, 429, 494
Construction operator, 278, 347, 391, 433, 434, 485, 495, 497, 501, 503–506, 508, 671, 733
Contact hyperfine interaction, 71, 73, 201
Continuity equation, 3, 5
Continuous Fock representation, 494–501
Conventional alloy analogy, 471, 473, 483
Cooper pair creation operator, 560
Coordination number, 468, 647, 649
Core electrons, 388, 525
Correlated electron hopping, 435, 473
energy, 153, 154
function, 236, 238, 239, 271, 301, 436, 439, 441, 465, 481, 529, 531, 535, 560, 639
Correspondence principle, 9
Coulomb gauge, 9, 10, 68, 72
Coulomb integral, 146, 191
Covalent bonding, 188
CPA equation, 472, 473
Creation operator, 177, 226, 277, 278, 323, 391, 495, 496, 504, 511, 560
Criterion for ferromagnetism, 182, 402, 457–461, 463
Critical exponent, 228, 269, 270, 299, 405, 622, 623, 624
Critical phenomena, 234
Critical region, 299, 368, 381, 623
Curie constant, 24, 161, 165, 173, 181, 300, 306, 311, 319, 485, 608, 615, 619, 621
Curie law, 24, 161, 165, 170, 173, 245, 420, 566, 567, 606, 607
Curie–Weiss law, 183, 184, 227, 300, 308, 321, 371, 372, 381, 484, 615, 620
Current density of polarization charges, 3
Cyclic invariance of trace, 517, 529, 728, 729

Index
Index

Cyclotron frequency, 105, 127, 128
Cyclotron mass, 126–127
Cyclotron orbit, 126

D
Darwin term, 44, 73, 76
d-band degeneracy, 393
Degeneracy of the Landau levels, 106, 593
Degenerate electron gas, 118
Degree of degeneracy, 107, 109, 110, 128, 129, 593
de Haas-von Alphen effect, 113, 121–134
Delta function, 505, 518, 532, 548, 549, 550, 555
Density
  correlation, 436
  parameter, 151, 152
Diagram technique, 443
Diamagnetic susceptibility, 88, 134, 585
Diamagnetism, 15, 85–136, 175, 596
Dielectric function, 520–523
Dipolar hyperfine interaction, 69, 70, 73
Dipole–dipole interaction, 179
Dipole interaction, 179, 180, 280–281, 345, 346, 347, 349, 350, 351, 385, 667
Dipole moment, 3, 23, 63
Dirac equation, 28–34, 38, 45
  for an electron in an electromagnetic field, 30
  for a free particle, 30
Dirac identity, 354, 455, 534, 538, 540
Dirac picture, 516
Dirac spin operator, 33
Dirac’s vector model, 195–200
Direct Coulomb interaction, 148
Direct terms, 229, 393
Discrete Fock representation, 501–506
Distinguishable particles, 149, 492
Double exchange, 217–226
Double exchange Hamiltonian, 223, 225
Double–hopping correlation, 465
Dressed skeleton diagrams, 442
d-states, 392
Dynamical mean-field theory (DMFT), 450, 476, 478, 479, 480
Dynamic susceptibility, 14
Dyson equation, 439, 441, 442, 448, 449, 454, 477, 480, 547
Dyson–Maleev transformation, 329

E
Easy axis, 310, 311, 312, 313, 316, 341
Easy direction, 310, 315, 316, 337
Effective Hamiltonian, 187, 195, 200, 207, 222, 428, 429
Effective Heisenberg Hamiltonian, 216
Effective magneton number, 165
Effective mass approximation, 207, 209
Effective masses, 104, 113, 120, 121, 127, 207, 209, 545, 561
Eigenenergies of the transfer matrix, 243
Eigenspace, 75, 196, 197, 200
Electric displacement, 522
Electron hopping, 217, 421, 422, 423, 427, 431, 435, 465, 473
Electron–phonon interaction, 389
Electron polarization, 468
Electron spin, 28, 34, 35, 37, 39, 41, 45, 71, 76, 91, 106, 123, 139, 187, 200, 201, 202, 211, 212, 218, 427, 431, 484, 486, 487
Elementary excitations, 277, 291, 337, 353, 354, 523
Energy gap, 340, 427, 734, 735
Energy renormalization, 545
Entropy, 19, 24, 98, 134, 137, 173, 174, 239, 240, 243, 244, 269, 587, 606, 607, 610, 616
Entropy per spin, 243, 244
Equal-time correlations, 406, 407
Equation of motion method, 416, 451, 530, 553
EuO, 17, 176, 179, 230, 273, 335, 336, 628
EuSe, 176, 307, 309, 382, 644
EuTe, 176, 273, 307, 309, 310, 621
Exactly half-filled energy band, 427
Exchange corrected susceptibility, 154
Exchange corrections, 142–154
Exchange integral, 176, 191, 193, 210, 280, 287, 304, 309, 326, 335, 382, 384, 431, 543
Exchange interaction, 17, 142, 149, 154, 175–231, 279, 280, 293, 336, 337, 346, 357, 358, 359, 387
Exchange operator, 200, 216, 281
Exchange parameter, 182, 194, 298, 305, 312, 319
Exchange splitting, 397, 399, 435, 467, 468, 474, 485
Exchange terms, 229, 230, 281, 393
Excitation energy, 294, 322, 542, 544

F
Families of loops, 258, 259
Fermi
dge, 97, 111, 130, 139, 468, 481, 482, 551
energy, 92, 97, 124, 134, 152, 186, 398, 399, 402, 403, 459, 461, 462, 591
function, 97, 98, 99, 110, 111, 115, 130, 140, 141, 143, 399, 419, 437, 444, 468, 541, 555, 679, 727
layer, 97, 99, 120, 140
operator, 226, 276
sea, 128, 130
sphere, 92, 93, 109, 129, 172, 203, 205, 551, 561
surface, 130, 131
temperature, 93
wavevector, 92, 551
Ferromagnet, 317–321, 336
Ferromagnetism, 17–18, 87, 175
Ferrite, 317
Ferroelectrics, 235
Ferromagnet with dipolar interaction, 345–351
Ferromagnetic saturation, 292, 323, 382, 383, 468, 474
Fine structure, 11, 45, 57, 72, 79, 156, 162, 163, 164, 166, 281
Finite lifetimes, 470, 471, 484, 485, 545, 552, 554
First law of thermodynamics, 19, 302
Fluctuation-dissipation theorem, 23, 271
Fock states, 503, 505, 513, 586, 713, 724, 725, 726, 727
Four-component theory, 41, 42
Fourier transformation, 265, 411, 445, 448, 452, 485, 518, 523, 527, 542, 550, 653, 697, 703
Four-spin correlation function, 271, 639
Free current density, 3, 7
Free energy, 19, 20, 21, 98, 137, 142, 173, 174, 178, 182, 226, 227, 239, 240, 253, 323, 361, 401, 431, 543, 559, 595, 606, 608, 611, 615, 616, 618, 634, 738
Free energy of the two-dimensional Ising model, 254–270
Free energy per spin, 242, 245, 255, 266–267, 634
Free enthalpy, 227, 569, 608, 617
Frustration, 201
4f-systems, 177, 201
δ-function, 113, 114, 119, 130, 141, 486
Fundamental commutation relations, 50, 82, 202, 277, 383, 491, 501, 508, 511, 540, 544, 733
rules, 497, 504
G
Garnet, 317
GdCl₃, 303, 304
Generalized susceptibility, 13
Gibbs–Duhem relation, 21
Grand canonical ensemble, 21, 22, 513, 525, 528, 586, 724
Grand canonical partition functions, 95, 104, 109, 134, 323, 525, 528, 725
Grand canonical potential, 21, 104, 109–117, 119, 121, 129, 130, 324, 350
Grid volume, 128, 586, 588
Ground state energy, 75, 151, 152, 153, 191, 192, 215, 216, 222, 322, 329, 339, 342, 349, 360, 384, 427, 513, 543, 690, 724
Ground state energy of the Jellium model, 152, 153
Ground state of the Jellium model, 151, 153
Group velocity, 124
G-type, 286, 306
H
Half-filled band, 403, 419, 427–431, 435, 462, 473, 480, 483, 706
Hamilton function, 270
Hamiltonian matrix, 220, 487, 680, 683
Hard direction, 281, 315
Harmonic approximation, 322, 345–351
Harmonic approximation for antiferromagnets, 336–345
Harmonic oscillator, 106, 276, 279, 323
Landau quantum number, 128, 130
Landé-factor, 56, 59
Landé’s g-factor, 11, 40, 233
Landé’s interval rule, 79, 170
Langevin function, 160, 181, 228, 596, 605, 622
Langevin paramagnetism, 16, 164, 165, 170, 173, 605
Larmor diamagnetism, 87–90, 134
Lattice dynamics, 388, 389
Lattice gas model, 235
Lattice potential, 91, 104, 145, 177, 389, 390, 506, 539, 541
Lattice structure, 307, 317, 389, 393, 469, 485, 556
Linear response theory, 515–523
Linear spin wave approximation, 322, 343, 383
Local diagrams, 450
Local exchange, 218
Local magnetism, 12, 177, 194, 201, 209
Local-moment magnetism, 177
Local propagator, 448, 449
Logarithmic divergence, 269
Longitudinal susceptibility, 519
Lorentz force, 7, 82, 574
Lower sub-band, 425, 426, 462
Low-temperature region, 334, 367–368, 380
Luttinger coupling, 77, 155
Luttinger sum rule, 481, 482
Luttinger theorem, 481

M
Macroscopic Maxwell’s equations, 2
Magnetic anisotropy, 281–283, 316
Magnetic insulators, 194, 210, 233, 234, 273, 387
Magnetic moment operator, 9
Magnetic moment of spin, 29, 41
Magnetic part of the specific heat, 328
Magnetic quantum number, 26, 51, 90, 158, 203
Magnetic stability, 468, 470, 483, 485, 520
Magnetic susceptibility tensor, 519
Magnetite, 317
Magnetization
  current density, 5, 7
curve, 182, 183, 184, 335, 336, 409, 468, 484
  per spin, 242, 243
Magnon
  interaction, 332
  occupation density, 544
  vacuum state, 323
Many-magnon states, 295
Material equations, 7, 522
Matsumbara propagator, 441
Maxwell–Boltzmann distribution, 97
Maxwell’s equations, 1, 2, 569
Mean field decoupling, 451
Mermin–Wagner theorem, 283–291, 298, 405, 410–415
Metal–insulator transitions, 395
Metallic bonding, 153
Method of double-time Green’s function, 351
Microscopic dipole density, 3
Microscopic Maxwell’s equations, 1
MnO structure, 307
Modified alloy analogy, 472, 473, 483
Modified perturbation theory, 479–482
Molecular Heisenberg model, 188
Moment method, 464, 465, 470
Monopole moment, 63
Mott–Hubbard insulator, 557
Mott transitions, 395
Multiple processes, 432
Multipole expansion, 62, 63

N
Narrow energy band, 387, 389–393, 395
Neel state, 337, 338, 342, 343, 344
Neel temperature, 18, 175, 306–308, 311, 317
NNSS structure, 307
Non-linear spin wave theory, 329
Non-local diagrams, 450
Non-locality, 450, 468
Non-orthogonality catastrophe, 192
Non-relativistic limit, 38, 41
Non-relativistic limit of the Dirac’s theory, 37, 39
Normal ordering, 278
Normal Zeeman effect, 61, 81, 158, 162, 164
N-particle state, 196, 197, 491, 492, 493, 494, 495, 501, 502, 504
lifetime, 554, 555
magnon, 294, 329
splitting, 467, 468, 473, 474
sub-bands, 425, 432, 436, 438, 451, 456
weight, 554, 555
Quenching, 201
Random phase approximation, 330, 353, 361
Recursion formula, 237, 366
Reduced matrix element, 54, 67
Relativistic electrons, 29, 82
Renormalized spin wave energy, 331
Renormalized spin waves, 329–336
Resonance energies, 549, 550, 551
Resonances, 71, 282, 481, 482, 484, 520, 523, 548, 549, 550, 551
Response functions, 13, 123, 515, 534, 537
Retarded Green's function, 352, 442, 451, 517, 519, 523, 528, 532, 538, 546
Riemann's $\zeta$-function, 99
Screening, 75, 90, 154, 395, 402, 520, 523
Scalar operator, 47, 53
Scalar product, 10, 42, 54, 55, 56, 58, 84, 188, 199, 207, 215, 217, 233, 274, 283, 284, 285, 494
Schrödinger picture, 516, 517
Schwarz inequality, 283, 285, 286
Screening, 75, 90, 154, 395, 402, 520, 523
Screening effects, 154, 395
SDA self-energy, 465, 470, 475
Second order perturbation theory, 200, 428, 431, 438, 444, 479, 630
Second order phase transitions, 484
Second order self-consistent perturbation theory, 443
Second quantization, 275, 390, 491–514, 721, 724
Secular equation, 192, 212, 428
$s$-electrons, 62, 69, 70, 71, 73, 75, 121, 155, 202, 203, 420
Self-energy part, 442
Semiclassical vector model, 221
$s$–$f$ interaction, 204
$s$–$f$ model, 177
Short-range ordering, 301
Single-impurity Anderson model, 476, 479, 480
Single-ion anisotropy, 282
Single step, 261, 262, 265
Skeleton diagram, 442, 443, 479, 480
Slater determinant, 502
Solvability condition, 59, 349
Sommerfeld expansion, 99–103, 141, 591
Sommerfeld model, 90–103, 104, 123, 129, 130, 131, 134, 135, 138, 139, 142, 143, 151, 152, 154, 172, 201, 387
Sommerfeld's fine structure constant, 11
Space of antisymmetric states, 493
Space of symmetric states, 493
Specific heat, 98, 102, 244, 268–269, 297, 301–303, 304, 313–315, 328, 340, 341
Specific heat of the antiferromagnet, 314
Spectral density ansatz, 441, 464
approach, 469
Spectral representation of the advanced Green's function, 533
Spectral representation of the retarded Green's function, 532
Spectral representation of the spectral density, 532, 533, 553
Spectral representation of the spectral density, 532, 533, 553
Spectral weights, 417, 432, 434, 438, 451, 457, 458, 464, 466, 473, 489, 545, 549, 554, 555, 561, 674, 737, 740
Spectroscopies, 523–528, 532, 534
Spherical harmonics, 53, 63, 64
Spherical multipole moments, 63
Spin $\frac{1}{2}$ particles, 29, 229
Spin correlation function, 236, 238, 271, 639
Index

Spin-dependent band shift, 177, 436, 460, 461, 464–470, 475, 480, 483, 485, 488, 489, 703
Spin deviation, 275, 277, 292, 294, 295, 322, 354
Spin disorder, 343
Spin-flip correlation, 436
Spin-flip operator, 274
Spin-flip terms, 296
Spin-flop field, 315–316, 341
Spin glass behaviour, 201
Spin–orbit coupling, 9, 12, 25, 29, 40–45, 57, 61, 75–76, 79, 156, 158, 162, 164–165, 281
Spin–orbit interaction, 25, 41, 43, 44, 57, 72, 74, 77, 78, 80, 83, 157, 158–164, 203, 280, 281
Spin-statistics theorem, 493
Spin wave approximation, 278, 322, 336, 341, 342, 343, 351, 375, 383, 384, 385, 662, 667
Spin wave branches, 340
Split-band regime, 473
Spontaneous ordering, 175, 464
Square lattice, 254, 255
Standard components, 52, 53, 54, 64, 66, 78, 83, 84
State with finite lifetime, 552
Static paramagnetic susceptibility, 461, 463, 484
Stationary state, 552, 553, 561, 740
Statistical operator, 516, 559, 586
Step function, 97, 143, 205, 517, 529, 532, 560
Stoke’s theorem, 133
Stoner approximation, 396, 486, 672
Stoner criterion, 186, 402, 404, 409, 415, 458, 460, 461
Stoner electron, 398
Strong-coupling limit, 432, 458
Strong-coupling regime, 427, 431–437, 438, 441, 464, 468
Strong ferromagnetism, 398
Sum rule, 425, 464, 481, 482, 536
Superconductor, 15, 291, 561
Superclosure, 194, 195, 209–216, 218, 221, 427
Susceptibility of the conduction electrons, 104, 117–121, 138
Symmetric decoupling, 373, 374
Symmetric triplet state, 187

T
Taylor expansion, 48, 102, 115, 140, 141, 268
Tensor
 operator, 52–53, 54, 64, 66, 83
of rank, 52, 66, 83
Term, 27, 28, 280
Thermal energy, 157, 161, 179, 295, 359
Thermodynamic expectation value, 332, 351, 353, 359, 372, 412, 413, 435, 541
Thermodynamic potential, 19, 21, 243, 252, 359–361
Third law of thermodynamics, 173, 244
Time evolution operator, 493
Time ordering operator, 529
Total angular momentum operator, 37
Transfer function, 241
Transfer integral, 214, 216, 219
Transfer matrix, 241, 243
Transfer matrix element, 213
Transfer matrix method, 240
Transition
metals, 16, 137, 210, 387, 389, 395, 402
operator, 523, 524, 525, 526
Translational symmetry, 85, 171, 239, 265,
297, 332, 353, 384, 396, 413, 417, 435,
452, 465, 466, 510, 522, 647, 665, 701
Transposition operator, 198, 199, 492
Transverse susceptibility, 520
Triangular inequality, 413
Tunnelling probability, 389
Two-component theory, 38, 41
Two dimensional Ising model, 245–270
Two-electron system, 186, 187, 195, 199, 423,
426
Two-magnon states, 330
Two-particle density of states, 524
Two-site Hubbard-model, 421, 424, 487, 488
Two-site model, 420–427, 432, 451, 456, 464,
487, 488
Tyablikov approximation, 353, 356
U
Uniaxial ferromagnet, 282
Upper sub-band, 425, 456
V
Vacuum state, 323, 495, 501, 504, 511
Valence electrons, 388
Valence mixture, 217, 317
van Vleck paramagnetism, 166–171
Variation ansatz, 190, 192
Variation method, 190
Vector operator, 48, 49, 52, 53, 54, 78, 82, 83
Vector potential, 9, 10, 67, 68, 72, 82, 104
Vertex, 256, 257, 442
Virtual hopping, 431
W
Wall, 247, 249, 250
Wannier functions, 508
Wave packet, 124, 492
Weak-coupling behaviour, 441, 475, 479, 481,
482, 484
Weak ferromagnetism, 398
Weight of the path, 261
Weiss ferromagnet, 180–184, 228, 298, 305,
397, 401, 621
Weiss model, 180–184, 230, 298, 395
Wigner–Eckart theorem, 45–56, 59, 60, 61, 64,
65, 66, 78, 162, 167, 168, 233, 280
Wigner–Seitz cell, 281, 598
X
XY-model, 233
Zeeman energy, 68, 156
Zeeman term, 58, 72, 106, 280, 281, 292
Zero-bandwidth limit, 417, 487
Z