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**APPLICATION**  
**OF DOUBLE-TIME**  
**THERMODYNAMIC**  
**GREEN FUNCTIONS**  
**TO SOLID STATE PHYSICS**

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# Chapter 1

## The Formalism of Green Functions

### 1.1 Introduction

Main purpose in quantum statistical mechanics is to calculate mean value (statistical average) of an observable physical quantity, if one deals with static (equilibrium) properties of the system under consideration, or time-dependent correlation functions, if one deals with a response of a system on an external dynamic perturbation.

For example, the problem can be put to calculate the mean value of the system's energy  $E$ , magnetization  $\mathbf{M}$ , electric current  $\mathbf{j}$ , *ets* which is equivalent to evaluating the static averages from Quantum Mechanical (QM) operators of these quantities, *e.g.*:

$$\langle \hat{A} \rangle = \text{Tr} (\hat{\rho} \hat{A}), \quad (1.1)$$

where  $\hat{A}$  is the QM operator of the observable physical quantity,  $\hat{\rho}$  is the equilibrium density matrix:  $\hat{\rho} = Q^{-1} \exp(-\hat{\mathcal{H}}/k_B T)$ ,  $Q = \text{Tr}(\exp(-\hat{\mathcal{H}}/k_B T))$ ,  $\hat{\mathcal{H}}$  is the Hamiltonian of the system,  $T$  is the absolute temperature, and  $k_B$  is the Boltzmann constant.

For nonequilibrium processes, *i.e.* dynamic processes under an external, time dependent perturbation, it is important to know **correlation functions (CF)** like

$$\langle \hat{A}(t) \hat{B}(t') \rangle = \text{Tr} (\hat{\rho} \hat{A}(t) \hat{B}(t')). \quad (1.2)$$

Here,  $\hat{A}$  and  $\hat{B}$  are QM operators of dynamic variables of a problem,  $\hat{A}(t) = e^{i\hat{\mathcal{H}}t} \hat{A} e^{-i\hat{\mathcal{H}}t}$  is the operator in the Heisenberg representation, hereafter we adopt the **Plank constant**  $\hbar = 1$ . The response of a system on an external dynamic perturbation can be expressed via the correlation functions.

These both, dynamic and static, problems are closely related to each other. For example, the average value of a certain physical quantity, or its average squared value, can be represented as particular cases of the correlation functions:  $\hat{B}(t') = 1$  for the first one, and  $\hat{B}(t') = \hat{A}(t)$  for the second one. From this observation we conclude that calculating CF we obtain the static and dynamic (kinetic) properties of a studied system as well.

## 1.2 Correlation Functions and their Spectral Representations

Note, first of all, that averaging in expression for CF (1.2) is performed over the equilibrium state with the total Hamiltonian in the density matrix definition. This immediately allows us to establish the symmetry relation which is:

- CF for the equilibrium state depends only on difference of arguments of the operators, entering in definition of CF (1.2).

**Proof.** Look at first that

$$\begin{aligned} \langle \widehat{A}(t)\widehat{B}(t') \rangle &= \text{Tr} \left( \widehat{\rho} \widehat{A}(t)\widehat{B}(t') \right) = Q^{-1} \text{Tr} \left( e^{-\widehat{H}/kT} e^{i\widehat{H}t} \widehat{A} e^{-i\widehat{H}t} e^{i\widehat{H}t'} \widehat{B} e^{-i\widehat{H}t'} \right) \quad (1.3) \\ &= Q^{-1} \text{Tr} \left( e^{-i\widehat{H}t'} e^{-\widehat{H}/kT} e^{i\widehat{H}t} \widehat{A} e^{-i\widehat{H}t} e^{i\widehat{H}t'} \widehat{B} \right) \end{aligned}$$

due to invariance of the trace with respect to cyclic transmutation of the operators under the trace. Then, due to commutativity of the first two exponential operators in the last bracket of Eq. (1.3) expression (1.3) becomes

$$\begin{aligned} Q^{-1} \text{Tr} \left( e^{-\widehat{H}/kT} e^{-i\widehat{H}t'} e^{i\widehat{H}t} \widehat{A} e^{-i\widehat{H}t} e^{i\widehat{H}t'} \widehat{B} \right) \\ &= Q^{-1} \text{Tr} \left( e^{-\widehat{H}/kT} e^{-i\widehat{H}t'+i\widehat{H}t} \widehat{A} e^{-i\widehat{H}t+i\widehat{H}t'} \widehat{B} \right) \\ &= Q^{-1} \text{Tr} \left( e^{-\widehat{H}/kT} e^{i\widehat{H}(t-t')} \widehat{A} e^{-i\widehat{H}(t-t')} \widehat{B} \right) \\ &= Q^{-1} \text{Tr} \left( e^{-\widehat{H}/kT} \widehat{A}(t-t') \widehat{B}(0) \right) \\ &= \langle \widehat{A}(t-t') \widehat{B}(0) \rangle, \quad (1.4) \end{aligned}$$

which proves the above symmetry relation statement.

When time arguments of the operators  $\widehat{A}$  and  $\widehat{B}$  coincide we get the equilibrium average of the product of the operators  $\widehat{A}$  and  $\widehat{B}$ .

Let us introduce spectral intensities of CFs according to following definitions:

$$\langle \widehat{A}(t)\widehat{B}(t') \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{AB}(\omega) e^{-i\omega(t-t')}, \quad (1.5)$$

$$\langle \widehat{B}(t')\widehat{A}(t) \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{BA}(\omega) e^{-i\omega(t-t')}. \quad (1.6)$$

Then, let us write down CF in the left-hand side of (1.5) and (1.6) via matrix elements of the constituent operators:

$$\langle \widehat{A}(t)\widehat{B}(t') \rangle = Q^{-1} \sum_{m,n} e^{-E_n/kT} \langle n | \widehat{A} | m \rangle \langle m | \widehat{B} | n \rangle e^{iE_n(t-t')} e^{-iE_m(t-t')}. \quad (1.7)$$

Here, we work in representation, where the Hamiltonian  $\widehat{H}$  is diagonal, so  $|n\rangle$  and  $E_n$  are eigenfunction and eigenvalue of the Hamiltonian, respectively. Denoting the matrix

elements as  $\langle n | \widehat{A} | m \rangle = A_{nm}$ , we obtain

$$\langle \widehat{A}(t) \widehat{B}(t') \rangle = Q^{-1} \sum_{m,n} e^{-E_n/kT} A_{nm} B_{mn} e^{-i(E_m - E_n)(t-t')}. \quad (1.8)$$

Comparing with Eq. (1.5) we establish that

$$J_{AB}(\omega) = \frac{2\pi}{Q} \sum_{m,n} e^{-E_n/kT} A_{nm} B_{mn} \delta(\omega - E_m + E_n). \quad (1.9)$$

Analogously,

$$\langle \widehat{B}(t') \widehat{A}(t) \rangle = Q^{-1} \sum_{m,n} e^{-E_n/kT} B_{nm} A_{mn} e^{i(E_m - E_n)(t-t')}. \quad (1.10)$$

Let us permute the indices  $n$  and  $m$  in (1.10),

$$\begin{aligned} \langle \widehat{B}(t') \widehat{A}(t) \rangle &= Q^{-1} \sum_{m,n} e^{-E_m/kT} B_{mn} A_{nm} e^{i(E_n - E_m)(t-t')} \\ &= Q^{-1} \sum_{m,n} e^{-E_m/kT} (e^{E_n/kT} e^{-E_n/kT}) A_{nm} B_{mn} e^{-i(E_m - E_n)(t-t')}, \end{aligned} \quad (1.11)$$

with obvious identity transformation from the first to the second line in (1.11). Then, we rewrite (1.11) as

$$= Q^{-1} \sum_{m,n} e^{-E_n/kT} e^{(E_n - E_m)/kT} A_{nm} B_{mn} e^{-i(E_m - E_n)(t-t')} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{BA}(\omega) e^{-i\omega(t-t')}. \quad (1.12)$$

Comparing both parts of (1.12) we conclude that

$$J_{BA}(\omega) = \frac{2\pi}{Q} \sum_{m,n} e^{-E_n/kT} A_{nm} B_{mn} e^{-\omega/kT} \delta(\omega - E_m + E_n). \quad (1.13)$$

Equations (1.9) and (1.13) allow to establish a relation between the spectral intensities of CFs, (1.5) and (1.6):

$$J_{BA}(\omega) = e^{-\omega/kT} J_{AB}(\omega). \quad (1.14)$$

Thus, Eqs. (1.9) and (1.13) solve the problem of finding the spectral intensities of correlation functions, and expression (1.14) establishes the important relation between them.

### 1.3 Definitions for Green Functions and their Spectral Representations

Let us introduce **Green functions (GFs)** by following definitions:

$$G_{\eta}^r(t-t') = -i\theta(t-t') \langle \widehat{A}(t) \widehat{B}(t') - \eta \widehat{B}(t') \widehat{A}(t) \rangle \quad (1.15)$$

is the *retarded* Green function of commutator ( $\eta = 1$ ) or anticommutator ( $\eta = -1$ ) type.

$$G_{\eta}^a(t-t') = i\theta(t'-t) \langle \widehat{A}(t) \widehat{B}(t') - \eta \widehat{B}(t') \widehat{A}(t) \rangle \quad (1.16)$$

is the *advanced* GF, and, at last,

$$G_{\eta}^c(t-t') = -i \left\langle T \hat{A}(t) \hat{B}(t') \right\rangle \quad (1.17)$$

is the *causal* GF.

In a general case, the averaging is over the equilibrium grand canonical ensemble.  $T$ -symbol in definition (1.17) means the time-ordered product defined as

$$T \hat{A}(t) \hat{B}(t') = \theta(t-t') \hat{A}(t) \hat{B}(t') + \eta \theta(t'-t) \hat{B}(t') \hat{A}(t). \quad (1.18)$$

Hereafter,

$$\theta(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases} \quad (1.19)$$

is the Heavyside step function.

Commonly accepted notations for these GFs are:

$$G_{\eta}^r(t-t') = \left\langle \left\langle \hat{A}(t) \mid \hat{B}(t') \right\rangle \right\rangle_{\eta}^r, \quad (1.20)$$

$$G_{\eta}^a(t-t') = \left\langle \left\langle \hat{A}(t) \mid \hat{B}(t') \right\rangle \right\rangle_{\eta}^a, \quad (1.21)$$

$$G_{\eta}^c(t-t') = \left\langle \left\langle \hat{A}(t) \mid \hat{B}(t') \right\rangle \right\rangle_{\eta}^c. \quad (1.22)$$

According to definitions (1.15)-(1.17) GFs depend on difference of the time variables. Define the spectral representation for the retarded GF by following relations:

$$G_{\eta}^r(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\eta}^r(\omega) e^{-i\omega(t-t')}, \quad (1.23)$$

$$G_{\eta}^r(\omega) = \int_{-\infty}^{\infty} dt G_{\eta}^r(t) e^{i\omega t}. \quad (1.24)$$

The spectral representations for the advanced and causal GFs are introduced by similar definitions.

## 1.4 The Relationship between Spectral Representations for the Retarded Green Function and Correlation Functions

Using (1.24) let us rewrite the expression for GF in detail:

$$G_{\eta}^r(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \left\{ -i\theta(t-t') \left[ \left\langle \hat{A}(t) \hat{B}(t') \right\rangle - \eta \left\langle \hat{B}(t') \hat{A}(t) \right\rangle \right] \right\}. \quad (1.25)$$



Substituting spectral representations for the both correlation functions in (1.25) according to (1.5) and (1.6) we get

$$\begin{aligned} G_\eta^r(\omega) &= -i \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \theta(t-t') \frac{1}{2\pi} \int_{-\infty}^{\infty} dE e^{-iE(t-t')} [J_{AB}(E) - \eta J_{BA}(E)] \quad (1.26) \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} dE J_{BA}(E) (e^{E/kT} - \eta) \int_{-\infty}^{\infty} d(t-t') e^{-i(\omega-E)(t-t')} \theta(t-t'). \end{aligned}$$

Changing the time variable in the last integral on  $\tau = t - t'$  we evaluate it as follows (see **Appendix** to this Chapter):

$$\int_{-\infty}^{\infty} d\tau e^{i(\omega-E)\tau} \theta(\tau) = \int_0^{\infty} d\tau e^{i(\omega-E)\tau} = \frac{i}{\omega - E + i\varepsilon}, \quad (1.27)$$

where  $\varepsilon = +0$  in order to ensure convergence on the upper limit of the integration. Substituting this equation into Eq. (1.26) we obtain:

$$G_\eta^r(\omega) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \frac{1}{\omega - E + i\varepsilon}. \quad (1.28)$$

Repeating similar calculations for the advanced GF  $G_\eta^a(\omega)$  we get:

$$G_\eta^a(\omega) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \frac{1}{\omega - E - i\varepsilon}. \quad (1.29)$$

We can join expressions (1.28) and (1.29) for the spectral densities of GFs:

$$G_\eta^r(\omega) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \frac{1}{\omega - E \pm i\varepsilon}, \quad (1.30)$$

with the superscript  $r$  or  $a$  standing for the sign "+" or "-" in the right-hand side of the equation, respectively. Moreover, we can consider the frequency  $\omega$  as a complex variable, *i.e.* extend the definition of the spectral densities of GFs on the complex plane of  $\omega$  :

$$G_\eta(\omega) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \frac{1}{\omega - E} = \begin{cases} G_\eta^r(\omega), & \text{Im } \omega > 0 \\ G_\eta^a(\omega), & \text{Im } \omega < 0 \end{cases} \quad (1.31)$$

This means that we have defined the nonanalytic function  $G_\eta(\omega)$  having discontinuity on the real axis.  $G_\eta^r(\omega)$  is the analytic continuation on the upper half-plane of the complex frequency  $\omega$ ,  $G_\eta^a(\omega)$  is the analytical continuation on the lower half-plane of complex  $\omega$ .

Expressions (1.28)-(1.31) allow us to establish a relation between the spectral densities of GFs and CFs. Let us calculate difference of GFs:

$$\begin{aligned}
& G_\eta(\omega + i\varepsilon) - G_\eta(\omega - i\varepsilon) \\
&= \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \left\{ \frac{1}{\omega - E + i\varepsilon} - \frac{1}{\omega - E - i\varepsilon} \right\} \\
&= \int_{-\infty}^{\infty} \frac{dE}{2\pi} J_{BA}(E) (e^{E/kT} - \eta) \{-2\pi i \delta(\omega - E)\} \\
&= -i (e^{\omega/kT} - \eta) J_{BA}(\omega).
\end{aligned} \tag{1.32}$$

Here we have used the following relation:

$$\lim_{\varepsilon \rightarrow +0} \frac{1}{\omega - E \pm i\varepsilon} = \frac{\mathcal{P}}{\omega - E} \mp i\pi \delta(\omega - E), \tag{1.33}$$

where  $\mathcal{P}$  means taking of the principal value of an integral, when (1.33) is used in an integrand together with a certain smooth function (see the proof of (1.33) in the **Appendix** to this Chapter). From (1.32) we get

$$J_{BA}(\omega) = i \frac{G_\eta^{AB}(\omega + i\varepsilon) - G_\eta^{AB}(\omega - i\varepsilon)}{e^{\omega/kT} - \eta}, \tag{1.34}$$

and then

$$\langle \widehat{B}(t') \widehat{A}(t) \rangle = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_\eta^{AB}(\omega + i\varepsilon) - G_\eta^{AB}(\omega - i\varepsilon)}{e^{\omega/kT} - \eta} e^{-i\omega(t-t')}. \tag{1.35}$$

Using relation (1.14) between  $J_{AB}(\omega)$  and  $J_{BA}(\omega)$  we obtain

$$\langle \widehat{A}(t) \widehat{B}(t') \rangle = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \{G_\eta^{AB}(\omega + i\varepsilon) - G_\eta^{AB}(\omega - i\varepsilon)\} \frac{e^{\omega/kT}}{e^{\omega/kT} - \eta} e^{-i\omega(t-t')}. \tag{1.36}$$

Expressions (1.34)-(1.36) establish the relation between the spectral densities of GFs and CFs, and give prescription for evaluating correlation functions provided that the spectral densities of corresponding Green functions are known (calculated in a certain approximations in general case).

## 1.5 The Dispersion Relations for Green Functions

Let us split GF (1.28) on the real and the imaginary parts using (1.33):

$$\begin{aligned}
G_\eta^r(\omega) &= \frac{1}{2\pi} \mathcal{P} \int_{-\infty}^{\infty} (e^{E/kT} - \eta) J_{BA}(E) \frac{dE}{\omega - E} - \frac{i}{2} J_{BA}(\omega) (e^{\omega/kT} - \eta) \\
&= \text{Re } G_\eta^r(\omega) + i \text{Im } G_\eta^r(\omega).
\end{aligned} \tag{1.37}$$

From the above we obtain

$$\text{Im } G_{\eta}^r(\omega) = -\frac{1}{2} J_{BA}(\omega)(e^{\omega/kT} - \eta), \quad (1.38)$$

and, consequently,

$$\frac{1}{2}(e^{\omega/kT} - \eta) J_{BA}(\omega) = -\text{Im } G_{\eta}^r(\omega). \quad (1.39)$$

Substituting (1.39) into the real part taken from Eq. (1.37) we get for the retarded GF

$$\text{Re } G_{\eta}^r(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \text{Im } G_{\eta}^r(E) \frac{dE}{E - \omega}. \quad (1.40)$$

Repeating the similar calculations for advanced GF (1.29) we make certain that both dispersion relations can be merged into a formula

$$\text{Re } G_{\eta}^{\pm}(\omega) = \pm \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \text{Im } G_{\eta}^{\pm}(E) \frac{dE}{E - \omega}, \quad (1.41)$$

which is the desired dispersion relation for the *retarded* (upper sign) and *advanced* (lower sign) GFs.

Proceeding from definition of causal GF (1.17)-(1.19) the dispersion relation can be obtained by the similar way for the *causal* Green function (L.D.Landau, 1955)

$$\text{Re } G_{\eta}^c(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{e^{E/kT} - \eta}{e^{E/kT} + \eta} \text{Im } G_{\eta}^c(E) \frac{dE}{E - \omega}. \quad (1.42)$$

## 1.6 Equation of Motion for Green Functions

Green functions (1.15)-(1.17) are defined for general operators  $\hat{A}$  and  $\hat{B}$  which obey the quantum mechanical equation of motion

$$i \frac{\partial \hat{A}}{\partial t} = [\hat{A}, \hat{\mathcal{H}}]. \quad (1.43)$$

Using (1.43) one can write down the equation of motion for the retarded GF (1.15):

$$\begin{aligned} i \frac{\partial G_{\eta}^r(t, t')}{\partial t} &= i \frac{\partial}{\partial t} \left\langle \left\langle \hat{A}(t) \mid \hat{B}(t') \right\rangle \right\rangle_{\eta}^r \\ &= \frac{\partial \theta(t - t')}{\partial t} \left\langle [\hat{A}(t), \hat{B}(t')] \right\rangle_{\eta} + \left\langle \left\langle i \frac{\partial \hat{A}(t)}{\partial t} \mid \hat{B}(t') \right\rangle \right\rangle_{\eta}^r, \end{aligned} \quad (1.44)$$

where  $\left\langle [\hat{A}(t), \hat{B}(t')] \right\rangle_{\eta}$  means the equilibrium statistical average of the commutator ( $\eta = 1$ ) or anticommutator ( $\eta = -1$ ) of operators  $\hat{A}(t)$  and  $\hat{B}(t')$ . As it can be deduced from the **Appendix** to Chapter 1,

$$\frac{\partial \theta(t)}{\partial t} = \delta(t), \quad \text{and} \quad \frac{\partial \theta(-t)}{\partial t} = -\frac{\partial \theta(t)}{\partial t} = -\delta(t), \quad (1.45)$$

where  $\delta(t)$  is the Dirac's delta-function. By inspection we conclude that the equation of motion for every of the GF from (1.15)-(1.17) has the same form:

$$i\frac{\partial G_\eta(t, t')}{\partial t} = \delta(t - t') \left\langle \left[ \widehat{A}, \widehat{B} \right] \right\rangle_\eta + \left\langle \left\langle \widehat{A}(t) \widehat{\mathcal{H}}(t) - \widehat{\mathcal{H}}(t) \widehat{A}(t) \mid \widehat{B}(t') \right\rangle \right\rangle_\eta. \quad (1.46)$$

In general case the right-hand side of equation (1.46) contains high-order GFs. For these new GFs it is necessary to write down equations which again may contain high order GFs in the general case. By this prescription a chain of coupled equations for GFs can be written down. In certain cases, the chain of equations is decoupled automatically due to commutation properties of operators. In other cases, decoupling procedures, which correspond to certain physical approximations, have to be developed. The decoupling procedure depends on the specific problem under consideration. In the next chapters we proceed to analyze physical models beginning from simplest ones, which can be solved *exactly*.

## 1.7 The Perturbation Theory for Green Functions

### 1.7.1 General perturbation theory for a self-energy

Let us assume that Hamiltonian of the system can be represented as follows:

$$\mathcal{H} = \mathcal{H}_0 + \varepsilon \mathcal{H}_1, \quad (1.47)$$

where the "zero-order" Hamiltonian  $\widehat{\mathcal{H}}_0$  satisfies a relation

$$[A, \mathcal{H}_0] = KA, \quad (1.48)$$

$\varepsilon$  is a small parameter of the perturbation series,  $K$  is a linear operator (we omit hereafter the "hat" over operators for brevity), and the operator  $A$  is a basic variable of the problem, the equation of motion for which reads:

$$i\frac{\partial}{\partial t} \langle\langle A|B \rangle\rangle = \delta(t - t') \langle[A, B]\rangle_\eta + \langle\langle [A, \mathcal{H}] | B \rangle\rangle. \quad (1.49)$$

After decomposition (1.47) the equation of motion for the operator  $A$  can be converted into the form ([6], §29),

$$i\frac{\partial A}{\partial t} = KA + \varepsilon R_1 A_1, \quad (1.50)$$

where  $R_1$  is also a linear operator, and  $A_1$  is a certain operator built of larger number of the second quantization operators. Then, equation of motion (1.49) generates an infinite set of equations

$$\begin{aligned} (E - K) \langle\langle A|B \rangle\rangle &= i \langle[A, B]\rangle_\eta + \varepsilon R_1 \langle\langle A_1|B \rangle\rangle, \\ (E - K_1) \langle\langle A_1|B \rangle\rangle &= i \langle[A_1, B]\rangle_\eta + \varepsilon R_2 \langle\langle A_2|B \rangle\rangle, \dots \end{aligned} \quad (1.51)$$

Let us introduce notations:

$$\langle\langle A|B \rangle\rangle \equiv G_1, \quad \langle\langle A_1|B \rangle\rangle = G_2, \dots \quad (1.52)$$

Then, set of equations (1.52) can be rewritten as follows:

$$\begin{aligned} L_1 G_1 &= I_1 + \varepsilon R_1 G_2, \\ L_2 G_2 &= I_2 + \varepsilon R_2 G_3, \dots \end{aligned} \quad (1.53)$$

The following development becomes more transparent, if Hamiltonian of the system can be represented as a Hamiltonian of free quasiparticles ( $\mathcal{H}_0$  in Eq. (1.47)), and an interaction between them, which can be treated as a perturbation ( $\varepsilon\mathcal{H}_1$  in Eq. (1.47)). Then,  $K$  in equations (1.51) is an energy of free quasiparticles, and  $R_1$  is an integral operator, the kernel of which is a matrix element of the interaction Hamiltonian. The analogous meaning can be extended on the operators  $K_1, R_2, \dots$ . In a general case, the operators  $L_n$  and  $I_n$  are functions of the small parameter  $\varepsilon$ :  $L_n = L_n(\varepsilon)$ ,  $I_n = I_n(\varepsilon)$ . The operator  $L_n$  can be decomposed on the operator of free quasiparticles,  $L_n^0$ , and the operator  $\varepsilon^m L_n^1$  depending on the perturbation parameter  $\varepsilon$ . The quantities  $I_n(\varepsilon)$  are correlation functions, which can be represented oftenly as a sum of correlation functions of the free quasiparticles,  $I_n^0$ , and so-called irreducible energy part proportional to the perturbation energy. The above decompositions can be summarized as follows:

$$\begin{aligned} L_n(\varepsilon) &= L_n^0 + \varepsilon L_n^1, \\ L_1 &\equiv L_1^0, \quad L_n^0 = \sum L_1, \\ I_n(\varepsilon) &= I_n^0 + O(\varepsilon). \end{aligned} \quad (1.54)$$

Let us denote by  $G_n^0$  a solution of the equation

$$L_n G_n^0 = I_n. \quad (1.55)$$

Now we would like to formulate perturbation method for the chain of equations of motion, (1.53). The parameter  $\varepsilon$  is considered as a small parameter  $\varepsilon \ll 1$ ,  $\mathcal{H}_0$  will be called Hamiltonian of free quasiparticles, and  $\mathcal{H}_1$  will be called Hamiltonian of interaction.

Poles of the Green function determine the energy of elementary excitations of a system. Then, system of equations (1.53) constitutes an expansion series on the poles of the Green functions, *i.e.* on inverse powers of the small parameter  $\varepsilon$ . To avoid obvious divergence of the series it is more instructive to build the expansion series for the *inverse* Green function. The expansion will have meaning of a power series in the small parameter  $\varepsilon$  which is convergent by definition. The Green function itself can be retrieved from the inverse one. This approach provides correct behavior of the Green functions in vicinity of their poles.

Let us define a mass operator,  $M_1$  (the self-energy operator), for the first Green function by equation

$$(L_1 - M_1) G_1 = I_1, \quad (1.56)$$

where  $L_1$  is the operator of free quasiparticles, and  $M_1$  includes the interaction energy. Comparing equation (1.56) with the first equation of (1.53) we may derive that

$$M_1 = \varepsilon R_1 G_2 G_1^{-1}, \quad (1.57)$$

where  $G_1^{-1}$  is inverse operator with respect to  $G_1$ . Define

$$X_1 = R_1 G_2 I_1^{-1}, \quad (1.58)$$

and substitute (1.56) into (1.57). Then, we have

$$M_1 = \varepsilon X_1 (L_1 - M_1), \quad (1.59)$$

from which we find

$$M_1 = (1 + \varepsilon X_1)^{-1} \varepsilon X_1 L_1. \quad (1.60)$$

Expression for self-energy (1.60) can be expanded in a series on the small parameter  $\varepsilon$ :

$$M_1 = \{ \varepsilon X_1 - (\varepsilon X_1)^2 + (\varepsilon X_1)^3 - \dots \} L_1, \quad (1.61)$$

where  $X_1$  is determined by expression (1.58). Expansion (1.61) makes sense far away from poles of the self-energy (1.60) given by:  $1 + \varepsilon X_1 = 0$ . In vicinity of the poles the self-energy  $M_1$  (1.60) can be approximated by

$$M_1 = \{ 1 - (1 + \varepsilon X_1)^{-1} \} L_1 \simeq - (1 + \varepsilon X_1)^{-1} L_1. \quad (1.62)$$

In vicinity of the poles of  $X_1$ ,  $\varepsilon X_1 \gg 1$ , so expansion (1.61) has no sense. The poles of  $X_1$  correspond to poles of the Green function  $G_2$  (see equation (1.58)), which, in turn, may depend on energy of the free particles and the interaction energy as well.

From system of equations (1.53) one can obtain:

$$\begin{aligned} G_2 &= G_2^0 + \varepsilon L_2^{-1} R_2 G_3 \\ &= G_2^0 + \varepsilon L_2^{-1} R_2 G_3^0 + \varepsilon^2 L_2^{-1} R_2 L_3^{-1} R_3 G_4^0 + \dots \end{aligned} \quad (1.63)$$

Substitution into (1.58) allows to represent  $X_1$  as a series in  $\varepsilon$ :

$$X_1 = R_1 G_2^0 I_1^{-1} + \varepsilon R_1 L_2^{-1} R_2 G_3^0 I_1^{-1} + \varepsilon^2 R_1 L_2^{-1} R_2 L_3^{-1} R_3 G_4^0 I_1^{-1} + \dots \quad (1.64)$$

Finally, this gives us expansion of the mass operator in powers of the interaction energy:

$$M_1 = \varepsilon M_1' + \varepsilon^2 M_1'' + \dots, \quad (1.65)$$

where

$$M_1' = R_1 G_2^0 I_1^{-1} L_1 = R_1 G_2^0 (G_1^0)^{-1}, \quad (1.66)$$

$$M_1'' = R_1 L_2^{-1} R_2 G_3^0 (G_1^0)^{-1} - R_1 G_2^0 (G_1^0)^{-1} L_1^{-1} R_1 G_2^0 (G_1^0)^{-1}. \quad (1.67)$$

For the spatially homogeneous systems the self energy (mass operator) is diagonal in the momentum representation. In the spectral-momentum ( $E - k$ ) representation the Green function reads:

$$G_k(E) = \frac{I_k}{E - K_k - \varepsilon M_k(E)}. \quad (1.68)$$

The energy of the elementary excitations is determined by poles of the Green function (1.68):

$$E = K_k + \varepsilon M_k(E). \quad (1.69)$$

In the zero-approximation on  $\varepsilon$  the excitation spectrum is equal to the (real) energy of free quasiparticles,  $E = K_k$ . The mass operator in a general case can be a complex function of the complex variable  $E = \omega + i\Gamma$ , where  $\Gamma$  is a small positive real:

$$M_k(\omega \pm i\Gamma) = M_k'(\omega, i\Gamma) \mp i M_k''(\omega, i\Gamma), \quad (1.70)$$

where  $M'_k$  and  $M''_k$  are real functions. Then, the real (dispersion) and imaginary (decay) parts of the excitations spectrum read:

$$\omega = K_k + \varepsilon M'_k(\omega, i\Gamma), \quad (1.71)$$

$$\Gamma = -\varepsilon M''_k(\omega, i\Gamma), \quad (1.72)$$

which, in fact, is a system of equations. If the decay is small ( $\Gamma \ll \omega$ ) the approximate expressions are as follows:

$$\omega \simeq K_k + \varepsilon M'_k(\omega, 0), \quad \Gamma \simeq -\varepsilon M''_k(\omega, 0). \quad (1.73)$$

For the spectral intensity we have

$$\begin{aligned} \left( e^{\frac{\omega}{k_B T}} - \eta \right) J_k(\omega) &= G_k(\omega + i\Gamma) - G_k(\omega - i\Gamma) \\ &= -iI_1(k) \frac{M''_k}{(\omega - \varepsilon M'_k)^2 + (\varepsilon M''_k)^2}. \end{aligned} \quad (1.74)$$

Finally, for the Green function we obtain:

$$G_k(E) \simeq \frac{I_k}{E - (K_k + \varepsilon M'_k) + i\varepsilon M''_k}. \quad (1.75)$$

### 1.7.2 A particular but important case of the perturbation theory (Ref. [8], §20)

Let us the Hamiltonian and the operator  $A$  satisfy Eqs. (1.48) and (1.49), and, in addition, the operator  $B$  satisfies a relation similar to (1.49):

$$[\mathcal{H}_0, B] = KB, \quad (1.76)$$

where  $K$  is a C-number, and  $i \langle [A, B] \rangle_\eta = 1$  (the standard situation when the  $A$  and  $B$  operators are creation and annihilation operators for fermions or bosons). Then, the equations of motion can be composed differentiating the operator  $A$  in the first, and the operator  $B$  in the second equation of motion:

$$(E - K) \langle \langle A|B \rangle \rangle = 1 + \varepsilon \langle \langle [A, \mathcal{H}_1] | B \rangle \rangle, \quad (1.77)$$

$$(E - K) \langle \langle A|B \rangle \rangle = 1 + \varepsilon \langle \langle A | [\mathcal{H}_1, B] \rangle \rangle. \quad (1.78)$$

Following, at first, line (1.77), and then, applying line (1.78) where we substituted  $[A, \mathcal{H}_1]$  instead of  $A$ , we get

$$(E - K) \langle \langle [A, \mathcal{H}_1] | B \rangle \rangle = i \langle \langle [A, \mathcal{H}_1], B \rangle \rangle_\eta + \varepsilon \langle \langle [A, \mathcal{H}_1] | [\mathcal{H}_1, B] \rangle \rangle. \quad (1.79)$$

Provided that  $\langle \langle [A, \mathcal{H}_1], B \rangle \rangle_\eta = 0$  we obtain from (1.77) and (1.79)

$$\langle \langle A|B \rangle \rangle = \frac{1}{E - K} + \frac{\varepsilon^2}{(E - K)^2} \langle \langle [A, \mathcal{H}_1] | [\mathcal{H}_1, B] \rangle \rangle. \quad (1.80)$$

If the above mentioned conditions are satisfied, equation (1.80) is exact. Then, compare it with the formally exact Dyson equation

$$\langle \langle A|B \rangle \rangle = \frac{1}{E - K - \Sigma(E)} \quad (1.81)$$

with the unknown for a moment self-energy  $\Sigma(E)$ . As we are interested in a case when the perturbation theory is applicable, expand Eq. (1.81) in a series of small  $\Sigma(E)$  and compare first two terms of the expansion with Eq. (1.80). The self-energy  $\Sigma(E)$  is then identified with the coefficient at  $(E-K)^{-2}$  in the second term of (1.80). At the moment, it is formally valid up to the second order of the perturbation theory on the small parameter  $\varepsilon$ , however, to prove this one needs to continue set of equations of motion (1.80) on one hand, and expand Dyson equation (1.81) in the perturbation series to higher terms in  $\varepsilon$  on the other hand. The latter expansion will contain perturbation terms in small  $\Sigma(E)$  as well as the expansion of  $\Sigma(E)$  itself on the small parameter  $\varepsilon$ . Comparing the two series term-by-term of the same order in  $\varepsilon$  one may deduce that  $\Sigma(E)$  can be written down as follows:

$$\Sigma(E) = \varepsilon^2 \langle\langle [A, \mathcal{H}_1] | [\mathcal{H}_1, B] \rangle\rangle^{irr}, \quad (1.82)$$

where the symbol "irr" (irreducible) means that terms containing singularities of the type  $(E-K)^{-n}$  ( $n$  is positive integer) should be excluded as they already had been excluded when formulating the Dyson equation (1.81). Formally, within the perturbation theory, Eq. (1.82) is exact. If the second order term is required only, it is a prescription how to find it neglecting in the r.h.s. the perturbation Hamiltonian in the density matrix.

## 1.8 Appendix

### 1.8.1 Calculation of the time integral in expression (1.26)

Let us check that the following integral represents the Heavyside  $\theta$ -function properties:

$$\lim_{\varepsilon \rightarrow +0} \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x+i\varepsilon} e^{-ixt} = \theta(t). \quad (1.83)$$

We use contour integration on the complex  $x$ -plane to evaluate the integral in (1.83):

$$\frac{i}{2\pi} \int_{path} \frac{dx}{x+i\varepsilon} e^{-ixt} = \lim_{R \rightarrow \infty} \frac{i}{2\pi} \int_{-R}^R \frac{dx}{x+i\varepsilon} e^{-ixt} + \lim_{R \rightarrow \infty} \frac{i}{2\pi} \int_{C_R} \frac{dx}{x+i\varepsilon} e^{-ixt}. \quad (1.84)$$

In this case the exponential in the integrand of (1.83) will provide convergence of the path integral, if we close the integration contour (see Fig.1.1) in the lower half-plane,  $\text{Im } x < 0$ :

$$\exp(-it[\text{Re}(x) + i \text{Im}(x)]) = \exp(-it \text{Re}(x)) \exp(t \text{Im}(x)). \quad (1.85)$$

It is clear that, when  $t > 0$  and  $\text{Im}(x) < 0$ ,  $\exp(t \text{Im}(x)) \rightarrow 0$ , when the radius  $R$  of  $C_R$  circle goes to infinity. So, upon  $R \rightarrow \infty$  the contribution of  $C_R$  to the contour integral vanishes, and we have from the residue theorem

$$\begin{aligned} \frac{i}{2\pi} \int_{path} \frac{dx}{x+i\varepsilon} e^{-ixt} &= \lim_{R \rightarrow \infty} \frac{i}{2\pi} \int_{-R}^R \frac{dx}{x+i\varepsilon} e^{-ixt} \\ &= -2\pi i \text{Res} \left[ \frac{i}{2\pi} \frac{1}{x+i\varepsilon} e^{-ixt}, -i\varepsilon \right]. \end{aligned} \quad (1.86)$$



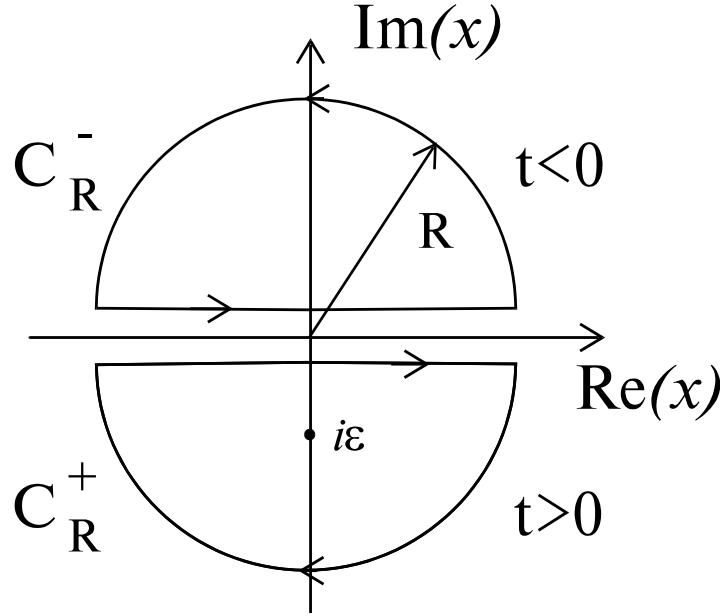


Figure 1.1: Integration paths in the expression (1.76).

”Minus” sign in the right-hand side of (1.86) is due to clockwise circling along the integration path. The residue in the right-hand side can be easily evaluated:

$$\text{Res} \left[ \frac{1}{x + i\varepsilon} e^{-ixt}, -i\varepsilon \right] = e^{-\varepsilon t}, \quad (1.87)$$

so

$$\begin{aligned} \lim_{\varepsilon \rightarrow +0} \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x + i\varepsilon} e^{-ixt} &= \lim_{R \rightarrow \infty} \frac{i}{2\pi} \int_{-R}^R \frac{dx}{x + i\varepsilon} e^{-ixt} \\ &= - \lim_{\varepsilon \rightarrow +0} 2\pi i \left( \frac{i}{2\pi} \right) e^{-\varepsilon t} = \lim_{\varepsilon \rightarrow +0} e^{-\varepsilon t} = 1. \end{aligned} \quad (1.88)$$

This means that  $\theta(t) = 1$  at  $t > 0$ .

Let us consider the case  $t < 0$ . In this case the integration path should be closed in the upper half-plane of the complex  $x$ -plane. Inspection of Figure 1 shows that there is no pole in the upper half-plane, so the residue in the right-hand side of the equation, similar to Eq. (1.86), is equal to zero. This means that the integral in (1.83) equals zero at  $t < 0$ , so  $\theta(t) = 0$  at  $t < 0$ .

Collecting the above findings we conclude that

$$\theta(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}, \quad (1.89)$$

which is the property of the Heavyside  $\theta$ -function.

Now we use integral representation for the  $\theta$ -function (1.83) for evaluating the integral over the time variable in (1.27):

$$\int_{-\infty}^{\infty} d\tau e^{i(\omega-E)\tau} \theta(\tau) = \frac{i}{2\pi} \iint_{-\infty}^{\infty} \frac{d\tau dx}{x + i\varepsilon} e^{i(\omega-E)\tau} e^{-ix\tau}. \quad (1.90)$$

Integrating first on  $\tau$ -variable we obtain:

$$\begin{aligned} & \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x+i\varepsilon} \int_{-\infty}^{\infty} d\tau e^{i(\omega-E-x)\tau} \\ &= \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x+i\varepsilon} (2\pi\delta(\omega-E-x)) = \frac{i}{\omega-E+i\varepsilon}, \end{aligned} \quad (1.91)$$

where we have used the integral representation for Dirac's  $\delta$ -function (1.97) and the property of functionals of smooth functions with  $\delta$ -function, described in detail in the following subsection of the Appendix. Formula (1.91) proves relation (1.27) of the main text.

### 1.8.2 Derivation of formula (1.33)

Note first of all that mathematically correct definition of the Dirac's  $\delta$ -function implies establishing of correspondence between the functional of certain smooth enough (doubly differentiable in the interval  $[a, b]$  specified below) function  $\varphi(x)$  and the value of this function for the zero-value argument, *i.e.*  $\varphi(0)$ :

$$\int_a^b \varphi(x)\delta(x)dx = \varphi(0), \quad (1.92)$$

$$0 \in [a, b]. \quad (1.93)$$

If the function  $\varphi(x)$  is represented by a constant one, for example,  $\varphi(x) = 1$ , the expression

$$\int_a^b \delta(x)dx = 1, \quad (1.94)$$

$$0 \in [a, b],$$

means the normalization relation for the  $\delta$ -function.

The "physical" definition of the  $\delta$ -function says that it is a function, which is equal to zero everywhere except the point, where its argument matches zero-value. In this point a value of the  $\delta$ -function is equal to infinity. In addition, the  $\delta$ -function is normalized to unity by relation (1.94). There exists another, and more close to our context, way to introduce the  $\delta$ -function as a limit of a certain sequence of functions, for example,

$$\lim_{\varepsilon \rightarrow +0} \frac{\varepsilon}{\pi} \frac{1}{\omega^2 + \varepsilon^2} = \lim_{\varepsilon \rightarrow +0} \delta(\omega, \varepsilon) = \delta(\omega). \quad (1.95)$$

Actually, the bell-shaped function under the  $\lim_{\varepsilon \rightarrow +0}$  operation (see Fig.1.2) becomes more narrow and high-peaked, once the value of  $\varepsilon$  decreases. At the same time,

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{\varepsilon}{\pi} \frac{d\omega}{\omega^2 + \varepsilon^2} &= \frac{\varepsilon}{\pi} \frac{1}{\varepsilon} \arctan \frac{\omega}{\varepsilon} \Big|_{-\infty}^{\infty} \\ &= \frac{1}{\pi} \left\{ \frac{\pi}{2} - \left( -\frac{\pi}{2} \right) \right\} = 1, \end{aligned} \quad (1.96)$$

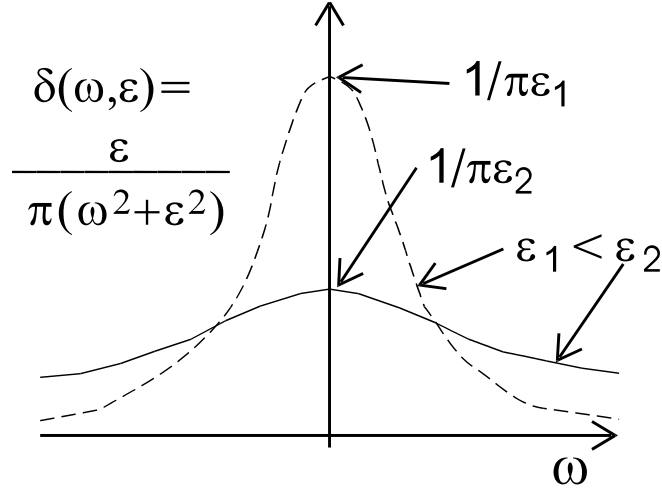


Figure 1.2: The function  $\delta(\omega, \varepsilon)$  in expressions (1.95)-(1.98).

from which we may conclude that the function  $\delta(\omega, \varepsilon)$  in Fig.1.2 is normalized to unity.

The definition of the  $\delta$ -function introduced by (1.95) allows to define the useful integral representation for the  $\delta$ -function

$$\delta(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} = \lim_{\varepsilon \rightarrow +0} \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-\varepsilon|t| + i\omega t} = \lim_{\varepsilon \rightarrow +0} \delta(\omega, \varepsilon). \quad (1.97)$$

The straightforward calculation yields

$$\delta(\omega, \varepsilon) = \frac{1}{2\pi} \left\{ \int_0^{\infty} dt e^{-\varepsilon t + i\omega t} + \int_{-\infty}^0 dt e^{+\varepsilon t + i\omega t} \right\} = \frac{\varepsilon}{\pi} \frac{1}{\omega^2 + \varepsilon^2}, \quad (1.98)$$

which, together with (1.95), proves (1.97).

Let us return now to our expression (1.33) and construct a functional with smooth function  $\varphi(\omega)$  :

$$\begin{aligned} & \int_{-\infty}^{\infty} d\omega \frac{\varphi(\omega)}{\omega - E \pm i\varepsilon} \\ &= \int_{-\infty}^{\infty} d\omega \varphi(\omega) \left\{ \frac{\omega - E}{(\omega - E)^2 + \varepsilon^2} \mp i \frac{\varepsilon}{(\omega - E)^2 + \varepsilon^2} \right\} \\ &= \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{\omega - E}{(\omega - E)^2 + \varepsilon^2} \mp i \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{\varepsilon}{(\omega - E)^2 + \varepsilon^2}. \end{aligned} \quad (1.99)$$

Let us take the limit  $\varepsilon \rightarrow 0$  of the above integrals:

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{\omega - E}{(\omega - E)^2 + \varepsilon^2} &= \mathcal{P} \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{1}{\omega - E} \\ &\equiv \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{\mathcal{P}}{\omega - E} \end{aligned} \quad (1.100)$$

by definition.

$$\lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{\varepsilon}{(\omega - E)^2 + \varepsilon^2} = \pi \int_{-\infty}^{\infty} d\omega \varphi(\omega) \delta(\omega - E) \quad (1.101)$$

according to (1.95).

Then, substituting (1.100) and (1.101) into (1.99) and collecting terms, we obtain

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} d\omega \varphi(\omega) \frac{1}{\omega - E \pm i\varepsilon} \\ &= \int_{-\infty}^{\infty} d\omega \varphi(\omega) \left\{ \frac{\mathcal{P}}{\omega - E} \mp i\pi\delta(\omega - E) \right\}, \end{aligned} \quad (1.102)$$

that proves relation (1.33) of the main text.

## 1.9 Problems

1. Prove the symmetry property relating the *retarded* and *advanced* GFs:

$$\left\langle \left\langle \hat{A} \mid \hat{B} \right\rangle \right\rangle_{\eta}^r(\omega) = \eta \left\langle \left\langle \hat{B} \mid \hat{A} \right\rangle \right\rangle_{\eta}^a(-\omega).$$

2. Reproduce the derivation of the dispersion relation for the *advanced* GF and confirm formula (1.41).
3. Derive dispersion relation (1.42) for the *causal* Green function.
4. By direct inspection prove that every type of GFs (*retarded*, *advanced* and *causal*) satisfies equation of motion (1.46).

# Chapter 2

## Application of Green Functions to Exactly Solvable Models

### 2.1 The Equilibrium Distributions for Ideal Quantum Gases

#### 2.1.1 The average number of free bosons in the state with given value of energy

Consider an ensemble of  $N$  free particles obeying the Bose-Einstein statistics. The Hamiltonian of this system is

$$\mathcal{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}, \quad \varepsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu, \quad (2.1)$$

where  $\mu$  is the chemical potential,  $b_{\mathbf{k}}^{\dagger}(b_{\mathbf{k}})$  is the creation (annihilation) operator of a boson with the energy  $\varepsilon_{\mathbf{k}}$ , the quantized values of which are classified by the momentum  $\mathbf{k}$ . For calculations we choose the *retarded, commutator*-type GF ( $\eta = 1$ ). The latter choice is based on the commutation properties of bosonic operators:

$$b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} - b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}} \equiv [b_{\mathbf{k}}, b_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'}; \quad (2.2)$$

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}] = [b_{\mathbf{k}}^{\dagger}, b_{\mathbf{k}'}^{\dagger}] = 0, \quad (2.3)$$

where

$$\delta_{\mathbf{k}\mathbf{k}'} = \begin{cases} 1, & \mathbf{k} = \mathbf{k}' \\ 0, & \mathbf{k} \neq \mathbf{k}' \end{cases}. \quad (2.4)$$

Let us write down the equation of motion for the GF

$$G_{\mathbf{k}}^r(t, t') = \left\langle \left\langle b_{\mathbf{k}} \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle^r = -i\theta(t - t') \left\langle b_{\mathbf{k}}(t) b_{\mathbf{k}}^{\dagger}(t') - b_{\mathbf{k}}^{\dagger}(t') b_{\mathbf{k}}(t) \right\rangle; \quad (2.5)$$

$$i \frac{\partial G_{\mathbf{k}}^r}{\partial t} = \delta(t - t') \left\langle [b_{\mathbf{k}}, b_{\mathbf{k}}^{\dagger}] \right\rangle + \left\langle \left\langle [b_{\mathbf{k}}, \mathcal{H}] \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle^r. \quad (2.6)$$

Then, we calculate the commutator which appears in the high-order GF (last term in the right-hand side of the above equation):

$$\begin{aligned} [b_{\mathbf{k}}, \mathcal{H}] &= \left[ b_{\mathbf{k}}, \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} \right] \\ &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left[ b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} \right] = \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left( b_{\mathbf{k}} b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} - b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}} \right). \end{aligned} \quad (2.7)$$

Interchanging first two operators in the first term of the bracket according to (2.2) we have:

$$\begin{aligned} &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left\{ \left( \delta_{\mathbf{k}\mathbf{k}'} + b_{\mathbf{k}'}^\dagger b_{\mathbf{k}} \right) b_{\mathbf{k}'} - b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}} \right\} \\ &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left\{ b_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} + b_{\mathbf{k}'}^\dagger b_{\mathbf{k}} b_{\mathbf{k}'} - b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}} \right\} = \varepsilon_{\mathbf{k}} b_{\mathbf{k}}, \end{aligned} \quad (2.8)$$

because  $b_{\mathbf{k}}$  and  $b_{\mathbf{k}'}$  in the last line commute in accordance with (2.3). Substituting (2.8) into (2.6) we obtain the equation of motion

$$i \frac{\partial G_{\mathbf{k}}^r}{\partial t} = \delta(t - t') + \varepsilon_{\mathbf{k}} G_{\mathbf{k}}^r. \quad (2.9)$$

It is convenient to perform Fourier-transformation of equation (2.9) according to definitions for  $G_{\mathbf{k}}^r(\tau)$

$$G_{\mathbf{k}}^r(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\mathbf{k}}^r(\omega) e^{-i\omega\tau}, \quad \tau = t - t', \quad (2.10)$$

and for the Dirac's delta-function  $\delta(\tau)$  (see also (1.97)),

$$\delta(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau}. \quad (2.11)$$

Substitution of (2.10) and (2.11) into (2.9) gives

$$i \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\mathbf{k}}^r(\omega) e^{-i\omega\tau} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} + \varepsilon_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{\mathbf{k}}^r(\omega) e^{-i\omega\tau}. \quad (2.12)$$

Taking the time-derivative of the exponential in the left-hand side of (2.12) and comparing the both sides of the above equation we obtain the equation

$$\omega G_{\mathbf{k}}^r(\omega) = 1 + \varepsilon_{\mathbf{k}} G_{\mathbf{k}}^r(\omega), \quad (2.13)$$

and, finally, the solution of equation (2.13):

$$G_{\mathbf{k}}^r(\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}}}. \quad (2.14)$$

The main purpose of these calculations is to compute the average number of free bosons in the state with the given energy  $\varepsilon_{\mathbf{k}}$ :

$$n_{\mathbf{k}} = \left\langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \right\rangle. \quad (2.15)$$

Using the definition of correlation functions (1.2), their symmetry property (1.4) and spectral representations (1.5), (1.6), we establish that

$$\begin{aligned} \langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \rangle &\equiv \langle b_{\mathbf{k}}^\dagger(t) b_{\mathbf{k}}(t) \rangle \\ &= \lim_{t' \rightarrow t} \langle b_{\mathbf{k}}^\dagger(t) b_{\mathbf{k}}(t') \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{b^\dagger b}(\omega). \end{aligned} \quad (2.16)$$

On the other hand, the spectral intensity of CF  $J_{b^\dagger b}(\omega)$  is connected with the spectral intensity of GF,  $G_{\mathbf{k}}^r(\omega) \equiv \left\langle \left\langle b_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \right\rangle \right\rangle_{\omega}^r$ , by relation (1.34). Making use solution (2.14) for the GF  $G_{\mathbf{k}}^r(\omega)$  and relation (1.34) we find that

$$\begin{aligned} J_{b^\dagger b}(\omega) &= i \frac{G_{\mathbf{k}}^r(\omega + i\varepsilon) - G_{\mathbf{k}}^r(\omega - i\varepsilon)}{e^{\omega/kT} - 1} \\ &= \frac{i}{e^{\omega/kT} - 1} \left\{ \frac{1}{\omega - \varepsilon_{\mathbf{k}} + i\varepsilon} - \frac{1}{\omega - \varepsilon_{\mathbf{k}} - i\varepsilon} \right\}. \end{aligned} \quad (2.17)$$

Realizing relation (1.33) as follows,

$$\frac{1}{\omega - \varepsilon_{\mathbf{k}} \pm i\varepsilon} = \frac{\mathcal{P}}{\omega - \varepsilon_{\mathbf{k}}} \mp i\pi\delta(\omega - \varepsilon_{\mathbf{k}}), \quad \varepsilon = +0, \quad (2.18)$$

we obtain the spectral density of CF

$$\begin{aligned} J_{b^\dagger b}(\omega) &= \frac{i}{e^{\omega/kT} - 1} \{-2i\pi\delta(\omega - \varepsilon_{\mathbf{k}})\} \\ &= \frac{2\pi\delta(\omega - \varepsilon_{\mathbf{k}})}{e^{\omega/kT} - 1}. \end{aligned} \quad (2.19)$$

With the spectral density found above, formula (2.16) immediately yields

$$\begin{aligned} n_{\mathbf{k}} &= \langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \rangle \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{2\pi\delta(\omega - \varepsilon_{\mathbf{k}})}{e^{\omega/kT} - 1} = \frac{1}{e^{\varepsilon_{\mathbf{k}}/kT} - 1}. \end{aligned} \quad (2.20)$$

It is just the Bose-Einstein distribution for a free boson gas. If the fixed total number of bosons  $N$  is considered, the chemical potential  $\mu$  can be calculated from the conventional normalization condition:

$$\sum_{\mathbf{k}} n_{\mathbf{k}} = N. \quad (2.21)$$

### 2.1.2 The physical meaning of the Green function's pole

Let us return to the problem of calculating the Bose-Einstein distribution function solved above. For Hamiltonian of free bosons (2.1) we have obtained retarded commutator GF (2.14). Inspection of solution for GF (2.14) shows that the pole of  $G_{\mathbf{k}}^r(\omega)$  is just the excitation spectrum of free bosons, i.e.  $\varepsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu$ . This statement has more general meaning: a pole of the Green function  $\left\langle \left\langle b_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \right\rangle \right\rangle_{\eta=1}^r$  yields the excitation spectrum of bosons

also, if they interact with other particles or excitations, or interactions exist between the bosons themselves. In general, a set of self-frequencies of the GF equations system (chain of equations for GFs) gives the excitation spectrum of interacting quasiparticles. Further, we will illustrate this statement by an exactly solvable example of the system consisting of two kinds of bosons, "a" and "b", interacting by means of operator form bilinear on creation and annihilation operators of "a" and "b" types (B.I. Kochelaev, Sov. Phys. - Dokl. **11**, 130 (1966); M.N. Aliev, B.I. Kochelaev, Izv. Vuzov - Fizika, **2**, 7 (1968)).

## 2.2 The System of Interacting Bosons of Two Kinds

### 2.2.1 The equation of motion and its solution

Let us suppose the Hamiltonian of the model in the form

$$\mathcal{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + \sum_{\mathbf{k}'} v_{\mathbf{k}'} \left( a_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'} + a_{\mathbf{k}'} b_{\mathbf{k}'}^{\dagger} \right), \quad (2.22)$$

where  $v_{\mathbf{k}}$  is assumed to be real, and  $v_{\mathbf{k}} \rightarrow 0$  as  $k \rightarrow 0$ . Making use of commutation relations (2.2)-(2.4) we write down the equation of motion for the retarded commutator type Green function  $G_{\mathbf{k}}(t, t') = \left\langle \left\langle b_{\mathbf{k}} \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle_{\eta=1}^r$ . In the following we shall omit for brevity the sub- and super-scripts in the definition of the GF:

$$i \frac{\partial G_{\mathbf{k}}(t, t')}{\partial t} = \delta(t - t') \left\langle \left[ b_{\mathbf{k}}, b_{\mathbf{k}}^{\dagger} \right] \right\rangle + \left\langle \left\langle [b_{\mathbf{k}}, \mathcal{H}](t) \mid b_{\mathbf{k}}^{\dagger}(t') \right\rangle \right\rangle. \quad (2.23)$$

After Fourier-transformation over the time variables we obtain for the above equation

$$E \left\langle \left\langle b_{\mathbf{k}} \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle_E = 1 + \varepsilon_{\mathbf{k}} \left\langle \left\langle b_{\mathbf{k}} \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle_E + v_{\mathbf{k}} \left\langle \left\langle a_{\mathbf{k}} \mid b_{\mathbf{k}}^{\dagger} \right\rangle \right\rangle_E, \quad (2.24)$$

where the following commutators have been utilized:

$$\begin{aligned} 1). \quad \left[ b_{\mathbf{k}}, \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'} \right] &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left\{ b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'} - b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'} b_{\mathbf{k}} \right\} \\ &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} \left\{ b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'} - (b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} - \delta_{\mathbf{k}\mathbf{k}'}) b_{\mathbf{k}'} \right\} \\ &= \sum_{\mathbf{k}'} \varepsilon_{\mathbf{k}'} b_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} = \varepsilon_{\mathbf{k}} b_{\mathbf{k}}, \end{aligned} \quad (2.25)$$

where commutativity of any couple of boson annihilation operators was used to interchange the last two operators in the first line of equation (2.25) and then, commutation relation (2.2) was used to interchange  $b_{\mathbf{k}'}^{\dagger}$  and  $b_{\mathbf{k}}$  in the second line of (2.25).

$$2). \quad \left[ b_{\mathbf{k}}, \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \right] = 0, \quad (2.26)$$

because the operators belonging to different kinds of bosons commute.

$$\begin{aligned} 3). \quad \left[ b_{\mathbf{k}}, \sum_{\mathbf{k}'} v_{\mathbf{k}'} b_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} \right] &= \sum_{\mathbf{k}'} v_{\mathbf{k}'} \left\{ b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} - b_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} b_{\mathbf{k}} \right\} \\ &= \sum_{\mathbf{k}'} v_{\mathbf{k}'} \left\{ b_{\mathbf{k}} b_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}'} - b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}} a_{\mathbf{k}'} \right\} \end{aligned} \quad (2.27)$$



with the second line obtained from the previous one by permutation of the annihilation operators in the last term of the first line in accordance with (2.3). Proceeding with commuting of  $b_{\mathbf{k}'}^\dagger$  and  $b_{\mathbf{k}}$  in the last term of the second line of (2.27) we get

$$= \sum_{\mathbf{k}'} v_{\mathbf{k}'} \left\{ b_{\mathbf{k}} b_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} - \left( b_{\mathbf{k}} b_{\mathbf{k}'}^\dagger - \delta_{\mathbf{k}\mathbf{k}'} \right) a_{\mathbf{k}'} \right\} = v_{\mathbf{k}} a_{\mathbf{k}}.$$

And, the last contribution is

$$4). \quad \left[ b_{\mathbf{k}}, \sum_{\mathbf{k}'} v_{\mathbf{k}'} b_{\mathbf{k}'} a_{\mathbf{k}'}^\dagger \right] = 0 \quad (2.28)$$

because of commutation relation (2.3).

The inspection of equation (2.24) shows that a new Green function appeared in the right-hand side of the equation, it is  $\langle\langle a_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E$ . For this GF we have to write down the equation of motion,

$$E \langle\langle a_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E = \omega_{\mathbf{k}} \langle\langle a_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E + v_{\mathbf{k}} \langle\langle b_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E, \quad (2.29)$$

in close analogy with derivation of Eq. (2.24). The inspection of equation (2.29) shows that its right-hand side does not contain new GFs. It means that the chain of equations for GFs is truncated automatically. Actually, the Hamiltonian (2.22) is a bilinear form of creation and annihilation operators, and, according to the Bogolyubov theorem, it can be always diagonalized exactly (for example, by the Bogolyubov canonical transformation) ([6], §13).

### 2.2.2 The excitation spectrum

The self-frequencies (energies) of the system of equations ((2.24) plus (2.29)),

$$\begin{aligned} (E - \varepsilon_{\mathbf{k}}) \langle\langle b_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E - v_{\mathbf{k}} \langle\langle a_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E &= 1, \\ -v_{\mathbf{k}} \langle\langle b_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E + (E - \omega_{\mathbf{k}}) \langle\langle a_{\mathbf{k}} | b_{\mathbf{k}}^\dagger \rangle\rangle_E &= 0, \end{aligned} \quad (2.30)$$

can be obtained equating the main determinant of (2.30) to zero:

$$\begin{vmatrix} E - \varepsilon_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{\mathbf{k}} & E - \omega_{\mathbf{k}} \end{vmatrix} = E^2 - E(\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}) + \varepsilon_{\mathbf{k}}\omega_{\mathbf{k}} - v_{\mathbf{k}}^2 = 0. \quad (2.31)$$

Solutions of this equation are

$$E_{1,2} = \frac{\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}}{2} \pm \sqrt{\frac{(\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}})^2}{4} + v_{\mathbf{k}}^2}, \quad (2.32)$$

which represent the excitations spectrum of interacting bosons of two kinds.

Suppose that the free bosons have energy dispersion laws, as indicated in Figure 2.1:  $\varepsilon_{\mathbf{k}} = \varepsilon_0 = \text{const}$ , and  $\omega_{\mathbf{k}}$  is linear on  $k$ . There exists  $k$ -value  $-k_0$ , at which the dispersion laws experience crossing, and the system has doubly degenerate value of energy in the absence of interaction given by the last term of Hamiltonian (2.22). Let us now consider

the behavior of *exact* self-energies (2.32) at small momentum  $k$ , large momentum  $k$  (will be defined below), and at the crossing point momentum  $k = k_0$ .

1). *Small momentum values*  $k \rightarrow 0$ .

$v_{\mathbf{k}}^2 \ll \left(\frac{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}}{2}\right)^2$ , so expanding the square root in (2.32) one obtains

$$E_{1,2} \simeq \frac{\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}}{2} \pm \left| \frac{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}}{2} \right| \left\{ 1 + \frac{1}{2} \left( \frac{2v_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}} \right)^2 \right\}. \quad (2.33)$$

For the case under consideration, at  $k \rightarrow 0$ ,  $\varepsilon_{\mathbf{k}} > \omega_{\mathbf{k}}$  (see Fig. 2.1), so  $|\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}| =$

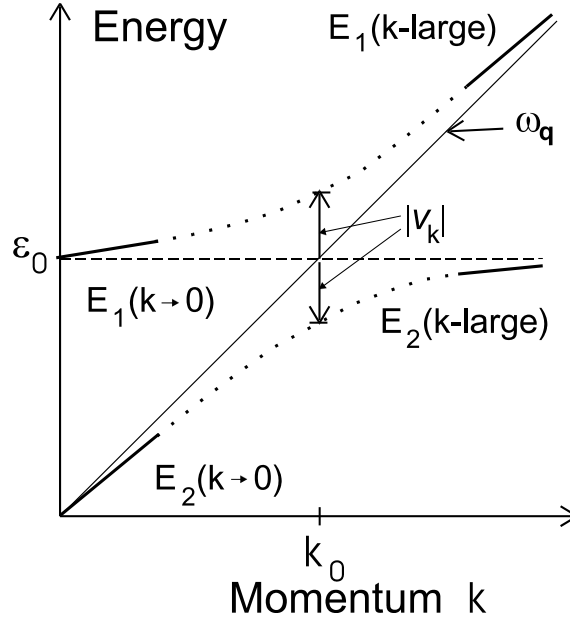


Figure 2.1: Dispersion laws and the solutions for the interacting bosons (see the text for details).

$\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}} > 0$ . With this remark we have

$$E_{1,2} \simeq \frac{\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}}{2} \pm \left\{ \frac{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}}{2} + \frac{v_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}} \right\}, \quad (2.34)$$

from which we obtain

$$E_1(\mathbf{k}) \simeq \varepsilon_{\mathbf{k}} + \frac{v_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}} = \varepsilon_0 + \frac{v_{\mathbf{k}}^2}{\varepsilon_0}, \quad (2.35)$$

$$E_2(\mathbf{k}) \simeq \omega_{\mathbf{k}} - \frac{v_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}} = \omega_k - \frac{v_{\mathbf{k}}^2}{\varepsilon_0}. \quad (2.36)$$

The energy correction is small for the solution  $E_1$ , but it is very essential for the solution  $E_2$ , because  $\omega_k \rightarrow 0$  at  $k \rightarrow 0$ . These solutions are indicated in the Figure by bold solid lines.

2). *Large enough momentum values*, so that  $\omega_k \gg \varepsilon_0$ .

If the condition  $v_{\mathbf{k}}^2 \ll \left(\frac{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}}{2}\right)^2$  fulfils, then expansion (2.33) is valid again, but  $|\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}| = \omega_{\mathbf{k}} - \varepsilon_{\mathbf{k}} > 0$ . With this remark we have for the energy roots:

$$\begin{aligned} E_{1,2} &\simeq \frac{\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}}{2} \pm \frac{\omega_{\mathbf{k}} - \varepsilon_{\mathbf{k}}}{2} \left\{ 1 + \frac{1}{2} \left( \frac{2v_{\mathbf{k}}}{\varepsilon_{\mathbf{k}} - \omega_{\mathbf{k}}} \right)^2 \right\} \\ &= \frac{\varepsilon_{\mathbf{k}} + \omega_{\mathbf{k}}}{2} \pm \left\{ \frac{\omega_{\mathbf{k}} - \varepsilon_{\mathbf{k}}}{2} + \frac{v_{\mathbf{k}}^2}{\omega_{\mathbf{k}} - \varepsilon_{\mathbf{k}}} \right\}, \end{aligned} \quad (2.37)$$

from which

$$E_1(\mathbf{k}) \simeq \omega_k + \frac{v_{\mathbf{k}}^2}{\omega_k - \varepsilon_0}, \quad (2.38)$$

$$E_2(\mathbf{k}) \simeq \varepsilon_0 - \frac{v_{\mathbf{k}}^2}{\omega_k - \varepsilon_0}. \quad (2.39)$$

The solutions are indicated in Figure 2.1 by bold solid lines.

3). *The crossing point:*  $\mathbf{k} = \mathbf{k}_0$ , at which  $\omega_k = \varepsilon_{\mathbf{k}} = \varepsilon_0$ .

Applying these equalities to *exact* expression (2.32) for the self-energies we obtain

$$E_{1,2}(\mathbf{k}) \simeq \varepsilon_0 \pm |v_{\mathbf{k}_0}|, \quad (2.40)$$

which indicates the lift-off of degeneracy at the crossing point by the perturbation  $\propto v_{\mathbf{k}_0}$ . Solutions (2.40) are indicated in Fig. 2.1 by arrows. The dot curves interpolate qualitatively our small momentum and large momentum solutions, including the particular points at  $k = k_0$ .

Note in conclusion that at small and large values of momentum  $k$  the interaction  $\propto v_{\mathbf{k}}$  does not change appreciably the nature of initial excitations of the system, but only introduces corrections corresponding to the second order perturbation theory. At the momentum range around the energy of the crossing point the excitations are equally mixed, so we have collective excitations of the system consisting of two kinds of interacting bosons. Let us emphasize here that we did not take care about the crossing point when deriving the equations of motion for the Green functions, though we would have been applied the quantum mechanical perturbation theory for the degenerate case solving this problem in the frame of the conventional quantum mechanics approach. This is because of exact solvability of the model, and exact commutation relations that have been used upon solution of the model.

## 2.3 The Average Value of $S^z$ in an External DC Magnetic Field for $S=1/2$

Next example illustrates an application of the GF technique to spin-systems: the system of noninteracting  $S = 1/2$  spins in the external DC magnetic field of the magnitude  $H$ . The Hamiltonian of the system is

$$\mathcal{H} = -g\mu_B H \sum_i S_i^z, \quad (2.41)$$

where  $\mu_B$  is the Bohr magneton, and  $g \simeq 2.0$  is the spectroscopic g-factor.

We have to calculate  $\langle S_i^z \rangle$  - the equilibrium expectation value of the operator  $S_i^z$ . For this purpose let us recover at first commutation relations for the spin operators:

$$\begin{aligned} [S_i^+, S_j^-] &= 2S_i^z \delta_{ij}; & [S_i^z, S_j^\pm] &= \pm S_i^\pm \delta_{ij}, \\ S_i^\pm &= S_i^x \pm iS_i^y. \end{aligned} \quad (2.42)$$

Then, for the squared operator of a particular spin we establish

$$\mathbf{S}_i^2 = S(S+1) = (S_i^z)^2 + \frac{1}{2} (S_i^+ S_i^- + S_i^- S_i^+). \quad (2.43)$$

For the spin value  $S = 1/2$ ,  $S(S+1) = 3/4$ ,  $(S_i^z)^2 = 1/4$ , from which we get the *anticommutator*

$$S_i^+ S_i^- + S_i^- S_i^+ = 1. \quad (2.44)$$

Together with *commutation* relations (2.42), Eq. (2.44) gives the system of equations for determining of  $S_i^z$  :

$$\begin{aligned} S_i^+ S_i^- + S_i^- S_i^+ &= 1, \\ S_i^+ S_i^- - S_i^- S_i^+ &= 2S_i^z, \end{aligned} \quad (2.45)$$

from which we obtain our basic operator equation

$$S_i^z = S_i^+ S_i^- - \frac{1}{2}. \quad (2.46)$$

Averaging over the equilibrium statistical ensemble immediately gives us

$$\langle S_i^z \rangle = \langle S_i^+ S_i^- \rangle - \frac{1}{2}, \quad (2.47)$$

where  $\langle S_i^+ S_i^- \rangle$  can be evaluated using general definitions of CFs (1.5), (1.6), the relation between GF with coinciding time-arguments, and the spectral density of CF, similar to (2.16):

$$\langle S_i^+ S_i^- \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{+-}(\omega), \quad (2.48)$$

with  $J_{+-}(\omega)$  standing instead of  $J_{S^+S^-}(\omega)$ . For calculating the spectral intensity  $J_{+-}(\omega)$  we have to evaluate the Green function (see Eq. (1.34))

$$\langle\langle S_i^-(t) S_i^+(t') \rangle\rangle_{\eta=1}^r = G_{-+}(t, t'), \quad (2.49)$$

the superscript and subscript in the left-hand side show us that we have chosen the *retarded, commutator*-type Green function.

According to prescription (1.46) the equation of motion for  $G_{-+}(t, t')$  is

$$i \frac{\partial}{\partial t} G_{-+}(t, t') = -2 \langle S^z \rangle \delta(t - t') + \omega_0 G_{-+}(t, t'), \quad (2.50)$$

where we have defined for brevity

$$\omega_0 = -g\mu_B H, \quad (2.51)$$

and dropped the site subscript in  $\langle S^z \rangle$ . After the Fourier transformation over the time variable we get

$$\omega G_{-+}(\omega) = -2 \langle S^z \rangle + \omega_0 G_{-+}(\omega), \quad (2.52)$$

from which the solution for the GF spectral density comes as follows:

$$G_{-+}(\omega) = -\frac{2 \langle S^z \rangle}{\omega - \omega_0}. \quad (2.53)$$

Next step is evaluation of the spectral density  $J_{+-}(E)$  for CF by means of (1.34):

$$J_{+-}(\omega) = i \frac{G_{-+}(\omega + i\varepsilon) - G_{-+}(\omega - i\varepsilon)}{e^{\omega/kT} - 1}. \quad (2.54)$$

Substitution of (2.53) into (2.54) gives

$$\begin{aligned} J_{+-}(\omega) &= i \frac{-2 \langle S^z \rangle}{e^{\omega/kT} - 1} \left\{ \frac{1}{\omega - \omega_0 + i\varepsilon} - \frac{1}{\omega - \omega_0 - i\varepsilon} \right\} \\ &= -\frac{4\pi \langle S^z \rangle \delta(\omega - \omega_0)}{e^{\omega/kT} - 1}. \end{aligned} \quad (2.55)$$

According to (2.48)

$$\begin{aligned} \langle S^+ S^- \rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left( -\frac{4\pi \langle S^z \rangle}{e^{\omega/kT} - 1} \right) \delta(\omega - \omega_0) \\ &= -\frac{2 \langle S^z \rangle}{e^{\omega_0/kT} - 1}, \end{aligned} \quad (2.56)$$

and then, according to (2.47),

$$\langle S^z \rangle = -\frac{1}{2} - \frac{2 \langle S^z \rangle}{e^{\omega_0/kT} - 1}, \quad (2.57)$$

so we get the equation for finding  $\langle S^z \rangle$ . The solution is straightforward:

$$\langle S^z \rangle = -\frac{1}{2} \tanh \frac{\omega_0}{2k_B T} \equiv \frac{1}{2} \tanh \frac{g\mu_B H}{2k_B T}, \quad (2.58)$$

which is well-known result for  $\langle S^z \rangle$  at  $S = 1/2$ .

## 2.4 Problems

1. Derive the distribution function for free fermions

$$n_{\mathbf{k}} = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{e^{\varepsilon_{\mathbf{k}}/kT} + 1}$$

using the retarded GF of the *anticommutator* type.

2. Solve the problem of interacting bosons of two types for more general Hamiltonian of interaction between bosons:

$$\mathcal{H}_{int} = \sum_{\mathbf{k}'} \left( v_{\mathbf{k}'} a_{\mathbf{k}'}^\dagger b_{\mathbf{k}'} + v_{\mathbf{k}'}^* a_{\mathbf{k}'} b_{\mathbf{k}'}^\dagger + u_{\mathbf{k}'} a_{\mathbf{k}'} b_{\mathbf{k}'} + u_{\mathbf{k}'}^* a_{\mathbf{k}'}^\dagger b_{\mathbf{k}'}^\dagger \right).$$

Take the excitation spectra of the noninteracting bosons same as in the solved problem. Analyze the excitations spectrum in particular cases of small, large momentum and at the crossing point.

3. Derive the expression for the average value of  $S^z$  in an external DC magnetic field for  $S=1/2$  (2.58) using the *anticommutator*-type retarded Green function for spin operators.

# Chapter 3

## Magnetism of Solids in the Heisenberg Model

### 3.1 Heisenberg Ferromagnet in the Molecular-Field Approximation

#### 3.1.1 The molecular-field approximation

Consider lattice of spins  $S = 1/2$  interacting by means of the Heisenberg scalar exchange

$$\mathcal{H} = \omega_0 \sum_i S_i^z - \frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i \mathbf{S}_j. \quad (3.1)$$

The first term represents the energy of spins in an external DC magnetic field, the second one is the Heisenberg scalar exchange interaction between the spins. The sign of the interaction  $J_{ij}$  is positive, indicating the *ferromagnetic* type of coupling between spins.

The molecular-field approximation implies that:

- a) the two-particle operators in (3.1) should be transformed into single-particle ones, considering average value of one of the operators in a product instead of the operator one;
- b) fluctuations of the average values from site to site of magnetic ions lattice should be neglected.

Actually,

$$\mathbf{S}_i \mathbf{S}_j = S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+), \quad (3.2)$$

$$S_i^z S_j^z \longrightarrow \langle S_i^z \rangle S_j^z + S_i^z \langle S_j^z \rangle, \quad (3.3)$$

$$S_i^+ S_j^- \longrightarrow \langle S_i^+ \rangle S_j^- + S_i^+ \langle S_j^- \rangle, \quad (3.4)$$

$$S_i^- S_j^+ \longrightarrow \langle S_i^- \rangle S_j^+ + S_i^- \langle S_j^+ \rangle, \quad (3.5)$$

and, at last,

$$\langle S_i^z \rangle = \langle S_j^z \rangle = \langle S^z \rangle \quad (3.6)$$

is independent on the site label. For isotropic ferromagnet in an external DC magnetic field applied in the  $z$ -direction, the average transverse magnetization is equal to *zero*. This means that

$$\langle S_i^\pm \rangle = \langle S^\pm \rangle = 0, \quad (3.7)$$

so Hamiltonian (3.1) in the *molecular-field approximation* transforms to

$$\begin{aligned}\mathcal{H}_{mf} &= \omega_0 \sum_i S_i^z - \frac{1}{2} \langle S^z \rangle \sum_{i,j} J_{ij} (S_i^z + S_j^z) \\ &= \omega_0 \sum_i S_i^z - \langle S^z \rangle \sum_{i,j} J_{ij} S_j^z.\end{aligned}\quad (3.8)$$

The last equality follows from the symmetry property of the exchange,  $J_{ij} = J_{ji}$ . The second term can be decomposed by the following way:

$$\begin{aligned}\sum_{i,j} J_{ij} S_j^z &= \sum_j S_j^z \sum_i J_{ji} \\ &= J_0 \sum_j S_j^z,\end{aligned}\quad (3.9)$$

where we have denoted

$$J_0 = \sum_i J_{ji}, \quad (3.10)$$

which does not depend on the site label  $j$  for a regular lattice of spins. Thus, the Hamiltonian takes its final form:

$$\mathcal{H}_{mf} = \omega_0 \sum_i S_i^z - \langle S^z \rangle J_0 \sum_j S_j^z. \quad (3.11)$$

Observing Hamiltonian (3.11) one can point out that it is diagonal in the  $S^z$ -representation, so the magnetization can be computed considering the conventional thermodynamic expressions for the statistical sum and its derivatives. It is actually the case, however, as we shall see below, derivation of the equation for the average magnetization by Green functions is not more difficult than the traditional thermodynamic one.

### 3.1.2 The spectral intensity of a Green function

We recall, at first, the *commutation* relations for the spin operators:

$$\begin{aligned}[S_i^+, S_j^-] &= 2S_i^z \delta_{ij}; & [S_i^z, S_j^\pm] &= \pm S_i^\pm \delta_{ij}, \\ S_i^\pm &= S_i^x \pm iS_i^y.\end{aligned}\quad (3.12)$$

For the spin value  $S = 1/2$ ,  $S(S+1) = 3/4$ ,  $(S_i^z)^2 = 1/4$ , from which we get the *anticommutator*

$$S_i^+ S_i^- + S_i^- S_i^+ = 1. \quad (3.13)$$

Together with *commutation* relations (3.12), Eq. (3.13) gives the system of equations for determining of  $S_i^z$ :

$$\begin{aligned}S_i^+ S_i^- + S_i^- S_i^+ &= 1, \\ S_i^+ S_i^- - S_i^- S_i^+ &= 2S_i^z.\end{aligned}\quad (3.14)$$

Let us write down now the equation of motion for the *commutator*-type Green function  $\langle\langle S_i^-(t) | S_i^+(t') \rangle\rangle$  using general prescription (1.46):

$$i \frac{\partial}{\partial t} \langle\langle S_i^-(t) | S_i^+(t') \rangle\rangle = -2 \langle S^z \rangle \delta(t-t') + \omega_0 \langle\langle S_i^-(t) | S_i^+(t') \rangle\rangle - J_0 \langle S^z \rangle \langle\langle S_i^-(t) | S_i^+(t') \rangle\rangle. \quad (3.15)$$



Performing the Fourier transformation on the time variables by the rule

$$G_{\eta}^r(t-t') = \int_{-\infty}^{\infty} \frac{dE}{2\pi} G_{\eta}^r(E) e^{-iE(t-t')}, \quad (3.16)$$

we obtain from (3.15)

$$E \langle \langle S_i^- | S_i^+ \rangle \rangle_E = -2 \langle S^z \rangle + \omega_0 \langle \langle S_i^- | S_i^+ \rangle \rangle_E - J_0 \langle S^z \rangle \langle \langle S_i^- | S_i^+ \rangle \rangle_E. \quad (3.17)$$

From (3.17) the spectral intensity of GF  $\langle \langle S_i^- | S_i^+ \rangle \rangle_E$  can be found as follows

$$\begin{aligned} \langle \langle S_i^- | S_i^+ \rangle \rangle_E &= \frac{-2 \langle S^z \rangle}{E - \omega_0 + \langle S^z \rangle J_0} \\ &= -\frac{2 \langle S^z \rangle}{E - \omega_J}, \end{aligned} \quad (3.18)$$

where we have introduced

$$\omega_J = \omega_0 - \langle S^z \rangle J_0, \quad (3.19)$$

which is the excitation spectrum of the spin-system.

### 3.1.3 The equation for the spontaneous magnetization

According to (1.34) we evaluate the spectral intensity of correlation function  $\langle S_i^+(t) S_i^-(t) \rangle - J_{S^+ S^-}(E) \equiv J_{+-}(E)$  :

$$\begin{aligned} J_{+-}(E) &= -i \frac{2 \langle S^z \rangle}{e^{E/kT} - 1} (-2\pi i \delta(E - \omega_J)) \\ &= -\frac{4\pi \langle S^z \rangle \delta(E - \omega_J)}{e^{E/kT} - 1}, \end{aligned} \quad (3.20)$$

from which the equal-time correlation function (the average value of the operators product) can be computed as follows:

$$\begin{aligned} \langle S_i^+ S_i^- \rangle &= \int \frac{dE}{2\pi} J_{+-}(E) \\ &= -2 \langle S^z \rangle \int dE \frac{\delta(E - \omega_J)}{e^{E/kT} - 1} = -\frac{2 \langle S^z \rangle}{e^{\omega_J/kT} - 1}. \end{aligned} \quad (3.21)$$

Then, using commutation and anticommutation relations for  $S = 1/2$  (3.14) we get the operator equality

$$S_i^+ S_i^- = \frac{1}{2} + S_i^z, \quad (3.22)$$

from which one can obtain after the thermodynamic averaging

$$\langle S_i^z \rangle = \langle S_i^+ S_i^- \rangle - \frac{1}{2}. \quad (3.23)$$

After the substitution of (3.21) into (3.23) we get

$$\langle S_i^z \rangle = -\frac{1}{2} - \frac{2 \langle S^z \rangle}{e^{\omega_J/kT} - 1}, \quad (3.24)$$

which is the equation for finding  $\langle S_i^z \rangle$ . After a little algebra one can obtain the transcendental equation for evaluation the average spin value per magnetic lattice site  $\langle S^z \rangle \equiv \langle S_i^z \rangle$ :

$$\langle S^z \rangle \coth \frac{\omega_0 - \langle S^z \rangle J_0}{2k_B T} = -\frac{1}{2}. \quad (3.25)$$

This equation defines the magnetic ordering temperature in the molecular-field approximation, and the temperature dependence of the average spin value (or magnetization by virtue of  $g\mu_B \langle S^z \rangle N/V = M^z$ ) per magnetic lattice site as well.

### 3.1.4 The ferromagnetic transition temperature

The main feature of equation (3.25) is that it allows the nonzero magnetization to appear even in the **absence** of the external DC magnetic field, *i.e.*  $\omega_0 = 0$ . This happens at certain finite temperature, which can be found from (3.25), and we shall refer it as the magnetic ordering temperature  $T_{c0}$ . To prove this statement, let us note that at temperatures close to  $T_{c0}$  the magnetization vanishes:  $\langle S^z \rangle_{T \rightarrow T_{c0}} \rightarrow 0$ . Then, the hyperbolic cotangent can be expanded in power series for a small value of the argument

$$\coth x \simeq \frac{1}{x} + \frac{x}{3}. \quad (3.26)$$

Keeping the first term in (3.26) we transform equation (3.25) to

$$\langle S^z \rangle \coth \frac{\langle S^z \rangle J_0}{2k_B T} \Big|_{\langle S^z \rangle \rightarrow 0} = \frac{2k_B T_{c0}}{J_0} = \frac{1}{2}. \quad (3.27)$$

From (3.27) the relation between  $J_0$  and  $T_{c0}$  immediately follows,

$$k_B T_{c0} = \frac{J_0}{4}, \quad (3.28)$$

which determines the magnetic ordering temperature  $T_{c0}$  of a ferromagnet in the *molecular-field approximation*.

Let us compare (3.28) with the well-known expression for the Curie-Weiss temperature  $\theta$  in the high-temperature approximation

$$k_B \theta = J_0 \frac{S(S+1)}{3} \Big|_{S=1/2} = \frac{J_0}{4}. \quad (3.29)$$

From the above expressions we conclude that  $T_{c0}$  in the *molecular field approximation* coincides with the Curie-Weiss temperature  $\theta$ .

### 3.1.5 Temperature dependence of magnetization

Let us now investigate the temperature behavior of  $\langle S^z \rangle$  at high ( $T \rightarrow T_{c0}$ ) and low ( $T \rightarrow 0K$ ) temperatures.

1). *High temperatures:*  $T_{c0} - T \ll T_{c0}$  ( $|\langle S^z \rangle| \ll 1$ ).

The temperature dependence of the average magnetization near  $T_{c0}$  can be found by keeping both terms in Eq. (3.26):

$$\langle S^z \rangle \left( \frac{2k_B T}{\langle S^z \rangle J_0} + \frac{\langle S^z \rangle J_0}{6k_B T} \right) = \frac{1}{2}, \quad (3.30)$$

or

$$\frac{2k_B T}{J_0} + \frac{\langle S^z \rangle^2 J_0}{6k_B T_{c0}} = \frac{1}{2}, \quad (3.31)$$

where we have neglected the difference between  $T$  and  $T_{c0}$  in the second term of the left-hand side of the equation upon going from (3.30) to (3.31). This is because of  $\langle S^z \rangle^2 \ll 1$  factor in this term. From Eq. (3.31) we obtain for  $\langle S^z \rangle^2$ :

$$\begin{aligned} \langle S^z \rangle^2 &= \frac{6k_B T_{c0}}{J_0} \left( \frac{1}{2} - \frac{2k_B T}{J_0} \right) \\ &= \frac{3}{4} \left( 1 - \frac{T}{T_{c0}} \right), \end{aligned} \quad (3.32)$$

where we have used expression (3.28) for  $T_{c0}$  for substitution in the first line of (3.32). As equation (3.25) at  $\omega_0 = 0$  is even with respect to the sign of  $\langle S^z \rangle$ , **hereafter we shall search for the positive-sign solution** for this equation implying a modulus of  $\langle S^z \rangle$  instead of  $\langle S^z \rangle$ . Thus, from (3.32) we finally find

$$\langle S^z \rangle = \frac{\sqrt{3}}{2} \sqrt{1 - \frac{T}{T_{c0}}}, \quad (3.33)$$

which is the square root temperature behavior of  $\langle S^z \rangle$  and  $M^z$  near  $T_{c0}$ . Taking the derivative of  $\langle S^z \rangle$  with respect to temperature

$$\frac{\partial \langle S^z \rangle}{\partial T} = -\frac{\sqrt{3}}{4T_{c0}} \frac{1}{\sqrt{1 - \frac{T}{T_{c0}}}} \Bigg|_{T \rightarrow T_{c0}} \rightarrow -\infty \quad (3.34)$$

we conclude that the magnetization approaches zero with *infinite* derivative on  $T$ . It means that  $\langle S^z \rangle$  grows with infinite slope upon changing the temperature just below  $T_{c0}$ . This behavior is indicated on Figure 3.1 by the bold solid curve.

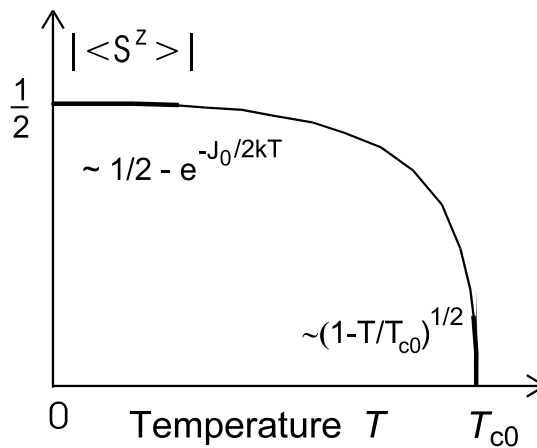


Figure 3.1: The temperature dependence of  $\langle S^z \rangle$  in the molecular-field approximation.

2). *Low temperatures:* ( $T \rightarrow 0K$ ,  $J_0 \gg k_B T$ ).

At low temperatures the average value of  $\langle S^z \rangle$  does not go far from its limiting magnitude  $S = 1/2$ . So we can represent

$$\langle S^z \rangle = \frac{1}{2} - \delta, \quad (3.35)$$

where  $\delta \ll 1/2$ . Substitution of (3.35) into (3.25) (recall that we consider the case of  $\omega_0 = 0$ ) gives

$$\left(\frac{1}{2} - \delta\right) \coth \left\{ \frac{\left(\frac{1}{2} - \delta\right) J_0}{2k_B T} \right\} = \frac{1}{2}. \quad (3.36)$$

At low temperatures  $k_B T \ll J_0$ , so we can use the expansion of  $\coth(x)$  at large  $x$ :

$$\coth(x)|_{x \rightarrow \infty} \simeq 1 + 2e^{-2x}. \quad (3.37)$$

Substituting (3.37) into (3.36) we get:

$$\left(\frac{1}{2} - \delta\right) \left(1 + 2e^{-2\frac{\left(\frac{1}{2} - \delta\right) J_0}{2k_B T}}\right) = \frac{1}{2}, \quad (3.38)$$

from which the equation

$$e^{-\frac{J_0}{2k_B T}} (1 - 2\delta) e^{\delta \frac{J_0}{k_B T}} - \delta = 0 \quad (3.39)$$

follows. This equation can be analyzed for cases, when  $\delta \frac{J_0}{k_B T} \ll 1$  and  $\delta \frac{J_0}{k_B T} \geq 1$ , and we proceed with this analysis:

a) if  $\delta \frac{J_0}{k_B T} \ll 1$ , then

$$\exp\left(\delta \frac{J_0}{k_B T}\right) \simeq 1 + \delta \frac{J_0}{k_B T}. \quad (3.40)$$

Substituting (3.40) into (3.39) and collecting terms up to the first order in  $\delta$  we obtain

$$e^{-\frac{J_0}{2k_B T}} \left(1 + \delta \frac{J_0}{k_B T}\right) - 2\delta e^{-\frac{J_0}{2k_B T}} - \delta = 0, \quad (3.41)$$

from which the solution for  $\delta$  follows

$$\delta \simeq \frac{e^{-\frac{J_0}{2k_B T}}}{1 - \frac{J_0}{k_B T} e^{-\frac{J_0}{2k_B T}}}. \quad (3.42)$$

This solution, according to definition (3.35), finally gives for  $\langle S^z \rangle$  :

$$\langle S^z \rangle \simeq \frac{1}{2} - \frac{e^{-\frac{J_0}{2k_B T}}}{1 - \frac{J_0}{k_B T} e^{-\frac{J_0}{2k_B T}}}. \quad (3.43)$$

In (3.42) we have neglected the term  $2e^{-\frac{J_0}{2k_B T}}$  in the denominator as compared with the kept term  $\frac{J_0}{k_B T} e^{-\frac{J_0}{2k_B T}}$ , because  $\frac{J_0}{k_B T} \gg 1$  in the low-temperature case under the consideration.

Formula (3.43) predicts the exponential approaching by  $\langle S^z \rangle$  the limiting value  $1/2$ , because the denominator of (3.43) approaches unity as  $T \rightarrow 0K$  ( $xe^{-x}|_{x \rightarrow \infty} \rightarrow 0$ ).

b) if  $\delta \frac{J_0}{k_B T} \geq 1$ , or  $\delta \geq \frac{k_B T}{J_0}$ , then the equation for  $\langle S^z \rangle$  remains transcendental, but Eq. (3.39), rewritten as

$$\delta = e^{-\frac{J_0}{2k_B T}} (1 - 2\delta) e^{\delta \frac{J_0}{k_B T}}, \quad (3.44)$$

together with the above condition  $\delta \geq \frac{k_B T}{J_0}$  defines the inequality

$$e^{-\frac{J_0}{2k_B T}} (1 - 2\delta) e^{\delta \frac{J_0}{k_B T}} \geq \frac{k_B T}{J_0}. \quad (3.45)$$

As  $0 < 2\delta \ll 1$ , from (3.45) we obtain more strong inequality,

$$e^{-\frac{J_0}{2k_B T}} e^{\delta \frac{J_0}{k_B T}} > \frac{k_B T}{J_0}, \quad (3.46)$$

which cannot be satisfied anyway because of the following reasons: Let us recall first that the initial condition,

$$\delta \frac{J_0}{k_B T} \geq 1, \quad (3.47)$$

means that

$$e^{\delta \frac{J_0}{k_B T}} > 2. \quad (3.48)$$

The inequality (3.46) can be rewritten in the new variable  $x = \frac{J_0}{2k_B T}$  as follows:

$$2xe^{-x} e^{2x\delta} > 1. \quad (3.49)$$

Together with Eq. (3.48) and the basic assumptions,

$$\begin{aligned} \delta &\ll 1/2, \\ x &\gg 1, \end{aligned} \quad (3.50)$$

it forms the coupled set of inequalities, which can never be satisfied.

Thus, expression (3.43) defines the temperature dependence of the average single-site spin value for low temperatures. This behavior is indicated in Fig. 3.1 by the bold solid curve in the area of low temperatures.

In conclusion, we have to emphasize that the *molecular-field approximation* predicts the exponential approaching of the saturation value by  $\langle S^z \rangle$  as the temperature approaches absolute zero. Contrary to this conclusion, experiment shows the power-law temperature behavior of  $\langle S^z \rangle$ :  $\langle S^z \rangle \simeq \frac{1}{2} - \alpha T^{\frac{3}{2}}$  - the Bloch's law. Thus, we note the discrepancy between the temperature behavior of  $\langle S^z \rangle$  in the *molecular-field approximation* and in experiments.

### 3.1.6 Problems

1. Solve numerically transcendental equation for  $\langle S^z \rangle$  (3.25) ( $\omega_0 = 0$ ) in the entire temperature range  $T \in [0, T_{c0}]$ . Draw the curve of the temperature dependence of the "exact" numerical  $|\langle S^z \rangle|$ , and of the approximate solutions for  $|\langle S^z \rangle|$  near absolute zero and near  $T_{c0}$  by computer.

## 3.2 Heisenberg Ferromagnet in the Random Phase Approximation

### 3.2.1 Basic formulations and the spectral intensity of a Green function

Let us recall the Hamiltonian of the Heisenberg ferromagnet

$$\mathcal{H} = \omega_0 \sum_i S_i^z - \frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i \mathbf{S}_j. \quad (3.51)$$

Now, we do not introduce any approximations to the Hamiltonian (3.51), and proceed with introducing the *commutator-type* retarded Green function

$$\langle\langle S_f^-(t) | S_g^+(t') \rangle\rangle = -i\theta(t-t') \langle [S_f^-(t), S_g^+(t')] \rangle_{\eta=1}^r. \quad (3.52)$$

For the above GF the equation of motion can be written down by general prescription (1.46):

$$E \langle\langle S_f^- | S_g^+ \rangle\rangle_E = -2\delta_{fg} \langle S_f^z \rangle + \omega_0 \langle\langle S_f^- | S_g^+ \rangle\rangle_E - \sum_j J_{fj} \langle\langle S_f^- S_j^z - S_j^- S_f^z | S_g^+ \rangle\rangle_E. \quad (3.53)$$

Inspection of (3.53) shows that a new Green function appears in the right-hand side of the equation. According to the general formulation of the Green function method we have to write down equation(s) of motion for the new GF(s) and so on, but we shall do an approximation just in equation (3.53), and show that it will give nontrivial improvement of the molecular-field approximation, providing the correct temperature behavior of magnetization at low temperatures:  $M_z \propto T^{3/2}$ .

Let us note that in the ferromagnetic state, at temperatures not very close to the transition temperature  $T_c$  (actually, at  $T \leq 0.7T_c$ ), almost all magnetic moments are aligned in one direction, so the magnetization only slightly deviates from its saturation value. Then, we replace the operator  $S_f^z$  in GFs by its average value  $\langle S_f^z \rangle$ , and neglect fluctuations of the staggered magnetization from one lattice site to the other:  $\langle S_f^z \rangle \rightarrow \langle S^z \rangle$ . This approximation is called random phase, or Tyablikov approximation [3]. Equation (3.53) may be rewritten as follows

$$E \langle\langle S_f^- | S_g^+ \rangle\rangle_E = -2\delta_{fg} \langle S^z \rangle + \omega_0 \langle\langle S_f^- | S_g^+ \rangle\rangle_E - \sum_j J_{fj} \langle S^z \rangle \left\{ \langle\langle S_f^- | S_g^+ \rangle\rangle_E - \langle\langle S_j^- | S_g^+ \rangle\rangle_E \right\}. \quad (3.54)$$

This equation is integral over the spatial variable. In order to solve it we perform the Fourier transformation over the spatial variables. Noting at first that GFs depend on the difference of spatial arguments (*e.g.*,  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ ) due to translational invariance of the problem, we define

$$\langle\langle S_f^- | S_g^+ \rangle\rangle_E = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, E) e^{i\mathbf{k}\mathbf{r}_{fg}}. \quad (3.55)$$

Then, we substitute the Fourier-transforms of fashion (3.55) for all terms in Eq. (3.54) and obtain

$$E \sum_{\mathbf{k}} G(\mathbf{k}, E) e^{i\mathbf{k}\mathbf{r}_{fg}} = -2 \langle S^z \rangle \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{fg}} + \omega_0 \sum_{\mathbf{k}} G(\mathbf{k}, E) e^{i\mathbf{k}\mathbf{r}_{fg}} - \frac{1}{N} \sum_j \langle S^z \rangle \sum_{\mathbf{k}} J_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{fj}} \sum_{\mathbf{k}'} \left\{ e^{i\mathbf{k}'\mathbf{r}_{fg}} - e^{i\mathbf{k}'\mathbf{r}_{jg}} \right\} G(\mathbf{k}', E) \quad (3.56)$$

Using

$$\frac{1}{N} \sum_j e^{i(\mathbf{k}' - \mathbf{k})\mathbf{r}_{jg}} = \delta_{\mathbf{k}'\mathbf{k}} \quad (3.57)$$

by definition we can transform the last term of Eq. (3.56) as follows

$$\begin{aligned} & \frac{1}{N} \sum_j \langle S^z \rangle \sum_{\mathbf{k}} J_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{fj}} \sum_{\mathbf{k}'} \left\{ e^{i\mathbf{k}'\mathbf{r}_{fg}} - e^{i\mathbf{k}'\mathbf{r}_{jg}} \right\} G(\mathbf{k}', E) \\ &= + \langle S^z \rangle \sum_{\mathbf{k}} \sum_{\mathbf{k}'} J_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_f} G(\mathbf{k}', E) e^{i\mathbf{k}'\mathbf{r}_{fg}} \delta_{\mathbf{k}\mathbf{0}} \\ & \quad - \langle S^z \rangle \sum_{\mathbf{k}} \sum_{\mathbf{k}'} J_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_f} G(\mathbf{k}', E) e^{-i\mathbf{k}'\mathbf{r}_g} \delta_{\mathbf{k}\mathbf{k}'} \\ &= \langle S^z \rangle \sum_{\mathbf{k}'} J_0 G(\mathbf{k}', E) e^{i\mathbf{k}'\mathbf{r}_{fg}} - \langle S^z \rangle \sum_{\mathbf{k}} J_{\mathbf{k}} G(\mathbf{k}, E) e^{i\mathbf{k}\mathbf{r}_{fg}}, \end{aligned} \quad (3.58)$$

where we have defined  $J_0 \equiv J_{\mathbf{k}=\mathbf{0}}$ . Changing the variable  $\mathbf{k}' \rightarrow \mathbf{k}$  in the first term of (3.58) and observing the same structure of all terms of Eq. (3.56) we conclude, that because of arbitrary volume under consideration and, consequently, the arbitrary set of  $\mathbf{k}$  values, the integrands of the both sides of Eq. (3.56) are equal, *i.e.*

$$(E - \omega_0) G(\mathbf{k}, E) = -2 \langle S^z \rangle - J_0 \langle S^z \rangle G(\mathbf{k}, E) + J_{\mathbf{k}} \langle S^z \rangle G(\mathbf{k}, E). \quad (3.59)$$

From (3.59) the spectral intensity of the GF  $G(\mathbf{k}, E)$  can be immediately obtained

$$G(\mathbf{k}, E) = -\frac{2 \langle S^z \rangle}{E - \omega_0 + \langle S^z \rangle (J_0 - J_{\mathbf{k}})}. \quad (3.60)$$

### 3.2.2 The excitations spectrum

The pole of the spectral intensity (3.60) of GF gives us the excitation spectrum of the interacting spin-system

$$E \equiv E_{\mathbf{k}} = \omega_0 - \langle S^z \rangle (J_0 - J_{\mathbf{k}}), \quad (3.61)$$

which has dispersion (dependence on  $\mathbf{k}$ ), as opposed to (3.19) - the dispersionless excitation spectrum of the Heisenberg ferromagnet in the molecular-field approximation. In the absence of an external DC magnetic field  $\omega_0 = 0$ , and the excitation spectrum reads

$$E_{\mathbf{k}} = -\langle S^z \rangle (J_0 - J_{\mathbf{k}}) = -\langle S^z \rangle \sum_j J_{ij} (1 - e^{-i\mathbf{k}\mathbf{r}_{ij}}). \quad (3.62)$$

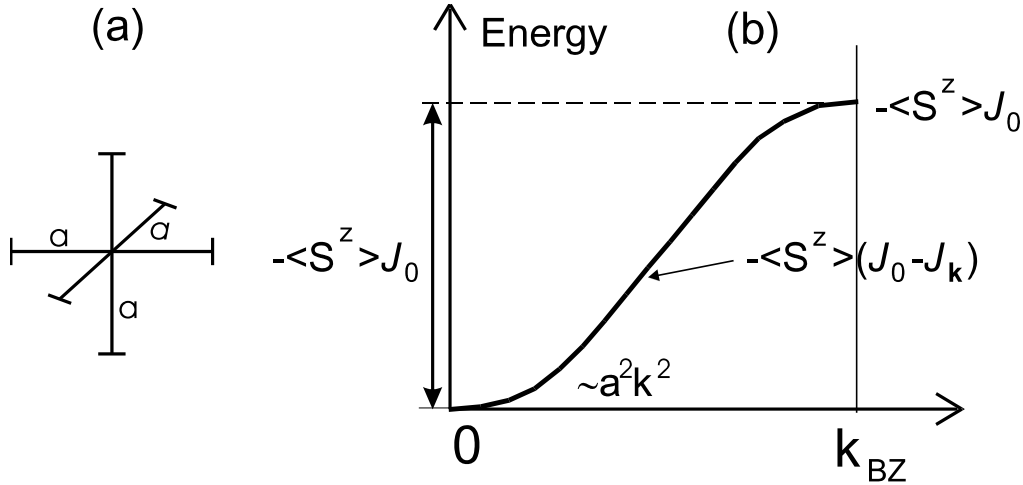


Figure 3.2: The picture of the nearest neighbors in the magnetic lattice (a) and the excitation spectrum (b).

In further calculations we assume the *nearest neighbors exchange* with an exchange integral between nearest magnetic moments equal to  $J$ , the *simple cubic lattice* with 6 nearest neighbors for any particular local spin, and with the lattice spacing equal to  $a$  (see Figure 3.2a). With these assumptions, for the excitation spectrum we have

$$\begin{aligned} E_{\mathbf{k}} &= -J \langle S^z \rangle \left\{ 6 - \left( e^{-ik_x a} + e^{ik_x a} + e^{-ik_y a} + e^{ik_y a} + e^{-ik_z a} + e^{ik_z a} \right) \right\} \\ &= -2J \langle S^z \rangle \left\{ 3 - \cos(k_x a) - \cos(k_y a) - \cos(k_z a) \right\} \end{aligned} \quad (3.63)$$

for an arbitrary  $\mathbf{k}$  value. Actually, (3.62) and (3.63) represent the *band of excitations*, as it is shown in Figure 3.2b. From expression (3.63) it can be easily seen that the band width is given by (recall that  $\langle S^z \rangle < 0$ )

$$-6J \langle S^z \rangle = -J_0 \langle S^z \rangle. \quad (3.64)$$

At small values of the momentum  $\mathbf{k}$  ( $k_\alpha a \ll 1$ ) we may expand the cosines in (3.63) in power series, thus obtaining

$$E_{\mathbf{k}}|_{small \mathbf{k}} \simeq -\langle S^z \rangle J k^2 a^2, \quad (3.65)$$

which represents the parabolic dispersion law for the excitations near the bottom of the band. As we shall see below, the dispersion (and gapless) character of the excitation spectrum in the random phase approximation will ensure correct temperature behavior of the spontaneous magnetization at low temperatures.

### 3.2.3 The equation for the spontaneous magnetization

In this subsection we use spectral intensity of GF (3.60) obtained before to derive the equation for the spontaneous magnetization (or the averaged  $z$ -projection of a spin) below the ferromagnetic transition temperature  $T_c$ , which also has to be found from this equation. First of all, we calculate the spectral intensity of the correlation function -



$J_{+-}(\mathbf{k}, E) \equiv J_{S^+S^-}(\mathbf{k}, E)$  making use of our general expression (1.34):

$$\begin{aligned} J_{+-}(\mathbf{k}, E) &= -i \frac{2\langle S^z \rangle}{e^{E/kT} - 1} \left\{ \frac{1}{E - E_{\mathbf{k}} + i\varepsilon} - \frac{1}{E - E_{\mathbf{k}} - i\varepsilon} \right\} \\ &= -i \frac{2\langle S^z \rangle}{e^{E/kT} - 1} \{-2\pi i \delta(E - E_{\mathbf{k}})\} = -\frac{4\pi \langle S^z \rangle}{e^{E/kT} - 1} \delta(E - E_{\mathbf{k}}). \end{aligned} \quad (3.66)$$

Having  $J_{+-}(\mathbf{k}, E)$  we can calculate the *equal-time* correlation function (the averaged product),

$$\begin{aligned} \langle S_f^+(t) S_g^-(t) \rangle_{\mathbf{k}} &\equiv \langle S_f^+ S_g^- \rangle_{\mathbf{k}} \\ &= \int \frac{dE}{2\pi} J_{+-}(\mathbf{k}, E) = -\frac{2\langle S^z \rangle}{e^{E_{\mathbf{k}}/kT} - 1}. \end{aligned} \quad (3.67)$$

After that we can find the *single-site* correlation function (single-site averaged product), which is, in fact, the *single-site static correlation function*  $\langle S_f^+ S_f^- \rangle$  (see equation (3.55)):

$$\langle S_f^+ S_f^- \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle S_f^+ S_f^- \rangle_{\mathbf{k}} = -\frac{2\langle S^z \rangle}{N} \sum_{\mathbf{k}} \frac{1}{e^{E_{\mathbf{k}}/kT} - 1}. \quad (3.68)$$

Then, by averaging and combining commutation and anticommutation relations (3.14) we obtain

$$\langle S_f^z \rangle \equiv \langle S^z \rangle = \langle S_f^+ S_f^- \rangle - \frac{1}{2}, \quad (3.69)$$

from which we arrive to the transcendental equation for the average  $z$ -projection of a single spin on a magnetic lattice site using single-site GF (3.68):

$$\frac{\langle S^z \rangle}{N} \sum_{\mathbf{k}} \coth \frac{E_{\mathbf{k}}}{2k_B T} = -\frac{1}{2}, \quad (3.70)$$

where the following identity had been used upon derivation of (3.70),

$$\frac{1}{N} \sum_{\mathbf{k}} 1 = 1. \quad (3.71)$$

### 3.2.4 The ferromagnetic transition temperature

For calculating the magnetic transition temperature, similar to the case of Heisenberg ferromagnet in the molecular-field approximation, we take into account that  $\langle S^z \rangle$  vanishes as temperature approaches  $T_c$  from below. In the absence of a magnetic field ( $\omega_0 = 0$ ):

$$\langle S^z \rangle \coth \frac{E_{\mathbf{k}}}{2k_B T} \Big|_{T \rightarrow T_c} = -\frac{2k_B T_c}{J_0 - J_{\mathbf{k}}}. \quad (3.72)$$

Substituting (3.72) into equation (3.70) we get

$$\frac{1}{2} = \frac{2k_B T_c}{N} \sum_{\mathbf{k}} \frac{1}{J_0 - J_{\mathbf{k}}}, \quad (3.73)$$

from which we find

$$k_B T_c = \frac{1}{4} \left\{ \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{J_0 - J_{\mathbf{k}}} \right\}^{-1}. \quad (3.74)$$

As  $|J_0 - J_{\mathbf{k}}| < |J_0|$ , then  $T_c$  in the interpolation random-phase approximation is **lower** than in the molecular-field approximation:  $T_{c0} = J_0/4$ . Actually, for simple cubic (SC) lattice

$$\begin{aligned} k_B T_c &= \frac{1}{4} \left\{ \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{2J(3 - \cos k_x a - \cos k_y a - \cos k_z a)} \right\}^{-1} \\ &= \frac{1}{4} \left\{ \frac{V}{(2\pi)^3} \iiint_{-\pi/a}^{\pi/a} \frac{dk_x dk_y dk_z}{2J(3 - \cos k_x a - \cos k_y a - \cos k_z a)} \right\}^{-1} \\ &= \frac{1}{2} \frac{(2\pi)^3}{V} J a^3 \left\{ \iiint_{-\pi}^{\pi} \frac{dx dy dz}{3 - \cos x - \cos y - \cos z} \right\}^{-1} \\ &= 4\pi^3 J W^{-1}, \end{aligned} \quad (3.75)$$

where

$$W = \iiint_{-\pi}^{\pi} \frac{dx dy dz}{3 - \cos x - \cos y - \cos z} \quad (3.76)$$

is well known Watson integral (*Handbook of mathematical functions*, ed. by M. Abramovitz and I.A. Stegun, NBS, 1964). The result of the integration is known:

$$W = 32\pi \left( 18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6} \right) \mathbf{K}^2 \left[ \left( 2 - \sqrt{3} \right) \left( \sqrt{3} - \sqrt{2} \right) \right], \quad (3.77)$$

and  $\mathbf{K}(x)$  is the elliptic function. Evaluating the elliptic function for the particular argument,

$$\mathbf{K}^2 [0.0851642] \simeq [1.606]^2 = 2.57924, \quad (3.78)$$

we get for the Watson integral

$$W \simeq 4\pi \cdot 10.4. \quad (3.79)$$

For transition temperature (3.75) we obtain

$$k_B T_c \simeq J \frac{\pi^2}{10.4} \simeq 0.95J, \quad (3.80)$$

or

$$k_B T_c \simeq 0.95 \frac{J_0}{6} \quad (3.81)$$

(compare this result with  $k_B T_{c0} = J_0/4$  obtained before in the molecular-field approximation).

### 3.2.5 Temperature dependence of $\langle S^z \rangle$ near $T_c$ ( $T_c - T \ll T_c$ )

For deriving an equation which governs the temperature dependence of  $\langle S^z \rangle$  near the transition temperature  $T_c$ , given by (3.81), we keep two terms of the hyperbolic cotangent expansion in the power series at small  $\langle S^z \rangle$  (see (3.26) in Eq. (3.70)):

$$\langle S^z \rangle \coth \frac{E_{\mathbf{k}}}{2k_B T} \simeq -\frac{2k_B T}{J_0 - J_{\mathbf{k}}} - \frac{\langle S^z \rangle^2 (J_0 - J_{\mathbf{k}})}{6k_B T_c}. \quad (3.82)$$

Again, as in the case of the molecular-field approximation, we replaced  $T$  by  $T_c$  in the second term of the right-hand side of Eq. (3.82), because  $\langle S^z \rangle^2 \ll 1$ . Substituting (3.82) into (3.70) we obtain

$$\frac{k_B T}{2} \left( \frac{1}{N} \sum_{\mathbf{k}} \frac{4}{J_0 - J_{\mathbf{k}}} \right) + \frac{\langle S^z \rangle^2}{6k_B T_c} \frac{1}{N} \sum_{\mathbf{k}} (J_0 - J_{\mathbf{k}}) = \frac{1}{2}. \quad (3.83)$$

The multiplier in the large brackets of the first term is  $T_c^{-1}$ , according to (3.74). In the second term

$$\frac{1}{N} \sum_{\mathbf{k}} J_0 = J_0 \frac{1}{N} \sum_{\mathbf{k}} 1 = J_0 \quad (3.84)$$

according to (3.71), and

$$\frac{1}{N} \sum_{\mathbf{k}} J_{\mathbf{k}} \equiv J(\mathbf{r}_{ij} = 0) \equiv 0, \quad (3.85)$$

because it represents the exchange interaction of magnetic moment with itself. Substituting (3.84) and (3.85) into (3.83) we get

$$\frac{T}{2T_c} + \frac{J_0 \langle S^z \rangle^2}{6k_B T_c} = \frac{1}{2}, \quad (3.86)$$

from which we find

$$|\langle S^z \rangle| = \sqrt{\frac{3k_B T_c}{J_0}} \sqrt{1 - \frac{T}{T_c}}. \quad (3.87)$$

Recalling from (3.80) and (3.81) that

$$k_B T_c \simeq \frac{J_0}{6} \quad (3.88)$$

we finally obtain

$$|\langle S^z \rangle| \simeq \frac{1}{\sqrt{2}} \sqrt{1 - \frac{T}{T_c}}. \quad (3.89)$$

Differentiating (3.89) on temperature

$$\frac{\partial |\langle S^z \rangle|}{\partial T} = -\frac{1}{2\sqrt{2}T_c} \frac{1}{\sqrt{1 - \frac{T}{T_c}}} \Big|_{T \rightarrow T_c} \rightarrow -\infty \quad (3.90)$$

we check again that  $\langle S^z \rangle$  approaches zero at  $T_c$  with infinite derivative on  $T$ .

### 3.2.6 Low temperature behavior of $\langle S^z \rangle$ ( $T \ll T_c$ )

Let us assume that temperature  $T$  is low enough, so that  $k_B T \ll J_0$ , and  $|\langle S^z \rangle|$  is close to its saturation value  $= 1/2$ . We introduce the deviation of  $\langle S^z \rangle$  from  $(-1/2)$  by

$$\delta = \langle S^z \rangle + \frac{1}{2}, \quad (3.91)$$

and substitute it into the equation for  $\langle S^z \rangle$ , which may be obtained from equations (3.68) and (3.69), and is equivalent to Eq. (3.70):

$$\delta = \frac{2}{N} \left( \frac{1}{2} - \delta \right) \sum_{\mathbf{k}} \left\{ \exp \left[ \frac{\left( \frac{1}{2} - \delta \right) (J_0 - J_{\mathbf{k}})}{k_B T} \right] - 1 \right\}^{-1}. \quad (3.92)$$

We will get the first nonvanishing approximation for  $\delta$  if we set  $\delta = 0$  in the right-hand side of Eq. (3.92):

$$\delta = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{e^{(J_0 - J_{\mathbf{k}})/2k_B T} - 1}. \quad (3.93)$$

For the nearest neighbors interaction, and the simple cubic lattice, we have from (3.63) for the excitation spectrum at  $T \rightarrow 0$

$$E_{\mathbf{k}} = J \{ 3 - \cos(k_x a) - \cos(k_y a) - \cos(k_z a) \}, \quad (3.94)$$

and from (3.65) for the small momentum ( $k_{\alpha} a \ll 1$ )

$$E_{\mathbf{k}}|_{small \mathbf{k}} \simeq \frac{1}{2} J k^2 a^2 \equiv \frac{J_0}{12} k^2 a^2. \quad (3.95)$$

To evaluate the sum in (3.93) let us change it to integration over the Brillouin Zone (BZ) by

$$\frac{1}{N} \sum_{\mathbf{k}} \longrightarrow \frac{V}{(2\pi)^3} \int_{\Omega_{\mathbf{k}}} d\mathbf{k}, \quad (3.96)$$

where  $V$  is the actual volume of the specimen, and  $\Omega_{\mathbf{k}}$  is the volume of BZ. Then, Eq. (3.93) becomes

$$\delta = \frac{V}{(2\pi)^3} \int_0^{k_{BZ}} \frac{d\mathbf{k}}{e^{E_{\mathbf{k}}/k_B T} - 1}. \quad (3.97)$$

In further calculations we shall use long wave-length approximation (3.95) for the excitations spectrum, and change  $k_{BZ}$  on  $\infty$ , because at low temperatures, due to  $\exp(E_{\mathbf{k}}/k_B T)$  in denominator of (3.95), only the low-energy states in band (3.94) are populated. These states correspond to small  $k$  (see Fig. 3.2b), and detailed  $E_{\mathbf{k}}$  behavior at the upper integration limit is unimportant because of negligible contribution to the integral. With this remark we continue the evaluation of (3.97):

$$\begin{aligned} \delta &= \frac{V}{(2\pi)^3} \int_0^{\infty} \frac{4\pi k^2 dk}{e^{Jk^2 a^2 / 2k_B T} - 1} \\ &= \frac{1}{2\pi^2} \left( \frac{2k_B T}{J} \right)^{\frac{3}{2}} \int_0^{\infty} \frac{x^2 dx}{e^{x^2} - 1}, \end{aligned} \quad (3.98)$$

where we have changed variable by  $x^2 = \frac{Jk^2 a^2}{2k_B T}$ . The remaining integral in (3.98) can be found in the tables of integrals, or by expanding the integrand in power series, integrating term by term and summing the obtained series. The result is

$$= \frac{1}{2\pi^2} \left( \frac{2k_B T}{J} \right)^{\frac{3}{2}} \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right) \propto T^{\frac{3}{2}}. \quad (3.99)$$

Finally, we get for  $\langle S^z \rangle$

$$\langle S^z \rangle \simeq -\frac{1}{2} + \frac{1}{2\pi^2} \left( \frac{2k_B T}{J} \right)^{\frac{3}{2}} \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right), \quad (3.100)$$

where  $\Gamma(x)$  and  $\zeta(x)$  are the Euler's gamma-function and the Riemann's zeta-function, respectively. From (3.99) and (3.100) we learn that at low temperatures the deviation of  $|\langle S^z \rangle|$  value from its saturation value,  $1/2$ , reveals the power-law behavior  $\propto T^{\frac{3}{2}}$  (Bloch's law), which corresponds to experiments.

In the intermediate range of temperatures, equation (3.70) for  $\langle S^z \rangle$  can be solved numerically.

### 3.2.7 Problems

1. Reproduce equation of motion (3.53).
2. Evaluate the integral over the variable  $x$  in Eq. (3.98).
3. Solve numerically equation (3.70) for the nearest neighbors exchange and simple cubic lattice. Approximate the sum by the integral on momentum over the BZ. Draw the temperature dependence of  $|\langle S^z \rangle|$ .



# Chapter 4

## Ferromagnetic Transition Metals in the Spin-Wave (Magnon) Approximation

It is well known that the electrical and magnetic properties of transition metals strongly depend on an unfilled electron shells ( $d$  or  $f$ ) of the atoms with the non-compensated spin [4,8]. Experience shows that in spite of some changes, which occur with unfilled electron shells of atoms during their association into a crystal, the individuality of these electrons in a metal conserve in a considerable degree indicating their substantial localization near the lattice points.

The exchange interaction between electrons of the unfilled shells oftenly results in a transition to ferromagnetic state, while their metallic properties ascribe with the former valence electrons, forming the system of mobile (itinerant) conduction electrons (called  $s$ -electrons).

In this chapter we will examine a model of transition metal based on the  $s$ - $d$  exchange interaction between localized " $d$ " and itinerant  $s$ -electrons. The system of  $d$ -electrons is considered in the spin-wave approximation. Using the method of Green functions we compute the equilibrium distribution functions for spin waves (magnons) and the conduction electrons (fermions). Then, the interaction between magnons and fermions is considered.

### 4.1 The Hamiltonian of Electron System in Transition Metals

In accordance with the model declared above, let us distinguish two groups of electrons:  $d$ -electrons of the unfilled  $3d$  shells and conduction electrons ( $s$ ). Hereafter the electrons of the unfilled shells we will designate by index  $d$ . The " $s$ - $d$  exchange interaction" indicates interaction of the itinerant conduction electrons with the localized electrons of unfilled  $3d$ -shells. We describe the latter electrons by atomic localized functions, and the conduction electrons by Bloch functions:

$$\varphi_{\mathbf{k}\sigma}(\mathbf{r}, s) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) \chi_{\sigma}(s) = \psi_{\mathbf{k}}(\mathbf{r}) \chi_{\sigma}(s), \quad (4.1)$$

where  $\chi_\sigma(s)$  is the so-called spin wave function of electron. Spin index  $\sigma$  can take two values,  $\sigma = \pm 1/2$ . Let us ascribe for the certainty that  $\sigma = +1/2 = \downarrow$  - corresponds to spin-down projection, and  $\sigma = -1/2 = \uparrow$  - to spin-up projection.

The operator of the  $s - d$ -exchange interaction can be written down in the form

$$\mathcal{H}_{sd} = -2 \sum_j I(\mathbf{r} - \mathbf{R}_j) (\mathbf{s} \cdot \mathbf{S}_j), \quad (4.2)$$

where  $\mathbf{s}$ ,  $\mathbf{r}$  and  $\mathbf{S}_j$ ,  $\mathbf{R}_j$  are the spin operators and the radius-vectors of the conduction electron and the total spin of a paramagnetic ion in the site  $\mathbf{R}_j$ ,  $I(\mathbf{r} - \mathbf{R}_j)$  is the exchange integral.

Hamiltonian (4.2) in the second quantization representation for conduction electrons has the form

$$\mathcal{H}_{sd} = -2 \sum_j \sum_{\mathbf{k}\mathbf{k}'\alpha\beta} \mathbf{S}_j \langle \mathbf{k}\alpha | I(\mathbf{r} - \mathbf{R}_j) \mathbf{s} | \mathbf{k}'\beta \rangle c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\beta}, \quad (4.3)$$

where  $c_{\mathbf{k}\alpha}^\dagger$  and  $c_{\mathbf{k}'\beta}$  are the creation and annihilation operators for conduction electrons in the states  $\mathbf{k}\alpha$  and  $\mathbf{k}'\beta$ . Here  $\alpha$  and  $\beta$  are also spin indices, which possess properties of  $\sigma$ . Commutation relations for this operators are given by

$$\begin{aligned} \{c_{\mathbf{k}\alpha}, c_{\mathbf{k}'\beta}^\dagger\} &\equiv c_{\mathbf{k}\alpha} c_{\mathbf{k}'\beta}^\dagger + c_{\mathbf{k}'\beta}^\dagger c_{\mathbf{k}\alpha} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\beta}, \\ \{c_{\mathbf{k}\alpha}, c_{\mathbf{k}'\beta}\} &= \{c_{\mathbf{k}\alpha}^\dagger, c_{\mathbf{k}'\beta}^\dagger\} = 0. \end{aligned}$$

Using multiplicativity of the spin and coordinate parts of function (4.1) and the translational invariance in the regular lattice  $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} - \mathbf{R}_j)$  (where  $\mathbf{R}_j$  is any vector of the lattice), matrix element (4.3) can be written down as

$$\langle \mathbf{k}\alpha | I(\mathbf{r} - \mathbf{R}_j) \mathbf{s} | \mathbf{k}'\beta \rangle = \frac{1}{N} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{R}_j} I(\mathbf{k}, \mathbf{k}') \langle \alpha | \mathbf{s} | \beta \rangle, \quad (4.4)$$

where  $2 \langle \alpha | \mathbf{s} | \beta \rangle$  are the Pauli matrices  $\sigma_{\alpha\beta}$ .  $I(\mathbf{k}, \mathbf{k}')$  is the  $s$ - $d$  exchange integral,

$$I(\mathbf{k}, \mathbf{k}') = \iint \mathbf{k}(\mathbf{r}) w^*(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \psi_{\mathbf{k}'}(\mathbf{r}') w(\mathbf{r}) d\mathbf{r} d\mathbf{r}', \quad (4.5)$$

where  $w(\mathbf{r})$  is the atomic function of  $d$  electron,  $V(\mathbf{r} - \mathbf{r}')$  is the potential of Coulomb interaction between  $s$  and  $d$  electrons.

Usually,  $I(\mathbf{k}, \mathbf{k}')$  enters into expressions for different physical quantities with values of  $\mathbf{k}$  and  $\mathbf{k}'$  close to the Fermi momentum  $k_F$ , since the conduction electrons in the metal are strongly degenerate. If we assume, that in a metal  $k \sim k_F$ ,  $k' = (k - q) \sim k_F$ , then  $I(\mathbf{k}, \mathbf{k}')$  depends weakly on momentum, so it is possible to admit  $I(\mathbf{k}, \mathbf{k} - \mathbf{q}) \approx I(k_F, k_F) = I$ .

According to different estimations the absolute value of  $I$  is by two orders less than the Fermi energy  $\varepsilon_F$ . In these conditions the parameter  $I/\varepsilon_F \ll 1$ , so at calculations of the thermodynamic and kinetic characteristics, the  $s$ - $d$  interaction can be considered as a perturbation.

Taking into account the above discussion  $s$ - $d$  Hamiltonian (4.3) can be represented in the form of

$$\mathcal{H}_{sd} = -I \sum_{j\mathbf{q}\mathbf{k}} \sum_{\alpha\beta} e^{-i\mathbf{q}\mathbf{R}_j} \mathbf{S}_j c_{\mathbf{k}\alpha}^\dagger \sigma_{\alpha\beta} c_{\mathbf{k}-\mathbf{q}\beta}, \quad (4.6)$$



or, realizing the matrix elements for spin operators (3.12), one obtains

$$\mathcal{H}_{sd} = -I \sum_{j\mathbf{q}\mathbf{k}} e^{-i\mathbf{q}\mathbf{R}_j} \left[ c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}-\mathbf{q}\downarrow} S_j^- + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}-\mathbf{q}\uparrow} S_j^+ + \left( c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}-\mathbf{q}\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}-\mathbf{q}\downarrow} \right) S_j^z \right]. \quad (4.7)$$

The complete Hamiltonian of the electronic system of transition metal consists of three contributions,  $\mathcal{H} = \mathcal{H}_s + \mathcal{H}_d + \mathcal{H}_{sd}$ , where  $\mathcal{H}_s$  is the Hamiltonian of conduction electrons, which in framework of the second quantization can be written down in the form

$$\mathcal{H}_s = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - SI - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \quad (4.8)$$

Here  $\varepsilon_{\mathbf{k}}$  is the energy of conduction electron in a metal without  $s$ - $d$  interaction,  $SI$  is an additive term representing spin-independent contribution from the exchange Hamiltonian, leading to the identical shift of the conduction electrons energy for both projections of the spin,  $\mu$  is the chemical potential.

The Hamiltonian  $\mathcal{H}_d$  for the localized moments of "magnetic" electrons is examined in the approximation of interaction between  $d$  electrons of the adjacent ions (compare with Hamiltonian of the Heisenberg model (3.1))

$$\mathcal{H}_d = -J \sum_{j\rho} \mathbf{S}_j \mathbf{S}_{j+\rho}, \quad (4.9)$$

where  $\rho = |\boldsymbol{\rho}|$  is the absolute value of vector, connecting  $j$ -ion with its nearest neighbors,  $J$  is the integral of direct exchange between the nearest neighbors,  $\mathbf{S}_j$  is the operator of localized spins. For determining the spectrum of the localized magnetic moments it is convenient to write down Hamiltonian (4.9) in the form (see (3.2) for details):

$$\mathcal{H}_d = -J \sum_{j\rho} S_j^z S_{j+\rho}^z - \frac{1}{2} J \sum_{j\rho} (S_j^+ S_{j+\rho}^- + S_j^- S_{j+\rho}^+). \quad (4.10)$$

The Hamiltonian  $\mathcal{H} = \mathcal{H}_s + \mathcal{H}_d + \mathcal{H}_{sd}$  was proposed for the first time in the work by S.V. Vonsovskii and E.A. Turov (S.V. Vonsovskii and E.A. Turov. On the exchange interaction of valence and internal electrons in crystals (s-d exchange model of transition crystals). ZhETF **24**, N3, p.419-428 (1953) (in Russian)).

## 4.2 Spin-Wave Approximation

To proceed further towards finding the eigenvalues of the Hamiltonian  $\mathcal{H}_d$  we introduce Holstein-Primakoff-Izyumov representation for the spin operators (see [6], §5):

$$\begin{aligned} S_j^+ &= (2S)^{1/2} \left( 1 - \frac{d_j^\dagger d_j}{2S} \right)^{1/2} d_j, & S_j^- &= (2S)^{1/2} d_j^\dagger \left( 1 - \frac{d_j^\dagger d_j}{2S} \right)^{1/2}, \\ S_j^z &= S - d_j^\dagger d_j. \end{aligned} \quad (4.11)$$

Here, the operators  $d_j$  and  $d_j^\dagger$  obey the commutation relations

$$d_i d_j - d_j d_i = 0, \quad (4.12)$$

$$d_i d_j^\dagger - d_j^\dagger d_i = \left( 1 - \frac{2S+1}{(2S)!} d_i^{\dagger 2S} d_i^{2S} \right) \delta_{ij}. \quad (4.13)$$

Relationship (4.12) has bosonic nature, however, relationship (4.13) is more complicated, it depends on the value of spin  $S$ . In particular case of  $S = 1/2$ , (4.13) converts to the fermionic commutation relation

$$d_j d_j^\dagger + d_j^\dagger d_j = 1 \quad (S = 1/2). \quad (4.14)$$

In a case of large spin  $S \gg 1$  the last term in (4.13) can be neglected, and (4.13) acquires the bosonic nature

$$d_j d_j^\dagger - d_j^\dagger d_j = 1. \quad (S \gg 1). \quad (4.15)$$

In the case of the bosonic commutation relations of operators  $d_j$  and  $d_j^\dagger$ , the eigenvalues of operator  $n_j = d_j^\dagger d_j$  are integer:  $0, 1, 2, \dots, 2S$ . The operator  $n_j$  describes deviations from the maximum projection of the spin in site  $j$ . In the ground state of ferromagnetic material all spins of  $d$ -shells align in one direction, so they have maximum projection  $S$  on the quantization axis  $Oz$ . If deviations from the ground state are small, the average value of the operator  $n_j$  must be small

$$\langle n_j \rangle = \langle d_j^\dagger d_j \rangle \ll 2S. \quad (4.16)$$

In this case (4.11) takes the form

$$S_j^+ = (2S)^{1/2} d_j, \quad S_j^- = (2S)^{1/2} d_j^\dagger, \quad S_j^z = S - d_j^\dagger d_j. \quad (4.17)$$

With the same degree of accuracy it is possible to disregard the last term in (4.13). Thus, the operators  $d_j$  and  $d_j^\dagger$  with condition (4.16) are approximately boson operators. This approximation is called *spin-wave approximation*.

Let us consider the total Hamiltonian  $\mathcal{H}_d$  of a ferromagnetic metal in this approximation. In the Fourier-representation of the operators  $d_j$  and  $d_j^\dagger$ ,

$$d_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_j} d_{\mathbf{q}}, \quad d_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\mathbf{R}_j} d_{\mathbf{q}}^\dagger, \quad (4.18)$$

the Hamiltonian  $\mathcal{H}_d$  takes the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' + \mathcal{H}'', \quad (4.19)$$

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}^\sigma c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} d_{\mathbf{q}}^\dagger d_{\mathbf{q}}, \quad (4.20)$$

$$\mathcal{H}' = -I (2NS)^{1/2} \sum_{\mathbf{k}\mathbf{q}} \left( c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}\downarrow} d_{\mathbf{q}}^\dagger + c_{\mathbf{k}+\mathbf{q}\downarrow}^\dagger c_{\mathbf{k}\uparrow} d_{\mathbf{q}} \right), \quad (4.21)$$

$$\mathcal{H}'' = I \sum_{\mathbf{k}\mathbf{q}\mathbf{p}} \left( c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}+\mathbf{q}-\mathbf{p}\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}+\mathbf{q}-\mathbf{p}\downarrow} \right) d_{\mathbf{q}}^\dagger d_{\mathbf{p}}, \quad (4.22)$$

where

$$\varepsilon_{\mathbf{k}}^\sigma = \varepsilon_{\mathbf{k}} - 2SI\delta_{\sigma\uparrow} - \mu \quad (4.23)$$

is the energy of  $s$  electrons with the spin  $\sigma = \pm 1/2$  denoted also as  $\downarrow\uparrow$ ;

$$\omega_{\mathbf{q}} = 2S(J_0 - J_{\mathbf{q}}), \quad (4.24)$$

is the excitation spectrum of spin waves with quasi-momentum  $\mathbf{q}$ , appearing in the system of  $d$ -electrons under the action of the direct exchange.

The diagonal part of the Hamiltonian,  $\mathcal{H}_0$ , represents the energy of elementary excitations of the system of spin waves and conduction electrons, moreover, the latter ones acquire magnetic bias due to saturated magnetization of the  $d$ -electrons. Thus, the spectrum of the elementary excitations of the electronic system of ferromagnetic metal contains two branches - Fermi (conduction electrons) and Bose (spin waves).

The interaction of  $s$  and  $d$  electrons in the adopted approximation leads to two effects: 1) change in energy of  $s$  electrons (second term in (4.23)) and 2) their interaction with spin waves, causing transitions between the unperturbed levels of the system: (a) operator  $\mathcal{H}'$  describes processes of inelastic scattering, with which spin waves can be created and annihilated; (b) operator  $\mathcal{H}''$  describes processes of the elastic scattering of the spin waves on conduction electrons. However, in these processes the operators  $\mathcal{H}'$ ,  $\mathcal{H}''$  conserve the total spin of the electronic system of metal. The operators  $\mathcal{H}'$ ,  $\mathcal{H}''$  provide also conservation of the particles quasi-momentum during collisions of elementary excitations.

### 4.3 The Distribution Functions for Conduction Electrons and Magnons in the First Order Perturbation Theory

For different applications it is not sufficient to know the energy spectrum of a system. Some correlation functions, distribution functions, and averages of the dynamic variables of the system could be interesting.

As an example, let us calculate the equilibrium distribution functions for the conduction electrons and spin waves being the statistical averages of the appropriate occupation numbers,

$$n_{\mathbf{k}}^{\sigma} = \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle, \quad n_{\mathbf{q}} = \langle d_{\mathbf{q}}^{\dagger} d_{\mathbf{q}} \rangle. \quad (4.25)$$

First, we introduce the appropriate Fermi and Bose Green functions:

$$\langle\langle c_{\mathbf{k}\sigma}(t) | c_{\mathbf{k}\sigma}^{\dagger}(t') \rangle\rangle, \quad \langle\langle d_{\mathbf{q}}(t) | d_{\mathbf{q}}^{\dagger}(t') \rangle\rangle. \quad (4.26)$$

Then, we write down equations of motion (see (1.47)) for them, using Hamiltonian (4.19),

$$i \frac{\partial}{\partial t} \langle\langle c_{\mathbf{k}\sigma}(t) | c_{\mathbf{k}\sigma}^{\dagger}(t') \rangle\rangle = \delta(t - t') + \langle\langle [c_{\mathbf{k}\sigma}(t), \mathcal{H}(t)] | d_{\mathbf{q}}^{\dagger}(t') \rangle\rangle, \quad (4.27)$$

$$i \frac{\partial}{\partial t} \langle\langle d_{\mathbf{q}}(t) | d_{\mathbf{q}}^{\dagger}(t') \rangle\rangle = \delta(t - t') + \langle\langle [d_{\mathbf{q}}(t), \mathcal{H}(t)] | d_{\mathbf{q}}^{\dagger}(t') \rangle\rangle. \quad (4.28)$$

After calculation of the commutators we realize that other composite Green functions appear in the right-hand side of Eqs. (4.27) and (4.28):

$$\langle\langle c_{\mathbf{k}\downarrow} c_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \rangle\rangle, \quad (4.29)$$

$$\left\langle\left\langle d_{\mathbf{q}} d_{\mathbf{q}}^{\dagger} c_{\mathbf{k}\downarrow} c_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle, \quad \left\langle\left\langle c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle. \quad (4.30)$$

The time variables are not shown for simplicity. We decouple the chain of equations using approximations:

$$\begin{aligned} \left\langle\left\langle d_{\mathbf{q}} d_{\mathbf{q}}^{\dagger} c_{\mathbf{k}\downarrow} c_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle &\cong n_{\mathbf{q}} \left\langle\left\langle c_{\mathbf{k}\downarrow} c_{\mathbf{k}-\mathbf{q}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle, \\ \left\langle\left\langle c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle &\cong n_{\mathbf{k}}^{\sigma} \left\langle\left\langle d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle, \end{aligned} \quad (4.31)$$

where the occupation numbers,  $n_{\mathbf{k}}^{\sigma}$  and  $n_{\mathbf{q}}$ , determined by (4.25), should be so far considered as unknown variables.

With the aid of (4.31) the chain of equations for the Green's functions is converted into the closed system of three equations:

$$i \frac{\partial}{\partial t} \left\langle\left\langle c_{\mathbf{k}\sigma} | c_{\mathbf{k}\sigma}^{\dagger} \right\rangle\right\rangle = \delta(t-t') + (\tilde{\varepsilon}_{\mathbf{k}}^{\sigma} - \mu) \left\langle\left\langle c_{\mathbf{k}\sigma} | c_{\mathbf{k}\sigma}^{\dagger} \right\rangle\right\rangle, \quad (4.32)$$

$$i \frac{\partial}{\partial t} \left\langle\left\langle d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle = \delta(t-t') + \left[ \omega_{\mathbf{q}} - I \sum_{\mathbf{k}} (n_{\mathbf{k}}^{\uparrow} - n_{\mathbf{k}}^{\downarrow}) \right] \left\langle\left\langle d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle + \quad (4.33)$$

$$+ I (2NS)^{1/2} \left\langle\left\langle c_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle, \quad (4.34)$$

$$\begin{aligned} i \frac{\partial}{\partial t} \left\langle\left\langle c_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle &= (\tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^{\downarrow} - \tilde{\varepsilon}_{\mathbf{k}}^{\uparrow}) \left\langle\left\langle c_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow}^{\dagger} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle + \\ &+ I (2NS)^{1/2} (n_{\mathbf{k}}^{\uparrow} - n_{\mathbf{k}+\mathbf{q}}^{\downarrow}) \left\langle\left\langle d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle, \end{aligned} \quad (4.35)$$

where

$$\tilde{\varepsilon}_{\mathbf{k}}^{\sigma} = \varepsilon_{\mathbf{k}} - 2\sigma SI \left( 1 - \frac{1}{S} \sum_{\mathbf{q}} n_{\mathbf{q}} \right). \quad (4.36)$$

We find solution of the system of equations making use of Fourier transformation (see Subsections 3.1.2 and 3.2.2). We obtain for the Fourier-transforms of the Green's functions

$$\left\langle\left\langle c_{\mathbf{k}\sigma} | c_{\mathbf{k}\sigma}^{\dagger} \right\rangle\right\rangle_E = \frac{1}{E - \tilde{\varepsilon}_{\mathbf{k}}^{\sigma} + \mu}, \quad (4.37)$$

$$\left\langle\left\langle d_{\mathbf{q}} | d_{\mathbf{q}}^{\dagger} \right\rangle\right\rangle_E = \frac{1}{E - \omega_{\mathbf{q}} + \Delta - P_{\mathbf{q}}(E)}, \quad (4.38)$$

where

$$\Delta = I \sum_{\mathbf{k}} (n_{\mathbf{k}}^{\uparrow} - n_{\mathbf{k}}^{\downarrow}), \quad (4.39)$$

$$P_{\mathbf{q}}(E) = 2NSI^2 \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}^{\uparrow} - n_{\mathbf{k}+\mathbf{q}}^{\downarrow}}{E - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^{\downarrow} + \tilde{\varepsilon}_{\mathbf{k}}^{\uparrow}}. \quad (4.40)$$

With the aid of identity (1.33) it is easy to show, that

$$P_{\mathbf{q}}(E \pm i\varepsilon) = P_{\mathbf{q}}(E) \mp i\gamma_{\mathbf{q}}(E), \quad (4.41)$$

where

$$\gamma_{\mathbf{q}}(E) = 2\pi N S I^2 \sum_{\mathbf{k}} \left( n_{\mathbf{k}}^{\uparrow} - n_{\mathbf{k}+\mathbf{q}}^{\downarrow} \right) \delta \left( E - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^{\downarrow} + \tilde{\varepsilon}_{\mathbf{k}}^{\uparrow} \right). \quad (4.42)$$

Now we can determine distribution functions (4.25). From (4.37), utilizing (1.6) at  $t = t'$  and spectral theorem (1.34), we find

$$n_{\mathbf{k}}^{\sigma} = \frac{1}{\exp [(\tilde{\varepsilon}_{\mathbf{k}}^{\sigma} - \mu) / k_B T] + 1}. \quad (4.43)$$

It is the Fermi distribution function for  $s$  electrons, energy of which (4.36) is modified by  $s - d$ - interaction. Analogously, for the distribution function of magnons, from (4.38), making use of relationships (4.41) and (4.42), we obtain

$$n_{\mathbf{q}} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dE}{e^{E/k_B T} - 1} \frac{\gamma_{\mathbf{q}}(E)}{(E - \omega_{\mathbf{q}} + \Delta - P_{\mathbf{q}}(E))^2 + \gamma_{\mathbf{q}}^2(E)}. \quad (4.44)$$

This expression is the superposition of Bose elementary excitations with the resonance intensity and damping by  $\gamma_{\mathbf{q}}(E)$ . In the case of small damping the resonance function under the integral has sharp maximum at the point  $E = \tilde{\omega}_{\mathbf{q}}$ , determined from the equation

$$\tilde{\omega}_{\mathbf{q}} - \omega_{\mathbf{q}} + \Delta - P_{\mathbf{q}}(\tilde{\omega}_{\mathbf{q}}) = 0. \quad (4.45)$$

If one neglects the damping  $\gamma_{\mathbf{q}}(E)$  in Eq. (4.44), the Lorentzian reduces to the delta-function  $\delta(E - \tilde{\omega}_{\mathbf{q}})$ . Then, distribution function (4.44) becomes the Bose-type distribution:

$$n_{\mathbf{q}} = \frac{1}{\exp [\tilde{\omega}_{\mathbf{q}} / k_B T] - 1}. \quad (4.46)$$

Consequently, the quantities  $\tilde{\omega}_{\mathbf{q}}$  and  $\tilde{\varepsilon}_{\mathbf{k}}^{\sigma}$  make sense of the energies of elementary excitations.

## 4.4 The Energy of Conduction Electrons in the Second Order Perturbation Theory

In the previous section the equilibrium distribution function for conduction electrons was calculated in the approximation equivalent to the first order of perturbation theory with respect to the  $s - d$  interaction. Now we will consider high orders. Using decoupling of the complex Green functions of type (4.31), it is possible to obtain the closed system of equations for Green's functions of the following form:

$$i \frac{\partial}{\partial t} \langle \langle c_{\mathbf{k}\uparrow} | c_{\mathbf{k}\uparrow}^{\dagger} \rangle \rangle = \delta(t - t') + (\tilde{\varepsilon}_{\mathbf{k}}^{\uparrow} - \mu) \langle \langle c_{\mathbf{k}\uparrow} | c_{\mathbf{k}\uparrow}^{\dagger} \rangle \rangle - \quad (4.47)$$

$$- I (2NS)^{1/2} \sum_{\mathbf{q}} \langle \langle c_{\mathbf{k}+\mathbf{q}\downarrow} d_{\mathbf{q}}^{\dagger} | c_{\mathbf{k}\uparrow}^{\dagger} \rangle \rangle, \quad (4.48)$$

$$i \frac{\partial}{\partial t} \langle \langle c_{\mathbf{k}\downarrow} | c_{\mathbf{k}\downarrow}^{\dagger} \rangle \rangle = \delta(t - t') + (\tilde{\varepsilon}_{\mathbf{k}}^{\downarrow} - \mu) \langle \langle c_{\mathbf{k}\downarrow} | c_{\mathbf{k}\downarrow}^{\dagger} \rangle \rangle - \quad (4.49)$$

$$- I (2NS)^{1/2} \sum_{\mathbf{q}} \langle \langle c_{\mathbf{k}-\mathbf{q}\uparrow} d_{\mathbf{q}} | c_{\mathbf{k}\downarrow}^{\dagger} \rangle \rangle, \quad (4.50)$$

$$i\frac{\partial}{\partial t} \left\langle \left\langle c_{\mathbf{k}-\mathbf{q}\uparrow} d_{\mathbf{q}} | c_{\mathbf{k}\downarrow}^\dagger \right\rangle \right\rangle = \left( \tilde{\varepsilon}_{\mathbf{k}-\mathbf{q}}^\uparrow + \omega_{\mathbf{q}} - \Delta \right) \left\langle \left\langle c_{\mathbf{k}-\mathbf{q}\uparrow} d_{\mathbf{q}} | c_{\mathbf{k}\downarrow}^\dagger \right\rangle \right\rangle - \quad (4.51)$$

$$-I(2NS)^{1/2} \left( 1 + n_{\mathbf{q}} - n_{\mathbf{k}-\mathbf{q}}^\uparrow \right) \left\langle \left\langle c_{\mathbf{k}\downarrow} | c_{\mathbf{k}\downarrow}^\dagger \right\rangle \right\rangle, \quad (4.52)$$

$$i\frac{\partial}{\partial t} \left\langle \left\langle c_{\mathbf{k}+\mathbf{q}\downarrow} d_{\mathbf{q}}^\dagger | c_{\mathbf{k}\uparrow}^\dagger \right\rangle \right\rangle = \left( \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^\downarrow - \omega_{\mathbf{q}} + \Delta \right) \left\langle \left\langle c_{\mathbf{k}+\mathbf{q}\downarrow} d_{\mathbf{q}}^\dagger | c_{\mathbf{k}\uparrow}^\dagger \right\rangle \right\rangle - \quad (4.53)$$

$$-I(2NS)^{1/2} \left( n_{\mathbf{q}} + n_{\mathbf{k}+\mathbf{q}}^\downarrow \right) \left\langle \left\langle c_{\mathbf{k}\uparrow} | c_{\mathbf{k}\uparrow}^\dagger \right\rangle \right\rangle, \quad (4.54)$$

where  $\tilde{\varepsilon}_{\mathbf{k}}^\sigma$  and  $\omega_{\mathbf{q}}$  are given by formulas (4.23) and (4.24), respectively. The energy shift  $\Delta$  is determined by formula (4.39). From this system of four equations for the Fourier components of the Green's functions we obtain the following expression for the Green function  $\left\langle \left\langle c_{\mathbf{k}\sigma} | c_{\mathbf{k}\sigma}^\dagger \right\rangle \right\rangle_E$ :

$$\left\langle \left\langle c_{\mathbf{k}\sigma} | c_{\mathbf{k}\sigma}^\dagger \right\rangle \right\rangle_E = \frac{1}{E - \tilde{\varepsilon}_{\mathbf{k}}^\sigma - M_{\mathbf{k}}^\sigma(E)}, \quad (4.55)$$

where

$$M_{\mathbf{k}}^\uparrow(E) = 2NSI^2 \sum_{\mathbf{q}} \frac{n_{\mathbf{q}} + n_{\mathbf{k}+\mathbf{q}}^\downarrow}{E - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^\downarrow + \omega_{\mathbf{q}} - \Delta}, \quad (4.56)$$

$$M_{\mathbf{k}}^\downarrow(E) = 2NSI^2 \sum_{\mathbf{q}} \frac{1 + n_{\mathbf{q}} - n_{\mathbf{k}-\mathbf{q}}^\uparrow}{E - \tilde{\varepsilon}_{\mathbf{k}-\mathbf{q}}^\uparrow - \omega_{\mathbf{q}} + \Delta} \quad (4.57)$$

are the mass operators or self-energy parts.

For finding the distribution functions it is necessary to use spectral theorem, having preliminarily separated (see (1.33)) the real and imaginary parts in the expression

$$M_{\mathbf{k}}^\sigma(E - \sigma i 2\varepsilon) = \text{Re}(M_{\mathbf{k}}^\sigma(E)) + \sigma i 2\Gamma_{\mathbf{k}}^\sigma(E). \quad (4.58)$$

For  $\Gamma_{\mathbf{k}}^\sigma(E)$  we obtain:

$$\Gamma_{\mathbf{k}}^\uparrow(E) = 2\pi NSI^2 \sum_{\mathbf{q}} \left( n_{\mathbf{q}} + n_{\mathbf{k}+\mathbf{q}}^\downarrow \right) \delta \left( E - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}}^\downarrow + \omega_{\mathbf{q}} - \Delta \right), \quad (4.59)$$

$$\Gamma_{\mathbf{k}}^\downarrow(E) = 2\pi NSI^2 \sum_{\mathbf{q}} \left( 1 + n_{\mathbf{q}} - n_{\mathbf{k}-\mathbf{q}}^\uparrow \right) \delta \left( E - \tilde{\varepsilon}_{\mathbf{k}-\mathbf{q}}^\uparrow - \omega_{\mathbf{q}} + \Delta \right). \quad (4.60)$$

These functions describe damping of  $s$ -electrons with each spin alignment under the effect of their collisions with spin waves. Based on (1.35) we obtain the distribution function

$$n_{\mathbf{k}}^\sigma = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dE}{e^{E/k_B T} + 1} \frac{\Gamma_{\mathbf{k}}^\sigma(E)}{[E - \tilde{\varepsilon}_{\mathbf{k}}^\sigma - M_{\mathbf{k}}^\sigma(E) + \mu]^2 + \Gamma_{\mathbf{k}}^{\sigma 2}(E)}. \quad (4.61)$$

If the damping  $\Gamma_{\mathbf{k}}^\sigma(E)$  and the mass operator  $M_{\mathbf{k}}^\sigma(E)$  are neglected, Eq. (4.61) reduces to the Fermi function (4.43).

Thus, the  $s$ - $d$  interaction leads not only to magnetic biasing of  $s$ -electrons, but also to their damping. The first effect appears in the first order of the perturbation theory, and the second one - in the second order. In other words, the energy shift of conduction electron levels is proportional to  $I$ , and the damping - to  $I^2/\mu$ . On the other hand, conduction electrons act on the spin waves too. They shift the energy of magnons and give rise to their damping (see Eqs (4.40) and (4.42)), the latter is proportional to  $I^2/\mu$ .

# Chapter 5

## Localized Magnetic Moments in Metals

In the early sixties there were carried out systematic experimental investigations of magnetism of  $3d$ -ions dissolved in various **nonmagnetic** elemental metals and metallic compounds. It was found that in dilute solutions of iron, cobalt and nickel the appearance of a magnetic moment on a transition ion depends on the host metal, and the moments observed differ greatly from one solute to the other. In 1961, P. Anderson (Phys. Rev. **124**, 41 (1961)) proposed an interpretation of the localized magnetic moment formation on ions of transition groups ( $3d$ ), dissolved in a nonmagnetic host metal. The model Hamiltonian proposed by Anderson is often referred as the *Anderson Hamiltonian*.

### 5.1 The Anderson Hamiltonian and Basic Equations

Assume that there exists an ion with one orbital state of  $d$ -electron,  $\varphi_d$ , which may be filled by an electron with either spin projection ('+' - "up" or '-' - "down"). If the spin-up electron fills this state, then another electron with the spin-down projection will experience Coulomb repulsion from the first one, when trying to fill in the same orbital state. Therefore, if we denote the energy of spin-up filled state below the Fermi energy as  $E$ , then the energy of the spin-down state will be  $E + U$  (see Fig. 5.1 below), where  $U$  is the energy of  $d - d$  Coulomb repulsion (actually it is the atomic Coulomb repulsion energy). If  $U$  is large enough, the level  $E + U$  will be well above the Fermi energy, and this level will be empty provided that mixing with electrons of the host metal conduction band is neglected. Thus, on the site, occupied by impurity  $3d$ -ion, the magnetic moment appears which corresponds to one electron per orbital state  $\varphi_d$ .

Interaction of  $d$ -electrons with conduction electrons of a host metal (will be referred as  $s$ -electrons) increases energy of the lower-energy state and decreases energy of the upper lying state (*i.e.* decreases the initial splitting  $U$  between these states). At the same time, it introduces the life-time broadening of these states. Eventually, the residence of  $d$ -electrons on their ions becomes unstable, and it is no longer possible to maintain a localized moment. Because of interaction (covalent mixing) of  $d$ - and  $s$ - electrons the stability of the localized  $d$ -state becomes cooperative phenomenon. In addition,  $d$ -state with particular spin projection may have a non-integer occupation number. It means that the valence can be non-integer.

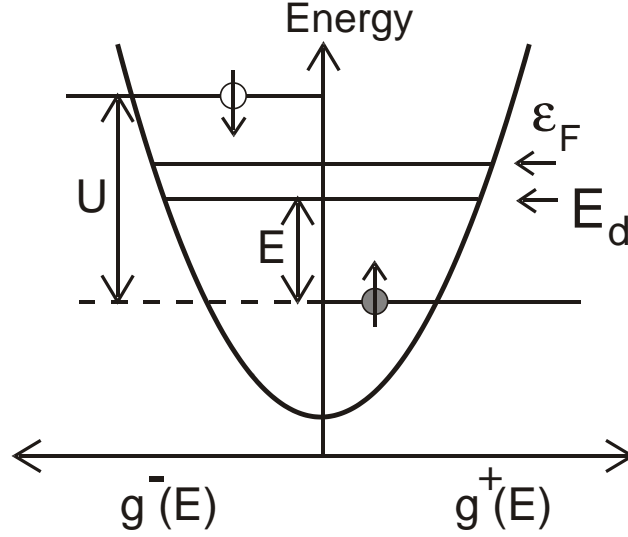


Figure 5.1: Unperturbed energy levels in the absence of  $s - d$  mixing.

The model can be summarized by writing down the Hamiltonian:

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + E (n_d^+ + n_d^-) + U n_d^+ n_d^- + \sum_{\mathbf{k}} V_{\mathbf{k}} (c_{\mathbf{k}\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{\mathbf{k}\sigma}), \quad (5.1)$$

where  $\varepsilon_{\mathbf{k}}$  is the energy of conduction electrons of the host metal,  $n_{\mathbf{k}\sigma} = c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$  is the particle number operator for momentum  $\mathbf{k}$  and spin projection  $\sigma$ , and  $c_{\mathbf{k}\sigma}^\dagger$  ( $c_{\mathbf{k}\sigma}$ ) is the creation (annihilation) operator for the conduction band electrons.  $E$  is the unperturbed energy of the  $d$ -state,  $n_d^\sigma = d_\sigma^\dagger d_\sigma$  is the particle number operator for the  $d$ -state and spin projection  $\sigma$ , and  $d_\sigma^\dagger$  ( $d_\sigma$ ) is the creation (annihilation) operator for the  $d$ -state electrons. The energies  $\varepsilon_{\mathbf{k}}$  and  $E$  are measured with respect to the chemical potential  $\mu$ . Commutation relations for fermions (either  $c$ - or  $d$ -types) read

$$\begin{aligned} \{c_{i\sigma}, c_{j\sigma'}^\dagger\} &\equiv c_{i\sigma} c_{j\sigma'}^\dagger + c_{j\sigma'}^\dagger c_{i\sigma} = \delta_{ij} \delta_{\sigma\sigma'}, \\ \{c_{i\sigma}, c_{j\sigma'}\} &= \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0. \end{aligned} \quad (5.2)$$

If potential  $V_{\mathbf{k}} = 0$ , then, for  $E + U > \mu$ , the energy level  $E + U$  is empty, and the magnetic moment arises at a  $d$ -ion site. If  $E + U < \mu$ , then electron states with the both spin projections are occupied, and localized moment at  $d$ -site is absent. If the  $sd$ -mixing interaction exists, the average number of electrons with spin projection  $\sigma$  at  $d$ -site,  $\langle n_d^\sigma \rangle = \langle d_\sigma^\dagger d_\sigma \rangle$ , can have non-integer values, and the value of the magnetic moment at the site is defined by the expression

$$m = \frac{1}{2} (\langle n_d^+ \rangle - \langle n_d^- \rangle). \quad (5.3)$$

For calculation of the local  $d$ -site magnetic moment we introduce an *anticommutator*-type Green function

$$G_d^\sigma(t, t') = \langle\langle d_\sigma(t) | d_\sigma^\dagger(t') \rangle\rangle. \quad (5.4)$$

Fourier-transform of equation of motion for the Green function  $G_d^\sigma(t, t')$  reads

$$\omega \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega = 1 + E \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega + U \langle\langle n_d^{-\sigma} d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega + \sum_{\mathbf{k}} V_{\mathbf{k}} \langle\langle c_{\mathbf{k}\sigma} | d_\sigma^\dagger \rangle\rangle_\omega, \quad (5.5)$$



the kinetic energy of the band  $s$ -electrons does not contribute to the equation of motion. Following Anderson we make decoupling by the (Hartree-Fock) approximation

$$\langle\langle n_d^{-\sigma} d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega \simeq \langle n_d^{-\sigma} \rangle \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega, \quad (5.6)$$

after which equation of motion (5.5) reads

$$(\omega - \varepsilon_\sigma) \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega = 1 + \sum_k V_k \langle\langle c_{k\sigma} | d_\sigma^\dagger \rangle\rangle_\omega, \quad (5.7)$$

where

$$\varepsilon_\sigma = E + U \langle n_d^{-\sigma} \rangle. \quad (5.8)$$

Equation of motion (5.5) contains new Green function  $\langle\langle c_{k\sigma} | d_\sigma^\dagger \rangle\rangle_\omega$ , the equation of motion for which reads

$$\omega \langle\langle c_{k\sigma} | d_\sigma^\dagger \rangle\rangle_\omega = \varepsilon_k \langle\langle c_{k\sigma} | d_\sigma^\dagger \rangle\rangle_\omega + V_k \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega. \quad (5.9)$$

The unperturbed energy of  $d$ -states, and Coulomb repulsion do not contribute equation of motion (5.9). Observation of equations (5.7) and (5.9) shows that the chain of equations is closed by decoupling (5.6). Now, we can find the desired Green function from equations (5.7) and (5.9):

$$G_d^\sigma(\omega) = \langle\langle d_\sigma | d_\sigma^\dagger \rangle\rangle_\omega = \frac{1}{\omega - \varepsilon_\sigma - \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k}}. \quad (5.10)$$

## 5.2 The Self-Consistency Equations for Particle Numbers at $d$ -Sites

The spectral intensity of correlation function  $\langle d_\sigma^\dagger d_\sigma \rangle$ ,  $J_{d^\dagger d}^\sigma(\omega)$ , can be found by the standard way, (1.34):

$$\begin{aligned} J_{d^\dagger d}^\sigma(\omega) &= \frac{i}{e^{\omega/kT} + 1} (G_d^\sigma(\omega + i\delta) - G_d^\sigma(\omega - i\delta))|_{\delta \rightarrow +0} \\ &= \frac{i}{e^{\omega/kT} + 1} \left\{ \frac{1}{\omega + i\delta - \varepsilon_\sigma - \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k + i\delta}} \right. \\ &\quad \left. - \frac{1}{\omega - i\delta - \varepsilon_\sigma - \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k - i\delta}} \right\}. \end{aligned} \quad (5.11)$$

The integral terms in the denominators of the fractions have finite *Real* and *Imaginary* parts (see below), which give the *Real* and *Imaginary* contributions to the excitation spectrum. That is why we can omit  $\pm i\delta$  contribution to the frequency  $\omega$  in other terms. The integral terms can be decomposed as follows

$$\begin{aligned} \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k \pm i\delta} &= \mathcal{P} \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k} \mp i\pi \sum_k |V_k|^2 \delta(\omega - \varepsilon_k) \\ &\equiv \Delta E \mp i\Gamma, \end{aligned} \quad (5.12)$$

where  $\Delta E(\omega) = \mathcal{P} \sum_k |V_k|^2 \frac{1}{\omega - \varepsilon_k}$  is a shift of the energy  $\varepsilon_\sigma$ , and  $\Gamma(\omega) \simeq \pi \langle |V_k|^2 \rangle_{av} \rho_0(\omega)$  is a width of this energy level. Here,  $\langle |V_k|^2 \rangle_{av}$  is an average value of the squared interaction potential between local  $d$ -electrons and itinerant  $s$ -electrons over the isoenergetic surface of the energy equal to  $\omega$ ,  $\rho_0(\omega)$  is the (unperturbed) density of states in the conduction band. Finally, we have for the spectral intensity

$$\begin{aligned} J_{d^\dagger d}^\sigma(\omega) &= \frac{i}{e^{\omega/kT} + 1} \left\{ \frac{1}{\omega - \varepsilon_\sigma - \Delta E + i\Gamma} - \frac{1}{\omega - \varepsilon_\sigma - \Delta E - i\Gamma} \right\} \\ &= \frac{1}{e^{\omega/kT} + 1} \frac{2\Gamma}{(\omega - \varepsilon_\sigma - \Delta E)^2 + \Gamma^2}, \end{aligned} \quad (5.13)$$

from which we find the average number of electrons with spin projection  $\sigma$  on the  $d$ -level of the site according to prescription (1.34), (1.35):

$$\langle n_d^\sigma \rangle = \langle d_\sigma^\dagger d_\sigma \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{d^\dagger d}^\sigma(\omega). \quad (5.14)$$

At temperature of absolute zero only the energies (frequencies in the chosen units)  $\omega < \mu$  are populated (this is defined by the Fermi distribution function  $n(\omega) = \frac{1}{e^{\omega/kT} + 1}$ , which enters the spectral intensity (5.13)), so for  $\langle n_d^\sigma \rangle$  we obtain

$$\langle n_d^\sigma \rangle = \int_{-\infty}^{\mu} \frac{d\omega}{\pi} \frac{\Gamma(\omega)}{(\omega - \varepsilon_\sigma - \Delta E(\omega))^2 + \Gamma^2(\omega)}. \quad (5.15)$$

The density of  $d$ -states can be found making use of the formula

$$\begin{aligned} g_d^\sigma(\omega) &= \frac{i}{2\pi} (G_d^\sigma(\omega + i\delta) - G_d^\sigma(\omega - i\delta)) \\ &= \frac{1}{\pi} \frac{\Gamma(\omega)}{(\omega - \varepsilon_\sigma - \Delta E(\omega))^2 + \Gamma^2(\omega)}. \end{aligned} \quad (5.16)$$

The total density of states for  $s$ - and  $d$ -electrons is shown on Fig. 5.2. As a result of mixing of localized and itinerant electrons, two (broadened) energy levels appear ("virtual states") which depend on  $\langle n_d^\sigma \rangle$  by the self-consistent way. The shifted positions of the levels can be found by simultaneous solution of equations set (5.15), which reads

$$\begin{aligned} \langle n_d^+ \rangle &= \int_{-\infty}^{\mu} \frac{d\omega}{\pi} \frac{\Gamma}{(\omega - E - U \langle n_d^- \rangle - \Delta E)^2 + \Gamma^2} \\ \langle n_d^- \rangle &= \int_{-\infty}^{\mu} \frac{d\omega}{\pi} \frac{\Gamma}{(\omega - E - U \langle n_d^+ \rangle - \Delta E)^2 + \Gamma^2}. \end{aligned} \quad (5.17)$$

The number of localized electrons per site is given by the obvious relation

$$n_d = n = \langle n_d^+ \rangle + \langle n_d^- \rangle, \quad (5.18)$$

and the magnetic moment per site by (5.3). If solution of the equations gives  $\langle n_d^+ \rangle = \langle n_d^- \rangle$ , then  $m = 0$ , which means that magnetic moment at the site is absent. Eqs. (5.17) are basic equations of the problem.

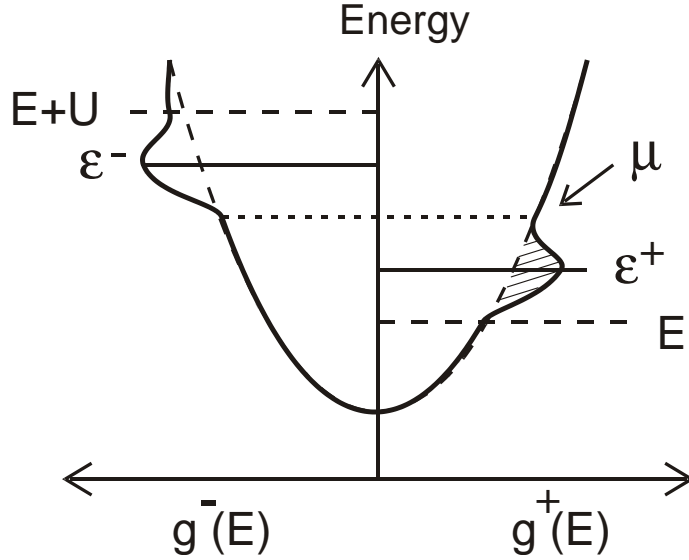


Figure 5.2: Density of states in the magnetic case. The "humps" at  $E + U \langle n_d^+ \rangle$  and  $E + U \langle n_d^- \rangle$  are the "virtual"  $d$ -levels of width  $2\Gamma$  for down and up spins, respectively.

### 5.3 Criterion of Magnetic Moment Formation

The criterion of formation of the localized moment at a  $d$ -site can be derived by combined analysis of equations (5.3), (5.17) and (5.18). From (5.3) and (5.18) it follows that

$$\langle n_d^+ \rangle = \frac{n_d}{2} + m, \quad \langle n_d^- \rangle = \frac{n_d}{2} - m, \quad (5.19)$$

from which the right-hand sides of self-consistency equations (5.17) can be represented in the form of functions of  $n_d$  and  $m$ :

$$\begin{aligned} \langle n_d^+ \rangle &= f \left( E + \frac{U}{2} n_d - Um \right), \\ \langle n_d^- \rangle &= f \left( E + \frac{U}{2} n_d + Um \right). \end{aligned} \quad (5.20)$$

Therefore, the equation for  $m$  reads

$$m = \frac{1}{2} \left[ f \left( E + \frac{U}{2} n_d - Um \right) - f \left( E + \frac{U}{2} n_d + Um \right) \right]. \quad (5.21)$$

Let us imagine that we solve equation (5.21) graphically. The left-hand side of Eq. (5.21) is the linear function of  $m$ , that is the straight line with the unit slope. To have nontrivial solution for  $m$  the initial (at  $m \rightarrow 0$ ) slope of the right-hand side function of  $m$  must exceed unity. Visual analysis of Eqs. (5.17) shows that their right-hand sides approach zero when  $m \rightarrow \infty$ , then the asymptotics of the right-hand side of Eq. (5.21) at  $m \rightarrow \infty$  is zero. It means that the curve, representing the right-hand side of Eq. (5.21), intersects the straight line, representing the left-hand side of Eq. (5.21), at least once. Therefore, we can write

$$\left. \frac{\partial f \left( E + \frac{U}{2} n_d \pm Um \right)}{\partial m} \right|_{m \rightarrow 0} = \pm U \frac{\partial f}{\partial E}, \quad (5.22)$$

and the condition that the slope of the right-hand side of (5.21) exceeds unity reads

$$-\frac{1}{2}U \frac{\partial f}{\partial E} - \frac{1}{2}U \frac{\partial f}{\partial E} > 1. \quad (5.23)$$

If energies involved in the physics of the problem are close to the Fermi energy  $\varepsilon_F$ , all functions entering the above relations can be approximated by their values at the Fermi energy. Then,

$$\frac{\partial f}{\partial E} = - \int_{-\infty}^{\varepsilon_F} d\omega \frac{\partial g_d^\sigma(\omega)}{\partial \omega} = -g_d^\sigma(\varepsilon_F), \quad (5.24)$$

where  $g_d^\sigma(\omega)$  is the density of states (5.16), and the criterion of magnetic moment formation (5.23) reads

$$U g_d^\sigma(\varepsilon_F) > 1. \quad (5.25)$$

## 5.4 The Analysis of Magnetic-Nonmagnetic Transition Curve

Neglecting the frequency (energy) dependence of the quantities  $\Delta E(\omega)$  and  $\Gamma(\omega)$  in (5.17) we can evaluate the integrals

$$\begin{aligned} \langle n_d^+ \rangle &= \frac{1}{\pi} \operatorname{arccot} \frac{E - \varepsilon_F + U \langle n_d^- \rangle}{\Gamma}, \\ \langle n_d^- \rangle &= \frac{1}{\pi} \operatorname{arccot} \frac{E - \varepsilon_F + U \langle n_d^+ \rangle}{\Gamma}. \end{aligned} \quad (5.26)$$

System of transcendental equations (5.26) are the basic set of equations of the theory. To demonstrate their meaning we plot typical magnetic situation in Fig. 5.2. We show the two virtual states in terms of their distributions (density of states)  $g_d^\sigma(\omega)$ . The filled portions of the two distributions of  $d$ -states are shaded.

Before giving physical discussion of these localized moment states let us analyze system of equations (5.26). We introduce the dimensionless parameter

$$y = U/\Gamma, \quad (5.27)$$

the ratio of the Coulomb repulsion to the width of the virtual state. When  $y$  is large, correlation is large, and localization is easy, while  $y$  small represents the nonmagnetic situation. The parameter

$$x = (\varepsilon_F - E)/U \quad (5.28)$$

is also useful:  $x = 0$  means the empty  $d$ -state is right at the Fermi level, while  $x = 1$  puts  $E + U$  at the Fermi level.  $x = 1/2$ , when  $E$  and  $E + U$  are symmetrically disposed about the Fermi level, is the most favorable case for magnetism. Inserting (5.27) and (5.28) into (5.26), and dropping angular brackets, we rewrite these equations in new variables

$$\pi n_d^\pm = \operatorname{arccot} [y (n_d^\mp - x)]. \quad (5.29)$$

Let us investigate some special cases:

*A: Magnetic limit:*  $y \gg 1$ ,  $x$  is not small or too near 1.

Then, the arccotangent is either close to zero or to  $\pi$ , and  $n_d^\pm$  is near zero or one. Assume that  $n_d^+ \sim 1$  and  $n_d^- \sim 0$ . Therefore,

$$\begin{aligned}\pi n_d^+ &\simeq \pi - \frac{1}{y(x - n_d^-)}, \\ \pi n_d^- &\simeq \frac{1}{y(n_d^+ - x)}.\end{aligned}\quad (5.30)$$

These equations can be approximately solved to obtain:

$$\begin{aligned}x(1 - n_d^+) &= (1 - x)n_d^- \simeq \left[ \pi y \left( 1 - \frac{1}{\pi x y (1 - x)} \right) \right]^{-1}, \\ 2m &= n_d^+ - n_d^- \simeq 1 - [\pi x y (1 - x) - 1]^{-1}.\end{aligned}\quad (5.31)$$

*B: Nonmagnetic cases.*

We may assume that  $n_d^+ = n_d^- = n$ . Then, Eq. (5.29) becomes

$$\cot(\pi n) = y(n - x). \quad (5.32)$$

In the simplest subcase,  $n$  will not be far from  $1/2$  - the virtual state lying within a width of the Fermi level - so that

$$\cot(\pi n) \simeq \pi(1/2 - n), \quad (5.33)$$

and

$$n \simeq \frac{1}{2} \left[ \frac{1 + 2xy/\pi}{1 + y/\pi} \right]. \quad (5.34)$$

We see that  $n$  tends to take on the value  $1/2$ , meaning that the effective energy level stays near the Fermi level. The effective energy of the  $d$  state with respect to the Fermi level is

$$E_{eff} = U(n - x) = U \frac{1 - 2x}{1 + y/\pi} = y \Gamma \frac{1 - 2x}{1 + y/\pi}. \quad (5.35)$$

This is a very good approximation when  $y$  is small or, when  $x$  is reasonably close to  $1/2$ , for all relevant  $y$ .

In the opposite limit ( $y$  is largest, and  $x$  is near 1 or 0) the most interesting region is  $x$  near 0 (result for  $x \simeq 1$  is symmetric),  $y$  quite large. Here

$$\cot(\pi n) \simeq 1/\pi n, \quad (5.36)$$

and we have

$$y(n - x) \simeq 1/\pi n. \quad (5.37)$$

Solving the equation by successive approximations we get

$$n \simeq (\pi y)^{-1/2} + \frac{1}{2}x + \dots \quad (5.38)$$

*C. The transition curve.*

It is interesting to trace out the transition curve from magnetic to nonmagnetic behavior. It is obvious that on the transition curve  $n_d^+ = n_d^-$ , so the equation (5.32) is one condition on the curve.

The second one may be obtained by differencing Eqs. (5.26):

$$\frac{\pi}{\sin^2(\pi n_c)} = y_c. \quad (5.39)$$

Here the subscript  $c$  refers to the values on the critical curve of transition to the magnetic state. Equations (5.32) and (5.39) can not be solved in a simple form for  $y_c$  as a function of  $x$ , but can be expressed simply in terms of  $n_c$  and  $x$ :

$$\sin(2\pi n_c) = 2\pi(n_c - x). \quad (5.40)$$

From Eqs. (5.39) and (5.40) we can obtain the following approximations for  $x \simeq 1/2$  and

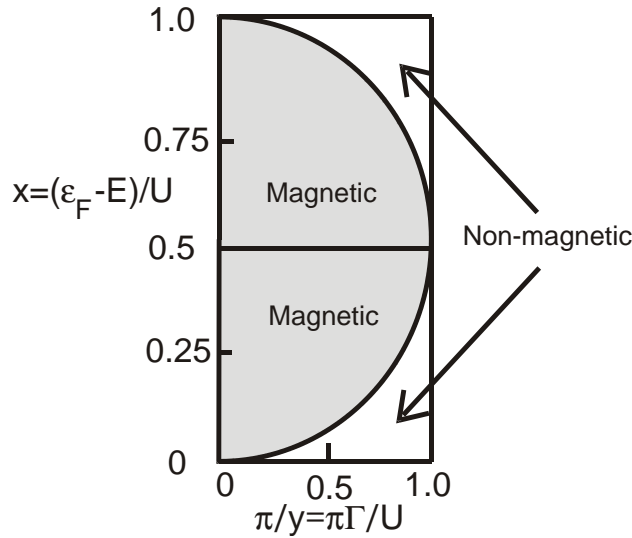


Figure 5.3: Regions of magnetic and nonmagnetic behavior. Curve gives  $x_c$  versus  $\pi/y_c = \pi\Gamma/U$ .

$x \simeq 0$ :

$$y_c \simeq \pi + \frac{1}{4}\pi^3 \left(x - \frac{1}{2}\right)^2 + \dots, \quad x \simeq 1/2, \quad (5.41)$$

and

$$y_c^3 \simeq \frac{4\pi}{9x^2} + \dots, \quad x \simeq 0. \quad (5.42)$$

The above results are summarized in Fig. 5.3, which gives the transition curve as a function of  $x$  and  $\pi/y$ .

## 5.5 Problems

1. Reproduce equations of motion (5.5) and (5.9).
2. Derive relations (5.30)-(5.42).

# Chapter 6

## Band Structure of Solids in the Hubbard Model, Metal-Insulator Transition

### 6.1 The Hamiltonian of the Model and Basic Equations

Let us assume that a crystal consists of ions each having the relevant atomic level, containing a single orbital state overlapping in certain degree with neighboring ones. The Hamiltonian for this ensemble of  $N$  overlapping  $3d$  atomic states is

$$\mathcal{H} = \varepsilon_0 \sum_{i,\sigma} n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_{j,\sigma} n_{j\sigma} n_{j-\sigma}, \quad (6.1)$$

which is commonly called "Hubbard Hamiltonian" because of valuable analysis of the model (6.1) by J. Hubbard in "Electron correlations in narrow electron bands":

- 1) Proc. Roy. Soc., 1963, **A276**, p.238-257;
- 2) Proc. Roy. Soc., 1963, **A277**, p.237-259;
- 3) Proc. Roy. Soc., 1964, **A281**, p.401-419.

The first term describes single-electron atomic levels of energy  $\varepsilon_0$ , the second term is the "hopping" energy, describing the movement of electrons from site to site due to overlapping, and the third term is the single-site Coulomb repulsion,  $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ ,  $\sigma$  is the spin-projection index.

Every atom at a site can exist: in the state without electron on it - an empty state; in the state with one electron with spin projection  $\sigma$ ; in the state with two electrons on the site having the opposite spin projections. The state with two electrons per site is forbidden by the Pauli principle, if the spin projections of electrons are same. When these atoms are collected in a crystal, electrons can hop from site to site because of overlapping of orbital states forming the band for conduction. The band-width  $W$  as wide as large the matrix of the hopping term from a site to the neighboring one,  $t_{ij} = t$ , and number of nearest neighbors  $Z$  is large:  $W \simeq 2tZ$  (factor 2 comes from the spin-projection summation). This picture is not complete, as the Coulomb repulsion has not been taken into account. If the single-site repulsion is strong enough, it will prevent the electron hopping, creating the strong potential barrier for the electron movement. All these properties can be treated on the basis of excitation spectrum - band structure of the model (6.1).

For obtaining the excitation spectrum let us recall first of all that the Green function of the type:  $\ll a_k | a_k^\dagger \gg_{\eta=-1}^r$  gives the single-particle excitation spectrum of a fermion system. For the investigation of model (6.1) we introduce the anticommutator-type retarded Green function

$$G_{ij\sigma}(t-t') = \ll a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \gg_{-1}^r. \quad (6.2)$$

The equation of motion for GF (6.2) follows from the general equation of motion (1.46) (we omit GF indices in the right-hand side of (6.2) for brevity)

$$i \frac{\partial}{\partial t} G_{ij\sigma}(t-t') = \delta(t-t') \langle \{ a_{i\sigma}, a_{j\sigma}^\dagger \} \rangle + \ll [a_{i\sigma}(t), \mathcal{H}] | a_{j\sigma}^\dagger(t') \gg. \quad (6.3)$$

Now, we have to calculate the commutator in the second term of the right-hand side of Eq. (6.3), but before let us recall for convenience the commutation relations for fermions (5.2):

$$\begin{aligned} \{ a_{i\sigma}, a_{j\sigma'}^\dagger \} &\equiv a_{i\sigma} a_{j\sigma'}^\dagger + a_{j\sigma'}^\dagger a_{i\sigma} = \delta_{ij} \delta_{\sigma\sigma'}, \\ \{ a_{i\sigma}, a_{j\sigma'} \} &= \{ a_{i\sigma}^\dagger, a_{j\sigma'}^\dagger \} = 0. \end{aligned} \quad (6.4)$$

Making use of (6.4) we calculate first of all

$$\begin{aligned} \left[ a_{i\sigma}, \varepsilon_0 \sum_{l,\sigma'} n_{l\sigma} \right] &\equiv \varepsilon_0 \left[ a_{i\sigma}, \sum_{l,\sigma'} a_{l\sigma'}^\dagger a_{l\sigma'} \right] \\ &= \varepsilon_0 \sum_{l,\sigma'} \left\{ a_{i\sigma} a_{l\sigma'}^\dagger a_{l\sigma'} - a_{l\sigma'}^\dagger a_{l\sigma'} a_{i\sigma} \right\} \\ &= \varepsilon_0 \sum_{l,\sigma'} \left\{ a_{i\sigma} a_{l\sigma'}^\dagger a_{l\sigma'} + \left( \delta_{il} \delta_{\sigma\sigma'} - a_{i\sigma} a_{l\sigma'}^\dagger \right) a_{l\sigma'} \right\} \\ &= \varepsilon_0 \sum_{l,\sigma'} \delta_{il} \delta_{\sigma\sigma'} a_{l\sigma'} = \varepsilon_0 a_{i\sigma}. \end{aligned} \quad (6.5)$$

Next term of the commutator is

$$\begin{aligned} \left[ a_{i\sigma}, \sum_{l,m,\sigma'} t_{lm} a_{l\sigma'}^\dagger a_{m\sigma'} \right] &= \sum_{l,m,\sigma'} t_{lm} \left\{ a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} - a_{l\sigma'}^\dagger a_{m\sigma'} a_{i\sigma} \right\} \\ &= \sum_{l,m,\sigma'} t_{lm} \left\{ a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} + a_{l\sigma'}^\dagger a_{i\sigma} a_{m\sigma'} \right\} \\ &= \sum_{l,m,\sigma'} t_{lm} \left\{ a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} + \left( \delta_{il} \delta_{\sigma\sigma'} - a_{i\sigma} a_{l\sigma'}^\dagger \right) a_{m\sigma'} \right\} \\ &= \sum_{l,m,\sigma'} t_{lm} \delta_{il} \delta_{\sigma\sigma'} a_{m\sigma'} = \sum_m t_{im} a_{m\sigma}. \end{aligned} \quad (6.6)$$

The last term of the commutator is

$$\begin{aligned} \left[ a_{i\sigma}, \frac{U}{2} \sum_{j,\sigma'} n_{j\sigma'} n_{j-\sigma'} \right] &= \frac{U}{2} \sum_{j,\sigma'} [a_{i\sigma}, n_{j\sigma'} n_{j-\sigma'}] \\ &= \frac{U}{2} \sum_{j,\sigma'} \{ a_{i\sigma} n_{j\sigma'} n_{j-\sigma'} - n_{j\sigma'} n_{j-\sigma'} a_{i\sigma} \}. \end{aligned} \quad (6.7)$$



Before development of (6.7) let us point out, as a result of calculation of (6.5), that

$$[a_{i\sigma}, n_{l\sigma'}] = \delta_{il}\delta_{\sigma\sigma'}a_{i\sigma}. \quad (6.8)$$

Using this relation we commute first two operators in the first term of (6.7), and then, second and third operators in the second term of the resulting expression:

$$\begin{aligned} a_{i\sigma}n_{j\sigma'}n_{j-\sigma'} - n_{j\sigma'}n_{j-\sigma'}a_{i\sigma} &= (\delta_{ij}\delta_{\sigma\sigma'}a_{i\sigma} + n_{j\sigma'}a_{i\sigma})n_{j-\sigma'} - n_{j\sigma'}n_{j-\sigma'}a_{i\sigma} \\ &= \delta_{ij}\delta_{\sigma\sigma'}a_{i\sigma}n_{j-\sigma'} + n_{j\sigma'}(\delta_{ij}\delta_{\sigma-\sigma'}a_{i\sigma} + n_{j-\sigma'}a_{i\sigma}) \\ -n_{j\sigma'}n_{j-\sigma'}a_{i\sigma} &= \delta_{ij}\delta_{\sigma\sigma'}a_{i\sigma}n_{j-\sigma'} + \delta_{ij}\delta_{\sigma-\sigma'}n_{j\sigma'}a_{i\sigma}. \end{aligned}$$

Substituting the above result into (6.7) we have finally

$$\left[ a_{i\sigma}, \frac{U}{2} \sum_{j,\sigma'} n_{j\sigma'} n_{j-\sigma'} \right] = U n_{i-\sigma} a_{i\sigma}. \quad (6.9)$$

Taking into account that the first term in (6.3) is the expectation value of commutation relation (6.4) we obtain the equation of motion

$$\begin{aligned} i \frac{\partial}{\partial t} \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} + \varepsilon_0 \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &\quad + \sum_m t_{im} \left\langle \left\langle a_{m\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &\quad + U \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle. \end{aligned} \quad (6.10)$$

Observation of equation (6.10) shows that it contains a new Green function (last term of the equation). For this new Green function we have to write down the equation of motion

$$\begin{aligned} i \frac{\partial}{\partial t} \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \left\langle \left\{ n_{i-\sigma} a_{i\sigma}, a_{j\sigma}^\dagger \right\} \right\rangle \\ &\quad + \left\langle \left\langle [n_{i-\sigma} a_{i\sigma}, \mathcal{H}](t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle, \end{aligned} \quad (6.11)$$

and then, calculate the terms in the right-side of Eq. (6.11).

$$\left\{ n_{i-\sigma} a_{i\sigma}, a_{j\sigma}^\dagger \right\} = n_{i-\sigma} \left\{ a_{i\sigma}, a_{j\sigma}^\dagger \right\} = n_{i-\sigma} \delta_{ij} \quad (6.12)$$

due to commutativity of the operator  $n_{i-\sigma}$  with creation and annihilation operators because of spin indices. Next contribution is the first term of the commutator in (6.11):

$$\begin{aligned} \left[ n_{i-\sigma} a_{i\sigma}, \varepsilon_0 \sum_{l,\sigma'} n_{l\sigma'} \right] &= \varepsilon_0 \sum_{l,\sigma'} \{ n_{i-\sigma} a_{i\sigma} n_{l\sigma'} - n_{l\sigma'} n_{i-\sigma} a_{i\sigma} \} \\ &= \varepsilon_0 \sum_{l,\sigma'} \{ n_{i-\sigma} (\delta_{il}\delta_{\sigma\sigma'} a_{i\sigma} + n_{l\sigma'} a_{i\sigma}) - n_{l\sigma'} n_{i-\sigma} a_{i\sigma} \} \\ &= \varepsilon_0 n_{i-\sigma} a_{i\sigma} + \varepsilon_0 \sum_{l,\sigma'} [n_{i-\sigma}, n_{l\sigma'}] a_{i\sigma}. \end{aligned} \quad (6.13)$$

Here the commutator of particle number operators has appeared, we calculate it separately in a general form:

$$[n_{m\sigma}, n_{l\sigma'}] = n_{m\sigma} n_{l\sigma'} - n_{l\sigma'} n_{m\sigma} = a_{m\sigma}^\dagger a_{m\sigma} n_{l\sigma'} - n_{l\sigma'} n_{m\sigma},$$

for commuting  $a_{m\sigma}$  and  $n_{l\sigma'}$  in the first term we use relation (6.8)

$$\begin{aligned}
&= a_{m\sigma}^\dagger (\delta_{lm} \delta_{\sigma\sigma'} a_{m\sigma} + n_{l\sigma'} a_{m\sigma}) - n_{l\sigma'} n_{m\sigma} \\
&= \delta_{lm} \delta_{\sigma\sigma'} n_{m\sigma} + a_{m\sigma}^\dagger a_{l\sigma'}^\dagger a_{l\sigma'} a_{m\sigma} - n_{l\sigma'} n_{m\sigma} \\
&= \delta_{lm} \delta_{\sigma\sigma'} n_{m\sigma} - a_{l\sigma'}^\dagger (\delta_{lm} \delta_{\sigma\sigma'} - a_{l\sigma'} a_{m\sigma}^\dagger) a_{m\sigma} - n_{l\sigma'} n_{m\sigma} \\
&= \delta_{lm} \delta_{\sigma\sigma'} n_{m\sigma} - \delta_{lm} \delta_{\sigma\sigma'} a_{l\sigma'}^\dagger a_{m\sigma} + a_{l\sigma'}^\dagger a_{l\sigma'} a_{m\sigma}^\dagger a_{m\sigma} - n_{l\sigma'} n_{m\sigma} = 0.
\end{aligned}$$

From these derivations we conclude that particle number operators commute irrelevant to values of their indices:

$$[n_{m\sigma}, n_{l\sigma'}] = 0. \quad (6.14)$$

For the experienced enough reader it is obvious that, if at least one subscript index in (6.14) is different in  $n_{m\sigma}$  and  $n_{l\sigma'}$ , then, because of commutation relation (6.4), these operators commute. Otherwise, if  $m = l$  and  $\sigma = \sigma'$  a particle number operator commute with itself. As a result, we cancel the last term in Eq. (6.13) and finally obtain

$$\left[ n_{i-\sigma} a_{i\sigma}, \varepsilon_0 \sum_{l,\sigma'} n_{l\sigma'} \right] = \varepsilon_0 n_{i-\sigma} a_{i\sigma}. \quad (6.15)$$

Next term of the right hand side of (6.11) comes from the commutator with the hopping term of (6.1):

$$\begin{aligned}
&\left[ n_{i-\sigma} a_{i\sigma}, \sum_{l,m,\sigma'} t_{lm} a_{l\sigma'}^\dagger a_{m\sigma'} \right] \\
&= \sum_{l,m,\sigma'} t_{lm} \left\{ n_{i-\sigma} a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} - a_{l\sigma'}^\dagger (\delta_{im} \delta_{-\sigma\sigma'} a_{m\sigma'} + n_{i-\sigma} a_{m\sigma'}) a_{i\sigma} \right\} \\
&= \sum_{l,m,\sigma} t_{lm} \left\{ n_{i-\sigma} a_{i\sigma} a_{l\sigma}^\dagger a_{m\sigma} - \delta_{im} \delta_{-\sigma\sigma'} a_{l\sigma'}^\dagger a_{m\sigma'} a_{i\sigma} + a_{l\sigma'}^\dagger n_{i-\sigma} a_{i\sigma} a_{m\sigma'} \right\}. \quad (6.16)
\end{aligned}$$

Before proceeding further we calculate at first the commutator:

$$\begin{aligned}
\left[ a_{i\sigma}^\dagger, n_{j\sigma'} \right] &= a_{i\sigma}^\dagger a_{j\sigma'}^\dagger a_{j\sigma'} - a_{j\sigma'}^\dagger a_{j\sigma'} a_{i\sigma}^\dagger \\
&= a_{i\sigma}^\dagger a_{j\sigma'}^\dagger a_{j\sigma'} - a_{j\sigma'}^\dagger \left( \delta_{ij} \delta_{\sigma\sigma'} - a_{i\sigma}^\dagger a_{j\sigma'} \right) \\
&= -\delta_{ij} \delta_{\sigma\sigma'} a_{i\sigma}^\dagger. \quad (6.17)
\end{aligned}$$

Using (6.17) we continue calculations in (6.16):

$$\begin{aligned}
&\sum_{l,m,\sigma'} t_{lm} \left\{ n_{i-\sigma} a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} - \delta_{im} \delta_{-\sigma\sigma'} a_{l\sigma'}^\dagger a_{m\sigma'} a_{i\sigma} + \left( -\delta_{il} \delta_{-\sigma\sigma'} a_{l\sigma'}^\dagger + n_{i-\sigma} a_{l\sigma'}^\dagger \right) a_{i\sigma} a_{m\sigma'} \right\} \\
&= \sum_{l,m,\sigma'} t_{lm} \left\{ n_{i-\sigma} a_{i\sigma} a_{l\sigma'}^\dagger a_{m\sigma'} - \delta_{im} \delta_{-\sigma\sigma'} a_{l\sigma'}^\dagger a_{m\sigma'} a_{i\sigma} - \delta_{il} \delta_{-\sigma\sigma'} a_{l\sigma'}^\dagger a_{i\sigma} a_{m\sigma'} \right. \\
&\quad \left. + n_{i-\sigma} \left( \delta_{il} \delta_{\sigma\sigma'} - a_{i\sigma} a_{l\sigma'}^\dagger \right) a_{m\sigma'} \right\} \\
&= -\sum_l t_{li} a_{l-\sigma}^\dagger a_{i-\sigma} a_{i\sigma} - \sum_m t_{mi} a_{i-\sigma}^\dagger a_{i\sigma} a_{m-\sigma} + \sum_m t_{mi} n_{i-\sigma} a_{m\sigma}, \quad (6.18)
\end{aligned}$$

where we have used the symmetry property,  $t_{mi} = t_{im}$ . Changing the summation index  $m$  on  $l$  we obtain finally

$$\begin{aligned} \left[ n_{i-\sigma} a_{i\sigma}, \sum_{l,m,\sigma'} t_{lm} a_{l\sigma'}^\dagger a_{m\sigma'} \right] &= \\ &= \sum_l t_{li} \left\{ n_{i-\sigma} a_{l\sigma} - a_{l-\sigma}^\dagger a_{i-\sigma} a_{i\sigma} - a_{i-\sigma}^\dagger a_{i\sigma} a_{l-\sigma} \right\}. \end{aligned} \quad (6.19)$$

At last, the term in the right-hand side of commutator in (6.11), which comes from the Coulomb single-site repulsion, is

$$\begin{aligned} \left[ n_{i-\sigma} a_{i\sigma}, \frac{U}{2} \sum_{j,\sigma'} n_{j\sigma'} n_{j-\sigma'} \right] &= \frac{U}{2} \sum_{j,\sigma'} \{ n_{i-\sigma} a_{i\sigma} n_{j\sigma'} n_{j-\sigma'} - n_{j\sigma'} n_{j-\sigma'} n_{i-\sigma} a_{i\sigma} \} \\ &= \frac{U}{2} \sum_{j,\sigma'} \{ n_{i-\sigma} (\delta_{ij} \delta_{\sigma\sigma'} a_{i\sigma} + n_{j\sigma'} a_{i\sigma}) n_{j-\sigma'} - n_{j\sigma'} n_{j-\sigma'} n_{i-\sigma} a_{i\sigma} \} \\ &= \frac{U}{2} \sum_{j,\sigma'} \{ \delta_{ij} \delta_{\sigma\sigma'} n_{i-\sigma} a_{i\sigma} n_{j-\sigma'} - n_{j\sigma'} n_{j-\sigma'} n_{i-\sigma} a_{i\sigma} \\ &\quad + n_{i-\sigma} n_{j\sigma'} (\delta_{ij} \delta_{\sigma-\sigma'} a_{i\sigma} + n_{j-\sigma'} a_{i\sigma}) \} \\ &= \frac{U}{2} \sum_{j,\sigma'} \{ \delta_{ij} \delta_{\sigma\sigma'} n_{i-\sigma} a_{i\sigma} n_{j-\sigma'} + \delta_{ij} \delta_{\sigma-\sigma'} n_{i-\sigma} n_{j\sigma'} a_{i\sigma} \}, \end{aligned} \quad (6.20)$$

where we have used the commutation property of the particle number operators (6.14) for cancelling the two terms in (6.20). Then, we note that operators  $a_{i\sigma}$  and  $n_{j-\sigma'}$  in the first term of (6.20) commute because of different spin indices ruled by  $\delta_{\sigma\sigma'}$  factor in this term:

$$\left[ n_{i-\sigma} a_{i\sigma}, \frac{U}{2} \sum_{j,\sigma'} n_{j\sigma'} n_{j-\sigma'} \right] = U n_{i-\sigma}^2 a_{i\sigma}. \quad (6.21)$$

We can further simplify contribution (6.21) by observing that  $n_{i-\sigma}^2 = n_{i-\sigma}$ , because the eigenvalues of the operator  $n_{i\sigma}$  are equal to 0 or 1:  $n_{i\sigma} |0_{i\sigma}\rangle = 0$ , and  $n_{i\sigma}^2 |0_{i\sigma}\rangle = 0$  too, but  $n_{i\sigma} |1_{i\sigma}\rangle = 1 \cdot |1_{i\sigma}\rangle$ , and  $n_{i\sigma}^2 |1_{i\sigma}\rangle = n_{i\sigma} \cdot 1 \cdot |1_{i\sigma}\rangle = 1 \cdot |1_{i\sigma}\rangle$ . After this remark we can collect all terms of the commutator in the equation of motion: (6.12), (6.15), (6.19), (6.21), and substitute them into (6.11). As a result we get the following equation

$$\begin{aligned} i \frac{\partial}{\partial t} \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} \langle n_{i-\sigma} \rangle + (\varepsilon_0 + U) \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &\quad + \sum_l t_{li} \left\langle \left\langle \left( n_{i-\sigma} a_{l\sigma} - a_{l-\sigma}^\dagger a_{i-\sigma} a_{i\sigma} \right. \right. \right. \\ &\quad \left. \left. \left. - a_{i-\sigma}^\dagger a_{i\sigma} a_{l-\sigma} \right) (t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle. \end{aligned} \quad (6.22)$$

This equation contains **three** new Green functions, for which we can write down their equations of motion. This routine is infinite, and we have to introduce a certain approximation to decouple, or to truncate, the infinite system of equations. To brighten up possible ways for the decoupling approximation we first collect the obtained equations of motion and then consider some limiting cases of the problem under investigation.

$$\begin{aligned}
i \frac{\partial}{\partial t} \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} + \varepsilon_0 \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\
&+ \sum_m t_{im} \left\langle \left\langle a_{m\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\
&+ U \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle, \tag{6.23}
\end{aligned}$$

$$\begin{aligned}
i \frac{\partial}{\partial t} \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} \langle n_{i-\sigma} \rangle + (\varepsilon_0 + U) \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\
&+ \sum_l t_{li} \left\{ \left\langle \left\langle (n_{i-\sigma} a_{l\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \right. \\
&- \left\langle \left\langle (a_{l-\sigma}^\dagger a_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\
&\left. - \left\langle \left\langle (a_{i-\sigma}^\dagger a_{i\sigma} a_{l-\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \right\}. \tag{6.24}
\end{aligned}$$

## 6.2 The Atomic Limit of the Hubbard Model

Let us assume for the moment that atomic wave functions do not overlap. This means that the hopping amplitude  $t_{ij}=0$ , and there is no carriers movement from one site to the others. Then, taking the limit  $t_{ij} \rightarrow 0$  in Eqs. (6.23) and (6.24), we obtain the following closed system of equations

$$\begin{aligned}
i \frac{\partial}{\partial t} \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} + \varepsilon_0 \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\
&+ U \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle, \tag{6.25}
\end{aligned}$$

$$\begin{aligned}
i \frac{\partial}{\partial t} \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &= \delta(t-t') \delta_{ij} \langle n_{i-\sigma} \rangle \\
&+ (\varepsilon_0 + U) \left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle. \tag{6.26}
\end{aligned}$$

Performing the Fourier transformation over time variables in equations (6.25) and (6.26) we get

$$(\omega - \varepsilon_0) \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij} + U \left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega, \tag{6.27}$$

$$(\omega - \varepsilon_0 - U) \left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij} \langle n_{i-\sigma} \rangle. \tag{6.28}$$

Substituting  $\left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega$ , expressed from Eq. (6.28), into (6.27) we obtain

$$\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \frac{\delta_{ij}}{\omega - \varepsilon_0} + U \frac{\langle n_{i-\sigma} \rangle \delta_{ij}}{(\omega - \varepsilon_0)(\omega - \varepsilon_0 - U)} \tag{6.29}$$

or

$$\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \frac{\langle n_{i-\sigma} \rangle \delta_{ij}}{(\omega - \varepsilon_0 - U)} + \frac{(1 - \langle n_{i-\sigma} \rangle) \delta_{ij}}{(\omega - \varepsilon_0)}. \tag{6.30}$$

If there is no magnetic ordering in the system, and both spin projections are equivalent, we may write  $\langle n_{i-\sigma} \rangle = \langle n_{i\sigma} \rangle = n/2$ , where  $n$  is the average concentration of carriers per site. Then we get

$$\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \frac{\delta_{ij} n/2}{(\omega - \varepsilon_0 - U)} + \frac{\delta_{ij} (1 - n/2)}{(\omega - \varepsilon_0)}. \quad (6.31)$$

Using expression (6.31) we can find the energy spectrum of excitations considering the poles of Eq. (6.31). These are  $\omega_1 = \varepsilon_0$  and  $\omega_2 = \varepsilon_0 + U$ . It means that under action of the Coulomb repulsion  $U$  in (6.1) the atomic level is split on two sub-levels with the energy difference  $U$  between them (see Fig. 6.1). Having obtained the spectral density

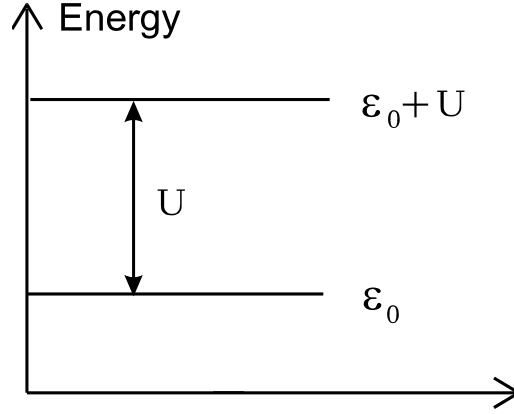


Figure 6.1: The energy levels in the atomic limit of the Hubbard model.

From  $\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega$ , (6.31) one can find the average number of particles of spin-projection  $\sigma$  on the site  $i$  by applying general formula (1.35):

$$\begin{aligned} \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle &= \langle n_{i\sigma} \rangle = \frac{n}{2} = \\ &= \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{e^{\omega/k_B T} + 1} \left\{ \left\langle \left\langle a_{i\sigma} | a_{i\sigma}^\dagger \right\rangle \right\rangle_{\omega+i\delta} - \left\langle \left\langle a_{i\sigma} | a_{i\sigma}^\dagger \right\rangle \right\rangle_{\omega-i\delta} \right\}. \end{aligned} \quad (6.32)$$

Substituting (6.31) into (6.32) and using formula (1.33) we obtain for  $\langle n_{i\sigma} \rangle$

$$\begin{aligned} \langle n_{i\sigma} \rangle &= \frac{n}{2} = \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{e^{\omega/k_B T} + 1} \left\{ -2\pi i \frac{n}{2} \delta(\omega - \varepsilon_0 - U) - 2\pi i \left(1 - \frac{n}{2}\right) \delta(\omega - \varepsilon_0) \right\} \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{e^{\omega/k_B T} + 1} \left\{ \frac{n}{2} \delta(\omega - \varepsilon_0 - U) + \left(1 - \frac{n}{2}\right) \delta(\omega - \varepsilon_0) \right\}. \end{aligned} \quad (6.33)$$

Let us rewrite Eq. (6.33) in the form

$$\langle n_{i\sigma} \rangle = \frac{n}{2} = \int_{-\infty}^{\infty} \frac{g_\sigma(\omega) d\omega}{e^{\omega/k_B T} + 1}, \quad (6.34)$$

where we have introduced the *density of states* (DOS)  $g_\sigma(\omega)$

$$g_\sigma(\omega) = \frac{n}{2}\delta(\omega - \varepsilon_0 - U) + \left(1 - \frac{n}{2}\right)\delta(\omega - \varepsilon_0). \quad (6.35)$$

Eq. (6.35) means that the electron (carrier) can be in the state with the energy  $\varepsilon_0 + U$  with probability  $n/2$ , and in the state with the energy  $\varepsilon_0$  with probability  $1 - n/2$ , so that the total probability to fill the either state is equal to unity. Observing set of equations (6.32)-(6.35) we derive the general formula for DOS expressed via Green functions:

$$g_\sigma(\omega) = \frac{i}{2\pi} \{G_\sigma(\omega + i\delta) - G_\sigma(\omega - i\delta)\}|_{\delta \rightarrow +0}, \quad (6.36)$$

where  $G_\sigma(\omega)$  is the spectral density of a single-particle Green function. Again, as the atomic state energy of an isolated atom is  $\varepsilon_0 = E_d - \mu$ , equations (6.33) and (6.34) can be considered as equations for finding the chemical potential  $\mu$ .

### 6.3 The Hartree-Fock Limit of the Hubbard Model

The limit opposite to the atomic one is the case  $t_{ij} \gg U$ , when electrons can easily move from site to site, and the band description is valid. In this limit we introduce a decoupling approximation in Eq. (6.23):

$$\left\langle \left\langle (n_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \simeq \langle n_{i-\sigma} \rangle \left\langle \left\langle (a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle. \quad (6.37)$$

Then, after the Fourier transformation we get from (6.23)

$$(\omega - \varepsilon_0) \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij} + \sum_m t_{im} \left\langle \left\langle a_{m\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega + U \langle n_{i-\sigma} \rangle \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega. \quad (6.38)$$

Performing the Fourier transformation over the spatial variables for every GF in Eq. (6.38) by the rule,

$$\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}r_{ij}} G_\sigma(\mathbf{k}, \omega), \quad (6.39)$$

where we introduced the momentum dependent spectral density  $G_\sigma(\mathbf{k}, \omega)$  for the spin projection  $\sigma$ , we come to equation

$$(\omega - \varepsilon_0 - U \langle n_{i-\sigma} \rangle) G_\sigma(\mathbf{k}, \omega) = 1 + t_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega). \quad (6.40)$$

$t_{\mathbf{k}}$  is the Fourier-transform of  $t_{ij}$  :

$$t_{ij} = \frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} e^{i\mathbf{k}r_{ij}}. \quad (6.41)$$

From (6.40) we obtain for the spectral density  $G_\sigma(\mathbf{k}, \omega)$ :

$$G_\sigma(\mathbf{k}, \omega) = \frac{1}{\omega - (\varepsilon_0 + t_{\mathbf{k}} + U \langle n_{i-\sigma} \rangle)}. \quad (6.42)$$

The pole of the spectral density (6.42),  $\omega = \varepsilon_0 + t_{\mathbf{k}} + U \langle n_{i-\sigma} \rangle$ , shows us that the excitation spectrum is a band (see Fig. 6.2) with the density of states given by

$$g_\sigma(\omega) = \frac{i}{2\pi N} \sum_{\mathbf{k}} (G_\sigma(\mathbf{k}, \omega + i\delta) - G_\sigma(\mathbf{k}, \omega - i\delta)). \quad (6.43)$$

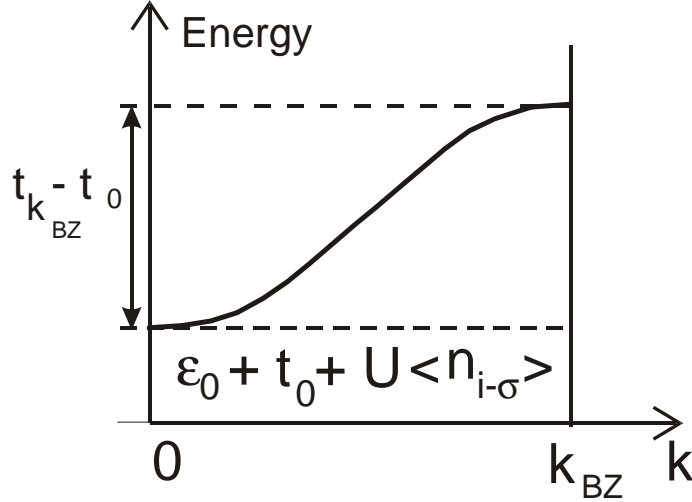


Figure 6.2: The excitation spectrum in the Hartree-Fock limit.

## 6.4 The Case when Both, Electron Hopping and Single-Site Correlations, are Important. Metal-Insulator (Semiconductor) Transition

Let us return again to our system of equations (6.23) and (6.24), and consider in detail the last term of Eq. (6.24) containing new Green functions. We intend to introduce approximations, which are called in scientific literature as "Hubbard-I approximations", in order to constrain the infinite chain of equations for Green functions by two equations, generated from Eqs. (6.23) and (6.24) by these approximations:

$$a) \left\langle \left\langle (n_{i-\sigma} a_{l\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \simeq \langle n_{i-\sigma} \rangle \left\langle \left\langle a_{l\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle; \quad (6.44)$$

$$\begin{aligned} b) \left\langle \left\langle (a_{l-\sigma}^\dagger a_{i-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &\simeq \langle a_{l-\sigma}^\dagger a_{i-\sigma} \rangle \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &\simeq \delta_{il} \langle a_{i-\sigma}^\dagger a_{i-\sigma} \rangle \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &= \delta_{il} \langle n_{i-\sigma} \rangle \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle; \end{aligned} \quad (6.45)$$

$$\begin{aligned} c) \left\langle \left\langle (a_{i-\sigma}^\dagger a_{i\sigma} a_{l-\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle &\simeq - \left\langle \left\langle (a_{i-\sigma}^\dagger a_{l-\sigma} a_{i\sigma})(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &\simeq -\delta_{il} \langle a_{i-\sigma}^\dagger a_{l-\sigma} \rangle \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle \\ &= -\delta_{il} \langle n_{i-\sigma} \rangle \left\langle \left\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \right\rangle \right\rangle. \end{aligned} \quad (6.46)$$

As it can be easily seen by observing the last term in Eq. (6.24) and the above approximations a) – c), contributions b) (6.45) and c) (6.46) cancel each other, so only the contribution a) holds in Eq. (6.24). Making use the Fourier-transformation over the time variable we rewrite Eqs. (6.23) and (6.24) as follows:

$$(\omega - \varepsilon_0) \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega - \sum_l t_{il} \left\langle \left\langle a_{l\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega - U \left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij}; \quad (6.47)$$

$$(\omega - \varepsilon_0 - U) \left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega - \langle n_{i-\sigma} \rangle \sum_l t_{il} \left\langle \left\langle a_{l\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij} \langle n_{i-\sigma} \rangle. \quad (6.48)$$

Then, GF  $\left\langle \left\langle n_{i-\sigma} a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega$  can be easily expressed from equation (6.48) and substituted into equation (6.47):

$$\begin{aligned} & (\omega - \varepsilon_0) \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega - \sum_l t_{il} \left\langle \left\langle a_{l\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega \\ & - \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \delta_{ij} - \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \sum_l t_{il} \left\langle \left\langle a_{l\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega = \delta_{ij}. \end{aligned} \quad (6.49)$$

Collecting terms in Eq. (6.49) we rewrite it as

$$\begin{aligned} & (\omega - \varepsilon_0) \left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega - \left\{ 1 + \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\} \sum_l t_{il} \left\langle \left\langle a_{l\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega \\ & = \delta_{ij} \left\{ 1 + \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\}. \end{aligned} \quad (6.50)$$

To solve equation (6.50) we perform Fourier-transformation over the space variables by the rule:

$$\begin{aligned} G_{ij}(\omega) &= \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} G(\mathbf{k}, \omega); \\ \delta_{ij} &= \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \equiv \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{ij}}. \end{aligned} \quad (6.51)$$

Making use of (6.51) for every space-dependent quantity in (6.50) we obtain

$$\begin{aligned} & (\omega - \varepsilon_0) \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{ij}} G_\sigma(\mathbf{k}, \omega) - \left\{ 1 + \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\} \sum_l \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{il}} t_{\mathbf{k}} \frac{1}{N} \sum_{\mathbf{k}'} e^{i\mathbf{k}'\mathbf{r}_{lj}} G_\sigma(\mathbf{k}', \omega) \\ & = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{ij}} \left\{ 1 + \frac{U \langle n_{i-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\}. \end{aligned} \quad (6.52)$$

Here we have introduced the space Fourier-transform of the spectral density  $\left\langle \left\langle a_{i\sigma} | a_{j\sigma}^\dagger \right\rangle \right\rangle_\omega$  denoted by  $G_\sigma(\mathbf{k}, \omega)$ . We consider the average particle number  $\langle n_{i-\sigma} \rangle$  to be independent on the site index  $i$ ,  $\langle n_{i-\sigma} \rangle = \langle n_{-\sigma} \rangle$ . Collecting exponentials in the last term of the left-hand side of Eq. (6.52) we get:

$$\begin{aligned} & \sum_l \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_{il}} t_{\mathbf{k}} \frac{1}{N} \sum_{\mathbf{k}'} e^{i\mathbf{k}'\mathbf{r}_{lj}} G_\sigma(\mathbf{k}', \omega) \\ & = \frac{1}{N^2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} t_{\mathbf{k}} G_\sigma(\mathbf{k}', \omega) e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_j} \sum_l e^{i(\mathbf{k}' - \mathbf{k})\mathbf{r}_l} \\ & = \frac{1}{N} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} t_{\mathbf{k}} G_\sigma(\mathbf{k}', \omega) e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_j} \delta_{\mathbf{k}\mathbf{k}'} \\ & = \frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega) e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}, \end{aligned} \quad (6.53)$$



where we have used the identity

$$\sum_l e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}_l} = N\delta_{\mathbf{k}\mathbf{k}'}. \quad (6.54)$$

Substitution of (6.53) into (6.52) gives

$$(\omega - \varepsilon_0)G_\sigma(\mathbf{k}, \omega) - t_{\mathbf{k}} \left\{ 1 + \frac{U \langle n_{-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\} G_\sigma(\mathbf{k}, \omega) = \left\{ 1 + \frac{U \langle n_{-\sigma} \rangle}{\omega - \varepsilon_0 - U} \right\} \quad (6.55)$$

or

$$G_\sigma(\mathbf{k}, \omega) = \left\{ \frac{1}{\omega - \varepsilon_0} + \frac{U \langle n_{-\sigma} \rangle}{(\omega - \varepsilon_0)(\omega - \varepsilon_0 - U)} \right\} + t_{\mathbf{k}} \left\{ \frac{1}{\omega - \varepsilon_0} + \frac{U \langle n_{-\sigma} \rangle}{(\omega - \varepsilon_0)(\omega - \varepsilon_0 - U)} \right\} G_\sigma(\mathbf{k}, \omega). \quad (6.56)$$

Comparing expression in the curly brackets in (6.56) with expression (6.29) we establish that it is just the spectral density of the Green function of the system in the *atomic limit*:

$$G_\sigma^a(\omega) = \left\{ \frac{1}{\omega - \varepsilon_0} + \frac{U \langle n_{-\sigma} \rangle}{(\omega - \varepsilon_0)(\omega - \varepsilon_0 - U)} \right\}. \quad (6.57)$$

The equation (6.56) then becomes

$$G_\sigma(\mathbf{k}, \omega) = G_\sigma^a(\omega) + G_\sigma^a(\omega)t_{\mathbf{k}}G_\sigma(\mathbf{k}, \omega), \quad (6.58)$$

from which we obtain

$$G_\sigma(\mathbf{k}, \omega) = \frac{G_\sigma^a(\omega)}{1 - t_{\mathbf{k}}G_\sigma^a(\omega)}. \quad (6.59)$$

The poles of Eq. (6.59) determine the excitation spectrum of the system under consideration:

$$t_{\mathbf{k}}G_\sigma^a(\omega) = 1,$$

or

$$t_{\mathbf{k}} \left\{ \frac{1}{\omega - \varepsilon_0} + \frac{U \langle n_{-\sigma} \rangle}{(\omega - \varepsilon_0)(\omega - \varepsilon_0 - U)} \right\} = 1. \quad (6.60)$$

Denoting  $\omega - \varepsilon_0 = x$  we derive from Eq. (6.60) the equation for finding  $x$ :

$$x^2 - x(U + t_{\mathbf{k}}) + Ut_{\mathbf{k}} \left( 1 - \frac{n}{2} \right) = 0. \quad (6.61)$$

$$\left( \langle n_{-\sigma} \rangle = \langle n \rangle = \frac{n}{2} \right)$$

Solutions for equation (6.61) are

$$x_{\pm} = \frac{U + t_{\mathbf{k}}}{2} \pm \sqrt{\left( \frac{U + t_{\mathbf{k}}}{2} \right)^2 - Ut_{\mathbf{k}} \left( 1 - \frac{n}{2} \right)} \quad (6.62)$$

or

$$\omega_{\pm} = \varepsilon_0 + \frac{U + t_{\mathbf{k}}}{2} \pm \sqrt{\left( \frac{U - t_{\mathbf{k}}}{2} \right)^2 + \frac{Ut_{\mathbf{k}}n}{2}}. \quad (6.63)$$

It is the general solution for the excitation spectrum in the *Hubbard-I* approximation.

Let us analyze it in the case when  $U \gg t_{\mathbf{k}}$  for every value of  $\mathbf{k}$ . We can expand the square root in (6.63). From the above inequality it follows that the first term in the root is larger than the second one:

$$\begin{aligned}\omega_{\pm} &= \varepsilon_0 + \frac{U + t_{\mathbf{k}}}{2} \pm \left| \frac{U - t_{\mathbf{k}}}{2} \right| \sqrt{1 + \frac{2Ut_{\mathbf{k}}n}{(U - t_{\mathbf{k}})^2}} \\ &\simeq \varepsilon_0 + \frac{U + t_{\mathbf{k}}}{2} \pm \left| \frac{U - t_{\mathbf{k}}}{2} \right| \left\{ 1 + \frac{Ut_{\mathbf{k}}n}{(U - t_{\mathbf{k}})^2} \right\}.\end{aligned}\quad (6.64)$$

Because of inequality  $U \gg t_{\mathbf{k}}$  we can replace the absolute value by parentheses in (6.64) and consider the two roots of (6.64):

$$\begin{aligned}\omega_+ &\simeq \varepsilon_0 + U + \frac{Ut_{\mathbf{k}}n}{2(U - t_{\mathbf{k}})} \approx \varepsilon_0 + U + t_{\mathbf{k}}\frac{n}{2}, \\ \omega_- &\simeq \varepsilon_0 + t_{\mathbf{k}} - \frac{Ut_{\mathbf{k}}n}{2(U - t_{\mathbf{k}})} \approx \varepsilon_0 + t_{\mathbf{k}}\left(1 - \frac{n}{2}\right).\end{aligned}\quad (6.65)$$

Band structure, corresponding to Eqs. (6.65), is displayed in Fig. 6.3. The band struc-

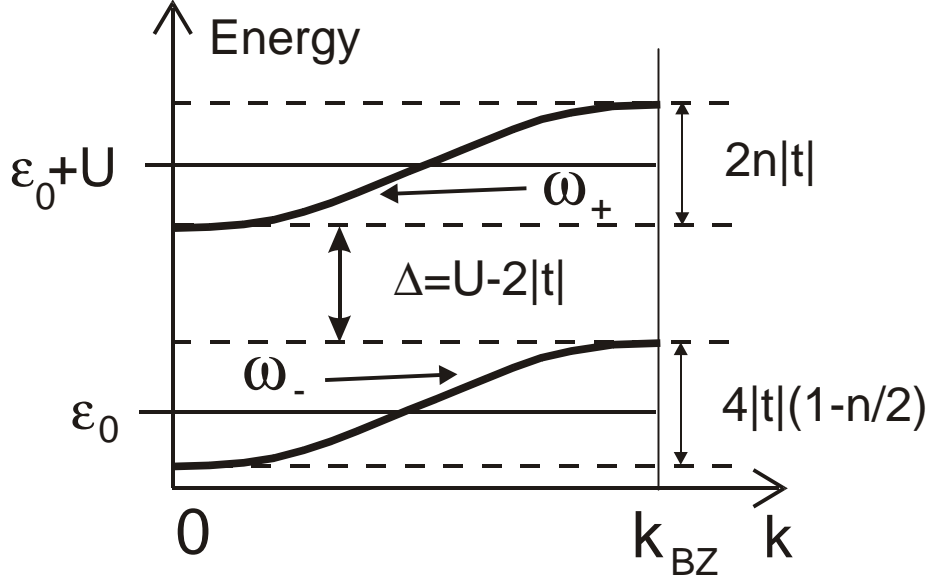


Figure 6.3: Band structure of the Hubbard model in the case when both, hopping and Coulomb repulsion, have been taken into account.

ture looks like two sub-bands, separated by the gap denoted by  $\Delta$ . We further analyze parameters of the band structure in more details. Assume that we have the simple cubic lattice with spacing  $a$  (see, for example, Fig. 3.2), and that hopping is important only between nearest neighbors:  $t_{i,i+1} = t < 0$ . Then, we find for  $t_{\mathbf{k}}$ :

$$\begin{aligned}t_{\mathbf{k}} &= \sum_{j(\text{nearest to } i)} t_{ij} e^{i\mathbf{k}\mathbf{r}_{ij}} = -|t| \{ e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a} \} \\ &= -2|t| \{ \cos k_x a + \cos k_y a + \cos k_z a \}.\end{aligned}\quad (6.66)$$

Let us choose that we observe the momentum dependence (dispersion) of the solutions for the energies (6.65) along the  $k_x$  direction, keeping  $\cos k_y a = \cos k_z a = 0$ . Then, we have for the bottom and top values of the band energies

$$\omega_+^{bottom} \simeq \varepsilon_0 + U + \frac{n}{2} t_{k_x=0} = \varepsilon_0 + U - n |t|, \quad (6.67)$$

$$\omega_+^{top} \simeq \varepsilon_0 + U + \frac{n}{2} t_{k_x=k_{BZ}} = \varepsilon_0 + U - \frac{n}{2} |t| \cos \pi = \varepsilon_0 + U + n |t|, \quad (6.68)$$

$$\omega_-^{bottom} \simeq \varepsilon_0 + \left(1 - \frac{n}{2}\right) t_{k_x=0} = \varepsilon_0 - 2 \left(1 - \frac{n}{2}\right) |t|, \quad (6.69)$$

$$\omega_-^{top} \simeq \varepsilon_0 + \left(1 - \frac{n}{2}\right) t_{k_x=k_{BZ}} = \varepsilon_0 + 2 \left(1 - \frac{n}{2}\right) |t|. \quad (6.70)$$

Thus, the upper sub-band width is  $2n |t|$ , the lower sub-band width is  $4 \left(1 - \frac{n}{2}\right) |t|$ . The gap value between the sub-bands is

$$\Delta = \omega_+^{bottom} - \omega_-^{top} = U - 2 |t|. \quad (6.71)$$

The bandwidths and the gap are indicated in Fig. 6.3. Equation (6.71) shows us that the **gap decreases** as the **hopping strength  $|t|$  increases**, but, according to the initial approximation ( $U \gg t_{\mathbf{k}}$ ),  $U$  must be  $> 2 |t|$ . If the system has the half-filled initial (nonsplit at  $U = 0$ ) band (it means that  $n = 1$  in the above expressions) the lower band is completely filled, but the upper band is empty, if  $\Delta \ll k_B T$ . Then, this band structure represents an insulator (semiconductor) at  $n = 1$ . So, the theory is able, at least in principle, to describe insulator (semiconductor)-metal (conductor) transition. This transition can be achieved applying the (hydrostatic) pressure to an insulating (semiconducting) compound.



# Chapter 7

## Magnetism of Strongly Correlated Electronic Systems

### 7.1 The Hamiltonian of $t - J$ Model

As it was shown in Chapter 6, the Hubbard model supposes the alternative approach to study the system of collective electrons with the Coulomb repulsion of two electrons with opposite spins at one site. Within the framework of this model the system can be investigated from the side of weak Coulomb interaction and from the side of strongly correlated limit. It appears, that at  $N_e \leq N$  or  $N_e \geq N$  ( $N_e$  - the number of collective electrons in the crystal,  $N$  - the number of sites) the latter case, *i.e.* the system of strongly correlated electrons, can be studied in more detail by means of a special Hamiltonian, which is derived from the Hamiltonian of the Hubbard model by expansion in a series on small parameter  $t/U \ll 1$ .

Suppose that  $N_e \leq N$ . The resulting Hamiltonian contains two terms. *The first term* presents the zero-order term with respect to small  $t/U$  and describes movement of the electrons from site to site in the system with infinitely high Coulomb repulsion  $U$ . In this case, electrons can hop from a site to the next free site only, since the state with two electrons per site is forbidden by the Pauli principle (the spin projections of electrons are the same) and by very high Coulomb repulsion  $U$  (the opposite spin projections). As a result, in the case  $U = \infty$  and  $N_e \leq N$  the average number of electrons per site cannot be more than 1.

*The second term* in expansion of the Hubbard Hamiltonian is linear on the small parameter  $t/U$ . It is responsible for indirect interaction between electrons of the nearest-neighbor sites of the crystal. This interaction originates from the virtual hopping of electron on the nearest-neighbor site which is occupied by an electron with the opposite spin. Such hopping is possible because  $U$  is finite quantity (though it is large in comparison with  $t$ ). As a result of hopping, the energy of such two sites system increases by  $U$ . Since it is not energetically favourable, the hopped electron jumps back to its site. Such jumps result in indirect interaction between the nearest-neighbor sites electrons with the opposite spins. Thus, from the point of view of magnetism, the second term of the Hubbard Hamiltonian expansion promotes antiferromagnetic ordering of strongly correlated system of electrons.

For the sake of convenience we recall here the Hamiltonian of the Hubbard model

(6.1),

$$\mathcal{H} = \varepsilon_0 \sum_{i,\sigma} n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_{j,\sigma} n_{j\sigma} n_{j-\sigma}. \quad (7.1)$$

Suppose the single-particle energy is measured with respect to  $\varepsilon_0$  ( $\varepsilon_0 = 0$ ), and take into account the nearest-neighbor hopping only ( $t_{ij} = -t$ ). Then, the expansion of the Hubbard Hamiltonian on small parameter  $t/U$  is given by

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} a_{i\sigma}^\dagger (1 - n_{i-\sigma}) a_{j\sigma} (1 - n_{j-\sigma}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (7.2)$$

plus higher on  $t/U$  order terms which we neglect because of smallness of the parameter  $t/U$ . In the above equation  $\langle ij \rangle$  denotes the nearest-neighbor sites,  $n_{i-\sigma} = a_{i-\sigma}^\dagger a_{i-\sigma}$  is the electron number operator at the site  $i$  and spin projection  $-\sigma$ ,

$$n_i = \sum_{\sigma} n_{i\sigma} \quad (7.3)$$

is operator of total number of electrons at the site  $i$ . At the same time, it is necessary to remember that at  $N_e \leq N$  the one site electron number is equal either zero, or unity. The states with two electrons per site are excluded from Hamiltonian (7.2). Thus, strictly speaking, we must understand behind the operator  $n_i$  in (7.2)

$$n_i = \sum_{\sigma} n_{i\sigma} (1 - n_{i-\sigma}). \quad (7.4)$$

The projection factors  $(1 - n_{i-\sigma})$  ensure elimination of double occupation of the site  $i$  by electrons with opposite spins. The role of the projection factors in the first term of (7.2) is the same.

The constant of indirect exchange interaction  $J$  is defined by expression

$$J = \frac{2t^2}{U}. \quad (7.5)$$

It follows that the second term in (7.2) is linear on the small parameter  $t/U$ .

Assuming that at the unit filling ( $N_e = N$ ) there is exactly one electron at each site, and neglecting an insignificant constant  $\frac{1}{4} n_i n_j$  in the second term of (7.2), we get

$$\mathcal{H}_E = J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j. \quad (7.6)$$

The Hamiltonian (7.6) is the Heisenberg model with the exchange interaction between neighboring spins. Since  $J > 0$ , it follows that there is an antiferromagnetic ordering of electrons in this case.

Hamiltonian (7.2) is the Hamiltonian of strongly correlated electrons. It is the Hamiltonian of the Hubbard model in the limit of strong Coulomb repulsion, and  $N_e \leq N$ . Model (7.2) is frequently referred to as  $t - J$  model, as the first term is proportional  $t$ , and the second one is proportional to  $J$ .

## 7.2 Hubbard Operators

It is convenient to express the  $t - J$  model Hamiltonian in terms of so-called Hubbard operators  $X_i^{pq}$  (or  $X$ -operators), where  $p$  and  $q$  are the numbers of one-site states. The  $X$ -operators mean operators of transfer of the  $i$  site from the state  $q$  to the state  $p$ ,

$$X_i^{pq} \equiv |pi\rangle\langle qi|. \quad (7.7)$$

It is easy to verify that number of the Hubbard operators equals nine when each site has three states:  $|0\rangle$  (without an electron),  $|\uparrow\rangle$  (spin up) and  $|\downarrow\rangle$  (spin down). For the  $t - J$  model we have eliminated one-site states with two electrons. The  $X$ -operators are neither Fermi nor Bose operators, but form a more complicated algebra with specific commutation relations and multiplication rules. There are four Fermi-like operators and five Bose-like operators. The Fermi-like  $X$ -operators are defined by relations

$$X_i^{0\sigma} = a_{i\sigma} (1 - n_{i-\sigma}); \quad X_i^{\sigma 0} = a_{i\sigma}^\dagger (1 - n_{i-\sigma}). \quad (7.8)$$

In the basis of functions  $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$  they take the form

$$\begin{aligned} X_i^{0+} &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, & X_i^{0-} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, \\ X_i^{+0} &= \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, & X_i^{-0} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}_i. \end{aligned} \quad (7.9)$$

It is seen that  $X_i^{0\sigma}$  ( $X_i^{\sigma 0}$ ) is the annihilation (creation) operator for the electron with spin  $\sigma$  at the site  $i$ , provided that there is no electron with the opposite direction of spin at this site.

From five of the Bose-like operators there are two,

$$\begin{aligned} X_i^{+-} &= a_{i\uparrow}^\dagger a_{i\downarrow}, & X_i^{-+} &= a_{i\downarrow}^\dagger a_{i\uparrow}, & (X_i^{\sigma\bar{\sigma}} &= a_{i\sigma}^\dagger a_{i\bar{\sigma}}, \text{ where } \bar{\sigma} = -\sigma), \\ X_i^{+-} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}_i, & X_i^{-+} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}_i, \end{aligned} \quad (7.10)$$

which are responsible for flip-flop of a spin at the site. The next three Bose-like operators are diagonal ones

$$\begin{aligned} X_i^{00} &= (1 - n_{i\uparrow})(1 - n_{i\downarrow}), & X_i^{++} &= n_{i\uparrow}(1 - n_{i\downarrow}), & X_i^{--} &= n_{i\downarrow}(1 - n_{i\uparrow}), \\ X_i^{00} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, & X_i^{++} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, & X_i^{--} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_i. \end{aligned} \quad (7.11)$$

One can see that there is only one nonzero matrix entry  $(X_i^{pq})_{pq} = 1$ , and  $(X_i^{pq})^\dagger = X_i^{qp}$ .

The operators  $X_i^{00}$ ,  $X_i^{++}$ ,  $X_i^{--}$  are responsible for the number of holes, number of electrons with spin  $\uparrow$  and number of electrons with spin  $\downarrow$ , respectively. Here, for any site  $i$  the equality takes place:

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} = 1, \quad (7.12)$$

which is the conservation rule.

The one-site Hubbard operators form an  $SU(n)$  Lie algebra ( $n = 3$  for the three-level  $t - J$  model) with the multiplication rules

$$X_i^{pq} X_i^{q'p'} = \delta_{qq'} X_i^{pp'}, \quad (7.13)$$

and the commutation relations

$$\left[ X_i^{pq}, X_i^{q'p'} \right]_{\pm} = X_i^{pp'} \delta_{qq'} \pm X_i^{q'q} \delta_{pp'}. \quad (7.14)$$

The different-site Hubbard operators can be either Bose-like or Fermi-like depending on the commutation relations which are written as follows

$$\left[ X_i^{pq}, X_{i'}^{q'p'} \right]_{\pm} = \left( X_i^{pp'} \delta_{qq'} \pm X_i^{q'q} \delta_{pp'} \right) \delta_{ii'}. \quad (7.15)$$

Here, the upper sign corresponds to the case when both operators in the left-hand side are Fermi-like, while the lower sign stands for the cases when at least one of them is Bose-like.

In terms of the  $X$ -operators the  $t - J$  model Hamiltonian can be rewritten as follows:

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} X_i^{\sigma 0} X_j^{0 \sigma} + J \sum_{\langle ij \rangle} (X_i^{-+} X_j^{+-} - X_i^{++} X_j^{--}). \quad (7.16)$$

Let's express now the Hamiltonian of the Hubbard model via the  $X$ -operators. In this case it is still necessary to consider states with two electrons per one site. As a result there are four states on each site:

$$|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle \quad (|0\rangle, |\sigma\rangle, |\bar{\sigma}\rangle, |2\rangle). \quad (7.17)$$

In such basis the  $X$ -operators are represented by fourth-order matrices with one of the matrix elements equal to unity, and the rest of matrix elements equal to zero. They include sixteen  $X$ -operators for the Hubbard's model with four states on one site. Nine of them are already familiar to us. In the new basis they have the same form but with added fourth line and fourth column with zero elements. This addition corresponds to joining the one-site functions of state with two electrons on a site. As the added line and column have zero matrix elements the physical meaning of the discussed nine  $X$ -operators does not depend on such adding.

Seven new operators are responsible for transitions of a site to or from the state with two electrons. Four of them are operators of the Fermi type:

$$\begin{aligned} X_i^{\sigma 2} &= a_{i\sigma}^{\dagger} a_{i\uparrow} a_{i\downarrow} = \sigma a_{i\bar{\sigma}} n_{i\sigma} \quad (\sigma = \pm 1), \\ X_i^{2\sigma} &= a_{i\downarrow}^{\dagger} a_{i\uparrow}^{\dagger} a_{i\sigma} = \sigma a_{i\bar{\sigma}}^{\dagger} n_{i\sigma}, \end{aligned} \quad (7.18)$$

where it has been taken into account that the operators of annihilation and creation of two electrons on one site have the form according to

$$X_i^{02} = a_{i\uparrow} a_{i\downarrow}, \quad X_i^{20} = a_{i\downarrow}^{\dagger} a_{i\uparrow}^{\dagger} \quad (X_i^{02} = \sigma a_{i\sigma} a_{i\bar{\sigma}}). \quad (7.19)$$

In the new basis the operators  $X_i^{\sigma 2}$ ,  $X_i^{2\sigma}$  are represented as follows

$$X_i^{+2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \quad X_i^{2+} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}_i,$$



$$X_i^{-2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \quad X_i^{2-} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}_i. \quad (7.20)$$

The operators  $X_i^{02}$ ,  $X_i^{20}$  are the Bose-like operators. The  $X$ -operators changing number of electrons by an odd number, are operators of the Fermi type, and the  $X$ -operators changing number of electrons by an even number, are of the Bose type. It is necessary to add to operators  $X_i^{02}$ ,  $X_i^{20}$  (7.19) one more Bose-like operator

$$X_i^{22} = n_{i\uparrow}n_{i\downarrow} = n_{i\sigma}n_{i\bar{\sigma}}. \quad (7.21)$$

It is diagonal operator responsible for the number of fillings of a site by two electrons. In the matrix representation these Bose-like operators are given by relations

$$X_i^{02} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}_i, \quad X_i^{20} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}_i, \quad X_i^{22} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_i. \quad (7.22)$$

Using expressions of the Fermi  $X$ -operators through  $a$ -operators, it is possible to derive the important relations between usual  $a$ -operators and  $X$ -operators of the Fermi type:

$$a_{i\sigma} = X_i^{0\sigma} + \bar{\sigma}X_i^{\bar{\sigma}2}, \quad a_{i\sigma}^\dagger = X_i^{\sigma 0} + \bar{\sigma}X_i^{2\bar{\sigma}}. \quad (7.23)$$

Note here that, if we define operators  $X_i^{02}$  and  $X_i^{20}$  as follows

$$X_i^{02} = a_{i\downarrow}a_{i\uparrow}, \quad X_i^{20} = a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger, \quad (7.24)$$

then

$$X_i^{\sigma 2} = \bar{\sigma}a_{i\bar{\sigma}}n_{i\sigma}, \quad X_i^{2\sigma} = \bar{\sigma}a_{i\bar{\sigma}}^\dagger n_{i\sigma} \quad (7.25)$$

and

$$a_{i\sigma} = X_i^{0\sigma} + \sigma X_i^{\bar{\sigma}2}, \quad a_{i\sigma}^\dagger = X_i^{\sigma 0} + \sigma X_i^{2\bar{\sigma}}. \quad (7.26)$$

This circumstance needs to be had in view upon manipulations with  $X$ -operators. The derived relations allow us to express the Hamiltonian of the Hubbard model through the  $X$ -operators. Substituting them into the formula (7.1) (taking into account that  $\varepsilon_0 = 0$  and  $\sum_{i,j} \Rightarrow \sum_{\langle ij \rangle}$ ) it is possible to get

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_{int}, \\ \mathcal{H}_0 &= U \sum_i X_i^{22}, \\ \mathcal{H}_{int} &= -t \sum_{\langle ij \rangle \sigma} (X_i^{\sigma 0} X_j^{0\sigma} + \bar{\sigma} X_i^{\sigma 0} X_j^{\bar{\sigma}2} + \bar{\sigma} X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{2\bar{\sigma}} X_j^{\bar{\sigma}2}). \end{aligned} \quad (7.27)$$

Such notations correspond to the choice of the term, responsible for the Coulomb repulsion, as a zero Hamiltonian. For any site we have

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} + X_i^{22} = 1. \quad (7.28)$$

### 7.3 Derivation of the $t - J$ Model Hamiltonian by Means of Operational Form of the Bogolyubov-Tyablikov Perturbation Theory

Let us derive the  $t - J$  model Hamiltonian from the Hubbard's Hamiltonian by expansion of the last in the series on small  $t/U$ . It can be made by means of the operational form of the Bogolyubov-Tyablikov perturbation theory.

Let's consider the Schrodinger equation irrespective of any model,

$$\left( \mathcal{H}_0 + \lambda \mathcal{H}' - \varepsilon \right) \psi = 0, \quad (7.29)$$

where  $\varepsilon$  is the eigenvalue,  $\psi$  is the corresponding eigenfunction, and  $\lambda$  is the small parameter ( $\lambda \ll 1$ ) selected from  $\mathcal{H}_{int}$  so, that

$$\lambda \mathcal{H}' = \mathcal{H}_{int} \quad (7.30)$$

is the small expansion parameter.

Let us  $\varepsilon_0$  be the least eigenvalue of operator  $\mathcal{H}_0$ , and  $\psi_0$  be the corresponding eigenfunction:

$$(\mathcal{H}_0 - \varepsilon_0) \psi_0 = 0. \quad (7.31)$$

Assume further that the level  $\varepsilon_0$  is  $N_0$ -fold multiply degenerate. Then,  $N_0$  functions  $\{\psi_0\}$  correspond to this level. Any linear combination of these functions is also an eigenfunction of the operator  $\mathcal{H}_0$  with the eigenvalue  $\varepsilon_0$ .

Suppose that all remaining levels  $\varepsilon_n$  (levels of the excited states) are separated by a finite gap from the level  $\varepsilon_0$ :

$$\varepsilon_n - \varepsilon_0 \geq \Delta > 0, \quad (7.32)$$

and they are  $N_n$  multiply degenerate ( $\Delta$  is some constant). For example, the nearest to  $\varepsilon_0$  the level  $\varepsilon_1$  is supposed  $N_1$  multiply degenerate. Any linear combination of  $N_1$  eigenfunctions  $\psi_1$  corresponding to this level has the eigenvalue  $\varepsilon_1$ .

Divide now the function  $\psi$  into two parts:

$$\psi = \psi_0 + \psi_{int}, \quad (7.33)$$

where  $\psi_{int}$  is the part of the function  $\psi$  caused by perturbation.  $\psi_{int} = 0$  at  $\lambda = 0$ .

Let us introduce an operator of projection  $P$  ( $P^2 = P$ ) such that

$$P\psi = \psi_0 \text{ and } [P, \mathcal{H}_0] = 0. \quad (7.34)$$

Then,

$$\psi_{int} = (1 - P) \psi. \quad (7.35)$$

Thus

$$P\psi_{int} = 0. \quad (7.36)$$

Substituting (7.33) into (7.29), we get

$$\left( \varepsilon - \mathcal{H}_0 - \lambda \mathcal{H}' \right) P\psi + \left( \varepsilon - \mathcal{H}_0 - \lambda \mathcal{H}' \right) \psi_{int} = 0. \quad (7.37)$$



which we have written out up to terms of the *first* order on  $\lambda$  ( $\mathcal{H}_{int} = \lambda\mathcal{H}'$ ).

We use now (7.50) for derivation of the  $t - J$  model Hamiltonian. Let us assume that the operators  $\mathcal{H}_0$  and  $\mathcal{H}_{int}$  in (7.50) look like (7.27), and  $\varepsilon_0$  is the  $\mathcal{H}_0$ 's least energy eigenvalue. It corresponds to the eigenfunction  $\psi_0$  with one-site states of the form  $|0\rangle$ ,  $|\uparrow\rangle$ ,  $|\downarrow\rangle$ , i.e. without a state with two electrons on a site. It is easy to see that  $\varepsilon_0 = 0$ .

Let us  $\varepsilon_1$  be the nearest to  $\varepsilon_0$  excited level that corresponds to the system states with two electrons on one site. It is obvious that  $\varepsilon_1 = U$ .

The levels  $\varepsilon_0$  and  $\varepsilon_1$  are degenerate. The sets of functions  $\psi_0$  and  $\psi_1$  correspond to them, accordingly. The eigenvalue  $\varepsilon_0$  corresponds to any linear combination of the functions  $\psi_0$  ( $\psi_1 \implies \varepsilon_1$ ).

The operator of projection  $P$  reads

$$P = \prod_i (1 - X_i^{22}) = \prod_i \left( X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} \right). \quad (7.51)$$

In fact, by virtue of identity

$$(1 - X_i^{22}) (1 - X_i^{22}) = (1 - X_i^{22}) \quad (7.52)$$

the operator  $P = \prod_i (1 - X_i^{22})$  is a projection operator. Secondly, this operator eliminates states with two electrons on a site. Indeed,

$$PX_i^{2\sigma} = PX_i^{22} = X_i^{22}P = X_i^{\sigma 2}P = 0. \quad (7.53)$$

Hence, at the action of the operator  $P$  on the full wave function  $\psi$  of the Hamiltonian  $\mathcal{H}$  we should derive function  $\psi_0$  which does not include one-site states with two electrons. Thus, first of relations (7.34) is fulfilled for operator (7.51) with interpretation which we give to the function  $\psi_0$ . Second of relations (7.34) follows immediately from (7.53). It is easy to see, that by virtue of (7.53)

$$P\mathcal{H}_{int}P\psi_0 = -t \sum_{\langle ij \rangle \sigma} X_i^{\sigma 0} X_j^{0\sigma} \psi_0, \quad (7.54)$$

that gives the first term of the  $t - J$  model Hamiltonian. Note that the state

$$(\mathcal{H}_{int} - P\mathcal{H}_{int}P)P\psi_0 = (\mathcal{H}_{int} - P\mathcal{H}_{int}P)\psi_0 \quad (7.55)$$

represents a linear combination of states with two electrons on one of sites of a crystal. Hence, it is the eigenstate of the operator  $\mathcal{H}_0$  with the eigenvalue  $\varepsilon_1 = U$ . Then, it follows that

$$(\mathcal{H}_0 - \varepsilon_0)^{-1} (\mathcal{H}' - P\mathcal{H}'P)P\psi_0 = \frac{1}{U} (\mathcal{H}' - P\mathcal{H}'P)P\psi_0. \quad (7.56)$$

In view of (7.56) the second term in (7.50) is represented as

$$-\frac{t^2}{U} P \sum_{\langle ij \rangle} \sum_{\langle i_1 j_1 \rangle} \sum_{\sigma\sigma_1} \bar{\sigma}\bar{\sigma}_1 X_i^{\sigma 0} X_j^{\sigma_2} X_{i_1}^{2\sigma_1} X_{j_1}^{0\sigma_1} P. \quad (7.57)$$

Making use of (7.53) we get

$$P(\mathcal{H}_{int} - P\mathcal{H}_{int}P) = -t \sum_{\langle ij \rangle \sigma} \bar{\sigma} X_i^{\sigma 0} X_j^{\sigma_2}, \quad (7.58)$$

and

$$(\mathcal{H}_{int} - P\mathcal{H}_{int}P)P = -t \sum_{\langle i_1 j_1 \rangle \sigma_1} \bar{\sigma}_1 X_{i_1}^{2\bar{\sigma}_1} X_{j_1}^{0\sigma_1}. \quad (7.59)$$

Expression (7.57) is not zero only in a case of  $j = i_1$ . Let still  $i = j_1$ . Taking into consideration (7.13), for acting by operator (7.57) on the function  $\psi_0$  we get

$$-\frac{t^2}{U} \sum_{\langle ij \rangle} \sum_{\sigma \sigma_1} \bar{\sigma} \sigma_1 X_i^{\sigma \sigma_1} X_j^{\bar{\sigma} \bar{\sigma}_1} \psi_0. \quad (7.60a)$$

After summing over the spin projections  $\sigma$  and  $\sigma_1$  this relation gives exactly the second term of the  $t - J$  model Hamiltonian:

$$J \sum_{\langle ij \rangle} (X_i^- + X_j^+ - X_i^{++} X_j^{--}), \quad J = \frac{2t^2}{U}. \quad (7.61)$$

In addition to instability with respect to ferromagnetic and antiferromagnetic orderings the  $t - J$  model describes a series of other properties. In particular, the non-phonon mechanisms of superconductivity in a system of itinerant electrons with the strong Coulomb repulsion can be investigated on the basis of  $t - J$  model.

## 7.4 The Hubbard Approximation

In the approach with a weak Coulomb interaction the band character of collective electrons does not differ so much in comparison with system of noninteracting band electrons. The effect of delocalization in this case is so great that the system cannot possess magnetic moment on a lattice site. Nucleation of the magnetic moment is possible only in a case of strong enough Coulomb repulsion. In this approach, the magnetic moment on a site, occupied by an electron, arises initially, and for ferromagnetism to appear, interaction between magnetic moments should be settled up.

The problem of existence and character of such interaction is extremely complicated and it is not solved completely up to now. Unlike Heisenberg model, the Hamiltonian of the Hubbard model does not contain in an explicit form neither magnetic moments nor interaction between them. This interaction, as well as magnetic moments, should manifest themselves in an indirect way.

For the system placed in an external magnetic field  $\mathbf{H}$  the Hamiltonian of the Hubbard model reads:

$$\mathcal{H} = \varepsilon_0 \sum_{i,\sigma} n_{i\sigma} - \frac{1}{2} H \sum_{i,\sigma} \sigma n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_{j,\sigma} n_{j\sigma} n_{j-\sigma}, \quad (\sigma = 1, \bar{\sigma} = -\sigma). \quad (7.62)$$

The Zeeman interaction with the external magnetic field is taken in terms of  $g\mu_B$ , where  $g$  is the electron  $g$ -factor,  $\mu_B$  is the Bohr magneton, i.e. it is supposed  $g\mu_B = 1$ . Assuming, that  $\langle a_{i\sigma}^\dagger a_{i\sigma} \rangle = \langle n_{i\sigma} \rangle$  does not depend on the site index, and  $m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle \neq 0$ , we investigate the electron spectrum of the system of strongly correlated electrons. We consider as we made, the single-particle electron Green function

$$G_{ij\sigma}(t - t') = \ll a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \gg_{\eta=-1}^r. \quad (7.63)$$

In further derivations we follow the subsection 5.4 where instead of  $\varepsilon_0$  we should take  $\varepsilon_0 - \frac{1}{2}H\sigma$ , and condition  $\langle n_\sigma \rangle = \langle n_{\bar{\sigma}} \rangle = \frac{n}{2}$  is relaxed.

The electron spectrum of two resulting bands looks like:

$$\omega_\sigma^\pm(\mathbf{k}) = \varepsilon_0 - \frac{1}{2}H\sigma + \frac{1}{2} \left\{ U + t_{\mathbf{k}} \pm \sqrt{(U - t_{\mathbf{k}})^2 + 4Ut_{\mathbf{k}} \langle n_{\bar{\sigma}} \rangle} \right\}. \quad (7.64)$$

In terms of this excitation spectrum, the single-particle Green function  $G_\sigma(\mathbf{k}, \omega)$  can be rewritten as:

$$G_\sigma(\mathbf{k}, \omega) = \frac{A_\sigma^-(\mathbf{k})}{\omega - \omega_\sigma^-(\mathbf{k})} + \frac{A_\sigma^+(\mathbf{k})}{\omega - \omega_\sigma^+(\mathbf{k})}, \quad (7.65)$$

where

$$A_\sigma^-(\mathbf{k}) = \frac{\omega_\sigma^-(\mathbf{k}) - U(1 - \langle n_{\bar{\sigma}} \rangle)}{\omega_\sigma^-(\mathbf{k}) - \omega_\sigma^+(\mathbf{k})}, \quad (7.66)$$

$$A_\sigma^+(\mathbf{k}) = \frac{\omega_\sigma^+(\mathbf{k}) - U(1 - \langle n_{\bar{\sigma}} \rangle)}{\omega_\sigma^+(\mathbf{k}) - \omega_\sigma^-(\mathbf{k})}, \quad (7.67)$$

and

$$A_\sigma^-(\mathbf{k}) + A_\sigma^+(\mathbf{k}) = 1. \quad (7.68)$$

It is seen to show that  $\omega_\sigma^-(\mathbf{k}) \leq U(1 - \langle n_{\bar{\sigma}} \rangle) \leq \omega_\sigma^+(\mathbf{k})$  and, hence,  $A_\sigma^\pm(\mathbf{k}) \geq 0$ .

It is visible that at any finite  $U$  the Hubbard bands  $\omega_\sigma^-(\mathbf{k})$  and  $\omega_\sigma^+(\mathbf{k})$  do not overlap. It can be verified that it is the case at  $U \gg W$ , however at  $U \ll W$  existence of the gap between the Hubbard subbands is incorrect from the physical point of view. From general considerations it follows that in presence of the Coulomb repulsion, the splitting of the initial conduction band  $t_{\mathbf{k}}$  should happen not at arbitrary  $U$ , but at  $U \gtrsim W$ . Hence, the Hubbard approximation strongly overestimates Coulomb correlations in case of weak coupling, and it provides qualitatively correct description of the band structure only in case  $U \gg W$ .

In the limiting case  $U \rightarrow \infty$  from (7.64) we get ( $H = 0$ )

$$\omega_\sigma^-(\mathbf{k}) = \varepsilon_0 + (1 - \langle n_{\bar{\sigma}} \rangle) t_{\mathbf{k}}, \quad \omega_\sigma^+(\mathbf{k}) = U + \langle n_{\bar{\sigma}} \rangle t_{\mathbf{k}}. \quad (7.69)$$

The spectrum in each subband differs from the spectrum of the system of noninteracting band electrons  $t_{\mathbf{k}}$  by factors:  $(1 - \langle n_{\bar{\sigma}} \rangle)$  - for the lower band and  $\langle n_{\bar{\sigma}} \rangle$  - for the upper band. As  $0 \leq \langle n_{\bar{\sigma}} \rangle \leq 1$  and  $0 \leq (1 - \langle n_{\bar{\sigma}} \rangle) \leq 1$  it is seen that the bands are narrowed down in comparison with the unperturbed band  $t_{\mathbf{k}}$ . The summarized width of the bands is exactly equal to the width of the initial band with spectrum  $t_{\mathbf{k}}$ . This correlation narrowing of the Hubbard bands is the major peculiarity of the one-electron spectrum of strongly correlated electronic system.

Let's consider now a possibility of the ferromagnetic ordering of strongly correlated electronic system in the Hubbard approximation. As the tendency to the ferromagnetic ordering strengthens with increase in  $U$ , we shall discuss a limiting case  $U \rightarrow \infty$ . Making use of the electron-hole symmetry, and considering the case  $N_e \leq N$  we realize that, and hence, the chemical potential  $\mu$  should be within the limits of the lower Hubbard band. At  $U \rightarrow \infty$  for the one-electron Green function we have:

$$G_\sigma(\mathbf{k}, \omega) = \frac{1 - \langle n_{\bar{\sigma}} \rangle}{\omega + \frac{1}{2}\sigma H - (1 - \langle n_{\bar{\sigma}} \rangle) t_{\mathbf{k}}}. \quad (7.70)$$

Using this Green function and the general relation (2.16) we can find the spin-dependent particle density

$$\langle n_\sigma \rangle = (1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} f[\omega_\sigma(\mathbf{k})], \quad (7.71)$$

where

$$\omega_\sigma(\mathbf{k}) = (1 - \langle n_{\bar{\sigma}} \rangle) t_{\mathbf{k}} - \frac{1}{2} \sigma H. \quad (7.72)$$

Let us introduce definitions of the magnetization  $m$  (without factor 1/2) and the net particle density  $n$  by means of relations

$$m = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle, \quad n = \langle n \rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle. \quad (7.73)$$

Then, with the use of expression (7.71) we obtain equation for the magnetization,

$$m = \sum_{\sigma} \sigma (1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} f[\omega_\sigma(\mathbf{k})] \quad (7.74)$$

and equation for finding the chemical potential,

$$n = \sum_{\sigma} (1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} f[\omega_\sigma(\mathbf{k})], \quad (7.75)$$

where the factor  $(1 - \langle n_{\bar{\sigma}} \rangle)$  can be expressed as

$$1 - \langle n_{\bar{\sigma}} \rangle = 1 - \frac{1}{2} (n - \sigma m) \quad (7.76)$$

using (7.74) and (7.75). Differentiating  $m$  on  $H$ , and then supposing  $H \rightarrow 0$  and  $m \rightarrow 0$ , we obtain

$$\chi = \frac{(1 - \frac{1}{2}n)^2 \chi_0}{1 - n + (1 - \frac{1}{2}n)^2 \Lambda}, \quad (7.77)$$

where

$$\chi_0 = -\frac{1}{N} \sum_{\mathbf{k}} \frac{df[\omega(\mathbf{k})]}{d\omega(\mathbf{k})}, \quad (7.78)$$

$$\Lambda = -\frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} \frac{df[\omega(\mathbf{k})]}{d\omega(\mathbf{k})}, \quad (7.79)$$

and

$$\omega(\mathbf{k}) = \left(1 - \frac{1}{2}n\right) t_{\mathbf{k}} \quad (7.80)$$

is the spectrum of electrons in the paramagnetic phase.

The relation

$$n = \frac{2}{N} \sum_{\mathbf{k}} f[\omega(\mathbf{k})], \quad (7.81)$$

which follows from (7.75), has been used to derive equation (7.77) for the susceptibility. Equation (7.81) is the equation for finding the chemical potential in the paramagnetic phase.

At  $T = 0$  we get

$$\chi_0 = \frac{1}{1 - \frac{1}{2}n} \rho(\tilde{\varepsilon}_F), \quad (7.82)$$

$$\Lambda = \frac{1}{1 - \frac{1}{2}n} \tilde{\varepsilon}_F \rho(\tilde{\varepsilon}_F), \quad (7.83)$$

where

$$\tilde{\varepsilon}_F = \frac{\varepsilon_F}{1 - \frac{1}{2}n}. \quad (7.84)$$

Hence, at  $T = 0$  we have

$$\chi = \frac{(1 - \frac{1}{2}n) \rho(\tilde{\varepsilon}_F)}{1 - n + (1 - \frac{1}{2}n) \tilde{\varepsilon}_F \rho(\tilde{\varepsilon}_F)}. \quad (7.85)$$

From this expression it follows that the requirement of nucleation of ferromagnetism at  $T = 0$  at the condition of  $U \rightarrow \infty$  is determined by an inequality

$$1 - n + \left(1 - \frac{1}{2}n\right) \tilde{\varepsilon}_F \rho(\tilde{\varepsilon}_F) < 0. \quad (7.86)$$

For a band with constant density of states, the Fermi energy, found from (7.81), is given by expression

$$\varepsilon_F = \frac{1}{2}W \left( \frac{3}{2}n - 1 \right). \quad (7.87)$$

Then, after the sequential substitutions of (7.87) into (7.84) and (7.86) we obtain

$$1 - \frac{1}{2}n < 0. \quad (7.88)$$

We receive a condition which breaks down for  $n$  lying in the interval  $[0, 1]$ . In this case the expression for the susceptibility  $\chi$  takes the form:

$$\chi = \frac{2}{W}. \quad (7.89)$$

The similar result can be received also for the energy dependent density of states  $\rho(\varepsilon)$  in the simple cubic lattice. However, numerical calculations are necessary in this case.

Thus, we have obtained a somewhat unexpected result, implying that the Hubbard approximation does not lead to a ferromagnetism. The ferromagnetism at  $U \rightarrow \infty$ , at least, in systems with a constant density of states and in the simple cubic lattice, is not realized in the Hubbard approximation.

The reason of it lies in the fact that, in Hubbard approximation removal of the spin degeneracy at  $m \neq 0$  happens not due to spin-dependent shift of the conduction band centre (as in the Hartree-Fock approximation), but due to spin-dependent correlative narrowing of the conduction bandwidth. The location of the band centre in the Hubbard approximation does not depend on  $\sigma m$ , and the correlative narrowing alone does not suffice to the ferromagnetic state development.

Thus, from the physical point of view, the Hubbard approximation breaks down. It has also other shortcomings. Insufficiency of a physical picture in the Hubbard approximation is caused by its roughness. The corresponding decoupling is the elementary decoupling corresponding to the case of the strong Coulomb repulsion. For deriving a real physical picture more sophisticated decoupling is necessary.



## 7.5 Ferromagnetism in the $t - J$ Model. The Roth Approximation.

Let's introduce into the  $t - J$  model Hamiltonian a term responsible for interaction of the system with an external magnetic field  $H$ , and a term considering conservation of the particle number with a chemical potential  $\mu$ :

$$\mathcal{H} = \sum_{i\sigma} \varepsilon_{\sigma} X_i^{\sigma\sigma} - t \sum_{\langle ij \rangle \sigma} X_i^{\sigma 0} X_j^{0\sigma} + J \sum_{\langle ij \rangle} (X_i^{-+} X_j^{+-} - X_i^{++} X_j^{--}), \quad (7.90)$$

where

$$\varepsilon_{\sigma} = -\mu - \frac{1}{2}\sigma H. \quad (7.91)$$

Then, consider single-electron Green function

$$G_{ij\sigma}(t - t') = -i\theta(t - t') \langle \{ X_i^{0\sigma}(t), X_j^{\sigma 0}(t') \} \rangle = \ll X_i^{0\sigma}(t) | X_j^{\sigma 0}(t') \gg_{\eta=-1}^r, \quad (7.92)$$

the equation of motion for which is given by

$$i \frac{\partial}{\partial t} G_{ij\sigma}(t - t') = \langle F_i^{\sigma 0} \rangle \delta_{ij} \delta(t - t') + \ll [X_i^{0\sigma}, \mathcal{H}] (t) | X_j^{\sigma 0}(t') \gg, \quad (7.93)$$

where  $F_i^{\sigma 0} = X_i^{00} + X_i^{\sigma\sigma} = 1 - X_i^{\bar{\sigma}\bar{\sigma}}$  is an anticommutator of operators  $X_i^{0\sigma}$  and  $X_i^{\sigma 0}$ .

Let's consider an approximation, proposed originally by Laura Roth (Phys. Rev., 1969, **184**, p. 451) for solving the Hubbard model. In this approximation the commutator of the operator  $X_i^{0\sigma}$  with the Hamiltonian  $\mathcal{H}$  on the right-hand side of (7.92) is represented as

$$[X_i^{0\sigma}, \mathcal{H}] \cong \sum_{j'} (E_{ij'}^{\sigma} - \mu \delta_{ij'}) X_{j'}^{0\sigma}, \quad (7.94)$$

where  $E_{ij'}^{\sigma}$  is a  $c$ -number. Clearly, that at commutation of the operator  $X_i^{0\sigma}$  with the Hamiltonian  $\mathcal{H}$  we do not generally obtain an operator linear on  $X_i^{0\sigma}$ . Therefore, the Roth approximation for the  $E_{ij'}^{\sigma}$  calculation is inherently a decoupling of the equations chain for the function  $G_{ij\sigma}(t - t')$ .

Anticommuting the left-hand and right-hand parts of the equation (7.94) with the operator  $X_j^{\sigma 0}$

$$\{ [X_i^{0\sigma}, \mathcal{H}] | X_j^{\sigma 0} \} = (E_{ij}^{\sigma} - \mu \delta_{ij}) F_j^{\sigma 0}, \quad (7.95)$$

and averaging this equation by using a statistical operator with the full Hamiltonian  $\mathcal{H}$  we get

$$E_{ij}^{\sigma} - \mu \delta_{ij} = \frac{1}{1 - \langle n_{\bar{\sigma}} \rangle} \langle \{ [X_i^{0\sigma}, \mathcal{H}] | X_j^{\sigma 0} \} \rangle. \quad (7.96)$$

Having yielded necessary calculations in the right-hand side term of (7.96), and approximately supposing

$$\langle X_i^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \simeq \langle X_i^{\sigma\sigma} \rangle \langle X_j^{\sigma\sigma} \rangle = \langle n_{\sigma} \rangle^2, \quad (7.97)$$

in the limit  $U \rightarrow \infty$  ( $J = 0$ ) we obtain

$$E_{\sigma}(\mathbf{k}) = \theta_{\sigma} + (1 - \langle n_{\bar{\sigma}} \rangle) t_{\mathbf{k}}, \quad (7.98)$$

where

$$E_{ij}^{\sigma} = \frac{1}{N} \sum_{\mathbf{k}} E_{\sigma}(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}_{ij}}, \quad (7.99)$$

$$\theta_\sigma = -\frac{1}{2}\sigma H + \frac{t}{1 - \langle n_{\bar{\sigma}} \rangle} \sum_j D_{j\bar{\sigma}}, \quad (7.100)$$

$$D_{j\bar{\sigma}} = \langle X_j^{\sigma 0} X_i^{0\sigma} \rangle. \quad (7.101)$$

The second term in (7.98) represents the energy of the electron in the Hubbard approximation, and the first one does not depend on the momentum  $\mathbf{k}$  and gives the spin-dependent shift of the Hubbard band middle. As the correlator  $D_{j\sigma}$  is determined via the Green function

$$G_\sigma(\mathbf{k}, E) = \frac{1 - \langle n_{\bar{\sigma}} \rangle}{E + \mu - E_\sigma(\mathbf{k})}, \quad (7.102)$$

for  $\theta_\sigma$  it is possible to get

$$\theta_\sigma = -\frac{1}{2}\sigma H + \frac{t}{1 - \langle n_{\bar{\sigma}} \rangle} \vartheta_{\bar{\sigma}}, \quad (7.103)$$

where

$$\vartheta_{\bar{\sigma}} = -(1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} f [E_\sigma(\mathbf{k})]. \quad (7.104)$$

From expression (7.103) for  $\theta_\sigma$  it is seen that in this approximation the factor  $1/(1 - \langle n_{\bar{\sigma}} \rangle)$  depresses a stability of the paramagnetic state. In this case, the equations for magnetization and for chemical potential superficially coincide with the equations (7.74) and (7.75):

$$m = \sum_{\sigma} \sigma (1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} f [E_\sigma(\mathbf{k})], \quad (7.105)$$

$$n = \sum_{\sigma} (1 - \langle n_{\bar{\sigma}} \rangle) \frac{1}{N} \sum_{\mathbf{k}} f [E_\sigma(\mathbf{k})], \quad (7.106)$$

but, as  $E_\sigma(\mathbf{k})$  now contains  $\vartheta_{\bar{\sigma}}$ , it is necessary to complement equations (7.105) and (7.106) with equation (7.104). Thus, we have system of four self-consistent equations for definition of  $\vartheta_{\uparrow}$ ,  $\vartheta_{\downarrow}$ ,  $\mu$  and  $m$ . As a result, magnetization is determined as a function of temperature  $T$  and the electron concentration  $n$ .

The analysis shows, that, as well as in the Hubbard approximation, the value of  $\chi$  is positive at all  $n$  from the interval  $(0, 1)$  (at  $T \rightarrow 0$ ). However, unlike in the Hubbard approximation  $m = 0$ , in the considered approximation  $m = n$ , that seems to contradict the deduction about stability of the paramagnetic state with respect to the ferromagnetic ordering. This inconsistency is easily resolved if to recall that the general theory of phase transitions proposes two types instabilities of normal to condensed (in this case paramagnetic to ferromagnetic) phase. Phase transitions are called as first-order phase transitions if at some critical values of temperature  $T$  and concentration  $n$  (in a phase space  $T$  and  $n$  determine the phase transition curve) the first derivative of a thermodynamic potential on an external field (magnetization in our case) is not certain (for example, discontinuous). Here, the second derivative (susceptibility) is continuous functions of  $T$  and  $n$ . At the second-order phase transitions, first derivatives of a thermodynamic potential are continuous functions of  $T$  and  $n$ , and the second derivatives increase infinitely upon approaching the phase boundary. The results for  $\chi$  and  $m$  obtained above are consistent, if to suppose that the transition of the system from paramagnetic state to ferromagnetic one takes place as the first-order phase transition.

In the Roth approximation

$$\langle X_i^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \cong \langle X_i^{\sigma\sigma} \rangle \langle X_j^{\sigma\sigma} \rangle, \quad (7.107)$$

and the electronic spectrum  $E_\sigma(\mathbf{k})$  turns out to be complicated enough if  $J \neq 0$ . We present only final results concerning magnetic behaviour of the system in this approximation.

The concentration dependence of the inverse paramagnetic susceptibility at  $T = 0$  for a band with a constant density of states is shown in Fig. 7.1. It is given for various values of  $J/t$ . From Fig. 7.1 it is seen, that in the Roth approximation instability of a paramagnetic state with respect to ferromagnetism occurs in some concentration interval determined by values  $n$ , for which  $\chi^{-1} < 0$ . Temperature phase transition to the ferromagnetic state takes place here as a second-order phase transition. Area of concentrations for which  $\chi^{-1} < 0$  essentially depends on  $J$ . With increase of  $J$  this area narrows down to zero at  $J/t = 0.124$ .

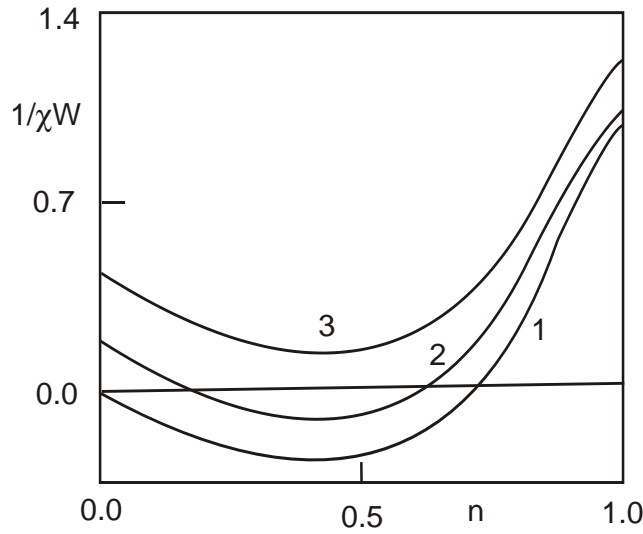


Figure 7.1: The concentration dependence of the inverse paramagnetic susceptibility at  $T = 0$ : 1 -  $J/t = 0$ , 2 -  $J/t = 0.05$ ,  $J/t = 0.16$ .

The phase diagram of the ferromagnetic state in a plane  $(J/t, n)$  at  $T = 0$  for a band with a constant density of states is given in Fig. 7.2. Curve 1 in this figure determines the phase area in which magnetization at  $T = 0$  is nonzero. At  $J = 0$ ,  $m = 0$  for all  $n$  in interval  $(0, 1)$ . With increase of  $J$  the ferromagnetic state deteriorates, completely vanishing at  $J/t = 0.124$ . Curve 2 in Fig. 7.2 separates areas I and II in which transition on temperature from the paramagnetic state takes place as a phase transition of the first and the second kind, respectively. In the Roth approximation an essential decrease of area I takes place at the expense of area II.

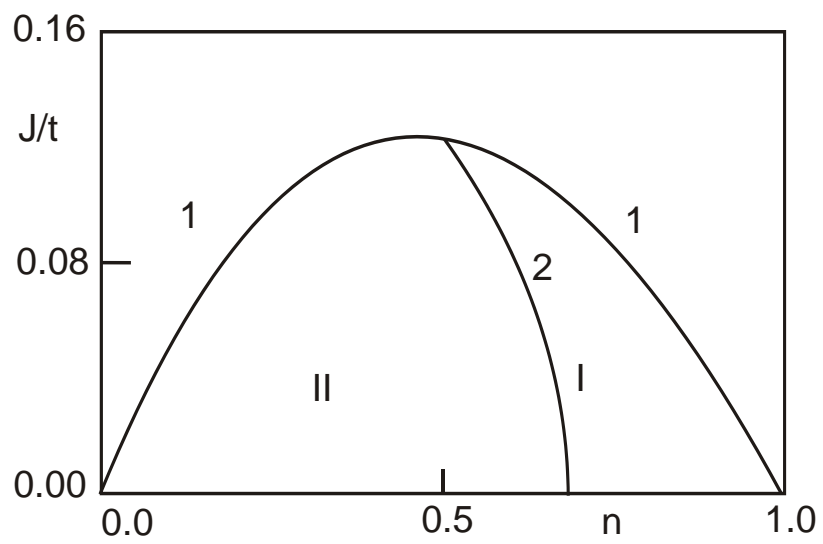


Figure 7.2: The phase diagram of the ferromagnetic state at  $T = 0$ .

# Chapter 8

## Application of Double-Time Green Functions to the Superconductivity Problem

### 8.1 The Hamiltonian and Equations of Motion for Green Functions

The starting point of the problem will be the BCS (Bardeen-Cooper-Schrieffer) Hamiltonian:

$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} - \frac{1}{2V} \sum_{\mathbf{k}, \mathbf{k}'} U(\mathbf{k}, \mathbf{k}') a_{\mathbf{k}\sigma}^\dagger a_{-\mathbf{k}-\sigma}^\dagger a_{-\mathbf{k}'-\sigma'} a_{\mathbf{k}'\sigma'}, \quad (8.1)$$

$$U(\mathbf{k}, -\mathbf{k}') = -U(\mathbf{k}, \mathbf{k}') = U(-\mathbf{k}, \mathbf{k}'). \quad (8.2)$$

In the above equations  $V$  is the volume of the system,  $\xi_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}\sigma} - \mu \equiv \xi_{\mathbf{k}}$  (when magnetic field is absent). Let us join the wave vector subscript and the spin-projection subscript into one subscript, say  $f = (\mathbf{k}, \sigma)$ . Then, the equation of motion for the annihilation operator reads

$$i \frac{\partial a_f}{\partial t} = [a_f, \mathcal{H}]. \quad (8.3)$$

We have to calculate contributions to the commutator, the first one comes from the kinetic energy term of the Hamiltonian:

$$\begin{aligned} \left[ a_f, \sum_{f'} \xi_{f'} a_{f'}^\dagger a_{f'} \right] &= \sum_{f'} \xi_{f'} \left\{ a_f a_{f'}^\dagger a_{f'} - a_{f'}^\dagger a_{f'} a_f \right\} \\ &= \sum_{f'} \xi_{f'} \left\{ \left( \delta_{ff'} - a_{f'}^\dagger a_f \right) a_{f'} - a_{f'}^\dagger a_{f'} a_f \right\} \\ &= \sum_{f'} \xi_{f'} \left\{ \delta_{ff'} a_{f'} + a_{f'}^\dagger a_f a_{f'} - a_{f'}^\dagger a_{f'} a_f \right\} = \xi_f a_f. \end{aligned} \quad (8.4)$$

Here, we have used the commutation relations (6.4) for fermions to permute annihilation and creation operators. Next contribution comes from commutation with the electron-electron attraction (BCS) term of the Hamiltonian:

$$\left[ a_f, \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} \right] = \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left[ a_f, a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} \right]$$

$$\begin{aligned}
&\equiv \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left\{ a_f a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} - a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} a_f \right\} \\
&= \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left\{ \left( \delta_{ff'} - a_{f'}^\dagger a_f \right) a_{-f'}^\dagger a_{-f''} a_{f''} - a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} a_f \right\} \\
&= \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left\{ \delta_{ff'} a_{-f'}^\dagger a_{-f''} a_{f''} - a_{f'}^\dagger \left( \delta_{f-f'} - a_{-f'}^\dagger a_f \right) a_{-f''} a_{f''} - a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} a_f \right\} \\
&= \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left\{ \delta_{ff'} a_{-f'}^\dagger a_{-f''} a_{f''} - \delta_{f-f'} a_{f'}^\dagger a_{-f''} a_{f''} \right. \\
&\quad \left. + a_{f'}^\dagger a_{-f'}^\dagger a_f a_{-f''} a_{f''} - a_{f'}^\dagger a_{-f'}^\dagger a_{-f''} a_{f''} a_f \right\} \\
&= \frac{1}{2V} \sum_{f', f''} U(\mathbf{k}', \mathbf{k}'') \left\{ \delta_{ff'} a_{-f'}^\dagger a_{-f''} a_{f''} - \delta_{f-f'} a_{f'}^\dagger a_{-f''} a_{f''} \right\} \\
&= \frac{1}{2V} \sum_{f''} U(\mathbf{k}, \mathbf{k}'') a_{-f}^\dagger a_{-f''} a_{f''} - \frac{1}{2V} \sum_{f''} U(-\mathbf{k}, \mathbf{k}'') a_{-f}^\dagger a_{-f''} a_{f''} \\
&= \frac{1}{V} \sum_{f'} U(\mathbf{k}, \mathbf{k}') a_{-f}^\dagger a_{-f'} a_{f'}. \tag{8.5}
\end{aligned}$$

In the 6-th line of Eq. (8.5) we have used the anticommutation relations (6.4) (second line) to cancel the terms in this line. In the 8-th line of (8.5) the symmetry properties of attraction potential (8.2) have been used to join the two terms into the final expression. With the above contributions equation of motion (8.3) reads

$$i \frac{\partial a_f}{\partial t} = \xi_f a_f - \frac{1}{V} \sum_{f'} U(\mathbf{k}, \mathbf{k}') a_{-f}^\dagger a_{-f'} a_{f'}. \tag{8.6}$$

Proceeding analogously with the creation operator we get

$$i \frac{\partial a_f^\dagger}{\partial t} = -\xi_f a_f^\dagger + \frac{1}{V} \sum_{f'} U(\mathbf{k}, \mathbf{k}') a_{f'}^\dagger a_{-f'}^\dagger a_{-f}. \tag{8.7}$$

Let us introduce the *anticommutator*-type Green function

$$G_f(t-t') = \left\langle \left\langle a_f(t) | a_f^\dagger(t') \right\rangle \right\rangle_{\eta=-1}. \tag{8.8}$$

Making use equation of motion (8.6) for the annihilation operator we write down equation of motion (8.8) for the Green function,

$$i \frac{\partial G_f(t-t')}{\partial t} = \delta(t-t') + \xi_f G_f(t-t') - \frac{1}{V} \sum_{f'} U(\mathbf{k}, \mathbf{k}') \left\langle \left\langle \left( a_{-f}^\dagger a_{-f'} a_{f'} \right) (t) | a_f^\dagger(t') \right\rangle \right\rangle. \tag{8.9}$$

In equation (8.9) a new Green function appeared

$$\Gamma_{ff'}(t-t') = \left\langle \left\langle \left( a_{-f}^\dagger a_{-f'} a_{f'} \right) (t) | a_f^\dagger(t') \right\rangle \right\rangle. \tag{8.10}$$

The equation of motion can be written down for this Green function as follows:

$$\begin{aligned}
i\frac{\partial\Gamma_{ff'}}{\partial t} &= -\delta(t-t')n_{-f}(\delta_{f,-f'}-\delta_{ff'})+(2\xi_{f'}-\xi_f)\Gamma_{ff'} \\
&\quad -\frac{1}{V}\sum_g U(f,g)\left\langle\left\langle\left(a_g^\dagger a_{-g}^\dagger a_{-f'} a_{f'} a_f\right)(t)\left|a_f^\dagger(t')\right.\right\rangle\right\rangle \\
&\quad -\frac{1}{V}\sum_g U(f',g)\left\langle\left\langle\left((1-n_{-f'}-n_{f'})a_{-f}^\dagger a_{-g} a_g\right)(t)\left|a_f^\dagger(t')\right.\right\rangle\right\rangle \\
&\quad -\frac{1}{V}\sum_g U(f',g)\Gamma_{fg}(\delta_{ff'}+\delta_{f,-f'}). \tag{8.11}
\end{aligned}$$

## 8.2 Basic Approximations and Solution of the Equations of Motion, the Excitations Spectrum

Looking at equation of motion (8.9) we note that the Green function  $\Gamma_{ff'}$  enters the equation with the factor  $V^{-1}$ , that is why at  $V \rightarrow \infty$  this term vanishes, if only in  $\sum_g$  an infinite number of terms will not balance the infinite increase of a volume, providing convergence of the term to a finite value. Thus, we may drop the terms containing  $\delta_{ff'}$  and  $\delta_{f,-f'}$  in the equations of motion. Next, taking into account that the average values of the particle numbers are finite at  $V \rightarrow \infty$ , we may introduce an approximation, which decouples the infinite chain of equations of motion for the Green functions

$$\begin{aligned}
&\left\langle\left\langle\left((1-n_{-f'}-n_{f'})a_{-f}^\dagger a_{-g} a_g\right)(t)\left|a_f^\dagger(t')\right.\right\rangle\right\rangle \\
&\simeq (1-\bar{n}_{-f'}-\bar{n}_{f'})\left\langle\left\langle\left(a_{-f}^\dagger a_{-g} a_g\right)(t)\left|a_f^\dagger(t')\right.\right\rangle\right\rangle, \tag{8.12}
\end{aligned}$$

where  $\bar{n}_{f'}$  is the average number of particles in the state labeled by  $f'$ . Then, equations of motion (8.9) and (8.11) read:

$$i\frac{\partial G_f}{\partial t} = \delta(t-t') + \xi_f G_f - \frac{1}{V}\sum_{f'} U(f,f')\Gamma_{ff'}, \tag{8.13}$$

$$\begin{aligned}
i\frac{\partial\Gamma_{ff'}}{\partial t} &= (2\xi_{f'}-\xi_f)\Gamma_{ff'} - \frac{1}{V}\sum_g U(f,g)\left\langle\left\langle a_g^\dagger a_{-g}^\dagger a_{-f'} a_{f'} \right\rangle\right\rangle G_f \\
&\quad -\frac{1}{V}\sum_g U(f',g)(1-\bar{n}_{-f'}-\bar{n}_{f'})\Gamma_{fg}. \tag{8.14}
\end{aligned}$$

In the second term of the right-hand side of Eq. (8.14) we allowed existence of the average value  $\left\langle\left\langle a_g^\dagger a_{-g}^\dagger a_{-f'} a_{f'} \right\rangle\right\rangle$ , which does not vanish as a volume goes to infinity. Making use of the Fourier transformation by the rule

$$G_f(\tau) = \int_{-\infty}^{\infty} \frac{dE}{2\pi} G_f(E) e^{-iE\tau}, \tag{8.15}$$

we obtain from Eqs. (8.13) and (8.14)

$$EG_f = 1 + \xi_f G_f - \frac{1}{V} \sum_{f'} U(f, f') \Gamma_{ff'}, \quad (8.16)$$

$$\begin{aligned} E\Gamma_{ff'} &= (2\xi_{f'} - \xi_f) \Gamma_{ff'} - \frac{1}{V} \sum_g U(f, g) \langle a_g^\dagger a_{-g}^\dagger a_{-f'} a_{f'} \rangle G_f \\ &\quad - \frac{1}{V} \sum_g U(f', g) (1 - \bar{n}_{-f'} - \bar{n}_{f'}) \Gamma_{fg}, \end{aligned} \quad (8.17)$$

where we have dropped the frequency arguments in the functions for brevity. The above system of equations is integral, however, we can solve it making use the following approximations:

$$\langle a_g^\dagger a_{-g}^\dagger a_{-f'} a_{f'} \rangle \simeq A_g A_{f'} \quad (8.18)$$

and

$$\Gamma_{ff'} \simeq \Gamma_f A_{f'}, \quad (A_f^* = A_f). \quad (8.19)$$

Substitution into Eqs. (8.16) and (8.17) gives:

$$EG_f = 1 + \xi_f G_f - \frac{1}{V} \Gamma_f \sum_{f'} U(f, f') A_{f'}, \quad (8.20)$$

$$\begin{aligned} E\Gamma_f A_{f'} &= (2\xi_{f'} - \xi_f) \Gamma_f A_{f'} - \frac{1}{V} A_{f'} G_f \sum_g U(f, g) A_g \\ &\quad - \frac{1}{V} (1 - \bar{n}_{-f'} - \bar{n}_{f'}) \Gamma_f \sum_g U(f', g) A_g. \end{aligned} \quad (8.21)$$

Let us denote

$$-\frac{1}{V} \sum_{f'} U(f, f') A_{f'} = L_f, \quad (8.22)$$

then, we obtain:

$$(E - \xi_f) G_f - L_f \Gamma_f = 1, \quad (8.23)$$

$$(E + \xi_f) \Gamma_f - L_f G_f = \left( 2\xi_{f'} - \frac{1 - 2\bar{n}_{f'}}{A_{f'}} L_{f'} \right) \Gamma_f. \quad (8.24)$$

We suppose that

$$2\xi_{f'} - \frac{1 - 2\bar{n}_{f'}}{A_{f'}} L_{f'} = 0, \quad (8.25)$$

which is nothing, but gauge (like the Lorentz condition in classic electrodynamics). In this gauge we get the final form of the equations of motion:

$$\begin{aligned} (E - \xi_f) G_f - L_f \Gamma_f &= 1, \\ (E + \xi_f) \Gamma_f - L_f G_f &= 0. \end{aligned} \quad (8.26)$$



Solutions to equations (8.26) are

$$\begin{aligned} G_f(E) &= \frac{E + \xi_f}{E^2 - \xi_f^2 - L_f^2}, \\ \Gamma_f(E) &= \frac{L_f}{E^2 - \xi_f^2 - L_f^2}. \end{aligned} \quad (8.27)$$

Poles of the above Green functions define the excitation spectrum,

$$E_f^\pm \equiv \pm E_f = \pm \sqrt{\xi_f^2 + L_f^2}. \quad (8.28)$$

### 8.3 Spectral Intensities of the Correlation Functions and Gap in the Excitations Spectrum

It is convenient to expand  $G_f(E)$  and  $\Gamma_{ff'}(E)$  on simple fractions to write down

$$G_f(E) = \frac{1}{2} \left\{ \left( 1 + \frac{\xi_f}{E_f} \right) \frac{1}{E - E_f} + \left( 1 - \frac{\xi_f}{E_f} \right) \frac{1}{E + E_f} \right\}, \quad (8.29)$$

$$\Gamma_{ff'}(E) = \frac{L_f A_{f'}}{2E_f} \left\{ \frac{1}{E - E_f} - \frac{1}{E + E_f} \right\}. \quad (8.30)$$

Now it is easy to find spectral intensities of the above Green functions. First, we calculate

$$\left\langle a_f^\dagger(t') a_f(t) \right\rangle = \int_{-\infty}^{\infty} \frac{dE}{2\pi} I_f(E) e^{-iE(t-t')}, \quad (8.31)$$

where

$$I_f(E) = i \frac{G_f(E + i\delta) - G_f(E - i\delta)}{e^{E/k_B T} + 1}. \quad (8.32)$$

From Eqs. (8.29) and (8.32) we have

$$I_f(E) = \pi \left( 1 + \frac{\xi_f}{E_f} \right) \frac{\delta(E - E_f)}{e^{E_f/k_B T} + 1} + \pi \left( 1 - \frac{\xi_f}{E_f} \right) \frac{\delta(E + E_f)}{e^{-E_f/k_B T} + 1}. \quad (8.33)$$

The average number of particles  $\bar{n}_f$  is

$$\bar{n}_f = \left\langle a_f^\dagger a_f \right\rangle = \int_{-\infty}^{\infty} \frac{dE}{2\pi} I_f(E) = \frac{1}{2} \left\{ 1 - \frac{\xi_f}{E_f} \tanh \frac{E_f}{2k_B T} \right\}. \quad (8.34)$$

Second, for the Green function  $\Gamma_{ff'}(E)$  we introduce the spectral intensity of correlation function  $\tilde{I}_f(E)$  by

$$\begin{aligned} \left\langle a_f^\dagger(t') a_{-f}^\dagger(t') a_{-f'}(t) a_{f'}(t) \right\rangle &= A_{f'} A_f (t - t') \\ &= A_{f'} \int_{-\infty}^{\infty} \frac{dE}{2\pi} \tilde{I}_f(E) e^{-iE(t-t')}. \end{aligned} \quad (8.35)$$

From (8.30) one obtains for  $\tilde{I}_f(E)$ :

$$\tilde{I}_f(E) = \frac{\pi L_f}{E_f} \left\{ \frac{\delta(E - E_f)}{e^{E_f/k_B T} + 1} - \frac{\delta(E + E_f)}{e^{-E_f/k_B T} + 1} \right\}. \quad (8.36)$$

Assuming  $t = t'$  we find  $A_f$  :

$$A_f = \int_{-\infty}^{\infty} \frac{dE}{2\pi} \tilde{I}_f(E) = -\frac{L_f}{2E_f} \tanh \frac{E_f}{2k_B T}, \quad (8.37)$$

from which one can check the validity of gauge condition (8.25).

The quantity  $L_f$  plays the role of a gap in the excitation spectrum of a superconductor. Using expression (8.37) we obtain for  $L_f$

$$L_f = -\frac{1}{V} \sum_{f'} U(f, f') A_{f'} = \frac{1}{V} \sum_{f'} U(f, f') \frac{L_{f'}}{2E_{f'}} \tanh \frac{E_{f'}}{2k_B T}, \quad (8.38)$$

which is a well known equation for the gap in the BCS theory.

# Chapter 9

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