LECTURE NOTES ON STATISTICAL MECHANICS

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January 10, 2023

Contents

Preface

The present notes have been written on the basis of lectures and seminars given as an undergraduate course on Statistical Mechanics at the Department of Physics of National Research University Higher School of Economics in spring 2020 and 2021. The material of these notes is written for a reader familiar with the traditional courses of classical thermodynamics and non-relativistic quantum mechanics.

Chapter 1

Basics of Statistical Mechanics

Introduction

In this chapter we give a brief introduction for foundations of statistical mechanics and, then, apply the Gibbs method to the thermodynamics of ideal Fermi and Bose gases. Describing the ideal Fermi and Bose gases, we avoid the second quantization. In view of time limitations we do not discuss the thermodynamics of the ideal Boltzmann gas in detail. For the additional aspects of this chapter, we recommend the textbook [1].

1.1   The Gibbs distribution in the quantum statistical mechanics

1.1.1   Density matrix

Let us start from the stationary Schrödinger equation for eigen energies E_a and eigenstates $|a\rangle$ of the quantum mechanical Hamiltonian H:

$$H|a\rangle = E_a|a\rangle. \tag{1.1}$$

We assume that $\langle a|a'\rangle = \delta_{a,a'}$. An arbitrary stationary normalizable quantum state can be written as a linear combination of the eigenstates:

$$|\psi\rangle = \sum_a c_a|a\rangle, \qquad \sum_a |c_a|^2 = 1. \tag{1.2}$$

The quantum mechanical average of operator A in the state $|\psi\rangle$ can be written as

$$\langle\psi|A|\psi\rangle = \operatorname{Tr}\rho A \tag{1.3}$$

where we have introduced the matrix

$$\rho = |\psi\rangle\langle\psi| = \sum_{a,b} c_a c_b^*|a\rangle\langle b|. \tag{1.4}$$

The matrix ρ is the *density matrix* for a *pure state*, i.e., the state described by the wave function. The density matrix of the pure state satisfies the following relations: $\operatorname{Tr}\rho = 1$ and $\rho^2 = \rho$.

Now we extend the notion of the density matrix to a mixed state. Let us define the latter as follows: the system can be found with a probability p_j in a state $|\psi_j\rangle$ where $j = 1,\ldots,K$ and $\sum_{j=1}^K p_j = 1$. Then the quantum mechanical average of an operator A over the states $|\psi_j\rangle$ can naturally be defined as follows

$$\overline{A} = \sum_{j=1}^K p_j\langle\psi_j|A|\psi_j\rangle = \operatorname{Tr}\rho A, \qquad \rho = \sum_{j=1}^K p_j|\psi_j\rangle\langle\psi_j|. \tag{1.5}$$

Although the density matrix constructed in this way satisfies the normalization condition $\operatorname{Tr}\rho = 1$, one has now that $\rho^2 \neq \rho$ and $\operatorname{Tr}\rho^2 < 1$.

To describe the dynamics of the density matrix, let us start from a pure state. The state $|\psi\rangle$ obeys the time-dependent Schrödinger equation

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle. \tag{1.6}$$

This implies that $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ and, consequently, the time-dependent density matrix becomes $\rho(t) = e^{-iHt}\rho(0)e^{iHt}$. Therefore, it satisfies the following dynamical equation termed as the *Liouville* equation,

$$\partial_t \rho = i[\rho, H]. \tag{1.7}$$

The generic density matrix of the closed quantum system described by the Hamiltonian H should satisfy the Liouville equation. The stationary density matrix should commute with the Hamiltonian, $[\rho, H] = 0$, i.e., ρ should be a function of Hamiltonian H.

1.1.2 The Gibbs distribution

For many isolated quantum systems, the stationary density matrix is described by the so-called *Gibbs distribution* which can be written as

$$\rho = e^{-\beta H}/Z, \qquad Z = \operatorname{Tr} e^{-\beta H}. \tag{1.8}$$

Here $\beta \geqslant 0$ is a formal parameter with the dimensionality of inverse energy and called the *inverse temperature*. The normalization factor Z is termed as the *partition function*. Below with the exception of the last chapters, we will use the Gibbs density matrix alone. The quantum mechanical and thermal averages of some operator A are now defined according to $\langle A \rangle = \operatorname{Tr} \rho A$. In particular, the average energy E is given according to $E = \operatorname{Tr} \rho H$. We mention that sometimes the density matrix in the Gibbs form, (1.8), is termed as the *canonical distribution*. The normalization factor Z is referred to as the *canonical partition function*.

The quantum systems with the Gibbs density matrix are said to be in the *thermal equilibrium*. However, there is a number of isolated quantum systems which stationary density matrix does not have the Gibbs distribution. This phenomenon is termed as the absence of thermalization. The scenario of how it can happen will be described in Chapter 5.

1.1.3 Entropy

In order to construct the complete thermodynamic description of the quantum system, we need to introduce the notion of the *entropy* based on the density matrix. The standard way, suggested by von Neumann, is as follows

$$S = -\operatorname{Tr} \rho \ln \rho. \tag{1.9}$$

We remind that the entropy is an extensive quantity similar to the energy. As for the Gibbs distribution, there is no rigorous derivation of the von-Neumann

entropy. Below we provide two reasonings. The first motivation is purely classical. Let us consider the system consisting of K subsystems each characterising by a probability p_j. Then we expect that due to additivity, the entropy of subsystem consisting of subsystems 1 and 2 will equal a sum of entropies $s_1 + s_2$ whereas the associated probability will be a product $p_{12} = p_1 p_2$. If we choose $s_j = \ln 1/p_j$, then $s_{12} = s_1 + s_2 = \ln 1/p_{12}$. The average entropy of the full system is given as $S = \sum_{j=1}^{K} p_j s_j = -\sum_{j=1}^{K} p_j \ln p_j$. Since the eigenvalues λ_j of the density matrix has the properties analogous to classical probabilities, we can define the entropy of the quantum system as $S = -\sum_j \lambda_j \ln \lambda_j$ which is equivalent to Eq. (1.9).

We note that the von Neumann definition of the entropy encounters a problem with the second law of the thermodynamics which allows the entropy to increase. However, for some density matrix which obeys the Liouville equation (1.7), the entropy is conserved, $S(t) = S(0)$. There are several ways of solving this problem which are discussed in the current scientific literature (see for example, Ref. [2]).

1.1.4 Maximal entropy principle

The second motivation for the von Neumann definition of the entropy is associated with the maximal entropy principle. Alternatively, it can be considered as a motivation for the Gibbs distribution. Let us maximize the entropy (1.9) over all possible density matrices but under an additional condition $\mathrm{Tr}\, \rho H = E = \mathrm{const}$. In order to solve this maximization problem, let us introduce the Lagrange multiplier β and consider the functional $-\mathrm{Tr}\, \rho \ln \rho + \beta(E - \mathrm{Tr}\, \rho H)$. Varying it with respect to $\delta\rho$ (under condition $\mathrm{Tr}\, \delta\rho = 0$ due to the normalization constraint $\mathrm{Tr}\, \rho = 1$), we obtain

$$-\mathrm{Tr}\, \delta\rho \big(\ln \rho + \beta H\big) = 0 \qquad \Rightarrow \qquad \rho \propto e^{-\beta H}. \tag{1.10}$$

Therefore, the maximal entropy principle for the von Neumann entropy results in the Gibbs distribution.

1.1.5 Relation with the thermodynamics

Substituting the Gibbs distribution (1.8) into the definition of the von Neumann entropy (1.9), we find

$$S = \beta E + \ln Z. \tag{1.11}$$

Alternatively, we can derive exactly the same expression for the entropy from the partition function as ($T = 1/\beta$)

$$S = \frac{\partial(T \ln Z)}{\partial T}. \tag{1.12}$$

Let us define the *free energy* as $F = -T \ln Z$. Then Eq. (1.11) can be rewritten in the form of the standard thermodynamic relation between energy, free energy, temperature, and entropy:

$$F = E - TS. \tag{1.13}$$

Simultaneously, Eq. (1.12) acquires the form of the standard thermodynamic relation between the entropy and the free energy:

$$S = -\left(\frac{\partial F}{\partial T}\right)_V. \tag{1.14}$$

Here V denotes the volume and the subscript V indicates that the derivative is taken under assumption of the constant volume.

Truly speaking, above we did not discuss the volume occupied by the quantum system. For the quantum system occupied a finite volume, the energy spectrum will depend on the volume. The simplest example to represent this is a quantum particle in the cubic box of size L with the infinite potential barrier. A quantum mechanical force acting on the box boundary in eigenstate $|a\rangle$ is given as $-\partial E_a/\partial L$. Therefore, the average pressure can be defined as

$$P = -\frac{1}{Z}\sum_a \frac{\partial E_a}{\partial V}e^{-\beta E_a} = -\frac{1}{Z}\operatorname{Tr}\frac{\partial H}{\partial V}e^{-\beta H} = -\left(\frac{\partial F}{\partial V}\right)_T. \tag{1.15}$$

The above results have the following important implications:

- the von Neumann entropy is equivalent to the thermodynamic entropy;

- the canonical partition function Z determines the free energy F;

- the auxiliary parameter β^{-1} is the thermodynamic temperature T;

- F is the function of T and V and determines the entropy and pressure in the conventional thermodynamic way.

1.1.6 Systems with an arbitrary number of particles

The discussion above assumes the constant number of particles in the quantum system. Very often the quantum system interacts weakly with another system which implies an exchange of particles. At the same time, in all other respects the quantum system can be considered as isolated and in the thermal equilibrium. To find the proper density matrix for such situation, we can use the maximal entropy principle but now with two conditions: $\operatorname{Tr}\rho H = E = $ const and $\operatorname{Tr}\rho n = N = $ const, where n denotes the operator of the number of particles and N is the average number of particles. Then we introduce two Lagrange multipliers β

and μ, and consider the functional $-\operatorname{Tr}\rho\ln\rho+\beta(E-\operatorname{Tr}\rho H)+\beta\mu(\operatorname{Tr}\rho n-N)$. Varying it with respect to $\delta\rho$ (under condition $\operatorname{Tr}\delta\rho=0$ due to the normalization constraint $\operatorname{Tr}\rho=1$), we obtain

$$-\operatorname{Tr}\delta\rho\big(\ln\rho+\beta H-\beta\mu n\big)=0 \qquad \Rightarrow \qquad \rho\propto e^{-\beta H+\beta\mu n}. \qquad (1.16)$$

The density matrix

$$\rho = e^{-\beta H+\beta\mu n}/\mathcal{Z}, \qquad \mathcal{Z}=\operatorname{Tr}e^{-\beta H+\beta\mu n} \qquad (1.17)$$

is termed as the *grand canonical distribution*. We note that now the symbol Tr includes the summation over many-body states with all possible particle numbers. The grand partition function $\mathcal{Z}$ determines the *thermodynamic potential*:

$$\Omega = -T\ln\mathcal{Z}. \qquad (1.18)$$

The thermodynamic potential Ω is the function of T, V, and the *chemical potential* μ. The average number of particles can be found as

$$N = \operatorname{Tr}\rho\,n = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V}. \qquad (1.19)$$

Using Eq. (1.9), we find

$$S = \beta E - \beta\mu N - \beta\Omega = -\left(\frac{\partial\Omega}{\partial T}\right)_{V,\mu}. \qquad (1.20)$$

In addition, since the quantum mechanical expression for the average force as a derivative of the energy of the state is not distorted by the possibility of varying the number of particles, the pressure can be found as

$$P = -\left(\frac{\partial\Omega}{\partial V}\right)_{T,\mu}. \qquad (1.21)$$

Equation (1.20) relates the thermodynamic potential and the free energy (its definition $F = E - TS$ remains the same) as $F = \Omega + \mu N$. Taking into account Eq. (1.19), one can say that potentials Ω and F are related by the Legendre transform such that F is the function of T, V, and N. Then the chemical potential is determined as

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V}. \qquad (1.22)$$

Let us use the Legendre transform and introduce one more potential $\Phi = F + PV$. Then Φ is a function of T, P and N. The potential Φ should be an extensive

quantity but since T and P are not extensive quantities, we have $\Phi = \mu(T, P)N$. In other words, the chemical potential as a function of T and P is the potential Φ per one particle. Therefore, we can write $\mu N = F + PV$. Comparing this with the relation between F and Ω, we obtain a surprising relation between the thermodynamic potential, the pressure, and the volume:

$$\Omega = -PV. \tag{1.23}$$

This equation together with Eq. (1.19) determines the equation of state for the quantum system in the equilibrium, i.e., the relation between the pressure, the volume, the number of particles and the temperature. The typical problem of the statistical mechanics is to compute the thermodynamic potential Ω.

In addition to thermodynamic potentials E, Ω, F, and Φ, one can introduce one more potential called the enthalpy $W(S, P, N) = E + PV$ as a function of entropy S, pressure P and the particle number N.

> *Problem for the seminar 1:* Compute the free energy, the energy, and the entropy for the system of N independent spins $s = 1/2$ in the magnetic field.

> *Problem for the seminar 2:* Find the chemical potential and the pressure for the system of N independent spins $s = 1/2$ in the magnetic field.

> *Problem for the seminar 3:* Using the Jacobian method, prove that $C_P > C_V$ provided $(\partial P/\partial V)_T < 0$. Here C_P and C_V are the specific heats at the fixed pressure and volume, respectively.

> *Exercise 1:* Prove that the eigenvalues λ_m of the density matrix satisfy the relations: $0 \leqslant \lambda_m \leqslant 1$ and $\sum_m \lambda_m = 1$.

> *Exercise 2:* Demonstrate that the maximal value of the von Neumann entropy (1.9) is given by $\dim \rho$. Find the form of the density matrix which maximizes the entropy.

1.2 The thermodynamic fluctuations

1.2.1 Introduction

In the previous lecture we demonstrated that the approach based on the Gibbs form of the density matrix and the von Neumann definition of the entropy produces the description of the quantum system in terms of the average physical quantities equivalent to the traditional thermodynamics. In this lecture we will demonstrate how the thermodynamic fluctuations can be incorporated into the approach based on the Gibbs density matrix.

1.2.2 The Gibbs approach to thermodynamic fluctuations

Since the eigenvalues λ_j of the density matrix are within the range $0 \leqslant \lambda_j \leqslant 1$, one can interpret the Gibbs distribution (1.8) as a probability distribution for the Hamiltonian H. Then one can calculate the variance of energy as

$$\langle (\Delta E)^2 \rangle = \operatorname{Tr} \rho H^2 - (\operatorname{Tr} \rho H)^2 = \frac{\partial^2 \ln Z}{\partial \beta^2} = -\frac{\partial E}{\partial \beta}. \qquad (1.24)$$

We note that in this approach to the thermodynamic fluctuations, the temperature (or β) is the fixed parameter (Lagrange multiplier) forbidden to fluctuate. As in the previous lecture, the derivatives with respect to β (or T) are taken under natural assumption of constant volume V. Then, we find the following relation between the variance of the energy and the specific heat at constant volume:

$$\langle (\Delta E)^2 \rangle_V = T^2 C_V, \qquad C_V = T \left(\frac{\partial S}{\partial T} \right)_V. \qquad (1.25)$$

The result (1.25) demonstrates the important property of the thermodynamic fluctuations. Since the energy and entropy are extensive quantities, i.e., proportional to the number of particles N, the relative fluctuations of the energy are $\sqrt{\langle (\Delta E)^2 \rangle_V}/E \propto 1/\sqrt{N}$. Therefore, the thermodynamic fluctuations disappear in the thermodynamic limit $N \to \infty$.

Similar to the energy variance we can determine the variance for pressure fluctuations:

$$\langle (\Delta P)^2 \rangle_V = \frac{1}{Z} \sum_a e^{-\beta E_a} \left(\frac{\partial E_a}{\partial V} \right)^2 - \left(\frac{1}{Z} \sum_a e^{-\beta E_a} \frac{\partial E_a}{\partial V} \right)^2$$
$$= T \left(\frac{\partial P}{\partial V} \right)_T + T \operatorname{Tr} \left(\frac{\partial^2 H}{\partial V^2} \rho \right). \qquad (1.26)$$

In general, the last term cannot be expressed in terms of the average thermodynamic quantities and its derivatives. This is the well-known problem of applying the Gibbs approach for calculating the pressure fluctuations [3].

1.2.3 Thermodynamic fluctuations of quantum system in an external field

Let us consider quantum system in the presence of external field φ which couples linearly to the operator q such that the full Hamiltonian becomes $H = H_0 - q\varphi$. Then the average value of the operator q can be found from the Gibbs distribution

$$Q = \operatorname{Tr} \rho \, q = -\left(\frac{\partial F}{\partial \varphi}\right)_{T,V} \tag{1.27}$$

where F is the free energy depending on T, V, and φ. For example, in the problem of spins in the magnetic field, it is the magnetic field that plays a role of the external field. Now we can compute the variance of Q as

$$\langle (\Delta Q)^2 \rangle = \operatorname{Tr} \rho \, q^2 - (\operatorname{Tr} \rho \, q)^2 = T\chi_Q(\varphi), \qquad \chi_Q(\varphi) = \left(\frac{\partial Q}{\partial \varphi}\right)_{T,V}. \tag{1.28}$$

The quantity χ_Q is called the static susceptibility for the physical observable Q. We note that the validity of Eq. (1.28) for an arbitrary value of φ relies on the linear dependence of the Hamiltonian H on φ. We emphasize that Eq. (1.28) has the important implication for the variance of Q in the absence of the external field. The variance of Q at $\varphi = 0$ is determined by the static susceptibility $\chi_Q(0)$. The computation of $\chi_Q(0)$ requires only the knowledge of linear coupling between the system and the external field. This situation is referred to as the *linear response*.

Now let us develop scheme which will allow us to calculate the variance of Q without the explicit knowledge of the Gibbs distribution. Let us introduce the thermodynamic potential related to $F(\varphi)$ via the Legendre transform:

$$\tilde{F}(Q) = F(\varphi) + Q\varphi, \qquad \varphi = \left(\frac{\partial \tilde{F}}{\partial Q}\right)_{T,V}. \tag{1.29}$$

We can consider $\tilde{F}$ as a formal function of the instantaneous value of Q. Then we define the quantity termed as the *minimal work* for the fluctuations of the thermodynamic variable Q according to

$$U_{\min} = \tilde{F}(Q + \Delta Q) - \tilde{F}(Q) - \varphi(Q)\Delta Q. \tag{1.30}$$

We note that here φ is a function of Q as prescribed by Eq. (1.29). The minimal work $U_{\min}$ is a function of T, V, Q, and ΔQ. It has the following important property: its expansion in ΔQ starts from the quadratic term:

$$U_{\min}(\Delta Q) = \frac{1}{2\chi_Q}(\Delta Q)^2 + O\big((\Delta Q)^3\big). \tag{1.31}$$

Now, in order to reproduce the result (1.28), we can postulate that the distribution function governing the probability of the variable Q to be changed from Q to $Q + \Delta Q$ due to thermal fluctuations is given by the normal distribution:

$$\mathcal{P}_Q(\Delta Q) = \frac{\sqrt{T}}{\sqrt{2\pi\chi_Q}}\, e^{-U_{\min}(\Delta Q)/T}. \tag{1.32}$$

Then we find

$$\langle(\Delta Q)^2\rangle = \int\limits_{-\infty}^{\infty} dX\, X^2 \mathcal{P}_Q(X) = T\chi_Q. \tag{1.33}$$

We note that the statistics for the fluctuations of Q is not Gaussian in general. Thus the normal distribution (1.32) is an approximation in essence.

1.2.4 The Einstein approach to the thermodynamic fluctuations

As we have seen above, the thermodynamic fluctuations of the physical quantities coupled to the external fields are determined by the static susceptibilities. The latter can be calculated using the Gibbs statistical mechanics. Let us now formulate the similar approach to computing the thermodynamic fluctuations of the main physical parameters T, P, V, and S, which determine the thermodynamic state of the system. Let us consider the case of the system connected to the thermal reservoir keeping the temperature and pressure fixed in the system. Then the entropy and the volume of the system are able to fluctuate. In the full analogy with Eq. (1.30) we introduce the minimal work as

$$U_{\min} = E(S + \Delta S, V + \Delta V) - E(S, V) - T\Delta S + P\Delta V. \tag{1.34}$$

Expanding $U_{\min}$ to the second order in ΔS and ΔV, we find

$$U_{\min}(\Delta S, \Delta V) = \frac{1}{2}\left(\frac{\partial^2 E}{\partial S^2}\right)_V (\Delta S)^2 + \left(\frac{\partial^2 E}{\partial S \partial V}\right)\Delta S \Delta V$$
$$+ \frac{1}{2}\left(\frac{\partial^2 E}{\partial V^2}\right)_S (\Delta V)^2 + \ldots \tag{1.35}$$

In the same way as we have done in Eq. (1.32), we postulate that the joint probability distribution that governs the fluctuations of ΔS and ΔV is proportional to $\exp(-U_{\min}(\Delta S, \Delta V)/T)$. (Here it is necessary to take the normalization factor into account.) We mention that, in order the probability distribution to be normalizable, the minimal work $U_{\min}$ should be positive as a function of its arguments ΔS and ΔV. This requirement yields a number of relations on the derivatives of the thermodynamic quantities that coincide with the so-called thermodynamic inequalities. One example is the relation $C_V > 0$.

Equation (1.35) implies that the fluctuation of the entropy at the fixed volume becomes

$$\langle (\Delta S)^2 \rangle_V = T \left(\frac{\partial S}{\partial T} \right)_V = C_V. \tag{1.36}$$

We note that this result coincides with that derived above directly from the Gibbs distribution.

For computing of the thermal fluctuations of other observables, it is convenient to represent the expression for the minimal work (1.35) in the following symmetric form:

$$U_{\min} = \big(\Delta S \Delta T - \Delta P \Delta V \big)/2. \tag{1.37}$$

Although we have derived this expression for the entropy and volume fluctuations at the fixed temperature and pressure, one can use Eq. (1.37) for calculating the fluctuations of any pair of the thermodynamic variables. For example, expanding ΔT and ΔV in Eq. (1.37) to first order in ΔP and ΔS, we find

$$\langle (\Delta P)^2 \rangle = -T \left(\frac{\partial P}{\partial V} \right)_S. \tag{1.38}$$

It is worthwhile to mention that the result (1.26) of the Gibbs approach to the pressure fluctuations differs from the result (1.38) of the Einstein approach.

Now we explain the origin of the term *"the minimal work"* for $U_{\min}$. Let us consider an isolated system consisting of thermal reservoir and subsystem. The subsystem can perform a work on the body isolated from the subsystem and the reservoir. We assume that the reservoir has the temperature T_0 and pressure P_0 which are kept fixed since the effect of subsystem on the reservoir is negligible. The subsystem has the temperature T and the pressure P which can differ from T_0 and P_0. In the absence of the reservoir the work U performed by the body upon the subsystem during some process equals the energy difference ΔE of the subsystem in this process. In the presence of the reservoir we should take into account the work $P_0 \Delta V_0$ done by the reservoir and the heat $-T_0 \Delta S_0$ transferred from the reservoir to the subsystem. Eventually, we find $\Delta E = U - T_0 \Delta S_0 + P_0 \Delta V_0$. Assuming the conservation of volume of the system, i.e., using the relation $\Delta V_0 = -\Delta V$, we find $U = \Delta E + T_0 \Delta S_0 + P_0 \Delta V$. Due

to the second law of the thermodynamics the entropy variation of the isolated system is not negative, $\Delta S_0 + \Delta S \geqslant 0$. Therefore, we find that the minimal value of the work is given as $U_{\min} = \Delta E - T_0 \Delta S + P_0 \Delta V$. For spontaneous thermodynamic fluctuations, the reservoir is a large part of the very same system with the same temperature and pressure as the small subsystem, i.e., $T_0 = T$ and $P_0 = P$. Then $U_{\min}$ is given by Eq. (1.34).

1.2.5   Thermodynamic fluctuations in the grand canonical ensemble

In the grand canonical ensemble the number of particle can fluctuate. Using in this case the Gibbs distribution (1.17), we find

$$\langle (\Delta N)^2 \rangle_{T,V,\mu} = \operatorname{Tr} \rho\, n^2 - (\operatorname{Tr} \rho\, n)^2 = T \left(\frac{\partial N}{\partial \mu} \right)_{T,V}. \qquad (1.39)$$

We emphasize the resemblance of this result with the general result (1.28). The chemical potential plays a role of the external field conjugated to the number of particles.

   In the Einstein approach to the thermodynamic fluctuations the case of varying the number of particles does not require a special consideration. On can take the extensive character of the volume into account and transform fluctuations of the volume $\langle (\Delta V)^2 \rangle_T = -T(\partial V/\partial P)_T$ into those for the number of particles. In this way the expression (1.39) can be reproduced.

   We mention that the Einstein approach to the thermodynamic fluctuations is limited to the Gaussian approximation. The higher cumulants of the thermodynamic fluctuations must be computed from the Gibbs distribution. For example, the third cumulant of the number of particles, $C_N^{(3)} = \langle N^3 \rangle - 3 \langle N^2 \rangle \langle N \rangle + 2 \langle N \rangle^3$, is equal to $C_N^{(3)} = T^2 (\partial^2 N / \partial \mu^2)_{T,V}$. In other words, the thermodynamic potential $\Omega(\mu)$ is the cumulant generating function for the number of particles.

Problem for the seminar 4: For the system of N independent spins $s = 1/2$ in the magnetic field, compute the thermodynamic fluctuations of the energy and compare them with those for the specific heat.

Problem for the seminar 5: For the system of N independent spins $s = 1/2$ in the magnetic field, calculate the spin susceptibility and thermodynamic fluctuations of the magnetization. Check the validity of Eq. (1.28).

Problem for the seminar 6: Derive the expression for $U_{\min}$ as a function of ΔV and ΔT. Express in terms of T and V as independent thermodynamic variables the following averages: $\langle (\Delta T)^2 \rangle$, $\langle (\Delta V)^2 \rangle$, $\langle \Delta T \Delta V \rangle$, $\langle (\Delta P)^2 \rangle$, $\langle (\Delta S)^2 \rangle$, $\langle \Delta T \Delta P \rangle$, $\langle \Delta T \Delta S \rangle$, $\langle \Delta V \Delta P \rangle$, $\langle \Delta S \Delta P \rangle$, and $\langle \Delta V \Delta S \rangle$.

Exercise 3: Using the von Neumann definition of the entropy, prove that the variance of entropy S is given by the specific heat at the fixed volume, $\langle (\Delta S)^2 \rangle_V = C_V$.

Exercise 4: For the system of N independent spins $s = 1$ in the magnetic field, calculate the thermodynamic fluctuations of the energy and the magnetization. Compare the results with the expressions for the specific heat and spin susceptibility, respectively.

Exercise 5: Derive the expression for $U_{\min}$ as a function of ΔS and ΔP. Express via P and S as independent thermodynamic variables the following averages: $\langle (\Delta T)^2 \rangle$, $\langle (\Delta V)^2 \rangle$, $\langle \Delta T \Delta V \rangle$, $\langle (\Delta P)^2 \rangle$, $\langle (\Delta S)^2 \rangle$, $\langle \Delta T \Delta P \rangle$, $\langle \Delta T \Delta S \rangle$, $\langle \Delta V \Delta P \rangle$, $\langle \Delta S \Delta P \rangle$, and $\langle \Delta V \Delta S \rangle$.

1.3 Thermodynamics of an ideal Fermi gas

1.3.1 The Fermi-Dirac distribution

We consider an ideal Fermi gas in the grand canonical ensemble, i.e., at the given temperature and chemical potential. Our aim is to derive the general expression for the thermodynamic potential and the average number of fermions. To simplify the derivation, for a moment we put nonzero spin of fermions aside. From the physical viewpoint we consider the fully spin-polarized Fermi gas.

Let us start from the simplest situation of a single energy level ε_1 which can be populated by fermions. Due to the Pauli exclusion principle, this level can be either empty or occupied. Therefore, the grand canonical partition function acquires the following form: $\mathcal{Z}^{(1)} = 1 + e^{-\beta\varepsilon_1 + \beta\mu}$. Now let us add another level ε_2. Again due to the Pauli exclusion principle, we can have four different situations:

  (i) both levels are empty,

  (ii) level ε_1 is occupied whereas level ε_2 is empty,

  (iii) level ε_1 is empty whereas level ε_2 is occupied,

  (iv) both levels are occupied.

The grand canonical partition function becomes

$$\begin{aligned}
\mathcal{Z}^{(2)} &= 1 + e^{-\beta\varepsilon_1 + \beta\mu} + e^{-\beta\varepsilon_2 + \beta\mu} + e^{-\beta(\varepsilon_1 + \varepsilon_2) + 2\beta\mu} \\
&= \left(1 + e^{-\beta\varepsilon_1 + \beta\mu}\right)\left(1 + e^{-\beta\varepsilon_2 + \beta\mu}\right).
\end{aligned} \tag{1.40}$$

As one can see, the grand partition function $\mathcal{Z}$ factorizes into the product of independent factors for each energy level. The generalization to an arbitrary number of levels is obvious:

$$\mathcal{Z} = e^{-\beta\Omega} = \prod_{a,\sigma}\left(1 + e^{-\beta\varepsilon_{a,\sigma} + \beta\mu}\right). \tag{1.41}$$

Here a enumerates the orbital degrees of freedom and σ stands for the z-projection of the fermion spin. The number of particles can be extracted from Eq. (1.41) as

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V} = \sum_{a,\sigma} f_F(\varepsilon_{a,\sigma}), \qquad f_F(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}. \tag{1.42}$$

The function $f_F(\varepsilon)$ is called the *Fermi-Dirac distribution function*.

The Fermi-Dirac distribution function can be seen from another point of view. Due to the Pauli exclusion principle, the given single particle state can be empty or occupied by a fermion. Therefore, in order to describe a single fermion, the density matrix of size 2×2 is required. The result (1.41) suggests that the density matrix for the fermion system can be written as a tensor product of the 2×2 density matrices: $\rho = \prod_{a,\sigma} \otimes \rho_{a,\sigma}$ where $\operatorname{Tr} \rho_{a,\sigma} = 1$. Let us denote the eigenvalues of $\rho_{a,\sigma}$ as $n_{a,\sigma}$ and $1 - n_{a,\sigma}$. Then the entropy can be written as follows:

$$S = -\sum_{a,\sigma} \big[n_{a,\sigma} \ln n_{a,\sigma} + (1 - n_{a,\sigma}) \ln(1 - n_{a,\sigma}) \big]. \tag{1.43}$$

The quantity $n_{a,\sigma}$ is termed as the occupation number for an energy level $\varepsilon_{a,\sigma}$ and has a meaning of probability that the energy level is occupied. Then the number of particles and the energy become

$$N = \sum_{a,\sigma} n_{a,\sigma}, \qquad E = \sum_{\alpha,\sigma} \varepsilon_{a,\sigma} n_{a,\sigma}. \tag{1.44}$$

Now we can apply the maximal entropy principle: to maximize S over $n_{a,\sigma}$ under conditions that N and E are kept as fixed. The variation procedure for the functional $S + \beta\mu N - \beta E$ over $n_{a,\sigma}$ results in the optimal value of the occupation number given by the Fermi-Dirac distribution function, i.e., $n_{a,\sigma} = f_F(\varepsilon_{a,\sigma})$ realizes the maximal entropy principle.

1.3.2 Canonical partition function

Sometimes it is convenient to work at the fixed number of particles rather than at the fixed chemical potential. In order to derive the expression for the canonical partition function, let us first consider the case of two energy levels ε_1 and ε_2. Then from the first line of Eq. (1.40) the canonical partition functions can be read as

$$Z_{N=0} = 1, \quad Z_{N=1} = e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2}, \quad Z_{N=2} = e^{-\beta(\varepsilon_1+\varepsilon_2)}, \quad Z_{N>2} = 0. \tag{1.45}$$

In the general case, we can write the *Darwin-Fowler integral* for the canonical partition function

$$Z_N = e^{-\beta F} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N} \prod_{a,\sigma} \left(1 + e^{-\beta\varepsilon_{a,\sigma}+i\theta}\right) = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N - \beta\Omega(iT\theta)}. \tag{1.46}$$

For the large number of particles, one can perform the integral over angle θ by means of the saddle point method. Then, if we denote the saddle point value of

the angle θ as $\theta_s = -i\mu$, it will satisfy the standard relation between the number of particles and the chemical potential: $N = -\partial\Omega(\mu)/\partial\mu$. The free energy will also be given by the standard Legendre transform: $F = \Omega(\mu) + \mu N$. Below, we usually employ the fixed chemical potential condition instead of the fixed particle number one.

1.3.3 Density of states

In order to compute the thermodynamic quantities of various fermion systems, it is convenient to introduce the *density of states*:

$$g(\varepsilon) = \frac{1}{V} \sum_{a,\sigma} \delta\big(\varepsilon - \varepsilon_{a,\sigma}\big). \tag{1.47}$$

Then the thermodynamic potential and the number of particles can be written as follows:

$$\Omega = -TV \int d\varepsilon \, g(\varepsilon) \ln\big(1 + e^{-\beta\varepsilon + \beta\mu}\big), \quad N = V \int d\varepsilon \, g(\varepsilon) f_F(\varepsilon). \tag{1.48}$$

Using the thermodynamic relation $E = \Omega + TS + \mu N$, one finds the expression for the energy in agreement with Eq. (1.44):

$$E = V \int d\varepsilon \, g(\varepsilon) \, \varepsilon f_F(\varepsilon). \tag{1.49}$$

This expression for the energy allows us to write down the result for the specific heat:

$$C = V \int d\varepsilon \, g(\varepsilon) \, \varepsilon \frac{\partial f_F(\varepsilon)}{\partial T} \tag{1.50}$$

where the derivative with respect to temperature is taken under fixed chemical potential.

The density of states is determined by the energy spectrum of single-particle problem. Let us consider a particle in the one-dimensional quantum well of size L with the infinite walls. Then the eigen energies become $\varepsilon_n = \hbar^2\pi^2 n^2/(2mL^2)$ where m denotes the particle mass and $n = 1, 2, 3, \ldots$ It is instructive to compute the density of states in the thermodynamic limit $L \to \infty$:

$$g(\varepsilon) = \frac{g_s}{L} \sum_{n=1}^{\infty} \delta\big(\varepsilon - \varepsilon_n\big) \approx \frac{g_s}{L} \int_0^{\infty} dn \, \delta\big(\varepsilon - \varepsilon_n\big) = \frac{g_s\sqrt{m}}{\pi\hbar\sqrt{2\varepsilon}}\Theta(\varepsilon). \tag{1.51}$$

Here $\Theta(\varepsilon)$ stands for the Heaviside step function and $g_s = 2s + 1$ is the number of projections for the spin s fermions. We note that the density of states is independent of size L in the limit $L \to \infty$.

The result (1.51) can be derived in the different way. Let us consider free particle with momentum p in one spatial dimension. Then, if we write the density of states as follows:

$$g(\varepsilon) = g_s \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \, \delta \left(\varepsilon - \frac{p^2}{2m} \right), \qquad (1.52)$$

we obtain exactly the same result as given by Eq. (1.51). The generalization of Eq. (1.52) to the free motion of quantum particle in an arbitrary spatial dimension d reads

$$g(\varepsilon) = g_s \int \frac{d^d \boldsymbol{p}}{(2\pi\hbar)^d} \, \delta \left(\varepsilon - \frac{\boldsymbol{p}^2}{2m} \right). \qquad (1.53)$$

1.3.4 Chemical potential and the Fermi energy

As an instructive example simple in the mathematical treatment, we consider the thermodynamical properties of two-dimensional ideal Fermi gas. Using Eqs. (1.48) and (1.53), we find the number of particles as

$$N = \frac{g_s V m}{2\pi\hbar^2} \int\limits_{0}^{\infty} \frac{d\varepsilon}{e^{\beta\varepsilon - \beta\mu} + 1} = \frac{g_s m V T}{2\pi\hbar^2} \ln \left(1 + e^{\beta\mu} \right). \qquad (1.54)$$

Solving this equation for μ, we obtain

$$\mu(T) = T \ln \left(e^{E_F/T} - 1 \right), \qquad E_F = \frac{2\pi\hbar^2 N}{g_s m V}. \qquad (1.55)$$

The only characteristic energy scale $E_F = \mu(T = 0)$ is referred to as the *Fermi energy*. The importance of the Fermi energy is due to the following observation: at $T = 0$ the fermion occupation, $f_F(\varepsilon)$, for the state of energy ε equals 1 if $\varepsilon \leqslant E_F$ and 0 otherwise. In other words, all the states below the Fermi energy are occupied in ideal Fermi gas. Further we will discuss how this statement is affected by the fermion-fermion interactions. It is convenient to introduce the notion of the *Fermi momentum* equal to $p_F = \sqrt{2mE_F}$. Then at zero temperature the states of ideal Fermi gas with momentum $p \leqslant p_F$ are occupied whereas the states with $p > p_F$ are empty.

The dependence $\mu(T)$ is shown in Fig. 1.1a. The chemical potential is the monotonously decreasing function of temperature. This is not a common feature. For $d < 2$, the chemical potential $\mu(T)$ is a non-monotonous function of temperature. In the degenerate regime, $T \ll E_F$, the chemical potential can be written as

$$\mu(T) = E_F - T e^{-E_F/T} + \dots. \qquad (1.56)$$

We note that the temperature corrections to the zero temperature magnitude of chemical potential are exponentially small. This is a specific feature for the spatial $d = 2$ dimensions.

At temperature $T_0 = E_F / \ln 2$ the chemical potential vanishes, $\mu(T_0) = 0$. In the high temperature regime, $T \gg E_F$, the chemical potential is negative and can be approximated by

$$\mu(T) = -T \ln T / E_F. \tag{1.57}$$

1.3.5   Equation of state in $d = 2$

In order to find the equation of state for an ideal Fermi gas, we should calculate the thermodynamic potential, cf. Eq. (1.48). Again, we consider the case of the spatial $d = 2$ dimensions. Then, we obtain

$$P = \frac{g_s m T}{2\pi\hbar^2} \int\limits_0^\infty d\varepsilon \ln\left(1 + e^{\beta\mu - \beta\varepsilon}\right) = -\frac{g_s m T^2}{2\pi\hbar^2} \, \mathrm{li}_2\left(-e^{\beta\mu}\right). \tag{1.58}$$

Here we introduce the special function $\mathrm{li}_k(z) = \sum_{j=1}^\infty z^j / j^k$ known as *polylogarithm*. Using (1.55), we find the equation of state for ideal Fermi gas in the spatial $d = 2$ dimensions:

$$\frac{PV}{NT} = -\frac{T}{E_F} \, \mathrm{li}_2\left(1 - e^{E_F/T}\right). \tag{1.59}$$

Using the asymptotic expression $\mathrm{li}_2(-z) = -(\ln z)^2/2 - \pi^2/6$ at $z \gg 1$, we find the pressure of an ideal degenerate Fermi gas at $T \ll E_F$:

$$P = \frac{N E_F}{2V}\left(1 + \frac{\pi^2}{3}\frac{T^2}{E_F^2}\right). \tag{1.60}$$

In the opposite case of high temperatures, $T \gg E_F$, we can use the asymptotic expansion of the polylogarithm at $z \ll 1$: $\mathrm{li}_2(z) = z + z^2/4$. Then, we obtain the following equation of state at $T \gg E_F$:

$$PV = NT\left(1 + \frac{E_F}{4T}\right). \tag{1.61}$$

As one can see, it resembles the equation of state for an ideal Boltzmann gas with the correction corresponding to an additional pressure at a given temperature. This correction is an effect of the Fermi-Dirac statistics due to quantum mechanical exchange effects (the Pauli exclusion principle, in essence). The similarity of the equation of state at $T \gg E_F$ with that for the ideal Boltzmann

gas is not occasional. For $T \gg E_F$, the Fermi-Dirac distribution function can be approximated as $f_F(\varepsilon) \approx \exp(\beta\mu - \beta\varepsilon)$, i.e, it goes over the Boltzmann distribution. The overall behavior of the pressure as the temperature varies is shown in Fig. 1.1b. This behavior is not specific to the spatial $d = 2$ dimensions. In any dimension, the pressure of the ideal Fermi gas at a given temperature is larger than that for the ideal Boltzmann gas.

1.3.6 Specific heat

In order to determine the specific heat under the fixed volume we start from calculating the free energy via the relation $F = -PV + \mu N$. In the spatial $d = 2$ dimensions the explicit expression for the free energy reads:

$$F = \frac{NT^2}{E_F} \, \mathrm{li}_2 \left(1 - e^{E_F/T}\right) + NT \ln \left(e^{E_F/T} - 1\right) . \tag{1.62}$$

As it is expected, the free energy is proportional to the number of particles and depends on the single parameter T/E_F. Using the results for the chemical potential and pressure in the degenerate regime, we find the free energy at $T \ll E_F$:

$$F = \frac{NE_F}{2} - \frac{\pi^2}{6} \frac{NT^2}{E_F} . \tag{1.63}$$

Therefore, the specific heat at $T \ll E_F$ in the spatial $d = 2$ dimensions becomes

$$C_V = -T \left(\frac{\partial^2 F}{\partial T^2}\right)_V = \frac{\pi^2}{3} \frac{NT}{E_F} . \tag{1.64}$$

We emphasize that the specific heat is proportional to the temperature. This fact is a direct consequence from existence of the Fermi sphere. At low temperatures only a small fraction of fermions in the vicinity of the Fermi energy with energies $|\varepsilon - E_F| \lesssim T$ can participate in the heat transfer.

In the Boltzmann region, $T \gg E_F$, using Eqs. (1.57) and (1.61), we reproduce the result for the specific heat of an ideal Boltzmann gas: $C_V = N$. The temperature behavior of the specific heat is shown in Fig. 1.1c.

1.3.7 From an ideal Fermi to the Boltzmann gas

As we have seen above, the thermodynamic quantities of the ideal Fermi gas goes over to those of the ideal Boltzmann gas. Therefore, it is instructive to derive the canonical partition function of an ideal Bolzmann gas directly from Eq. (1.46). Let us rewrite Z_N as follows (here we assume that the energy spectrum
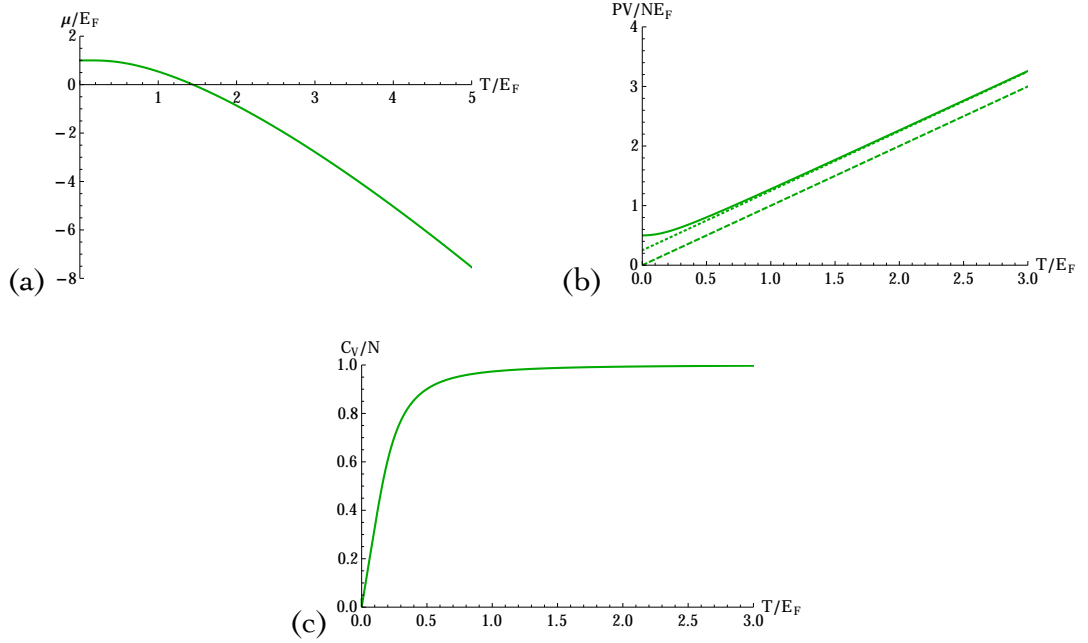
Figure 1.1: The temperature behavior of thermodynamic quantities in the two-dimensional ideal Fermi gas: (a) chemical potential, (b) pressure, and (c) specific heat.

is independent of the spin degrees of freedom):

$$Z_N = e^{-\beta\mu N} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N} \exp\left[g_s \sum_a \ln\left(1 + e^{-\beta\varepsilon_a + \beta\mu + i\theta}\right) \right]. \tag{1.65}$$

Now using the condition $\beta|\mu| \gg 1$, in the thermodynamic limit we can expand the logarithm to first order in its argument. Then, we find

$$Z_N \approx e^{-\beta\mu N} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N} \exp\left(g_s \sum_a e^{-\beta\varepsilon_a + \beta\mu + i\theta} \right) = e^{-\beta\mu N} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N}$$

$$\times \sum_{k=0}^{\infty} \left(g_s \sum_a e^{-\beta\varepsilon_a + \beta\mu} \right)^k \frac{e^{i\theta k}}{k!} = \frac{1}{N!} \left(\int d\varepsilon\, g(\varepsilon)\, e^{-\beta\varepsilon} \right)^N. \tag{1.66}$$

We mention the appearance of the factor $1/N!$ in the above expression for Z_N. The physical meaning of this factor is to involve the identity of particles. We

emphasize that this factor appears in the Fowler-Darwin formalism by its own nature.

Problem for the seminar 7: Compute the density of states for the free quantum particle in an arbitrary spatial dimension d, cf. Eq. (1.53).

Problem for the seminar 8: Compute the density of states of an ideal electron gas in the spatial $d = 2$ dimensions in the presence of the perpendicular magnetic field.

Problem for the seminar 9: Calculate the temperature correction to the chemical potential at $T \ll E_F$ for an ideal Fermi gas in $d \neq 2$ spatial dimensions.

Problem for the seminar 10: Compute the specific heat of ideal degenerate Fermi gas in an arbitrary spatial dimension.

Problem for the seminar 11: Compute the zero-field spin susceptibility of ideal electron gas in the spatial $d = 2$ dimensions.

Problem for the seminar 12: Compute the magnetization of ideal electron gas in the spatial $d = 2$ dimensions in the presence of the relatively strong perpendicular magnetic field $T \ll \mu_B B \ll E_F$.

Exercise 6: Calculate the density of states for a quantum particle in the three-dimensional box of size $L_x \times L_y \times L_z$ with the infinite walls in the thermodynamic limit $L_x, L_y, L_z \to \infty$.

Exercise 7: To find the change of the Fermi energy of an ideal gas of ^{3}He atoms after its full spin polarization by a magnetic field.

Exercise 8: Express the variance for the thermodynamic fluctuations of the number of particles in an ideal degenerate Fermi gas via the density of states at the Fermi energy, $g(E_F)$.

Exercise 9: Find the temperature at which the chemical potential of ideal electron gas in the spatial $d = 2$ dimensions vanishes in the presence of parallel magnetic field $\mu_B B \ll E_F$. (Take only the Zeeman effect of a magnetic field into account.)

Exercise 10: Compute the ratio $(C_P - C_V)/C_V$ for ideal degenerate Fermi gas in the spatial $d = 2$ dimensions.

1.4 Thermodynamics of an ideal Bose gas

1.4.1 The Bose-Einstein distribution

We consider an ideal Bose gas in the grand canonical ensemble, i.e., at the given temperature and chemical potential. Our aim is to derive the general expression for the thermodynamic potential and the average number of bosons. In order to simplify the derivation, we consider zero-spin bosons.

Let us start from simplest situation of a single energy level ε_1 which can be occupied by bosons. Due to the absence of the Pauli exclusion principle for bosons, this level can be empty, occupied by a single boson, occupied by two bosons, etc. Therefore, the grand canonical partition function acquires the following form: $\mathcal{Z}^{(1)} = \sum_{n=0}^{\infty} e^{-\beta\varepsilon_1 n + \beta\mu n} = (1 - e^{\beta\mu - \beta\varepsilon_1})^{-1}$. Now let us add one more level ε_2. Again due to the absence of the Pauli exclusion principle, we can have the following situation: the level ε_1 is occupied by n_1 bosons whereas the level ε_2 is occupied by n_2 bosons where $n_{1,2} = 0, 1, 2, \ldots$. The grand canonical partition function becomes

$$\mathcal{Z}^{(2)} = \sum_{n_{1,2}=0}^{\infty} e^{\beta\mu(n_1+n_2) - \beta(\varepsilon_1 n_1 + \varepsilon_2 n_2)} = \left(1 - e^{\beta\mu - \beta\varepsilon_1}\right)^{-1} \left(1 - e^{\beta\mu - \beta\varepsilon_2}\right)^{-1}.$$

(1.67)

As one can see, function $\mathcal{Z}$ factorizes as a product of the factors for each energy level. The generalization to an arbitrary number of levels is obvious:

$$\mathcal{Z} = e^{-\beta\Omega} = \prod_{a,\sigma} \left(1 - e^{-\beta\varepsilon_{a,\sigma} + \beta\mu}\right)^{-1}.$$

(1.68)

Here a enumerates the orbital degrees of freedom and σ stands for the z-projection of the spin of a boson. The number of particles can be extracted from Eq. (1.68) as

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V} = \sum_{a,\sigma} f_B(\varepsilon_{a,\sigma}), \qquad f_B(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}.$$

(1.69)

The function $f_B(\varepsilon)$ is called the *Bose-Einstein distribution function*.

It is instructive to formulate the derivation of the Bose-Einstein distribution function within the framework of the maximal entropy principle. Using the expression for the grand canonical partition function (1.68), we can compute the entropy as $-(\partial\Omega/\partial T)_{V,\mu}$. The result can be expressed in terms of the Bose-Einstein distribution function:

$$S = \sum_{a,\sigma} \left[\left(1 + f_B(\varepsilon_{a,\sigma})\right) \ln\left(1 + f_B(\varepsilon_{a,\sigma})\right) - f_B(\varepsilon_{a,\sigma}) \ln f_B(\varepsilon_{a,\sigma})\right].$$

(1.70)

Based on this observation, we can write the entropy of bosons in terms of the occupation number $n_{a,\sigma}$ for an energy level $\varepsilon_{a,\sigma}$:

$$S = -\sum_{\alpha,\sigma} \left[n_{a,\sigma} \ln n_{a,\sigma} - (1 + n_{a,\sigma}) \ln(1 + n_{a,\sigma}) \right]. \tag{1.71}$$

Maximizing the entropy S over $n_{a,\sigma}$ under the constant N and E, cf. (1.44), results in the Bose-Einstein distribution.

Introducing the density of states $g(\varepsilon)$, we can write the thermodynamic potential and the number of particles for an ideal Bose gas as follows:

$$\Omega = TV \int d\varepsilon \, g(\varepsilon) \ln \left(1 - e^{-\beta\varepsilon + \beta\mu} \right), \quad N = V \int d\varepsilon \, g(\varepsilon) f_B(\varepsilon). \tag{1.72}$$

Using the thermodynamic relation $E = \Omega + TS + \mu N$, one finds the expression for the energy:

$$E = V \int d\varepsilon \, g(\varepsilon) \, \varepsilon f_B(\varepsilon). \tag{1.73}$$

This expression for the energy allows us to write down the following result for the specific heat:

$$C = V \int d\varepsilon \, g(\varepsilon) \, \varepsilon \frac{\partial f_B(\varepsilon)}{\partial T} \tag{1.74}$$

where the derivative with respect to temperature is taken under the fixed chemical potential.

1.4.2   Canonical partition function

The canonical partition function for N bosons occupying the energy levels ε_a can be written in the obvious way:

$$Z_N = \sum_{\sum_\alpha n_\alpha = N} \prod_\alpha e^{-\beta\varepsilon_\alpha n_\alpha}. \tag{1.75}$$

As in the case of the Fermi gas, the canonical partition function can be related with the grand canonical partition function via the Darwin-Fowler integral:

$$Z_N = e^{-\beta F} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N} \prod_{a,\sigma} \left(1 - e^{-\beta\varepsilon_{a,\sigma} + i\theta} \right)^{-1} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\theta N - \beta\Omega(iT\theta)}. \tag{1.76}$$

For the large number of particles $N \gg 1$, the saddle point method applied to the integral over the angle θ provides us the standard relation $F = \Omega(\mu) + \mu N$ where $N = -\partial\Omega(\mu)/\partial\mu$.

1.4.3 Chemical potential in $d = 2$

Let us now compute the chemical potential dependence of two-dimensional ideal Bose gas as a function of temperature, particle number, and volume. Using Eqs. (1.72), we obtain the following result for the number of particles:

$$N = \frac{g_s V m}{2\pi\hbar^2} \int_0^\infty \frac{d\varepsilon}{e^{\beta\varepsilon - \beta\mu} - 1} = -\frac{g_s m V T}{2\pi\hbar^2} \ln\left(1 - e^{\beta\mu}\right). \qquad (1.77)$$

Here g_s involves the number of spin degenerate states of a boson. We emphasize that the number of particles is finite provided that chemical potential is *negative*, $\mu < 0$. Solving the above equation for μ, we obtain

$$\mu(T) = T \ln\left(1 - e^{-E_0/T}\right), \qquad E_0 = \frac{2\pi\hbar^2 N}{g_s m V}. \qquad (1.78)$$

We note that the chemical potential of an ideal Bose gas in $d = 2$ vanishes at $T = 0$. Although the characteristic energy scale E_0 has exactly the same expression as the Fermi energy, it has no such physical meaning. The chemical potential is the monotonously decreasing function of temperature (see Fig. 1.2a). In the degenerate region, $T \ll E_0$, the chemical potential can be written as

$$\mu(T) = -T e^{-E_0/T} + \dots. \qquad (1.79)$$

In the Boltzmann regime, $T \gg E_0$, the chemical potential is negative and can be approximated by

$$\mu(T) = -T \ln T/E_0. \qquad (1.80)$$

1.4.4 Equation of state in $d = 2$

In order to find the equation of state for an ideal Bose gas, we should calculate the thermodynamic potential, cf. Eq. (1.72). Again, we consider the case of the spatial $d = 2$ dimensions. Then, we obtain

$$P = -\frac{g_s m T}{2\pi\hbar^2} \int_0^\infty d\varepsilon \ln\left(1 - e^{\beta\mu - \beta\varepsilon}\right) = \frac{g_s m T^2}{2\pi\hbar^2} \text{li}_2\left(e^{\beta\mu}\right). \qquad (1.81)$$

Using (1.78), we find the equation of state for the ideal Bose gas in the spatial $d = 2$ dimensions:

$$\frac{PV}{NT} = \frac{T}{E_0} \text{li}_2\left(1 - e^{-E_0/T}\right). \qquad (1.82)$$

We note that, contrary to the case of the ideal Fermi gas, the argument of the polylogarithm is positive and smaller than unity. Expanding the argument of
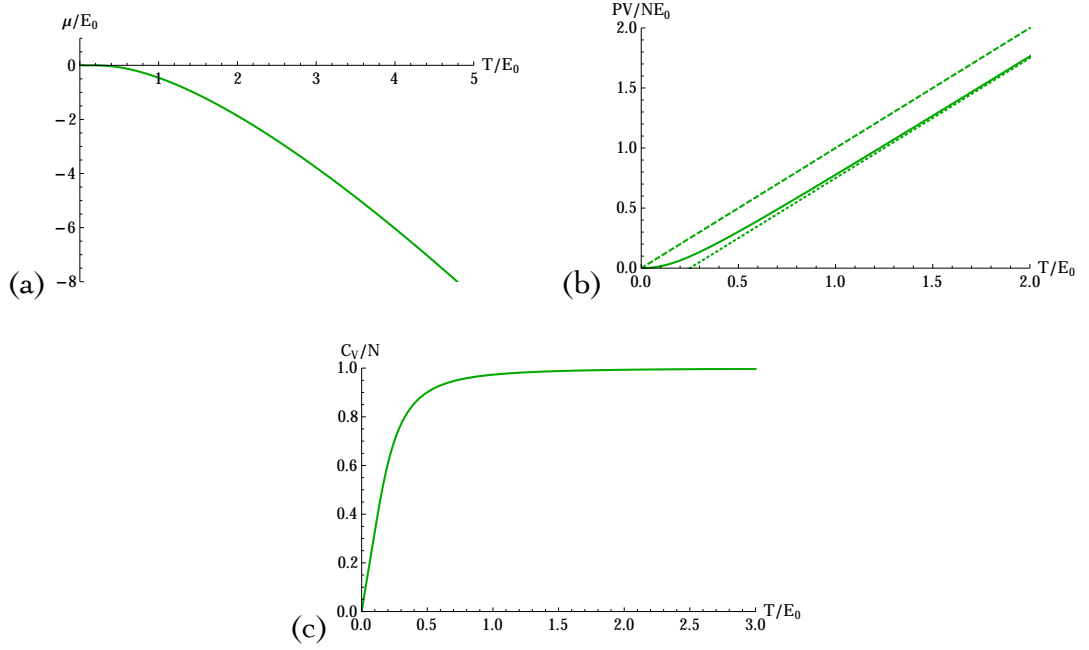
Figure 1.2: The temperature behavior of thermodynamic quantitiies in the ideal Bose gas: (a) chemical potential, (b) pressure, and (c) specific heat.

the polylogarithm in $\exp(-E_0/T)$, we find the pressure of an ideal degenerate Bose gas, $T \ll E_0$:

$$P = \frac{\pi^2}{6} \frac{NT^2}{VE_0}. \tag{1.83}$$

In the opposite case of high temperatures, $T \gg E_0$, we can use the asymptotic expansion of the polylogarithm at $z \ll 1$: $\mathrm{li}_2(z) = z + z^2/4$. Then, we obtain the following equation of state at $T \gg E_0$:

$$PV = NT \left(1 - \frac{E_0}{4T}\right). \tag{1.84}$$

As one can see, it resembles the equation of state for the ideal Boltzmann gas with the correction describing the pressure drop at the given temperature. This correction can be interpreted as a consequence of the effective attraction between bosons. The overall behavior of the pressure with varying the temperature is shown in Fig. 1.2b. This behavior is specific to the spatial $d = 2$ dimensions.

1.4.5 Specific heat

In order to find the specific heat at a fixed volume, we can compute the free energy via the relation $F = -PV + \mu N$. In the spatial $d = 2$ dimensions the explicit expression for the free energy of ideal Bose gas reads:

$$F = -\frac{NT^2}{E_0} \operatorname{li}_2 \left(1 - e^{-E_0/T}\right) + NT \ln \left(1 - e^{-E_0/T}\right). \qquad (1.85)$$

Like the case of fermions, the free energy of ideal Bose gas is proportional to the number of particles and depends on a single parameter T/E_0. Using the results for the chemical potential and pressure in the degenerate regime, we find the free energy at $T \ll E_0$:

$$F = -\frac{\pi^2}{6} \frac{NT^2}{E_0}. \qquad (1.86)$$

So, the specific heat of ideal Bose gas at $T \ll E_0$ in the spatial $d = 2$ dimensions becomes

$$C_V = -T \left(\frac{\partial^2 F}{\partial T^2}\right)_V = \frac{\pi^2}{3} \frac{NT}{E_0}. \qquad (1.87)$$

We note that this expression coincides with that for the Fermi gas. However, contrary to the Fermi gas, the linear temperature dependence for the specific heat in the ideal Bose gas takes place in the single $d = 2$ dimension.

In the Boltzmann regime, $T \gg E_0$, we reproduce the same result for the specific heat of ideal Boltzmann gas: $C_V = N$. The temperature dependence of the specific heat is shown in Fig. 1.2c.

1.4.6 The Bose-Einstein condensation in $d = 3$

The ideal Bose gas in the spatial $d = 3$ dimensions has an interesting physical phenomenon called *Bose-Einstein condensation*. Let us write the number of particles down:

$$N = \frac{g_s V (mT)^{3/2}}{\sqrt{2}\pi^2 \hbar^3} \int\limits_0^\infty \frac{dz \sqrt{z}}{e^{z - \beta\mu} - 1}. \qquad (1.88)$$

Here we use the density of states of free particles $g(\varepsilon) = g_s m^{3/2} \varepsilon^{1/2}/(\sqrt{2}\pi^2 \hbar^3)$ in $d = 3$. This integral has an interesting property. At $\mu = 0$ the right hand side of Eq. (1.88) becomes smaller with decreasing the temperature T whereas the left hand side, i.e., number of particles, remains unvaried. The chemical potential of ideal Bose gas in $d = 3$ vanishes for $T < T_{\text{BEC}}$. The Bose-Einstein condensation temperature, T_{BEC}, is determined from the integral in Eq. (1.88) at $\mu = 0$:

$$T_{\text{BEC}} = \frac{2\pi\hbar^2}{m} \left(\frac{N}{\zeta(3/2)g_s V}\right)^{2/3}. \qquad (1.89)$$

Here $\zeta(z) = \sum_{k=1}^{\infty} k^{-z}$ denotes the Riemann zeta function. At $T < T_{\text{BEC}}$ the finite fraction of bosons occupy the ground state. We say that these bosons are condensed or settled in the condensate. The number of bosons in the condensate is given as

$$N_0 = N\left[1 - (T/T_{\text{BEC}})^{3/2}\right]. \tag{1.90}$$

Evaluating the thermodynamic potential at $\mu = 0$, we obtain the following result for the pressure at $T < T_{\text{BEC}}$:

$$\frac{PV}{NT} = \frac{\zeta(5/2)}{\zeta(3/2)}\left(\frac{T}{T_{\text{BEC}}}\right)^{3/2}. \tag{1.91}$$

The pressure behavior as a function of temperature in the $d = 3$ case is similar that in the $d = 2$ case. In particular, the pressure is a continuous function of temperature and has no singularity at $T = T_{\text{BEC}}$. We mention that the pressure is volume-independent at $T < T_{\text{BEC}}$. This indicates that the specific heat at the fixed pressure is infinite for $T < T_{\text{BEC}}$.

> *Problem for the seminar 13:* Find the dependence of the chemical potential on the temperatures near the Bose-Einstein condensation temperature T_{BEC} in the spatial $d = 3$ dimensions.

> *Exercise 11:* Compute the variance of the thermodynamic fluctuations for the number of particles in the ideal degenerate Bose gas in the two-dimensional case.

> *Exercise 12:* Calculate the inverse compressibility $(\partial P/\partial V)_T$ of ideal degenerate Bose gas in $d = 2$.

> *Exercise 13:* Compute the specific heat at constant pressure of ideal Bose gas in the spatial $d = 2$ dimensions.

> *Exercise 14:* Compute the specific heat of ideal Bose gas at $T < T_{\text{BEC}}$ in the spatial $d = 3$ dimensions.

Exercise 15: Calculate the variance of the thermodynamic fluctuations for the number of particles in the ideal Bose gas near the Bose-Einstein condensation temperature T_{BEC} in the spatial $d = 3$ dimensions.

Chapter 2

Thermodynamics of quantum fluids

2.1 Weakly non-ideal Fermi gas

2.1.1 Introduction

In this lecture we consider the simplest model of interacting fermions. We compute the thermodynamic quantities to first order in the interaction strength.

2.1.2 Hamiltonian

We consider the interacting fermion system in the spatial $d = 3$ dimensions. We assume that fermions have spin $s = 1/2$ and interact via point-like interaction $U > 0$. The many-body Hamiltonian has the following form, $\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_{\text{int}}$, where

$$\mathscr{H}_0 = \sum_{\boldsymbol{p},\sigma} \varepsilon^{(0)}(p) a_{\boldsymbol{p}\sigma}^\dagger a_{\boldsymbol{p}\sigma}, \quad \mathscr{H}_{\text{int}} = \frac{U}{V} \sum_{\boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_3 + \boldsymbol{p}_4} a_{\boldsymbol{p}_1\uparrow}^\dagger a_{\boldsymbol{p}_2\downarrow}^\dagger a_{\boldsymbol{p}_3\downarrow} a_{\boldsymbol{p}_4\uparrow}. \quad (2.1)$$

Here $\varepsilon^{(0)}(p)$ denotes the bare spectrum which, we assume, to be quadratic, $\varepsilon^{(0)}(p) = p^2/2m$. The operator $a_{\boldsymbol{p}\sigma}^\dagger$ creates a fermion in a single particle state with momentum $\boldsymbol{p}$ and spin projection $\sigma = \uparrow, \downarrow$. The operator $a_{\boldsymbol{p}\sigma}$ annihilates a fermion from a single particle state with momentum $\boldsymbol{p}$ and spin projection σ. We remind that the creation and annihilation operators satisfy the following anti-commutation relation:

$$a_{\boldsymbol{p}\sigma}^\dagger a_{\boldsymbol{p}'\sigma'} + a_{\boldsymbol{p}'\sigma'} a_{\boldsymbol{p}\sigma}^\dagger = \delta_{\boldsymbol{p}\boldsymbol{p}'} \delta_{\sigma\sigma'}. \quad (2.2)$$

Also the following identity holds for:

$$\operatorname{Tr} a_{\boldsymbol{p}\sigma}^\dagger a_{\boldsymbol{p}'\sigma'} e^{-\beta\mathscr{H}_0 + \beta\mu\mathscr{N}} \Big/ \operatorname{Tr} e^{-\beta\mathscr{H}_0 + \beta\mu\mathscr{N}} = f_F\big(\varepsilon^{(0)}(p)\big) \delta_{\boldsymbol{p}\boldsymbol{p}'} \delta_{\sigma\sigma'}, \quad (2.3)$$

where $\mathscr{N}$ stands for the operator of the particle number: $\mathscr{N} = \sum_{\boldsymbol{p},\sigma} a_{\boldsymbol{p}\sigma}^\dagger a_{\boldsymbol{p}\sigma}$.

2.1.3   Thermodynamic potential

Our aim is to calculate first order interaction correction to the thermodynamic potential. We start from expanding the Gibbs weight $\mathscr{S} = \exp(-\beta\mathscr{H} + \beta\mu\mathscr{N})$ in powers of interaction constant U. Let us differentiate $\mathscr{S}$ with respect to β. Then we will find that it satisfies the following equation:

$$\frac{d\mathscr{S}}{d\beta} = -\big(\mathscr{H} - \mu\mathscr{N}\big)\mathscr{S}. \tag{2.4}$$

Now we seek for the solution of this equation as a power series in interaction part $\mathscr{H}_{\text{int}}$, $\mathscr{S} = \mathscr{S}_0 + \mathscr{S}_1 + \ldots$. Obviously, $\mathscr{S}_0 = \exp(-\beta\mathscr{H}_0 + \beta\mu\mathscr{N})$ whereas $\mathscr{S}_1$ satisfies the following equation:

$$\frac{d\mathscr{S}_1}{d\beta} = -\big(\mathscr{H}_0 - \mu\mathscr{N}\big)\mathscr{S}_1 - \mathscr{H}_{\text{int}}\mathscr{S}_0. \tag{2.5}$$

Its solution is given as

$$\mathscr{S}_1 = -e^{-\beta\mathscr{H}_0 + \beta\mu\mathscr{N}} \int\limits_0^\beta d\tau\, e^{\tau(\mathscr{H}_0 - \mu\mathscr{N})} \mathscr{H}_{\text{int}} e^{-\tau(\mathscr{H}_0 - \mu\mathscr{N})}. \tag{2.6}$$

The combination under the integral sign on the right hand side of Eq. (2.6) is very frequently used in the perturbation theory for the many-body Hamiltonians and is called the *interaction representation*.

Therefore, we obtain

$$e^{-\beta\Omega} = e^{-\beta\Omega_0} + \text{Tr}\, e^{-\beta\mathscr{H}_0 + \beta\mu\mathscr{N}} \int\limits_0^\beta d\tau\, e^{\tau(\mathscr{H}_0 - \mu\mathscr{N})} \mathscr{H}_{\text{int}} e^{-\tau(\mathscr{H}_0 - \mu\mathscr{N})} + \ldots \quad (2.7)$$

Here Ω_0 is the thermodynamic potential of the noninteracting system. Using the cyclic properties of trace operation, we find that

$$\Omega = \Omega_0 + \langle\mathscr{H}_{\text{int}}\rangle + \ldots, \tag{2.8}$$

where the average is taken with the Gibbs density matrix corresponding to the noninteracting Hamiltonian $\mathscr{H}_0$. Using Eq. (2.3), we find

$$\Omega(\mu) = \Omega_0(\mu) + \frac{U}{V}\left[\sum_p f_F\big(\varepsilon^{(0)}(p)\big)\right]^2 = \Omega_0(\mu) + \frac{U N_0^2(\mu)}{4V} \tag{2.9}$$

where $N_0(\mu) = -(\partial\Omega_0(\mu)/\partial\mu)_{T,V}$ stands for the number of particles as a function of the chemical potential in the absence of interaction. In order to find the

total energy, we should express the chemical potential in terms of the number of particles. Taking derivative with respect to μ for the both sides of Eq. (2.9) at fixed T and V, we find

$$N = N_0(\mu) - \frac{U N_0(\mu)}{2V} \frac{\partial N_0(\mu)}{\partial \mu} \approx N_0(\mu_0) + \frac{\partial N_0(\mu_0)}{\partial \mu_0}(\mu - \mu_0)$$
$$- \frac{U N_0(\mu_0)}{2V} \frac{\partial N_0(\mu_0)}{\partial \mu_0} + \dots \qquad (2.10)$$

Here μ_0 is the chemical potential in the absence of interaction, corresponding to the given number of particles: $N = N_0(\mu_0)$. Therefore, we find that the interaction shifts the chemical potential already in first order of perturbation theory:

$$\mu = \mu_0(N) + \frac{U N}{2V} + \dots \qquad (2.11)$$

Using the relation between the energy and the chemical potential, $\mu = (\partial E / \partial N)_{S,V}$, we obtain the total energy:

$$E = E_0(N) + \frac{U N^2}{4V} + \dots \qquad (2.12)$$

We note that the first-order correction to the energy is temperature-independent. Therefore, in first order in the interaction U the result for the specific heat remains the same as for an ideal Fermi gas.

It is instructive to introduce the scattering length a instead of the interaction potential U. To lowest order in the interaction U, i.e., in the Born approximation, the scattering length is given as $a = mU/(4\pi\hbar^2)$. Then using Eq. (2.12), we can write the ground state energy as

$$E(T = 0) = \frac{3 p_F^2 N}{10 m} \left[1 + \frac{10}{9\pi} \frac{p_F a}{\hbar} + \dots \right]. \qquad (2.13)$$

This result indicates that the expansion of the thermodynamic quantities in powers of interaction potential is justified while $p_F a/\hbar \ll 1$.

For the further details on weakly non-ideal Fermi gas, one can read the book [4].

Problem for the seminar 14: Find the Pauli spin susceptibility of the fermion system to first order in the interaction potential U. Express the result in terms of the scattering length.

Exercise 16: Find $\mathrm{Tr}\left[a_{\boldsymbol{p}\uparrow}^\dagger e^{\beta\varepsilon(p) a_{\boldsymbol{p}\uparrow}^\dagger a_{\boldsymbol{p}\uparrow}} a_{\boldsymbol{p}\uparrow} e^{-\beta\varepsilon(p) a_{\boldsymbol{p}\uparrow}^\dagger a_{\boldsymbol{p}\uparrow}} \right]$.

Exercise 17: Find the expression for $\mathscr{S}_2$.

Exercise 18: Express zero-temperature inverse compressibility $\partial P/\partial V$ in terms of derivative $\partial \mu/\partial N$.

Exercise 19: Find the pressure of the fermion system at zero temperature to first order in the interaction potential U. Express the result in terms of the scattering length.

2.2 Normal Fermi liquid

2.2.1 Introduction

In the previous lecture we demonstrated that the system with the weak fermion-fermion repulsive interaction is very similar to the ideal Fermi gas. Therefore, it is natural to formulate the theory of the interacting fermions in the way analogous to the ideal degenerate Fermi gas. Such theory, termed as the *Fermi liquid theory*, is developed by Lev Landau [5]. Although initially the Fermi liquid theory was developed as phenomenological, it was later confirmed by the microscopic theory for the spatial $d > 1$ dimension. We note that there are some subtleties in the spatial $d = 2$ dimension. In this lecture we consider the Fermi liquid for the spin $s = 1/2$ fermions in the spatial $d = 3$ dimension.

The Fermi liquid theory is based on the Hohenberg–Kohn theorem [6] which states that the ground state energy can unambiguously described by some functional depending on the distribution function alone. The Fermi liquid theory is the method to compute corrections of lowest order in temperature.

2.2.2 Main assumptions

The Fermi liquid phenomenology is based on several assumptions:

(i) The theory is specified in terms of *quasiparticles* replacing the real particles.

(ii) The quasiparticle distribution function is a matrix in the spin space: $\hat{n}(\boldsymbol{p})$ which is normalized by the condition:

$$\int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \, \mathrm{tr}\, \hat{n}(\boldsymbol{p}) = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \, n_{\sigma\sigma}(\boldsymbol{p}) = \frac{N}{V}. \qquad (2.14)$$

Here symbol tr stands for the trace in the spin space and the symbol $\sigma = \uparrow, \downarrow$ denotes the z-projection of the quasiparticle spin. We emphasize that N is the number of real fermions. The latter statement is an essence of the Luttinger theorem.

(iii) The ground state of the Fermi liquid can be represented with the physical picture similar to that of ideal Fermi gas. In the momentum space the quasiparticles occupy the states inside the Fermi sphere of radius p_F. The states outside the Fermi sphere with $p > p_F$ are unoccupied. The Fermi momentum has the same magnitude as for the ideal gas of the same number of real particles. In other words, the quasiparticle distribution function for the ground state has the step-like behavior analogous that in the ideal gas,

$$n_{\sigma\sigma'}^{(0)}(\boldsymbol{p}) = \Theta(p_F - p)\delta_{\sigma\sigma'}. \qquad (2.15)$$

In accordance with Eq. (2.14), the Fermi momentum is given by the relation of ideal Fermi gas:

$$p_F = (3\pi^2 \hbar^3 N/V)^{1/3}. \tag{2.16}$$

Here N/V is the density of the Fermi liquid.

(iv) Due to external perturbations the Fermi liquid can be driven from its ground state. Nevertheless, at zero temperature, $T = 0$, the energy E of such Fermi liquid remains some functional of distribution function $\hat{n}(\boldsymbol{p})$ as well. This is the statement of the *Kohn-Sham theorem*.

2.2.3 Effective mass

In order to trace the similarities between the Fermi liquid and ideal Fermi gas, it is convenient to introduce the *quasiparticle excitation energy*. This quantity can be determined as a variation in the total energy of the the Fermi liquid if one more quasiparticle is introduced into the liquid:

$$\varepsilon_{\sigma\sigma'}[n_{\sigma'\sigma}(\boldsymbol{p})] = \frac{1}{V}\frac{\delta E}{\delta n_{\sigma'\sigma}(\boldsymbol{p})}. \tag{2.17}$$

As stated in item (iv), the quasiparticle excitation energy is the functional of the quasiparticle distribution function $n_{\sigma'\sigma}(\boldsymbol{p})$. Since, according to assumption (iii), the quasiparticle distribution function in the ground state is uniquely determined by the quasiparticle momentum, the quasiparticle excitation energy, $\varepsilon_{\sigma\sigma'}^{(0)}$, in the ground state is a function of the momentum alone. Expanding this function near $p = p_F$, we find

$$\varepsilon_{\sigma\sigma'}^{(0)}(\boldsymbol{p}) = \varepsilon^{(0)}(p)\delta_{\sigma\sigma'}, \quad \varepsilon^{(0)}(p) = \left[\varepsilon_F + v_F(p - p_F)\right] + \dots. \tag{2.18}$$

Here ε_F denotes the magnitude of the quasiparticle energy at $p = p_F$, $\varepsilon_F = \varepsilon^{(0)}(p_F)$. Similarly to the ideal Fermi gas, coefficient v_F determines the velocity of quasiparticles at the Fermi level. This velocity is usually called *the Fermi velocity*. It is also convenient to introduce the effective mass: $m_* = p_F/v_F$. The magnitude of effective mass differs from the mass of real fermions and depends on the interaction between the particles in the liquid. As we will see below, the Fermi liquid in plenty of aspects can be treated as a Fermi gas with the energy spectrum $p^2/2m_*$.

2.2.4 The Landau f-function

In order to describe various physical effects in the Fermi liquid state perturbed from the ground state, we expand the total energy to second order in deviation

of the quasiparticle distribution function from the nonperturbed step-like one, $\delta n_{\sigma_1\sigma_2}(\boldsymbol{p}) = n_{\sigma_1\sigma_2}(\boldsymbol{p}) - n^{(0)}_{\sigma_1\sigma_2}(\boldsymbol{p})$,

$$
E = E_0 + V \sum_\sigma \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \left[\varepsilon^{(0)}(p) - \varepsilon_F\right]\delta n_{\sigma\sigma}(\boldsymbol{p}) + \frac{V}{2} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3}
$$
$$
\times \int \frac{d^3\boldsymbol{p'}}{(2\pi\hbar)^3} f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'})\delta n_{\sigma_2\sigma_1}(\boldsymbol{p})\delta n_{\sigma_3\sigma_4}(\boldsymbol{p'}) + \dots, \qquad (2.19)
$$

where E_0 means the total ground state energy. Here the function $f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'})$, called the *Landau f-function*, is the second variational derivative of the total energy at $\hat{n} = \hat{n}^{(0)}$:

$$
f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'}) = \frac{1}{V}\frac{\delta^2 E}{\delta n_{\sigma_2\sigma_1}(\boldsymbol{p})\delta n_{\sigma_3\sigma_4}(\boldsymbol{p'})} = \frac{\delta\varepsilon_{\sigma_1\sigma_2}(\boldsymbol{p})}{\delta n_{\sigma_3\sigma_4}(\boldsymbol{p'})}. \qquad (2.20)
$$

Since the Landau f-function is the second variational derivative of the total energy, it has the symmetric property: $f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'}) = f_{\sigma_4\sigma_1,\sigma_3\sigma_2}(\boldsymbol{p'},\boldsymbol{p})$.

Equation (2.20) implies that the energy of quasiparticle depends on its momentum as

$$
\varepsilon_{\sigma_1\sigma_2}(\boldsymbol{p}) \approx \left[\varepsilon_F + v_F(p - p_F)\right]\delta_{\sigma_1\sigma_2} + \int \frac{d^3\boldsymbol{p'}}{(2\pi\hbar)^3} f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'})\delta n_{\sigma_3\sigma_4}(\boldsymbol{p'}) + \dots
$$
$$
(2.21)
$$

In what follows, we deal only with the small perturbations $\delta\hat{n}$ of distribution function. For this reason, the absolute magnitudes of momenta $\boldsymbol{p}$ and $\boldsymbol{p'}$ can be put equal to the Fermi momentum, i.e. $p = p' = p_F$. Thus, only the dependence on the angle $\theta = \angle(\boldsymbol{p},\boldsymbol{p'})$ between the vectors $\boldsymbol{p}$ and $\boldsymbol{p'}$ proves to be essential. It is convenient to introduce the following parametrization,

$$
g(\varepsilon_F)f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p},\boldsymbol{p'}) = F^{(0)}(\theta)\delta_{\sigma_1,\sigma_2}\delta_{\sigma_3,\sigma_4} + F^{(\sigma)}(\theta)\boldsymbol{\sigma}_{\sigma_1,\sigma_2}\boldsymbol{\sigma}_{\sigma_3,\sigma_4}, \qquad (2.22)
$$

where $g(\varepsilon_F) = p_F m_*/(\pi^2\hbar^3)$ denotes the density of states at the Fermi energy ε_F and $\boldsymbol{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ denotes the vector of the Pauli matrices.

2.2.5 Relation between m_* and m

Surprisingly, the above assumptions and formulations are sufficient to derive the first non-trivial result. We will express the effective mass m^* of quasiparticles via genuine mass m of particles and the *Landau parameter* F_1.

Let us consider total quasiparticle momentum. We recall the following two points. First, the momentum of unit liquid volume equals the mass density flow.

Second, the number of quasiparticles equals the number of genuine particles. The total momentum of the liquid reads

$$\boldsymbol{P} = V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_\sigma \boldsymbol{p}\, n_{\sigma\sigma}(\boldsymbol{p}). \tag{2.23}$$

Now we compute the total quasiparticle current

$$\boldsymbol{J} = V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_{\sigma,\sigma'} \frac{\partial\varepsilon_{\sigma\sigma'}(\boldsymbol{p})}{\partial\boldsymbol{p}}\, n_{\sigma'\sigma}(\boldsymbol{p}). \tag{2.24}$$

Since the total number of quasiparticles is exactly the same as the total number of particles N and due to the continuity equation, the total quasiparticle current coincides with the total particle flow. Then we use the Galilean invariance relating the total particle momentum and the total particle current as $\boldsymbol{P} = m\boldsymbol{J}$. This relation yields the following identity:

$$V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_\sigma \boldsymbol{p}\, n_{\sigma\sigma}(\boldsymbol{p}) = mV \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_{\sigma,\sigma'} \frac{\partial\varepsilon_{\sigma\sigma'}(\boldsymbol{p})}{\partial\boldsymbol{p}}\, n_{\sigma'\sigma}(\boldsymbol{p}). \tag{2.25}$$

We note that, for an ideal Fermi gas with the quadratic spectrum, this identity is trivial. However, for the Fermi liquid this will result in non-trivial relation between m_* and m. Varying both sides of Eq. (2.25) with respect to $\delta n_{\sigma\sigma'}(\boldsymbol{p})$, we obtain

$$\int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_\sigma \boldsymbol{p}\, \delta n_{\sigma\sigma}(\boldsymbol{p}) = m \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_{\sigma,\sigma'} \frac{\partial\varepsilon_{\sigma\sigma'}(\boldsymbol{p})}{\partial\boldsymbol{p}}\, \delta n_{\sigma'\sigma}(\boldsymbol{p}) + m \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3}$$

$$\times \sum_{\sigma,\sigma',\sigma_1,\sigma_2} n_{\sigma'\sigma}(\boldsymbol{p}) \frac{\partial}{\partial\boldsymbol{p}} \int \frac{d^3\boldsymbol{p}'}{(2\pi\hbar)^3} f_{\sigma\sigma_1,\sigma'\sigma_2}(\boldsymbol{p},\boldsymbol{p}') \delta n_{\sigma_2\sigma_1}(\boldsymbol{p}'). \tag{2.26}$$

Since the above relation should hold for an arbitrary variation of the distribution function $\delta n_{\sigma\sigma'}(\boldsymbol{p})$, we find using the symmetry properties of the Landau f-function,

$$\frac{\boldsymbol{p}}{m}\delta_{\sigma_1\sigma_2} = \frac{\partial\varepsilon_{\sigma_1\sigma_2}(\boldsymbol{p})}{\partial\boldsymbol{p}} - \int \frac{d^3\boldsymbol{p}'}{(2\pi\hbar)^3} \sum_{\sigma,\sigma'} f_{\sigma_1\sigma,\sigma_2\sigma'}(\boldsymbol{p},\boldsymbol{p}') \frac{\partial}{\partial\boldsymbol{p}'} n_{\sigma'\sigma}(\boldsymbol{p}') \tag{2.27}$$

In the ground state we can use the relation $\partial n_{\sigma'\sigma}(\boldsymbol{p}')/\partial\boldsymbol{p}' = -\boldsymbol{p}'\delta(p'-p_F)\delta_{\sigma'\sigma}/p'$. Projecting Eq. (2.27) on the direction of $\boldsymbol{p}$ and choosing $p = p_F$, we obtain

$$\frac{m_*}{m} = 1 + \int\limits_0^\pi \frac{d\theta\sin\theta}{2} \cos\theta\, F^{(0)}(\theta). \tag{2.28}$$

It is convenient to expand $F^{(0/\sigma)}(\theta)$ in a series in the Legendre polynomials:

$$F^{(0/\sigma)}(\theta) = \sum_{l=0}^{\infty} (2l+1) F_l^{(0/\sigma)} P_l(\cos\theta). \tag{2.29}$$

Then we find

$$\frac{m_*}{m} = 1 + F_1^{(0)}. \tag{2.30}$$

The thermodynamic stability implies that $1 + F_l^{(0)} > 0$ [4], i.e., $m_* > 0$. In bulk ^{3}He the magnitudes of the Fermi-liquid parameters are known to be equal $F_0^{(\sigma)} \simeq -0.7$, $F_0^{(0)} \simeq 10.8$, and $F_1^{(0)} \simeq 2.08$.

2.2.6 Specific heat

As usual, the specific heat is related with with changing the total energy in the physical system as the temperature varies. The temperature variation results in changing the distribution function. Thus, the corresponding change in the total energy is determined by the quasiparticle energy, cf. Eq. (2.17). Therefore, at $T \to 0$ the specific heat of the Fermi liquid is given by the following expression, see Eq. (2.19),

$$C_V = V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \sum_{\sigma_1,\sigma_2} \left[\varepsilon_{\sigma_1\sigma_2}^{(0)}(\boldsymbol{p}) - \varepsilon_F \delta_{\sigma_1\sigma_2} \right] \frac{\partial}{\partial T} \delta n_{\sigma_2\sigma_1}(\boldsymbol{p}). \tag{2.31}$$

Due to term $\varepsilon_{\sigma_1\sigma_2}^{(0)}(\boldsymbol{p}) - \varepsilon_F \delta_{\sigma_1\sigma_2}$, the integral over momentum in Eq. (2.31) is restricted with the close vicinity to the Fermi momentum. It is natural to assume that the change of the distribution function due to temperature is similar to the ideal Fermi gas, i.e., can be described by the Fermi-Dirac distribution with some chemical potential variation $\Delta\mu$ and temperature T. We note that the chemical potential correction $\Delta\mu$ appears as a result of keeping the number of particles fixed (statement (ii)). Then, we can write

$$\delta n_{\sigma_2\sigma_1}(\boldsymbol{p}) = \delta_{\sigma_2\sigma_1} \left[\Delta\mu\, \delta(\varepsilon^{(0)}(p) - \varepsilon_F) - \frac{\pi^2 T^2}{6} \delta'(\varepsilon^{(0)}(p) - \varepsilon_F) \right]. \tag{2.32}$$

Here the dash denotes the derivative of the Dirac delta-function. We note that the conservation of the number of particles implies that $\Delta\mu \sim T^2$. Substituting Eq. (2.32) into Eq. (2.31), we find [$\xi = \varepsilon^{(0)}(p) - \varepsilon_F$]

$$C_V = -\frac{\pi^2}{3} V g(\varepsilon_F) \int d\xi \xi \frac{\partial}{\partial \xi} \delta(\xi) = \frac{\pi^2}{3} V g(\varepsilon_F) T = \frac{V p_F m_*}{3\hbar^3} T \tag{2.33}$$

where $g(\varepsilon_F)$ stands for the density of states at the Fermi momentum. We emphasize that result (2.33) is exactly the same as for the ideal Fermi gas on substituting $m \to m_*$.

Problem for the seminar 15: To express $\partial\mu/\partial N$ at zero temperature in terms of the function $F^{(0)}(\theta)$.

Problem for the seminar 16: To express the Pauli spin susceptibility of the Fermi liquid in terms of the function $F^{(\sigma)}(\theta)$.

Exercise 20: Using the results from the lecture on weakly non-ideal Fermi gas, determine the functions $F^{(0)}(\theta)$ and $F^{(\sigma)}(\theta)$ to first order in the interaction strength.

Exercise 21: Using the expression for the Landau f-function, determine $\partial P/\partial V$ to first order in interaction.

Exercise 22: Using the expression for the Landau f-function, determine the variance for thermodynamic fluctuations of the number of particles, $\langle(\Delta N)^2\rangle$ to first order in interaction at low temperatures.

Exercise 23: Using the following expression for the energy of electron system in the magnetic field at $T = 0$,

$$E = \frac{1}{2}E_0(N_\uparrow) + \frac{1}{2}E_0(N_\downarrow) + \frac{\mu_B B}{2}(N_\uparrow - N_\downarrow) + \frac{U}{V}N_\uparrow N_\downarrow,$$

find the spin susceptibility $\partial M/\partial B$ where $M = \mu_B(N_\uparrow - N_\downarrow)/2$ and $E_0(N)$ is the ideal Fermi gas energy.

2.3 Weakly non-ideal Bose gas

2.3.1 Introduction

In this lecture we consider simplest model of interacting bosons.

2.3.2 Hamiltonian

We consider the three-dimensional spinless bosons interacting via the repulsive contact interaction $U > 0$. The many-body Hamiltonian has the following form: $\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_{\text{int}}$, where

$$\mathscr{H}_0 = \sum_{\boldsymbol{p}} \varepsilon^{(0)}(p) b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}}, \quad \mathscr{H}_{\text{int}} = \frac{U}{2V} \sum_{\boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_3 + \boldsymbol{p}_4} b_{\boldsymbol{p}_1}^\dagger b_{\boldsymbol{p}_2}^\dagger b_{\boldsymbol{p}_3} b_{\boldsymbol{p}_4}. \tag{2.34}$$

Here $\varepsilon^{(0)}(p)$ denotes the bare spectrum assumed to be quadratic, $\varepsilon^{(0)}(p) = p^2/2m$. The operator $b_{\boldsymbol{p}}^\dagger$ creates a boson in the single particle state with momentum $\boldsymbol{p}$. The operator $b_{\boldsymbol{p}\sigma}$ annihilates a boson from single particle state with momentum $\boldsymbol{p}$. We remind that the creation and annihilation operators satisfy the following commutation relation,

$$b_{\boldsymbol{p}'} b_{\boldsymbol{p}}^\dagger - b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}'} = \delta_{\boldsymbol{p}\boldsymbol{p}'} \delta_{\sigma\sigma'}. \tag{2.35}$$

Also the following identity holds for,

$$\langle b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}'} \rangle = \text{Tr}\, b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}'} e^{-\beta \mathscr{H}_0} \Big/ \text{Tr}\, e^{-\beta \mathscr{H}_0} = f_B\big(\varepsilon^{(0)}(p)\big) \delta_{\boldsymbol{p}\boldsymbol{p}'}. \tag{2.36}$$

Hereafter we deal with the canonical ensemble keeping the constant number of particles N in mind.

2.3.3 Condensate

As we know, there is a phenomenon of Bose-Einstein condensation in the three-dimensional ideal Bose gas. Before diagonalizing the Hamiltonian $\mathscr{H}$, we should take an existence of condensate into account. This means that the occupation number of the zero-momentum many-body state, $p = 0$, is macroscopically large, i.e., $\langle b_0^\dagger b_0 \rangle = N_0 \sim N$. The convenient way to take this fact into account is to treat the creation and annihilation operators $b_0^\dagger$ and b_0 as real numbers but operators. They satisfy the relation

$$b_0^2 + \sum_{\boldsymbol{p} \neq 0} b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}} = N. \tag{2.37}$$

Also we assume that the number of particles in the states with $p > 0$ is small. Then, we can simplify the interaction Hamiltonian in the following way,

$$\mathscr{H}_{\mathrm{int}} \to \mathscr{H}_{\mathrm{int}}^{(2)} = \frac{U}{2V}b_0^4 + \frac{U}{2V}b_0^2 \sum_{\boldsymbol{p}\neq 0}\left[b_{\boldsymbol{p}}b_{-\boldsymbol{p}} + b_{\boldsymbol{p}}^\dagger b_{-\boldsymbol{p}}^\dagger + 4b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}}\right] + \cdots = \frac{UN^2}{2V}$$

$$+ \frac{UN}{2V}\sum_{\boldsymbol{p}\neq 0}\left[b_{\boldsymbol{p}}b_{-\boldsymbol{p}} + b_{\boldsymbol{p}}^\dagger b_{-\boldsymbol{p}}^\dagger + 2b_{\boldsymbol{p}}^\dagger b_{\boldsymbol{p}}\right] + \ldots \qquad (2.38)$$

Here we neglect the terms that contain either one or zero b_0. Also we have expressed b_0^2 in terms of particle number N using the relation (2.37). Now the total Hamiltonian $\mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}^{(2)}$ is quadratic in the creation and annihilation operators. However, $\mathscr{H}_{\mathrm{int}}^{(2)}$ contains the terms which do not conserve the number of bosons. This implies that $\mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}^{(2)}$ is not diagonal in the initial single particle basis.

2.3.4   Unitary transformation of the Hamiltonian

In order to diagonalize quadratic Hamiltonian $\mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}^{(2)}$, it is convenient to perform the unitary canonical transformation called the *Bogolubov transformation*. Let us introduce new creation and annihilation boson operators $\boldsymbol{\beta}_{\boldsymbol{p}}^\dagger$ and $\boldsymbol{\beta}_{\boldsymbol{p}}$ satisfying the commutation relation (2.35). Now we express the original boson creation and annihilation operators via the linear combinations of new ones

$$b_{\boldsymbol{p}} = u_p\boldsymbol{\beta}_{\boldsymbol{p}} + v_p\boldsymbol{\beta}_{-\boldsymbol{p}}^\dagger, \qquad b_{\boldsymbol{p}}^\dagger = u_p\boldsymbol{\beta}_{\boldsymbol{p}}^\dagger + v_p\boldsymbol{\beta}_{-\boldsymbol{p}}. \qquad (2.39)$$

Here u_p and v_p are real functions of the momentum. To fix them, we impose two conditions:

(i) operators $b_{\boldsymbol{p}}^\dagger$ and $b_{\boldsymbol{p}}$ satisfy the relation (2.35);

(ii) Hamiltonian $\mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}^{(2)}$ expressed in terms of operators $\boldsymbol{\beta}_{\boldsymbol{p}}^\dagger$ and $\boldsymbol{\beta}_{\boldsymbol{p}}$ does not contain terms like $\boldsymbol{\beta}_{\boldsymbol{p}}^\dagger\boldsymbol{\beta}_{-\boldsymbol{p}}^\dagger$ and $\boldsymbol{\beta}_{\boldsymbol{p}}\boldsymbol{\beta}_{-\boldsymbol{p}}$.

The requirement (i) results in the constraint: $u_p^2 - v_p^2 = 1$. This can be satisfied by an auxillary function θ_p such that $u_p = \cosh\theta_p$ and $v_p = \sinh\theta_p$. The second requirement determines the function θ_p as

$$\sinh 2\theta_p = -\frac{UN}{V\varepsilon(p)}, \quad \varepsilon(p) = \sqrt{(\varepsilon^{(0)}(p) + UN/V)^2 - (UN/V)^2}. \qquad (2.40)$$

The quadratic Hamiltonian becomes

$$\mathscr{H}_0 + \mathscr{H}_{\text{int}}^{(2)} = E_0 + \sum_{\boldsymbol{p}\neq 0} \varepsilon(p) \boldsymbol{\beta}_{\boldsymbol{p}}^{\dagger} \boldsymbol{\beta}_{\boldsymbol{p}},$$

$$E_0 = \frac{UN^2}{2V} + \frac{1}{2} \sum_{\boldsymbol{p}\neq 0} \left[\varepsilon(p) - \varepsilon^{(0)}(p) - \frac{UN}{V} \right]. \tag{2.41}$$

The form (2.41) of the quadratic Hamiltonian suggests that operators $\boldsymbol{\beta}_{\boldsymbol{p}}^{\dagger}$ creates and operator $\boldsymbol{\beta}_{\boldsymbol{p}}$ annihilates the quasiparticles with the energy $\varepsilon(p)$. The ground state energy is given by E_0. For the quadratic bare spectrum, $\varepsilon^{(0)}(p) = p^2/2m$, the quasiparticle energy has the following dependence on the momentum,

$$\varepsilon(p) = \sqrt{u^2 p^2 + \left(\frac{p^2}{2m} \right)^2} = \begin{cases} up, & p \ll \sqrt{aN/V} \\ p^2/(2m), & \sqrt{aN/V} \ll p. \end{cases} \tag{2.42}$$

Here we introduce the scattering length $a = mU/(4\pi\hbar^2)$. Therefore, the quasiparticle spectrum at small momentum has acoustic phonon dispersion with the sound velocity $u = \sqrt{4\pi aN/(m^2 V)}$. At large momentum the quasiparticle spectrum is almost the same as the bare one.

The ground state energy (2.41) can be expressed via the scattering length as [4]

$$E_0 = \frac{2\pi\hbar^2 a N^2}{mV} \left[1 + \frac{128}{15} \left(\frac{a^3 N}{\pi V} \right)^{1/2} \right]. \tag{2.43}$$

As one can see, the expansion in interaction is governed by the small parameter $a^3 N/V \ll 1$. Differentiating the ground state energy E_0 with respect to the number of particles, we find the chemical potential at zero temperature:

$$\mu(T = 0) = \frac{4\pi\hbar^2 a N}{mV} \left[1 + \frac{32}{3} \left(\frac{a^3 N}{\pi V} \right)^{1/2} \right]. \tag{2.44}$$

We emphasize that the chemical potential of non-ideal Bose at zero temperature is *positive*. As we will see below, this implies that not all the particles are in the condensate at zero temperature. Also we note that the small parameter of the theory can be written as a ratio $\mu(T = 0)/T_{\text{BEC}} \sim a(N/V)^{1/3} \ll 1$ (see Eq. (1.89)).

2.3.5 Specific heat

Using Eq. (2.41), we can write the total energy in the following form,

$$E = E_0 + V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \frac{\varepsilon(p)}{e^{\beta\varepsilon(p)} - 1}. \tag{2.45}$$

Approximating the quasiparticle spectrum by its small momentum asymptote, we find the total energy,

$$E = E_0 + \frac{\pi^2}{30} \frac{VT^4}{u^3}.$$

(2.46)

The evaluation of the integral in such approximation requires the characteristic thermal momentum T/u to be smaller than μ. This limits the applicability of Eq. (2.46) with low temperatures, $T \ll \mu(T = 0)$. The specific heat can be written as

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{2\pi^2}{15} \frac{VT^3}{u^3}.$$

(2.47)

2.3.6 The number of particles in the condensate

Using the relation (2.37), we can express the average number of particles in the condensate via the quasiparticle distribution function:

$$N_0 = b_0^2 = N - V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^2} \left[u_p^2 f_B(\varepsilon(p)) + v_p^2\big(f_B(\varepsilon(p)) + 1\big)\right].$$

(2.48)

Replacing the distribution function f_B with its zero magnitude at temperature $T = 0$, we obtain the number of particles in the condensate at zero temperature,

$$N_0(T = 0) = N - V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \frac{m^2 u^2}{2\varepsilon(p)[\varepsilon(p) + p^2/(2m) + mu^2]}$$
$$= N \left[1 - \frac{8}{3}\left(\frac{a^3 N}{\pi V}\right)^{1/2}\right].$$

(2.49)

As we have mentioned above, due to interparticle interaction the number of particles in the condensate at zero temperature is smaller than the total number of particles N. This effect is called the *depletion of condensate*.

2.3.7 The Gross–Pitaevskii equation

In the absence of the translation invariance it is convenient to develop another formulation of the theory of weakly non-ideal Bose gas at zero temperature. Let us introduce the operator $\Psi(\boldsymbol{r}) = \sum_{\boldsymbol{p}} b_{\boldsymbol{p}} e^{i\boldsymbol{pr}}/\sqrt{V}$. In the Heisenberg representation the operator $b_{\boldsymbol{p}}$ becomes time-dependent and satisfies the following equation:

$$\frac{db_{\boldsymbol{p}}}{dt} = i[\mathscr{H} - \mu\mathscr{N}, b_{\boldsymbol{p}}].$$

(2.50)

Using the commutation relation (2.35), we find

$$i\frac{db_{\boldsymbol{p}}}{dt} = \left(\varepsilon^{(0)}(p) - \mu\right)b_{\boldsymbol{p}} + \frac{U}{V}\sum_{\boldsymbol{p}+\boldsymbol{p}_2=\boldsymbol{p}_3+\boldsymbol{p}_4} b_{\boldsymbol{p}_2}^{\dagger}b_{\boldsymbol{p}_3}b_{\boldsymbol{p}_4}. \qquad (2.51)$$

This equation can be rewritten as the following equation for the operator $\Psi(\boldsymbol{r})$:

$$i\frac{d\Psi(\boldsymbol{r})}{dt} = \left(-\frac{\nabla^2}{2m} - \mu + V_{\text{ext}}(\boldsymbol{r})\right)\Psi(\boldsymbol{r}) + U\Psi^{\dagger}(\boldsymbol{r})\Psi^2(\boldsymbol{r}). \qquad (2.52)$$

Here we have used the quadratic bare spectrum and added the external confining potential $V_{\text{ext}}(\boldsymbol{r})$. At low temperatures the operator $\Psi(\boldsymbol{r})$ is dominated by its condensate part which can approximately be treated as a usual numerical variable $\Psi_0(\boldsymbol{r})$. The accurate consideration demonstrates that the interaction potential U should be substituted by the scattering length. Then, we arrive at the *Gross-Pitaevskii* equation for the *condensate wave function*

$$i\frac{d\Psi_0(\boldsymbol{r})}{dt} = \left(-\frac{\nabla^2}{2m} - \mu + V_{\text{ext}}(\boldsymbol{r})\right)\Psi_0(\boldsymbol{r}) + \frac{4\pi\hbar^2 a}{m}|\Psi_0(\boldsymbol{r})|^2\Psi_0(\boldsymbol{r}). \qquad (2.53)$$

In the absence of the external potential, the homogeneous solution Ψ_0 exists provided that the chemical potential equals $4\pi\hbar^2 a|\Psi_0|^2/m$. Comparing this expression with Eq. (2.44), we find that $|\Psi_0|^2$ is equal to the condensate density N_0/V.

> *Problem for the seminar 17:* Compute the ground state energy E_0 given by Eq. (2.41).

> *Problem for the seminar 18:* Compute the temperature dependence of the number of particles in condensate at $\mu(0) \ll T \ll T_{\text{BEC}}(an^{1/3})^{1/4}$.

> *Problem for the seminar 19:* Using the Gross-Pitaevskii equation, find the solution for a vortex and determine its energy.

> *Exercise 24:* Compute $\text{Tr}\left[b_{\boldsymbol{p}}^{\dagger}e^{-\beta\varepsilon(p)b_{\boldsymbol{p}}^{\dagger}b_{\boldsymbol{p}}/2}b_{\boldsymbol{p}}e^{-\beta\varepsilon(p)b_{\boldsymbol{p}}^{\dagger}b_{\boldsymbol{p}}/2}\right]/\text{Tr}\left[e^{-\beta\varepsilon(p)b_{\boldsymbol{p}}^{\dagger}b_{\boldsymbol{p}}}\right]$.

> *Exercise 25:* Determine the pressure of non-ideal Bose gas at zero temperature.

Exercise 26: Compute the zero-temperature sound velocity $c_s = \sqrt{-(V^2/(mN))\partial P/\partial V}$ in non-ideal Bose gas. To find its deviation from the velocity u.

Exercise 27: Find the dependence of the chemical potential on T at low temperatures, $T \ll \mu(T = 0)$.

Exercise 28: Determine the dependence of the number of particles in the condensate at low temperatures. To compare with the result for an ideal Bose gas.

Exercise 29: Using the Gross-Pitaevskii equation, determine the spectrum of weak modulation of the condensate wave function.

2.4 Superfluidity

2.4.1 Introduction

In this lecture we consider the phenomenon of superfluidity.

2.4.2 Criterion of superfluidity

The shape of the quasiparticle spectrum in liquid helium has been suggested by Lev Landau (see Fig. 2.1). For the small magnitudes of momentum, the spectrum is phonon-like and similar to the spectrum of non-ideal Bose gas, i.e. $\varepsilon_{\mathrm{ph}}(p) = up$. In contrast to the non-ideal Bose gas the spectrum in Fig. 2.1 has the minimum at nonzero momentum p_0. Near the minimum the quasiparticle spectrum can be approximated as $\varepsilon_{\mathrm{rot}}(p) = \Delta + (p - p_0)^2/(2m_{\mathrm{r}})$. The corresponding segment of the spectrum is called the *roton* spectrum. For the liquid helium, the parameters of the phonon and roton spectra are known to be as follows: $u \approx 240$ m/s, $\Delta \approx 8.6$ K, $m_{\mathrm{r}} \approx 0.14\, m_{^4\mathrm{He}}$, and $p_0/\hbar \approx 1.9 \cdot 10^8$ cm^{-1}.

Let us consider liquid helium flowing with some velocity in a capillary at zero temperature. The energy E and momentum $\boldsymbol{P}$ are related to the energy E_0 and momentum $\boldsymbol{P_0}$ in the coordinate frame where the liquid helium is at rest in the following way:

$$E = E_0 + \boldsymbol{P_0}\boldsymbol{v} + Mv^2/2, \quad \boldsymbol{P} = \boldsymbol{P_0} + M\boldsymbol{v}. \qquad (2.54)$$

Here M denotes the total mass of the liquid helium. Let us imagine that a quasiparticle with momentum p is created in the frame where the fluid is at rest. Then the energy and momentum of the liquid are equal to $E_0 = \varepsilon(p)$ and $P_0 = p$. Correspondingly, the energy of the fluid flowing with velocity $\boldsymbol{v}$ in the presence of a single quasiparticle is given as $E = \varepsilon(p) + \boldsymbol{p}\boldsymbol{v} + Mv^2/2$. Hence we can conclude that the energy of a quasiparticle in the fluid flowing at velocity $\boldsymbol{v}$ becomes $\varepsilon(p) + \boldsymbol{p}\boldsymbol{v}$. If this quantity is positive, the creation of quasiparticles is energetically unfavorable. Consequently, a quasiparticle in the flowing fluid can be created if its velocity v is larger than $\varepsilon(p)/p$ at least at some nonzero value of the momentum p. Therefore, there is no quasiparticle production in the fluid flowing at the velocities below the *critical velocity*,

$$v < v_{\mathrm{cr}} = \min_p[\varepsilon(p)/p]. \qquad (2.55)$$

The absence of quasiparticles at zero temperature suggests that the liquid can experience the frictionless flow, demonstrating the phenomenon of *superfluidity*.
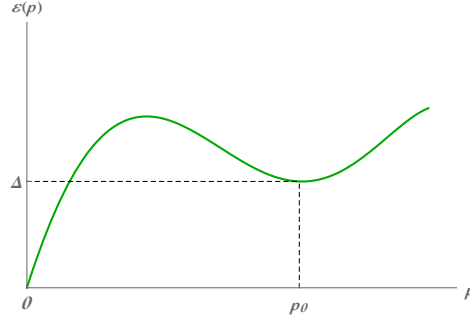
Figure 2.1: Sketch of the quasiparticle spectrum in the liquid helium. The linear part at $p \to 0$ corresponds to the phonon branch. The vicinity of the momentum p_0 describes the roton branch.

2.4.3   Density of the normal component

At nonzero temperature there is a finite number of excitations in the liquid. However, if condition (2.55) is fulfilled, there are no additional excitations which can be created. Let us assume that the fluid flows as a whole with velocity $\boldsymbol{v}_s$ whereas the gas of quasiparticles move at velocity $\boldsymbol{v}_n$. In the coordinate frame in which the liquid is at rest the quasiparticles move at velocity $\boldsymbol{v}_n - \boldsymbol{v}_s$. The quasiparticle with energy $\varepsilon(p)$ in the frame where the fluid is at rest can be produced with the probability $f_B(\varepsilon(p) - \boldsymbol{p}(\boldsymbol{v}_n - \boldsymbol{v}_s))$ since the probability is equal to $f_B(\varepsilon)$ for the quasiparticles at rest. Therefore, the total momentum of quasiparticles per unit volume becomes

$$\boldsymbol{P} = \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3}\boldsymbol{p}\, f_B\big(\varepsilon(p) - \boldsymbol{p}(\boldsymbol{v}_n - \boldsymbol{v}_s)\big). \qquad (2.56)$$

On the other hand, the total momentum can be written as the momentum per unit volume in the coordinate frame at which the liquid is at rest: $\boldsymbol{P} = \boldsymbol{j} - \rho\boldsymbol{v}_s$. Here ρ stands for the total density of the liquid and $\boldsymbol{j}$ denotes the momentum in the laboratory frame, so-called *mass flow*. In order to construct the expression for $\boldsymbol{j}$, we should take the following physical constraints into account:

(i) momentum $\boldsymbol{P}$ depends on the difference $\boldsymbol{v}_n - \boldsymbol{v}_s$;

(ii) mass flow $\boldsymbol{j}$ is a vector and should be a function of two vectors $\boldsymbol{v}_n$ and $\boldsymbol{v}_s$.

The only possibility is to set $\boldsymbol{j} = \rho_n\boldsymbol{v}_n + \rho_s\boldsymbol{v}_s$ where $\rho = \rho_n + \rho_s$; ρ_n and ρ_s are called *the density of the normal component* and *the superfluid density*, respectively. We note that, in general, the densities ρ_n and ρ_s are some scalar functions of the

relative or counterflow velocity $\boldsymbol{w} = \boldsymbol{v}_n - \boldsymbol{v}_s$. Expanding the right hand side of Eq. (2.56) in the limit $w \to 0$, we find

$$\rho_n = \frac{1}{3} \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} p^2 \left(-\frac{\partial f_B(\varepsilon)}{\partial \varepsilon} \right)_{\varepsilon = \varepsilon(p)}. \qquad (2.57)$$

The phase transition to the superfluid state from the normal state occurs at the so-called λ–*point* at which $\rho_s = \rho - \rho_n$ vanishes. The normal-superfluid transition temperature for the liquid helium is 2.17 K at zero pressure. In the superfluid phase, $\rho_s > 0$ and $\rho_s = \rho$ at $T = 0$.

2.4.4 Specific heat

Thermodynamics of superfluid liquid is determined by the quasiparticle excitations. Their free energy can be written as

$$F_{qp} = TV \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \ln \left[1 - e^{-\beta(\varepsilon(p) - \boldsymbol{p}\boldsymbol{w})} \right]. \qquad (2.58)$$

The following remark is in order here. The right hand side of the expression for F_{qp} resembles the thermodynamic potential of the Bose gas with zero chemical potential. This is not occasionally. The number of quasiparticles is determined by the extremum of their energy, i.e., the chemical potential of quasiparticles in the thermal equilibrium is zero, $\mu_{qp} = \partial E_{qp}/\partial N_{qp} = 0$. In the case of weakly non-ideal Bose gas we have checked it by the direct computation of the energy. For zero chemical potential, the thermodynamic potential and the free energy coincide. The energy of quasiparticles can be written as

$$E_{qp} = V \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3} \frac{\varepsilon(p) - \boldsymbol{p}\boldsymbol{w}}{e^{\beta(\varepsilon(p) - \boldsymbol{p}\boldsymbol{w})} - 1}. \qquad (2.59)$$

At zero relative velocity, $w = 0$, the phonon contribution to the energy is the same as in the non-ideal Bose gas, cf. Eq. (2.46).

Problem for the seminar 20: Show that the critical velocity to produce two excitations in superfluid exceeds that for the single one.

Problem for the seminar 21: Find the contributions to the normal density ρ_n from the phonon and roton parts of the spectrum.

Problem for the seminar 22: Calculate the roton contribution to specific heat at zero relative velocity.

Exercise 30: Show that the critical velocity is smaller than Δ/p_0. Use the condition $\Delta \ll p_0^2/m$.

Exercise 31: Find the critical velocity for a non-ideal Bose gas.

Exercise 32: Determine how the normal density depends on the relative velocity w, resulting from the sound segment of excitation spectrum.

Exercise 33: Determine how the normal density depends on the relative velocity w, resulting from the roton segment of excitation spectrum.

Exercise 34: Calculate the phonon contribution to specific heat as a function of relative velocity.

2.5 Superconductivity

2.5.1 Introduction

In this lecture we discuss the Bardeen–Cooper–Schrieffer (BCS) model and thermodynamic aspects of the superconductivity phenomenon.

2.5.2 The Cooper instability

Let us consider two electrons with the opposite spins and with the attraction between them in the vicinity of the Fermi surface. The two-particle Schrödinger equation reads

$$\left[-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) + U(\boldsymbol{r}_1 - \boldsymbol{r}_2)\right]\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \left(\delta\epsilon + \frac{p_F^2}{m}\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2). \quad (2.60)$$

We assume that the electrons have the opposite momenta $\boldsymbol{p}$ and $-\boldsymbol{p}$ such that the electron pair as a whole is at rest. Let two electrons are above the Fermi surface, i.e., the momentum corresponding to their relative motion satisfies the inequality, $p > p_F$. Also we assume that the attraction potential is constant, $U(\boldsymbol{r}_1 - \boldsymbol{r}_2) = -\lambda\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ with $\lambda > 0$. It is convenient to introduce the center-of-mass coordinate $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ and the relative coordinate $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. Then the Schrödinger equation for the Fourier transform of the wave function, $\tilde{\psi}(\boldsymbol{p}) = \int d^3\boldsymbol{r}\, e^{-i\boldsymbol{p}\boldsymbol{r}/\hbar}\psi(\boldsymbol{r})$, that describes the relative motion, can be written as follows,

$$\frac{p^2}{m}\tilde{\psi}(\boldsymbol{p}) - \frac{\lambda}{V}\sum_{\boldsymbol{p}'}\tilde{\psi}(\boldsymbol{p}') = \left(\delta\epsilon + \frac{p_F^2}{m}\right)\tilde{\psi}(\boldsymbol{p}). \quad (2.61)$$

To have nontrivial solution of the equation, the following relation should be fulfilled

$$1 = \sum_{\boldsymbol{p}}\frac{\lambda/V}{p^2/m - p_F^2/m - \delta\epsilon} = \frac{\lambda g(E_F)}{4}\int\limits_0^{\varepsilon_\Lambda}\frac{d\varepsilon}{\varepsilon - \delta\epsilon/2} = \frac{\lambda g(E_F)}{4}\ln\frac{\varepsilon_\Lambda}{-\delta\epsilon/2}. \quad (2.62)$$

Here $g(E_F) = p_F m/(\pi^2\hbar^3)$ denotes the density of states at the Fermi energy. We have here introduced the high energy cut-off ε_Λ to regularize the integral over energies. On the whole, we obtain that a pair of electrons with attraction has the negative binding energy $\delta\epsilon = -2\varepsilon_\Lambda\exp(-4/[\lambda g(\varepsilon_F)])$. This implies that an arbitrary weak attraction favors the creation of electron pairs with momenta $\boldsymbol{p}$ and $-\boldsymbol{p}$ near the Fermi surface. This phenomenon is referred to as *Cooper instability* and is analogous to the formation of a bound state in an arbitrary weak one-dimensional potential well.

2.5.3   The mean-field solution of BCS Hamiltonian

Motivated by the Cooper instability phenomenon, we simplify the Hamiltonian (2.1) and consider the following many-body Hamiltonian (it is known as the *Bardeen-Cooper-Schrieffer Hamiltonian*): $\mathscr{H}_{\mathrm{BCS}} = \mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}$, where

$$\mathscr{H}_0 = \sum_{\boldsymbol{p},\sigma} \varepsilon^{(0)}(p) a_{\boldsymbol{p}\sigma}^\dagger a_{\boldsymbol{p}\sigma}, \quad \mathscr{H}_{\mathrm{int}} = -\frac{\lambda}{V} \sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} a_{\boldsymbol{p}_1\uparrow}^\dagger a_{-\boldsymbol{p}_1\downarrow}^\dagger a_{\boldsymbol{p}_2\downarrow} a_{-\boldsymbol{p}_2\uparrow}. \qquad (2.63)$$

Here $\varepsilon^{(0)}(p)$ denotes the bare electron spectrum assume to be quadratic, $\varepsilon^{(0)}(p) = p^2/2m$. The operator $a_{\boldsymbol{p}\sigma}^\dagger$ creates a fermion in a single particle state with momentum $\boldsymbol{p}$ and spin projection $\sigma = \uparrow, \downarrow$. The operator $a_{\boldsymbol{p}\sigma}$ annihilates a fermion from the single particle state with momentum $\boldsymbol{p}$ and spin projection σ. The positive constant $\lambda = 4\pi\hbar^2|a|/m$ governs the magnitude of the attraction between the fermions and a stands for the negative scattering length.

Let us perform the canonical transformation of the fermion annihilation operators:

$$a_{\boldsymbol{p},\uparrow} = u_p \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow} + v_p \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow}^\dagger, \quad a_{\boldsymbol{p},\downarrow} = u_p \boldsymbol{\alpha}_{\boldsymbol{p},\downarrow} - v_p \boldsymbol{\alpha}_{-\boldsymbol{p},\uparrow}^\dagger. \qquad (2.64)$$

The creation operators transform accordingly. New operators $\boldsymbol{\alpha}_{\boldsymbol{p},\sigma}^\dagger$ and $\boldsymbol{\alpha}_{\boldsymbol{p},\sigma}$ satisfy the proper anti-commutation relations provided the following relation should hold for

$$u_p^2 + v_p^2 = 1. \qquad (2.65)$$

In order to resolve this constraint, we can use the parametrization: $u_p = \cos\theta_p$ and $v_p = \sin\theta_p$. Then we find

$$\mathscr{H} - \mu\mathscr{N} = 2\sum_{\boldsymbol{p}} \xi_p v_p^2 + \sum_{\boldsymbol{p},\sigma} \xi_p (u_p^2 - v_p^2) \boldsymbol{\alpha}_{\boldsymbol{p},\sigma}^\dagger \boldsymbol{\alpha}_{\boldsymbol{p},\sigma} + 2\sum_{\boldsymbol{p}} \xi_p u_p v_p \big(\boldsymbol{\alpha}_{\boldsymbol{p},\uparrow}^\dagger \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow}^\dagger$$

$$+ \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow} \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow}\big) - \frac{\lambda}{V} \sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} \mathscr{A}_{\boldsymbol{p}_1}^\dagger \mathscr{A}_{\boldsymbol{p}_2}, \qquad (2.66)$$

where $\xi_p = \varepsilon^{(0)}(p) - \mu$ and

$$\mathscr{A}_{\boldsymbol{p}} = u_p^2 \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow} \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow} - v_p^2 \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow}^\dagger \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow}^\dagger + u_p v_p \big(\boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow} \boldsymbol{\alpha}_{-\boldsymbol{p},\downarrow}^\dagger - \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow}^\dagger \boldsymbol{\alpha}_{\boldsymbol{p},\uparrow}\big). \qquad (2.67)$$

Now we assume that new operators $\boldsymbol{\alpha}_{\boldsymbol{p},\sigma}^\dagger$ and $\boldsymbol{\alpha}_{\boldsymbol{p},\sigma}$ describe annihilation and creation of non-interacting quasiparticles with some energies $\varepsilon_\sigma(p)$. Then we find the following average

$$\langle \mathscr{H} - \mu\mathscr{N} \rangle = 2\sum_{\boldsymbol{p}} \xi_p v_p^2 + \sum_{\boldsymbol{p},\sigma} \xi_p (u_p^2 - v_p^2) n_\sigma(p) - \Delta^2 V/\lambda, \qquad (2.68)$$

where $n_\sigma(p) = \langle \boldsymbol{\alpha}_{\boldsymbol{p},\sigma}^\dagger \boldsymbol{\alpha}_{\boldsymbol{p},\sigma} \rangle$ and

$$\Delta = \frac{\lambda}{V} \sum_{\boldsymbol{p}} u_p v_p \big(1 - n_\uparrow(p) - n_\downarrow(p) \big). \tag{2.69}$$

Next we minimize $\langle \mathscr{H} - \mu \mathscr{N} \rangle$ over θ_p at the fixed values of $n_\sigma(p)$ (i.e., at the constant entropy). The minimum corresponds to the following values of u_p and v_p:

$$u_p^2 = \frac{1}{2} \left(1 + \frac{\xi_p}{\sqrt{\Delta^2 + \xi_p^2}} \right), \quad v_p^2 = \frac{1}{2} \left(1 - \frac{\xi_p}{\sqrt{\Delta^2 + \xi_p^2}} \right). \tag{2.70}$$

For these values of u_p and v_p, the Hamiltonian (2.66) becomes

$$\mathscr{H} - \mu \mathscr{N} = E_0 + \mathscr{H}_{\mathrm{qp}}^{(0)} + \mathscr{H}_{\mathrm{qp}}^{(\mathrm{int})}, \tag{2.71}$$

where

$$\mathscr{H}_{\mathrm{qp}}^{(0)} = \sum_{\boldsymbol{p},\sigma} \varepsilon(p) \boldsymbol{\alpha}_{\boldsymbol{p},\sigma}^\dagger \boldsymbol{\alpha}_{\boldsymbol{p},\sigma}, \quad \varepsilon(p) = \sqrt{\Delta^2 + \xi_p^2},$$

$$E_0 = \sum_{\boldsymbol{p}} \big(\xi_p - \varepsilon(p) \big) + \sum_{\boldsymbol{p}} \frac{\Delta^2}{2\varepsilon(p)} \big(1 - n_\uparrow(p) - n_\downarrow(p) \big). \tag{2.72}$$

The Hamiltonian $\mathscr{H}_{\mathrm{qp}}^{(\mathrm{int})} = -(\lambda/V) \sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} \big(\mathscr{A}_{\boldsymbol{p}_1}^\dagger - \langle \mathscr{A}_{\boldsymbol{p}_1}^\dagger \rangle \big) \big(\mathscr{A}_{\boldsymbol{p}_2} - \langle \mathscr{A}_{\boldsymbol{p}_2} \rangle \big)$ describes the interaction of quasiparticles. It can safely be neglected. The quadratic Hamiltonian $\mathscr{H}_{\mathrm{qp}}^{(0)}$ suggests that the distribution functions of the quasiparticles are given as $n_\uparrow(p) = n_\downarrow(p) = f_F\big(\varepsilon(p) \big)$. The parameter Δ determines *the gap* in the quasiparticle spectrum and satisfies the *self-consistent equation* (cf. Eq. (2.69)):

$$\Delta = \frac{\lambda}{V} \sum_{\boldsymbol{p}} \frac{\Delta}{2\varepsilon(p)} \tanh \frac{\varepsilon(p)}{2T}. \tag{2.73}$$

Equations (2.72) and (2.73) constitute the mean–field solution of the BCS Hamiltonian. We mention that the BCS Hamiltonian can formally be solved exactly via the Bethe anzats method [7]. We note that the self-consistent equation can be written as $\Delta = -(\lambda/V) \sum_{\boldsymbol{p}} \langle a_{\boldsymbol{p}\uparrow} a_{-\boldsymbol{p}\downarrow} \rangle$. The average $\langle a_{\boldsymbol{p}\uparrow} a_{-\boldsymbol{p}\downarrow} \rangle$ is referred to as the *anomalous average*.

2.5.4 The ground state

The self-consistent gap equation, Eq. (2.73), has an obvious solution $\Delta = 0$. At the same time it has non-trivial solution as well. Let us find non-trivial solution

at $T = 0$. Then the gap equation becomes

$$1 = \frac{\lambda}{2} \int \frac{d^3 \boldsymbol{p}}{(2\pi\hbar)^3} \frac{1}{\sqrt{\Delta^2 + \xi_p^2}}. \tag{2.74}$$

Linearizing the bare spectrum near the Fermi energy, we can use approximation $\xi_p = v_F(p - p_F)$. Introducing the high energy cut-off for the integral over momentum, we find

$$1 = \frac{\lambda g(E_F)}{2} \int\limits_0^{\varepsilon_\Lambda} \frac{d\xi_p}{\sqrt{\Delta^2 + \xi_p^2}} \quad \rightarrow \quad \Delta(T = 0) = \Delta_0 = \varepsilon_\Lambda e^{-2/[\lambda g(E_F)]}. \tag{2.75}$$

In order to determine which solution $\Delta = 0$ or $\Delta = \Delta_0$ is realized, we should find a difference in the ground state energy for these solutions. This difference is called the *condensation energy*. The latter is given by

$$E_{\text{cond}} = E_0[\Delta_0] - E_0[0] = \sum_{\boldsymbol{p}} \left(\frac{\Delta_0^2}{2\varepsilon(p)} - \frac{\Delta_0^2}{\varepsilon(p) + |\xi_p|} \right) = -\frac{V g(E_F) \Delta_0^2}{2}$$

$$\times \int\limits_0^\infty \frac{dx(\sqrt{x^2 + 1} - x)}{\sqrt{x^2 + 1}(\sqrt{x^2 + 1} + x)} = -\frac{V g(E_F) \Delta_0^2}{4}. \tag{2.76}$$

Therefore, one can see that at $T = 0$ it is more energetically favorable to open the gap Δ_0 at the Fermi energy in the quasiparticle spectrum. One can demonstrate that the condensation energy decreases with increasing the temperature and vanishes at the critical temperature T_c.

We note that the quasiparticle spectrum $\varepsilon(p) = \sqrt{\Delta^2 + \xi_p^2}$ has nonzero critical velocity. Therefore, superfluidity is possible in the Fermi gas with attraction. Because of electron charge the superfluid properties affect the temperature behavior of the electrical resistivity. Below the critical temperature T_c the resistivity vanishes. This phenomenon is termed as *superconductivity*.

2.5.5 Specific heat

Using Eq. (2.72), the total energy can be written as

$$E = E_0 + 2 \sum_{\boldsymbol{p}} \varepsilon(p) f_F\big(\varepsilon(p)\big). \tag{2.77}$$

The specific heat can be obtained as follows

$$C_V = 2 \sum_{\boldsymbol{p}} \varepsilon(p) \frac{\partial f_F\big(\varepsilon(p)\big)}{\partial T}. \tag{2.78}$$

At low temperatures, $T \ll \Delta_0$, we can approximate the quasiparticle spectrum as $\varepsilon(p) \approx \Delta_0 + \xi_p^2/(2\Delta_0)$ and substitute the Fermi-Dirac distribution function by the Boltzmann distribution. Then we obtain

$$C_V = V g(E_F) \Delta_0 \frac{\partial}{\partial T} \int\limits_0^\infty d\xi_p e^{-\Delta_0/T - \xi_p^2/(2\Delta_0 T)} = V g(E_F) \sqrt{\frac{2\pi^3 \Delta_0^5}{T^3}} e^{-\Delta_0/T}.$$

(2.79)

Problem for the seminar 23: Find the temperature behavior of the gap and the condensation free energy near T_c.

Problem for the seminar 24: Find the magnitude of the jump in the specific heat at the transition temperature.

Exercise 35: Find the density of states of quasiparticles with the spectrum $\sqrt{\Delta^2 + \xi_p^2}$.

Exercise 36: Find the temperature behavior of the gap at low temperatures, $T \ll \Delta_0$.

Exercise 37: Show that Eq. (2.78) follows from $\partial E/\partial T$ as a result of the self-consistent equation.

Exercise 38: Find the critical velocity for the spectrum $\varepsilon(p) = \sqrt{\Delta^2 + \xi_p^2}$.

Exercise 39: Express the normal density in terms of the gap. Determine the behavior of the normal density at $T \to 0$ and $T \to T_c$.

2.6   The Luttinger liquid

2.6.1   Introduction

In this lecture we discuss the model of strongly interacting one-dimensional fermions which can be rewritten in the boson representation and, then, can exactly be solved. The additional details can be found in Refs. [8, 9].

2.6.2   Bosonization of non-interacting spinless 1D fermions

In the spatial $d = 1$ dimension the Fermi surface reduces to the two points $p = \pm p_F$ alone. One can describe the fermions near the Fermi point $p = p_F$ ($p = -p_F$) as the particles moving to the 'right' ('left'). The corresponding Hamiltonian for spinless fermions (for the spin effects, see Refs. [8, 9]) can be written as

$$\mathscr{H} - \mu\mathscr{N} = v_F \sum_{p,\eta=\pm} \left(\eta p - p_F\right) a^\dagger_{\eta,p} a_{\eta,p}. \tag{2.80}$$

Here the operators $a^\dagger_{+,p}$ and $a^\dagger_{-,p}$ create the right and left movers with momentum p, respectively. We emphasize that the Hamiltonian (2.80) is unbounded: there are states with arbitrary large negative energy. This unphysical assumption makes the model solvable by means of *bosonisation*. However, the unboundness of the spectrum can lead to divergences in some intermediate results. In order to treat them, we assume the cutoff momentum $p^{(+)}_\Lambda < p_F$ for the right movers such that all fermionic states with $p < p^{(+)}_\Lambda$ are occupied and $p^{(-)}_\Lambda > -p_F$ for the left movers such that all fermionic states with $p > p^{(-)}_\Lambda$ are occupied (see Fig. 2.2). At the end of all calculations the momentum $p^{(\eta)}_\Lambda$ should be put equal to $-\eta\infty$.

Let us now consider the density operator $\rho_\eta(q) = \sum_p a^\dagger_{\eta,p+q} a_{\eta,p}$. Its commutation relations can straightforwardly be calculated as

$$\left[\rho_{\eta_1}(q_1), \rho_{\eta_2}(q_2)\right] = \delta_{\eta_1,\eta_2} \sum_{p_1,p_2} \left[\delta_{p_1,p_2+q_2} a^\dagger_{\eta_1,p_1+q_1} a_{\eta_1,p_2} - \delta_{p_2,p_1+q_1} a^\dagger_{\eta_1,p_2+q_2} a_{\eta_1,p_1}\right]$$

$$= \delta_{\eta_1,\eta_2} \left[\sum_{p_2} a^\dagger_{\eta_1,p_2+q_1+q_2} a_{\eta_1,p_2} - \sum_{p_1} a^\dagger_{\eta_1,p_1+q_1+q_2} a_{\eta_1,p_1}\right] = 0. \tag{2.81}$$

This result that two density operators commute is obtained as a subtraction of two quantities. In the case $q_1 = -q_2$ the expectation value of each of two quantities is formally infinite. Therefore, special care to treat this case is necessary.
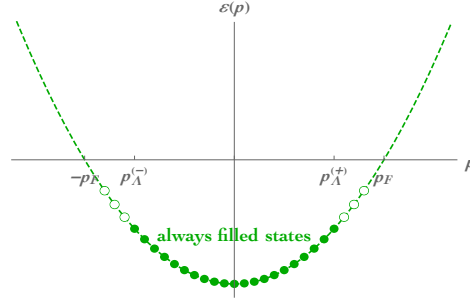
Figure 2.2: Sketch of the 1D fermion spectrum. The states between $p_\Lambda^{(-)} < p < p_\Lambda^{(+)}$ are always occupied by fermions.

We find (for $q > 0$)

$$\left[\rho_+(-q), \rho_+(q)\right] = \sum_{p_1, p_2} \left(a_{+,p_1-q}^\dagger a_{+,p_1} a_{+,p_2+q}^\dagger a_{+,p_2} - a_{+,p_2+q}^\dagger a_{+,p_2} a_{+,p_1-q}^\dagger a_{+,p_1} \right)$$

$$= \sum_{p_1, p_2} \delta_{p_2, p_1-q} \left(a_{+,p_1-q}^\dagger a_{+,p_2} - a_{+,p_2+q}^\dagger a_{+,p_1} \right) = \sum_{p_1} \left(\boldsymbol{n}_{+,p_1-q} - \boldsymbol{n}_{+,p_1} \right), \quad (2.82)$$

where $\boldsymbol{n}_{\eta,p} = a_{\eta,p}^\dagger a_{\eta,p}$. To proceed further, let us consider how the operator $\sum_{p_1} \left(\boldsymbol{n}_{+,p_1-q} - \boldsymbol{n}_{+,p_1} \right)$ acts on the vacuum state $|\text{vac}\rangle$,

$$\sum_{p_1} \left(\boldsymbol{n}_{+,p_1-q} - \boldsymbol{n}_{+,p_1} \right) |\text{vac}\rangle = \sum_{p_\Lambda^{(+)} \leqslant p < p_\Lambda^{(+)}+q} 1 |\text{vac}\rangle = \frac{qL}{2\pi\hbar} |\text{vac}\rangle, \quad (2.83)$$

where L denotes the length of the system. As one can check, the same result holds for the state with an arbitrary number of quasiparticles. Therefore, we derive the following commutation relation,

$$\left[\rho_+(-q), \rho_+(q)\right] = \frac{qL}{2\pi\hbar}. \quad (2.84)$$

In the similar way, one can compute the commutation relation for the left moving fermions. Finally, we can summarize the commutation relations as (for $q_2 > 0$),

$$\left[\rho_{\eta_1}(q_1), \rho_{\eta_2}(q_2)\right] = \delta_{\eta_1, \eta_2} \delta_{-q_1, q_2} \frac{\eta_2 q_2 L}{2\pi\hbar}. \quad (2.85)$$

We note that $\rho_\eta(-q) = [\rho_\eta(q)]^\dagger$. Similarly, we can find (for $q > 0$),

$$\left[\mathscr{H}, \rho_\eta(q)\right] = \eta v_F q \rho_\eta(q), \quad \left[\mathscr{H}, \rho_\eta(-q)\right] = -\eta v_F q \rho_\eta(-q). \quad (2.86)$$

The commutation relations (2.84) and (2.86) suggest that the density operators can be viewed as bosonic creation and annihilation operators (for $q > 0$):

$$\rho_+(q) = \sqrt{\frac{qL}{2\pi}}b^\dagger_{+,q}, \qquad \rho_+(-q) = \sqrt{\frac{qL}{2\pi}}b_{+,q},$$
$$\rho_-(-q) = \sqrt{\frac{qL}{2\pi}}b^\dagger_{-,q}, \qquad \rho_-(q) = \sqrt{\frac{qL}{2\pi}}b_{-,q}, \tag{2.87}$$

with the proper bosonic commutation relation $[b^\dagger_{\eta,q}, b_{\eta',q'}] = \delta_{\eta\eta'}\delta_{q,q'}$. Hamiltonian can be expressed as

$$\mathscr{H} - \mu\mathscr{N} = \sum_{\eta,q>0} v_F q\, b^\dagger_{\eta,q}b_{\eta,q}. \tag{2.88}$$

2.6.3   The interacting fermions: g-ology

Let us consider now the interaction between fermions. It has the standard form,

$$\mathscr{H}_{\text{int}} = \int dx_1 dx_2\, U(x_1 - x_2)\psi^\dagger(x_1)\psi(x_1)\psi^\dagger(x_2)\psi(x_2). \tag{2.89}$$

Here the real-space fermion creation and annihilation operators can be expressed in terms of $a^\dagger_{\eta,p}$ and $a_{\eta,p}$:

$$\psi^\dagger(x) = \sum_{\eta,p} e^{i(\eta p_F + p)x/\hbar}a^\dagger_{\eta,p}, \quad \psi(x) = \sum_{\eta,p} e^{-i(\eta p_F + p)x/\hbar}a_{\eta,p}. \tag{2.90}$$

Then we find that the operator corresponding to the electron density reads

$$\psi^\dagger(x)\psi(x) \approx \sum_{\eta,q} e^{iqx/\hbar}\rho_\eta(q). \tag{2.91}$$

Therefore the Hamiltonian $\mathscr{H}_{\text{int}}$ can be rewritten in terms of the density operators. We make the further simplification and consider the following interaction Hamiltonian,

$$\mathscr{H}^{(g)}_{\text{int}} = \frac{\pi g_2}{L}\sum_{\eta,q>0}\rho_\eta(q)\rho_{-\eta}(-q) + \frac{\pi g_4}{L}\sum_{\eta,q>0}\rho_\eta(q)\rho_\eta(-q), \tag{2.92}$$

where we assume g_2 and g_4 to be independent of transferred momentum. Finally, the Hamiltonian for the Luttinger liquid model written in terms of boson operators acquires the following form,

$$\mathscr{H}_{\text{LL}} = \sum_{\eta,q>0}(v_F + g_4)q\, b^\dagger_{\eta,q}b_{\eta,q} + \frac{g_2}{2}\sum_{\eta,q>0}q\big(b^\dagger_{\eta,q}b^\dagger_{-\eta,q} + b_{\eta,q}b_{-\eta,q}\big). \tag{2.93}$$

This quadratic bosonic Hamiltonian can be diagonalized using the canonical transformation,

$$b^\dagger_{\eta,q} = \cosh\theta_q \boldsymbol{\beta}^\dagger_{\eta,q} + \sinh\theta_q \boldsymbol{\beta}_{-\eta,q}, \quad b_{\eta,q} = \cosh\theta_q \boldsymbol{\beta}_{\eta,q} + \sinh\theta_q \boldsymbol{\beta}^\dagger_{-\eta,q}. \quad (2.94)$$

Expressing the Hamiltonian $\mathscr{H}_{\mathrm{LL}}$ in terms of new bosonic operators $\boldsymbol{\beta}^\dagger_{\eta,q}$ and $\boldsymbol{\beta}_{\eta,q}$, we can find θ_q from the condition that the non-diagonal terms $\boldsymbol{\beta}^\dagger_{\eta,q}\boldsymbol{\beta}^\dagger_{-\eta,q}$ and $\boldsymbol{\beta}_{\eta,q}\boldsymbol{\beta}_{-\eta,q}$ are canceled. The value of such θ_q is given as follows,

$$\cosh 2\theta_q = \frac{v_F + g_4}{u}, \quad \sinh 2\theta_q = -\frac{g_2}{u}, \quad u = \sqrt{(v_F + g_4)^2 - g_2^2}. \quad (2.95)$$

In terms of the new operators, the Hamiltonian reads

$$\mathscr{H}_{\mathrm{LL}} = E_{\mathrm{G}} + \sum_{\eta,q>0} uq\, \boldsymbol{\beta}^\dagger_{\eta,q}\boldsymbol{\beta}_{\eta,q}, \quad E_{\mathrm{G}} = \frac{1}{2}\sum_{q>0}(u - v_F - g_4)q. \quad (2.96)$$

Therefore, the interacting 1D fermions transform into the non-interacting bosonic quasiparticles moving at the renormalized velocity due to interaction.

In the Luttinger liquid theory the important parameter, termed as the *Luttinger liquid parameter*, is usually introduced. It is related with the parameter θ_q as follows

$$K = e^{2\theta_q} = \sqrt{\frac{v_F + g_4 - g_2}{v_F + g_4 + g_2}}. \quad (2.97)$$

The case $K = 1$ corresponds to the noninteracting fermions.

Problem for the seminar 25: Prove the following identity for non-interacting bosons with spectrum ω_q:

$$\left\langle e^{\sum_{q>0}(\alpha_q b_q + \beta_q b_q^\dagger)}\right\rangle = e^{\sum_{q>0}\langle(\alpha_q b_q + \beta_q b_q^\dagger)^2\rangle/2} = \exp\left(\frac{1}{2}\sum_{q>0}\alpha_q\beta_q \coth\frac{\hbar\omega_q}{2T}\right).$$

Problem for the seminar 26: Demonstrate that the annihilation operator for a right-side moving electron at a spatial point x can be written as $\psi_R(x) \sim e^{i\phi_R(x)}$, where

$$\phi_R(x) = \phi_{R,0} + \frac{\mathscr{N}_R x}{L} + i\sum_{q>0}\sqrt{\frac{2\pi}{qL}}\left(e^{-iqx}b^\dagger_{+,q} - e^{iqx}b_{+,q}\right).$$

To determine the commutation relation between $\phi_{R,0}$ and $\mathscr{N}_R$.

Problem for the seminar 27: Diagonalize the Luttinger liquid Hamiltonian
(2.93) in which the boson field has a spin $s = 1/2$ projection index:

$$\mathscr{H}_{\mathrm{LL}} = \sum_{\eta,\sigma,\sigma' q > 0} \left[(\delta_{\sigma,\sigma'} v_F + g_4) q\, b^\dagger_{\eta\sigma,q} b_{\eta\sigma',q} + \frac{g_2}{2} q \left(b^\dagger_{\eta\sigma,q} b^\dagger_{-\eta\sigma',q} + b_{\eta\sigma,q} b_{-\eta\sigma',q} \right) \right].$$

Exercise 40: Compute the commutation relation $\left[\mathscr{H}, \rho_\eta(q) \right]$ where
$\rho_\eta(q) = \sum_p a^\dagger_{\eta,p+q} a_{\eta,p}$ and $\mathscr{H} = v_F \sum_{p,\eta=\pm} \eta p a^\dagger_{\eta,p} a_{\eta,p}$.

Exercise 41: Compute the specific heat of one-dimensional bosons with
the Hamiltonian $\mathscr{H} = \sum_{q>0,\eta=\pm} v_F q b^\dagger_{\eta,q} b_{\eta,q}$ and compare it with the
specific heat of ideal one-dimensional Fermi gas at $T \ll E_F$.

Exercise 42: Demonstrate that the spatial representation of the density
operator of electrons moving to the right side has the following form:

$$\rho_R(x) = \sum_{q>0} \sqrt{\frac{qL}{2\pi}} \left[e^{iqx} b^\dagger_{+,q} + e^{-iqx} b_{+,q} \right] + \frac{\mathscr{N}_R}{L}.$$

where $\mathscr{N}_R$ is the operator of the total number of right movers.

Exercise 43: Compute the specific heat for the Luttinger liquid described
by the Hamiltonian

$$\mathscr{H}_{\mathrm{LL}} = \sum_{\eta,\sigma,\sigma' q > 0} \left[(\delta_{\sigma,\sigma'} v_F + g_4) q\, b^\dagger_{\eta\sigma,q} b_{\eta\sigma',q} + \frac{g_2}{2} q \left(b^\dagger_{\eta\sigma,q} b^\dagger_{-\eta\sigma',q} + b_{\eta\sigma,q} b_{-\eta\sigma',q} \right) \right].$$

Chapter 3

Phase transitions and critical phenomena

3.1 One-dimensional Ising model

In this lecture we consider consider the one-dimensional *Ising model* as simplest example of the analytically solvable model. More details on the analytically solvable models can be found in the book by R. Baxter [10].

3.1.1 Hamiltonian

We consider a chain of N interacting spins $s = 1/2$ in the magnetic field. We assume that the pairwise spin interaction involves the spin projection along the magnetic field. Then the Hamiltonian can be written as

$$\mathscr{H} = -\sum_{i=1}^{N-1} \left(J\sigma_i\sigma_{i+1} + h\frac{\sigma_i + \sigma_{i+1}}{2} \right) \tag{3.1}$$

where $(1/2)\sigma_i$ is the z component of the i-th spin. Since Hamiltonian $\mathscr{H}$ involves the z components of the spin operators, we can treat σ_i as numbers that can be equal to ± 1. The constants $J > 0$ and h play the role of ferromagnetic exchange interaction and magnetic field, respectively.

Before evaluating the partition function, the first question that should be addressed is that about the *boundary conditions*. The first type of the boundary conditions is the so-called the *periodic boundary conditions*:

$$\sigma_N = \sigma_1. \tag{3.2}$$

The periodic boundary conditions correspond to the system on a circle.

For the system determined on a segment, another type of boundary conditions is used, so-called the *free boundary conditions*. This conditions imply that spins σ_1 and σ_N can acquire all possible values ± 1.

Sometimes it is also convenient to use the so-called the *twisted boundary conditions*

$$\sigma_N = e^{i\alpha}\sigma_1, \tag{3.3}$$

where α is a free parameter.

In general, the properties of the system should be insensitive to the boundary conditions in the thermodynamic limit $N \to \infty$ with the exception of the systems with the infinite correlation length (see below).

3.1.2 Transfer matrix approach

The partition function of the model can be written as a sum of the Gibbs factors over all possible spin configurations $\{\sigma_i\}$: $Z = \sum_{\{\sigma_i\}} e^{-\beta\mathscr{H}}$. The number of such configurations is 2^N. Let us fix two neighboring spins at sites i and $i+1$: $\sigma_i = \sigma$ and $\sigma_{i+1} = \sigma'$. Then they enter the expression for the partition function as follows

$$Z = \sum_{\sigma\sigma'=\pm 1} \sum_{\{\sigma_j^z\}'} e^{\beta J\sigma_1\sigma_2 + \frac{\beta h}{2}(\sigma_1+\sigma_2)} \ldots e^{\beta J\sigma_{i-1}\sigma + \frac{\beta h}{2}(\sigma_{i-1}+\sigma)} \begin{pmatrix} e^{\beta J+\beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J-\beta h} \end{pmatrix}_{\sigma\sigma'}$$

$$\times e^{\beta J\sigma'\sigma_{i+2} + \frac{\beta h}{2}(\sigma'+\sigma_{i+2})} \ldots e^{\beta J\sigma_{N-1}\sigma_N + \frac{\beta h}{2}(\sigma_{N-1}+\sigma_N)}. \tag{3.4}$$

Here the dash in the sum means that the sites i and $i+1$ are elliminated. Now repeating the procedure, we find the following representation for the partition function:

$$Z = \sum_{\sigma_1,\sigma_N} (\mathscr{T}^L)_{\sigma_1\sigma_N}. \tag{3.5}$$

Here $L = N - 1$ is the dimensionless length of the system and the matrix

$$\mathscr{T} = \begin{pmatrix} e^{\beta J+\beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J-\beta h} \end{pmatrix} = e^{\beta J} \left(\cosh \beta h + \tau_z \sinh \beta h + \tau_x e^{-2\beta J} \right) \tag{3.6}$$

is referred to as the *transfer matrix*. Here τ_j are the Pauli matrices. We note that the summation over σ_1 and σ_N in Eq. (3.5) depends on the type of the boundary conditions chosen.

The representation (3.5) for the partition function in terms of the transfer matrix $\mathscr{T}$ simplifies the problem significantly. In order to evaluate the matrix product $\mathscr{T}^N$, it is convenient to diagonalize the transfer matrix $\mathscr{T}$. This can be

done by the orthogonal rotation

$$\mathscr{U} = e^{i\phi\tau_y}, \qquad \phi = \frac{1}{2}\arcsin\frac{e^{-2\beta J}}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \qquad (3.7)$$

such that

$$\mathscr{T} = \mathscr{U}^{-1}\Lambda\mathscr{U}, \qquad \Lambda = \mathrm{diag}\left\{\lambda_+, \lambda_-\right\}. \qquad (3.8)$$

The eigenvalues of the transfer matrix becomes

$$\lambda_\pm = e^{\beta J}\left(\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right). \qquad (3.9)$$

We note that $\lambda_+ \geqslant \lambda_-$.

3.1.3 Periodic boundary conditions

Let us start from the periodic boundary conditions (3.2). Then the partition function is given as

$$Z_{\mathrm{per}} = \mathrm{tr}\,\mathscr{T}^L = \lambda_+^L + \lambda_-^L. \qquad (3.10)$$

The free energy $F_{\mathrm{per}} = -T\ln Z_{\mathrm{per}}$ in the thermodynamic limit $N \to \infty$ becomes

$$\frac{F_{\mathrm{per}}}{L} = -T\left[\ln\lambda_+ + \frac{1}{L}\ln\left(1 + (\lambda_-/\lambda_+)^L\right)\right] \xrightarrow{L\to\infty} f = -J$$
$$-T\ln\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right). \qquad (3.11)$$

Now we can find the magnetization per site

$$m = \frac{M}{L} = -\frac{1}{L}\frac{\partial F_{\mathrm{per}}}{\partial h} = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}. \qquad (3.12)$$

The magnetization has non-analytic dependence at zero magnetic field $h = 0$ and zero temperature:

$$M(h \to 0^+)/L = \begin{cases} 0 & T > 0, \\ 1 & T = 0. \end{cases} \qquad (3.13)$$

This result indicates that the one-dimensional Ising model at zero magnetic field is always in the *paramagnetic state* at $T > 0$. At $T = 0$ the system goes over into the *ferromagnetic state*. This is a particular example of the *Mermin−Wagner* theorem.
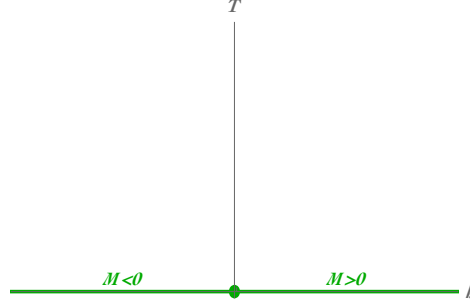
Figure 3.1: Sketch of the phase diagram of one-dimensional Ising model. The order phase exists at $T = 0$ only.

At $T = 0$ the free energy is given as

$$F_{\text{per}}(T = 0) = -L(J + |h|). \tag{3.14}$$

At $h = 0$ the free energy as a function of h has a cusp meaning the first-order phase transition between the phases with $M > 0$ and $M < 0$. The phase diagram of the Ising 1D model is shown in Fig. 3.1 .

For the finite-sized system, the correction to the free energy in the thermodynamic limit can be found by expanding the logarithm in Eq. (3.11) under assumption $\lambda_- < \lambda_+$. Then we find

$$F_{\text{per}} = fL - Te^{-L/\xi}, \qquad \xi = \frac{1}{\ln(\lambda_+/\lambda_-)}. \tag{3.15}$$

The length scale ξ can be associated with the correlation length. At $h = 0$ it diverges in the limit $T \to 0$: $\xi = \exp(2\beta J)/2$.

3.1.4   Twisted boundary conditions

Now let us compute the partition function of the one-dimensional Ising model with the twisted boundary conditions (3.3) with $\alpha = \pi$:

$$Z_{\text{twist}} = \text{tr } \mathscr{T}^L \tau_x. \tag{3.16}$$

By using the relation $\mathscr{U} \tau_x \mathscr{U}^{-1} = \sin 2\phi \tau_z + \cos 2\phi \tau_x$, we find

$$Z_{\text{twist}} = \sin 2\phi(\lambda_+^L - \lambda_-^L). \tag{3.17}$$

We mention that in zero magnetic field at $T \to 0$ and finite L the partition function is $Z_{\text{twist}} = 0$ (since $\lambda_+ = \lambda_-$).

The free energy with the twisted boundary conditions becomes

$$
\frac{F_{\text{twist}}}{L} = -T \ln \lambda_+ - \frac{T}{L} \ln \left[\sin 2\phi \left(1 - (\lambda_-/\lambda_+)^L \right) \right] \xrightarrow{L \to \infty} f
$$
$$
- \frac{T}{L} \ln \sin 2\phi + \frac{T}{L} e^{-L/\xi}. \tag{3.18}
$$

In the case of the twisted boundary conditions, on the contrary to the case of periodic boundary conditions, the finite size corrections to the free energy are not exponentially small.

Finally, we note that the transition between paramagnetic and ferromagnetic phases in the Ising 2D and 3D model occurs at the finite temperature. The 2D Ising model can be solved analytically.

> *Problem for the seminar 28:* Compute the density of the domain walls. To discuss the result at $h = 0$.

> *Problem for the seminar 29:* Find the correlation function $\langle \sigma_j \sigma_{j+n} \rangle = \text{Tr}[\sigma_j \sigma_{j+n} e^{-\beta \mathcal{H}}] / \text{Tr}\, e^{-\beta \mathcal{H}}$ in the thermodynamic limit.

> *Exercise 44:* Compute the spin susceptibility in the thermodynamic limit.

> *Exercise 45:* Find the entropy and specific heat at $h = 0$ in the thermodynamic limit.

> *Exercise 46:* Compute the variance of the thermodynamic fluctuations of the magnetization.

> *Exercise 47:* Compute the free energy $\tilde{F}$ as a function of the magnetization per spin, $m = M/L$ which is related with F via the Legendre transform.

3.2   The Landau theory of phase transitions

3.2.1   The mean-field approximation

Let us now consider the Ising model on the square lattice in the d dimensions. In order to treat the problem, we will use the mean-field approximation assuming the weak fluctuation limit. In particular, let us suppose that the average magnetic moment per spin is $m = \langle \sigma_i \rangle$. Then, we can rewrite the interaction term in the Hamiltonian as

$$\frac{J}{2} \sum_i \sum_{k=1}^{2d} \sigma_i \sigma_{i+k} = \frac{J}{2} \sum_{k=1}^{2d} \langle \sigma_i \rangle \langle \sigma_{i+k} \rangle + \frac{J}{2} \sum_{k=1}^{2d} \sigma_i \langle \sigma_{i+k} \rangle + \frac{J}{2} \sum_{k=1}^{2d} \langle \sigma_i \rangle \sigma_{i+k}$$

$$+ \frac{J}{2} \sum_{k=1}^{2d} \big(\sigma_i - \langle \sigma_i \rangle\big)\big(\sigma_{i+k} - \langle \sigma_{i+k} \rangle\big) \approx dNJm^2 + 2dJm \sum_i \sigma_i. \qquad (3.19)$$

Here in the last line we neglect the fluctuations of spin σ_i from its average value $\langle \sigma_i \rangle$. Then the Hamiltonian of the Ising model is reduced to the spin Hamiltonian in some effective magnetic field

$$\mathscr{H}_{\mathrm{MF}} = -dNJm^2 - \sum_i \big(2dJm + h\big)\sigma_i. \qquad (3.20)$$

The partition function and, consequently, the free energy can readily be computed as

$$F_{\mathrm{MF}} = -dNJm^2 - NT \ln\Big[2 \cosh \beta\big(2dJm + h\big)\Big]. \qquad (3.21)$$

Using the above expression for F_{MF}, we can calculate the magnetization per spin,

$$m = \langle \sigma_i \rangle = -\frac{1}{N}\frac{\partial F_{\mathrm{MF}}}{\partial h} = \tanh\Big[\beta\big(2dJm + h\big)\Big]. \qquad (3.22)$$

At zero magnetic field, $h = 0$, the solution of the self-consistent equation is temperature-dependent. There is the only solution $m = 0$ for $T > T_c = 2dJ$. For $T < T_c$, the other non-zero solutions exist. The non-zero solution $m = \pm m_0$ is more energetically favorable than the trivial solution with $m = 0$. At $T \to 0$ the non-trivial solution tends to unity, $m_0 \to 1$. At T close to T_c we can expand the right hand side of Eq. (3.22) in powers of m:

$$m = \frac{T_c m}{T} - \frac{1}{3}\left(\frac{T_c m}{T}\right)^3 + \dots \quad \Rightarrow \quad m = \pm m_0, \quad m_0 = \sqrt{3}\big(1 - T/T_c\big)^{1/2}. \qquad (3.23)$$

Therefore, we have a second-order phase transition at the *Curie temperature* T_c between the paramagnetic phase at $T > T_c$ and the ferromagnetic phase at $T < T_c$.

In the presence of magnetic field, just at the transition point $T = T_c$, the magnetization has a non-analytic behavior with h:

$$m_0(T = T_c) = \left(3h/T_c\right)^{1/3}. \tag{3.24}$$

3.2.2   The Landau expansion

Let us consider a ferromagnet near the Curie temperature where the second-order phase transition to paramagnetic state occurs. The ferromagnetic state is characterized by the finite magnetization $\boldsymbol{M}$ whereas in the paramagnetic state it vanishes. In the thermodynamic equilibrium the magnitude of magnetization M (we consider isotropic ferromagnet) is determined by the minimum of the Gibbs free energy $\Phi(T, P, M)$. In addition to magnetization M we characterize the ferromagnetic phase by temperature and pressure. Taking into account that magnetization M changes continuously across the transition, we expand $\Phi(T, P, M)$ in a power series in M:

$$\Phi(T, P, M) = \Phi_0(T, P) + \frac{1}{2}A(T, P)M^2 + \frac{1}{4}B(T, P)M^4 + \dots \tag{3.25}$$

There are no terms of odd powers in M due to the time reversal symmetry. We assume that the coefficient B is always positive. If it is negative, one should perform expansion to the next order, i.e., to take the term M^6 into account.

The magnitude of magnetization M can be found from the extremum condition for $\Phi(T, P, M)$:

$$\frac{\partial \Phi(T, P, M)}{\partial M} = A(T, P)M + B(T, P)M^3 = 0. \tag{3.26}$$

This equation has a trivial solution $M = 0$. In the case $A > 0$ this is the only minimum, i.e., the paramagnetic phase alone is realized. In the case $A < 0$ the other minimum is possible with $M = \pm M_0$, where $M_0 = \sqrt{|A|/B}$. The thermodynamic potential at this minimum is negative, $\Phi(T, P, M) - \Phi_0(T, P) = -A^2/(4B)$. Therefore, for $A < 0$ the ferromagnetic phase is more energetically favorable. The simplest conjecture, which one can make, is that coefficient $A(T, P)$ is a regular function of $T - T_c$ where the Curie temperature T_c is determined by the condition $A(T_c, P) = 0$, i.e., we can write

$$A(T, P) = a(P)(T - T_c), \qquad a > 0. \tag{3.27}$$

At the same time we can approximate the function $B(T, P)$ by its value at the transition point: $B(T, P) \approx B(T_c, P) \equiv B(P)$. Then the temperature dependence of the magnetization in the ferromagnet is given as

$$M_0 = \begin{cases} \sqrt{a/B}\sqrt{T_c - T}, & T < T_c, \\ 0, & T \geqslant T_c. \end{cases} \tag{3.28}$$

We emphasize that the $M_0(T)$ dependence reproduces that found in the mean field treatment of the Ising model.

Let us consider the magnetization in the magnetic field h. For definiteness, the ferromagnet is an infinite cylinder placed in the magnetic field parallel to the cylindrical axis. The free energy in the presence of an external magnetic field is given as:

$$F(T, P, M, h) = \Phi(T, P, M) - Mh - \frac{h^2}{8\pi}. \tag{3.29}$$

Now the equilibrium magnetization M is determined by the extremum of $F(T, P, M, h)$,

$$\frac{\partial \Phi(T, P, M)}{\partial M} = h. \tag{3.30}$$

It is worthwhile to mention that the free energy $F(T, P, M, h)$ satisfies the relation $(\partial F/\partial h)_M = -b/(4\pi)$ where $b = h + 4\pi M$ is the magnetic induction.

We note that the magnetization in the magnetic field h becomes non-zero at $T > T_c$. It can be found from the equation

$$a(T - T_c)M + BM^3 - h = 0. \tag{3.31}$$

At $T < T_c$ the $M(h)$ dependence has a hysteresis. For $T = T_c$, we find

$$M = (h/B)^{1/3}. \tag{3.32}$$

Again, we emphasize that this dependence is the same one obtained in the mean-field analysis of the Ising model. Comparing Eq. (3.32) with the expression for M_0, we find the characteristic magnetic field $h \sim B[a(T_c - T)/B]^{3/2}$.

3.2.3   Microscopic derivation of the Ginzburg-Landau theory

Let us consider the Ising model in the d dimensions on the crystalline lattice with coordination number z. The Hamiltonian is given as

$$\mathscr{H} = -\sum_{ij} J_{ij}\sigma_i\sigma_j \tag{3.33}$$

where the symmetric matrix J_{ij} describes the exchange interaction between spins $\sigma_i = \pm 1$. Let us use the identity

$$\left(\prod_{i=1}^{N}\int_{-\infty}^{\infty} dx_i\right)\exp\left[-\frac{1}{4}\sum_{ij} x_i(K^{-1})_{ij}x_j + \sum_i x_i a_i\right]$$

$$= (2\sqrt{\pi})^N \sqrt{\det K}\exp\left(\sum_{ij} a_i K_{ij} a_j\right). \tag{3.34}$$

Choosing $K_{ij} = \beta J_{ij}$, we can express the partition function of the Ising model as follows

$$Z = \frac{(4\pi)^{-N/2}}{\sqrt{\det K}} \left(\prod_{i=1}^{N} \int_{-\infty}^{\infty} dx_i \right) \exp\left[-\frac{1}{4} \sum_{ij} x_i (K^{-1})_{ij} x_j + \sum_i \ln\left(2\cosh x_i\right) \right]. \tag{3.35}$$

Now let us introduce new variable $\phi_i = \sum_j (K^{-1})_{ij} x_j / \sqrt{2}$ and expand the term $\ln\left(2\cosh x_i\right)$ in powers of ϕ_i. Then we obtain the approximate expression for the partition function

$$Z \approx 2^{N/2} \sqrt{\det K} \int D[\phi]\, e^{-\beta \mathscr{H}_{\text{eff}}[\phi]}, \qquad \int D[\phi] \equiv \prod_{i=1}^{N} \int_{-\infty}^{\infty} \frac{d\phi_i}{\sqrt{\pi}} \tag{3.36}$$

where the effective Hamiltonian reads

$$\mathscr{H}_{\text{eff}}[\phi] = \frac{1}{2} \sum_{ij} \phi_i \left[J_{ij} - \beta(J^2)_{ij} \right] \phi_j + \frac{\beta^3}{3} \sum_{ijklm} J_{ij} J_{ik} J_{il} J_{im} \phi_j \phi_k \phi_l \phi_m + \dots \tag{3.37}$$

For the sake of definiteness, we consider now a square lattice in the d dimensions and assume that the exchange interaction is non-zero for the neighboring spins alone. Then the Fourier transform of J_{ij} becomes

$$J_{\boldsymbol{q}} = \sum_j J_{jk} e^{i\boldsymbol{q}(\boldsymbol{r_j}-\boldsymbol{r_k})} = 2J \sum_{\alpha=1}^{d} \cos(q_\alpha \mathsf{a}) \approx J(2d - q^2 \mathsf{a}^2) + \dots \tag{3.38}$$

Here $\boldsymbol{r}_j$ is the vector from the origin to the position of the j-th spin and a is the lattice spacing. Introducing the Fourier transform for the variable ϕ_j:

$$\phi_j = \sum_{\boldsymbol{q}} \phi_{\boldsymbol{q}} e^{-i\boldsymbol{q}\boldsymbol{r}_j}, \tag{3.39}$$

we rewrite the effective Hamiltonian in the following form:

$$\mathscr{H}_{\text{eff}} = \frac{1}{2} \sum_{\boldsymbol{q}} (J_{\boldsymbol{q}} - \beta J_{\boldsymbol{q}}^2) |\phi_{\boldsymbol{q}}|^2 + \frac{\beta^3}{3} \sum_{\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3} J_{\boldsymbol{q}_1} J_{\boldsymbol{q}_2} J_{\boldsymbol{q}_3} J_{-\boldsymbol{q}_1-\boldsymbol{q}_2-\boldsymbol{q}_3} \phi_{\boldsymbol{q}_1} \phi_{\boldsymbol{q}_2}$$
$$\times \phi_{\boldsymbol{q}_3} \phi_{-\boldsymbol{q}_1-\boldsymbol{q}_2-\boldsymbol{q}_3}. \tag{3.40}$$

Here we use the relation $\phi_{-\boldsymbol{q}} = \phi_{\boldsymbol{q}}^*$. Using the expansion of $J_{\boldsymbol{q}}$ at small momenta, cf. Eq. (3.38), we obtain the effective Hamiltonian near $T = T_c = 2dJ$:

$$\mathscr{H}_{\text{eff}} = \frac{1}{2} \sum_{\boldsymbol{q}} \left(T - T_c + Jq^2 \mathrm{a}^2\right) |\phi_{\boldsymbol{q}}|^2 + \frac{2dJ}{3} \sum_{\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3} \phi_{\boldsymbol{q}_1} \phi_{\boldsymbol{q}_2} \phi_{\boldsymbol{q}_3} \phi_{-\boldsymbol{q}_1 - \boldsymbol{q}_2 - \boldsymbol{q}_3}.$$
(3.41)

Transforming into the real space representation, we write the effective Hamiltonian in terms of the continuous variable $\varphi(\boldsymbol{r}) = \mathrm{a}^{-d/2} \sum_{\boldsymbol{q}} \phi_{\boldsymbol{q}} \exp(i\boldsymbol{qr})$:

$$\mathscr{H}_{\text{eff}} = \frac{1}{2} \int d^d \boldsymbol{r} \left[\left(T - T_c\right) \varphi^2(\boldsymbol{r}) + b \left(\nabla \varphi\right)^2 + \frac{\lambda}{2} \varphi^4(\boldsymbol{r}) \right],$$
(3.42)

where $b = J\mathrm{a}^2$ and $\lambda = 4dJ\mathrm{a}^d/3$. Now in order to compute the partition function for the Ising model, one should integrate over all possible configurations of the field $\varphi(\boldsymbol{r})$, i.e., to compute the *functional integral*,

$$Z = \int D[\varphi] \, e^{-\mathscr{H}_{\text{eff}}/T}.$$
(3.43)

Integrating the spatially independent configurations φ, we find that $\ln Z \approx -\Phi(T, P, M)/T$ where $\Phi(T, P, M)$ is given by the Landau expansion (3.25).

3.2.4 The Ginzburg-Landau theory and the Ginzburg-Levanyuk criterion

Contrary to the Landau theory, the partition function is determined as a sum over all configurations $\varphi(\boldsymbol{r})$, cf. Eq. (3.43). This description is valid in vicinity of the transition temperature, $|T - T_c| \ll T_c$. Approximating the *functional integral* by its saddle point value, we obtain that the partition function is determined by the thermodynamic potential Φ coinciding formally with $\mathscr{H}_{\text{eff}}$. In the external magnetic field $h(\boldsymbol{r})$ the minimum of Φ is given by the solution of the corresponding Euler-Lagrange equation:

$$(T - T_c)\varphi - b\nabla^2 \varphi + \lambda\varphi^3 = h.$$
(3.44)

The comparison of the first and second terms in the left hand side of this equation implies an existence of the length scale $\xi \propto \sqrt{b/|T - T_c|}$ called the *correlation length*. The correlation length diverges at the transition point.

At $T > T_c$ we can neglect the third-order term in Eq. (3.44). Then, we find the linear relation between the magnetization and the magnetic field

$$\varphi(\boldsymbol{r}) = \int d^d \boldsymbol{r}' G_\chi(\boldsymbol{r} - \boldsymbol{r}') h(\boldsymbol{r}')$$
(3.45)

where the spin-spin correlation function is given as

$$G_\chi(\boldsymbol{r}) = \int \frac{d^d\boldsymbol{k}}{(2\pi)^d} G_\chi(\boldsymbol{k})e^{-i\boldsymbol{k}\boldsymbol{r}}, \qquad G_\chi(\boldsymbol{k}) = \frac{1}{T - T_c + bk^2}. \qquad (3.46)$$

We note that the spin susceptibility, discussed above, corresponds to $\chi = G_\chi(\boldsymbol{k} = 0)$. Evaluating the integral over $\boldsymbol{k}$, one finds that the spin susceptibility can be written as $G_\chi(\boldsymbol{r}) = b^{-1}\xi^{2-d}\mathcal{X}(r/\xi)$ where $\xi = \sqrt{b/(T - T_c)}$ and $\mathcal{X}(z) \propto \exp(-z)$ at $z \gg 1$.

Let us estimate the contribution to thermodynamic potential Φ from an inhomogeneous fluctuation of size $\varphi_0 \sim \sqrt{|T_c - T|/\lambda}$ and spatial extent of the order of the correlation length ξ: $\Phi_{\text{inhom}} \sim b\xi^d\varphi_0^2/\xi^2 \sim b^2\xi^{d-4}/\lambda$. This energy scale should be larger than the temperature in order to have the functional integral for the partition function governed by the saddle-point approximation. We note that at $d > 4$ this energy scale Φ_{inhom} decreases as we approach the transition temperature since ξ diverges. Therefore, at $d > 4$ the Ginzburg-Landau theory is the ultimate theory of the second-order phase transition. The latter has the mean-field character. The dimension $d = 4$ is termed as the *upper critical dimension*. For $d \leqslant 4$, we find the so-called the Ginzburg-Levanyuk criterion for applicability of the Ginzburg-Landau theory:

$$\xi^{-1} \gg (\lambda T_c/b^2)^{1/(4-d)} \quad \Rightarrow \quad \frac{|T - T_c|}{T_c} \gg \left(\frac{J}{T_c}\right)^{\frac{2-d}{4-d}}. \qquad (3.47)$$

Since $T_c = 2dJ$ for $d = 2$ and $d = 3$, the Ginzburg-Landau theory has no parametric range of its applicability for the Ising model.

We note that the Ginzburg-Landau theory can be developed for describing the superconducting transition in conventional superconductors with the anomalous average playing the role of the order parameter. In this case the region of applicability is wider. The fluctuation region is controlled by the small parameter $T_c/E_F \ll 1$.

Problem for the seminar 30: Find parallel spin susceptibility in zero magnetic field near the Curie temperature for the easy axis antiferromagnet.

Problem for the seminar 31: Compute the fluctuation correction to the specific heat above the transition, $T > T_c$.

Problem for the seminar 32: Find the variance for the fluctuations of the order parameter at $T > T_c$.

Exercise 48: Find the zero-field spin susceptibility $\chi = \lim\limits_{h \to 0} m/h$ in the paramagnetic phase close to T_c.

Exercise 49: Describe the hysteresis in $m(h)$ at $T < T_c$.

Exercise 50: Find the magnitude of the jump of the specific heat under constant pressure, C_P, at the transition temperature.

Exercise 51: Compute the spin susceptibility $\chi = \frac{\partial M}{\partial H}$ at zero magnetic field above and below T_c.

Exercise 52: Find the spin susceptibility and the correlation length at $T < T_c$.

3.3 Scaling ideas and renormalization group

3.3.1 Critical exponents

Although the Ginzburg-Landau theory is not applicable for describing the ferromagnetic–to–paramagnetic phase transition in the Ising model at $d < 4$ dimensions, it provides us the correct physical picture of the transition. The most important prediction is an existence of the divergent correlation length, $\xi(T \to T_c) \to \infty$. This fact implies the absence of any length scale at the phase transition and, as a consequence, power–law spatial behavior of correlation functions.

Let us formally define the following set of eight *critical exponents*:

(i) the correlation length exponents ν and μ which control the behavior of ξ in the absence of magnetic field: $\xi \sim |t|^{-\nu}$ where $t = (T - T_c)/T_c$, and at the transition point $T = T_c$ in the magnetic field : $\xi \sim h^{-\mu}$;

(ii) the order parameter exponents β and δ governing the behavior of the order parameter at $h = 0$: $\varphi \sim (-t)^{\beta}$, and at $T = T_c$: $\varphi \sim h^{1/\delta}$;

(iii) the specific heat exponents α and ε which control the contribution to the specific heat due to fluctuations at $h = 0$: $C_P \sim |t|^{-\alpha}$, and at $T = T_c$: $C_P \sim h^{-\varepsilon}$;

(v) the spin susceptibility exponent γ determing the behavior of χ at $h = 0$: $\chi \sim |t|^{-\gamma}$;

(vi) the exponent ζ which controls the behavior of the spin-spin correlation function at $T = T_c$ and $h = 0$: $G_\chi(\boldsymbol{r}) \sim r^{2-d-\zeta}$.

The Ginzburg-Landau theory predicts the following values of the exponents: $\nu = 1/2$, $\mu = 1/3$, $\beta = 1/2$, $\delta = 3$, $\alpha = 0$, $\varepsilon = 0$, $\gamma = 1$, $\zeta = 0$.

Remarkably, there is a set of general relations between the eight critical exponents. As in the Landau theory let us try to find the characteristic magnetic field which separates the regions of weak and strong magnetic field. Comparing $\varphi \sim (-t)^{\beta}$ with $\chi h \sim |t|^{-\gamma}h$, we find that the characteristic magnetic field behaves as $h_t \sim |t|^{\beta+\gamma}$. The similar estimate can be done by comparison of $\varphi \sim h^{1/\delta}$ with $\varphi \sim (-t)^{\beta}$. However, the latter estimate leads to $h_t \sim |t|^{\delta\beta}$. Assuming that there is only a single characteristic magnetic field in the problem, we obtain the relation between the critical exponents known as the *Widom relation*:

$$\delta\beta = \beta + \gamma. \tag{3.48}$$

Next, substituting $h_t \sim |t|^{\beta+\gamma}$ into the field-dependent expression for the correlation length and the specific heat and comparing the results with the temperature behavior, we obtain two more relations:

$$\mu(\beta + \gamma) = \nu, \qquad \varepsilon(\beta + \gamma) = \alpha. \tag{3.49}$$

Now we can estimate the specific heat as $C_P \sim V\varphi h_t/t^2 \sim |t|^{2\beta-\gamma-2}$. By comparing this behavior with the behavior $C_P \sim |t|^{-\alpha}$, we obtain the so-called *Essam-Fisher relation*:

$$\alpha + 2\beta + \gamma = 2. \tag{3.50}$$

Let us now estimate the spin susceptibility from the spin-spin correlation function: $\chi \sim \int d^d \boldsymbol{r} G_\chi(r)$. As we will see above, the function $G_\chi(r) \sim \exp(-r/\xi)$ for $r \gg \xi$. Therefore, we can expect that only the region $r < \xi$ contributes to the integral. Then, we find $\chi \sim \xi^{2-\zeta} \sim |t|^{-\nu(2-\zeta)}$. Hence we find the fifth relation

$$\gamma = \nu(2 - \zeta). \tag{3.51}$$

We note that the above five relations set three critical exponents unspecified. Also we mention that the critical exponents of the Ginzburg–Landau theory satisfy these five relations.

3.3.2   The scale invariance and scaling laws

Let us assume that the correlation length ξ is the single length scale in the fluctuation region of second-order phase transition. This assumption is termed as the *hypothesis of scale invariance* and is introduced by Kadanoff, Patashinskii, and Pokrovsky in 1966. In particular, this hypothesis implies that upon rescaling $\boldsymbol{r} \to \boldsymbol{r}/u$, one can change the temperature t to tu^{Δ_t}, magnetic field h to hu^{Δ_h} and the order parameter φ to $\varphi u^{\Delta_\varphi}$. Since the correlation length is the single length scale, it should transform in the same way as the length: $\xi \to \xi/u$. Since $\xi(tu^{\Delta_t}) \sim |t|^{-\nu}u^{-\nu\Delta_t}$, we find that the exponent $\Delta_t = 1/\nu$. In the similar way, one finds $\Delta_h = 1/\mu$. Also, the thermodynamic potential should be invariant with respect to the scale transformation. Estimating Φ as $V\varphi h$, we find the relation $\Delta_\varphi = d - \Delta_h = d - 1/\mu$.

Let us consider the order parameter $\varphi(t, h) = u^{-\Delta_\varphi}\varphi(tu^{1/\nu}, hu^{1/\mu})$. Now let us choose the specific magnidute of the scale transformation parameter, $u = h^{-\mu}$. Then we find

$$\varphi(t, h) = h^{\mu d-1}\varphi\big(th^{-\mu/\nu}, 1\big). \tag{3.52}$$

Setting $t = 0$, we obtain new relation between critical exponents:

$$\mu d - 1 = 1/\delta \tag{3.53}$$

which can be transformed into the relation

$$\nu d = 2 - \alpha. \tag{3.54}$$

We note that this relation (contrary to the five relations derived above) is not satisfied within the Ginzburg-Landau theory due to lack of scale invariance in this theory. Next we can rewrite Eq. (3.52) in the following scaling form:

$$\varphi(t, h) = h^{1/\delta} \mathcal{F}_\varphi\big(t/h^{1/(\beta\delta)}\big). \tag{3.55}$$

In the presence of non-zero h there is no reason to expect non-analytic behavior in t. Therefore, the function $\mathcal{F}_\varphi(X)$ is a regular function of its scaling argument. To be consistent with the behavior in weak magnetic fields, the function $\mathcal{F}_\varphi(X)$ should have the following asymptotic behavior:

$$\mathcal{F}_\varphi(X) \sim \begin{cases} (-X)^\beta, & X \to -\infty, \\ X^{-\gamma}, & X \to \infty. \end{cases} \tag{3.56}$$

For the two-dimensional Ising model, the set of critical exponents is known exactly: $\alpha = \varepsilon = 0$, $\nu = 1$, $\mu = 8/15$, $\gamma = 7/4$, $\beta = 1/8$, $\delta = 15$, and $\zeta = 1/4$. As one can check, they satisfy all the six relations.

3.3.3 The renormalization group

The hypothesis of the scale invariance allows us to establish the scaling form of all physical quantities. However, it does not permit to determine the values of the critical exponents. Using the property of the scale invariance, we can ask a question how the effective Hamiltonian

$$\mathscr{H}_{\text{eff}}[\varphi] = \frac{1}{2} \int d^d\boldsymbol{r} \left[\tau\varphi^2(\boldsymbol{r}) + \left(\nabla\varphi\right)^2 + \frac{\lambda}{2}\varphi^4(\boldsymbol{r}) \right] \tag{3.57}$$

is transformed under the scale transformation with $u = e^l$ where $l \to 0$. We note that τ plays the role of dimensionless temperature. To answer this question, we should perform several steps. We note that we changed a definition of the variable φ in comparison with one used in Eq. (3.42).

Firstly, let us split the variable $\varphi(\boldsymbol{r})$ into two parts:

$$\varphi(\boldsymbol{r}) = \underline{\varphi}(\boldsymbol{r}) + \overline{\varphi}(\boldsymbol{r}) \tag{3.58}$$

where

$$\underline{\varphi}(\boldsymbol{r}) = \int\limits_{0<k<\Lambda/u} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \varphi_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}}, \quad \overline{\varphi}(\boldsymbol{r}) = \int\limits_{\Lambda/u\leqslant k<\Lambda} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \varphi_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}}. \tag{3.59}$$

Here Λ is the ultra-violet cutoff of the order of inverse lattice spacing, $\Lambda \sim 1/a$. The contributions $\underline{\varphi}(\boldsymbol{r})$ and $\overline{\varphi}(\boldsymbol{r})$ are termed as *slow or long wave* component and *fast or short wave* component, respectively.

Secondly, we integrate out the fast components of the field and define new effective Hamiltonian

$$\mathscr{H}'_{\text{eff}}[\underline{\varphi}] = -T \ln \int D[\overline{\varphi}] e^{-\beta \mathscr{H}_{\text{eff}}[\underline{\varphi}+\overline{\varphi}]}. \tag{3.60}$$

Since the momenta in definition of $\underline{\varphi}$ are restricted within the range $0 < k < \Lambda/u$, we introduce the rescaled momentum $\underline{k} = uk$ and rescaled field $\tilde{\varphi}(\underline{k}) = u^{-\rho}\varphi(k)$. We note that in the real space this transformation corresponds to $\boldsymbol{r} \to \underline{\boldsymbol{r}} = \boldsymbol{r}/u$ and $\underline{\varphi}(\boldsymbol{r}) \to \tilde{\varphi}(\underline{\boldsymbol{r}}) = u^{d-\rho}\varphi(\boldsymbol{r})$. Then, we expect that $\mathscr{H}'_{\text{eff}}[\underline{\varphi}]$ has exactly the same form as $\mathscr{H}_{\text{eff}}[\tilde{\varphi}]$ but with τ and λ substituted by some functions $\tau(l)$ and $\lambda(l)$. This procedure is known as the *renormalization group*. This method has been used by L. Kadanoff and K. Wilson for describing the critical phenomena.

In order to demonstrate what we can gain from this renormalization procedure, let us consider the spin susceptibility. Since the latter is the spin-spin correlation function at $k = 0$, we, on the one hand, can calculate it from the initial effective Hamiltonian and, on the other hand, from the effective Hamiltonian $\mathscr{H}'_{\text{eff}}[\underline{\varphi}]$. Then using the relation between the susceptibility and the variance for the variable φ, cf. Eq. (1.33), $\langle \varphi^2 \rangle = T\chi/V$, we find

$$\chi(\tau, \lambda) = u^{2\rho-d}\chi(\tau(l), \lambda(l)). \tag{3.61}$$

3.3.4   The $4 - d$ expansion

For the further progress, one should determine the functions $\tau(l)$ and $\lambda(l)$. Near the upper critical dimension there is a systematic way to compute them. We write

$$\mathscr{H}_{\text{eff}}[\underline{\varphi} + \overline{\varphi}] = \mathscr{H}_{\text{eff}}[\underline{\varphi}] + \frac{1}{2} \int d^d\boldsymbol{r} \Big\{ \tau[\overline{\varphi}(\boldsymbol{r})]^2 + [\nabla\overline{\varphi}(\boldsymbol{r})]^2 + 3\lambda[\underline{\varphi}(\boldsymbol{r})]^2$$
$$\times [\overline{\varphi}(\boldsymbol{r})]^2 + 2\lambda\underline{\varphi}(\boldsymbol{r})[\overline{\varphi}(\boldsymbol{r})]^3 + \frac{\lambda}{2}[\overline{\varphi}(\boldsymbol{r})]^4 \Big\}. \tag{3.62}$$

Then we find $\mathscr{H}'_{\text{eff}}[\varphi]$ as a formal expansion in λ. We obtain to the second order in λ,

$$\mathscr{H}'_{\text{eff}}[\varphi] = \mathscr{H}_{\text{eff}}[\varphi] + \frac{3\lambda}{2} \int d^d\boldsymbol{r}[\underline{\varphi}(\boldsymbol{r})]^2 \langle[\overline{\varphi}(\boldsymbol{r})]^2\rangle - \frac{9\lambda^2\beta}{8} \int d^d\boldsymbol{r} \int d^d\boldsymbol{r}'[\underline{\varphi}(\boldsymbol{r})\underline{\varphi}(\boldsymbol{r}')]^2$$
$$\times \langle\langle[\overline{\varphi}(\boldsymbol{r})]^2[\overline{\varphi}(\boldsymbol{r}')]^2\rangle\rangle + \frac{\lambda^2\beta}{2} \int d^d\boldsymbol{r}\underline{\varphi}(\boldsymbol{r}) \int d^d\boldsymbol{r}'\underline{\varphi}(\boldsymbol{r}')\langle[\overline{\varphi}(\boldsymbol{r})]^3[\overline{\varphi}(\boldsymbol{r}')]^3\rangle$$
$$+ \frac{3\lambda^2\beta}{4} \int d^d\boldsymbol{r}[\underline{\varphi}(\boldsymbol{r})]^2 \int d^d\boldsymbol{r}'\langle\langle[\overline{\varphi}(\boldsymbol{r})]^2[\overline{\varphi}(\boldsymbol{r}')]^4\rangle\rangle \qquad (3.63)$$

where $\langle\langle AB\rangle\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle$. The brackets $\langle\ldots\rangle$ mean averaging with the effective Hamiltonian at $\lambda = 0$:

$$\langle O[\overline{\varphi}]\rangle = \int D[\overline{\varphi}]O[\overline{\varphi}]e^{-\beta\mathscr{H}^{(0)}_{\text{eff}}[\overline{\varphi}]} \bigg/ \int D[\overline{\varphi}]e^{-\beta\mathscr{H}^{(0)}_{\text{eff}}[\overline{\varphi}]},$$
$$\mathscr{H}^{(0)}_{\text{eff}}[\overline{\varphi}] = \frac{1}{2} \int d^d\boldsymbol{r}\Big\{\tau[\overline{\varphi}(\boldsymbol{r})]^2 + [\nabla\overline{\varphi}(\boldsymbol{r})]^2\Big\}. \qquad (3.64)$$

Now let us perform rescaling $\Lambda/u \to \Lambda$ by changing $k \to \underline{k} = uk$ and $\underline{\varphi}(k) \to \tilde{\varphi}(\underline{k}) = u^{-\rho}\varphi(k)$. To fix the magnitude of ρ, we impose the condition remaining the gradient term,

$$\int d^d\boldsymbol{r}[\nabla\overline{\varphi}(\boldsymbol{r})]^2 = u^{-d-2+2\rho} \int d^d\underline{\boldsymbol{r}}[\nabla\tilde{\varphi}(\boldsymbol{r})]^2, \qquad (3.65)$$

unvaried under such transformation, i.e., $\rho = (d+2)/2$. Performing such rescaling in the other terms, we find that $\mathscr{H}'_{\text{eff}}[\varphi]$ acquires the form of $\mathscr{H}_{\text{eff}}[\tilde{\varphi}]$ with

$$\tau \to \tau(l) = e^{2l}\tau + 3\lambda e^{2l}\langle[\overline{\varphi}(\boldsymbol{r})]^2\rangle,$$
$$\lambda \to \lambda(l) = e^{(4-d)l}\lambda - \frac{9\lambda^2 e^{(4-d)l}}{2T} \int d^d\boldsymbol{r}'\langle\langle[\overline{\varphi}(\boldsymbol{r})]^2[\overline{\varphi}(\boldsymbol{r}')]^2\rangle\rangle, \qquad (3.66)$$

to lowest order in λ. The averages in the above equations can be calculated as follows

$$\langle[\overline{\varphi}(\boldsymbol{r})]^2\rangle = \int\limits_{\Lambda/u<k<\Lambda} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{T}{\tau+k^2} = \frac{S_d\Lambda^d}{(2\pi)^d} \frac{T}{\tau+\Lambda^2}l,$$

$$\int d^d\boldsymbol{r}'\langle\langle[\overline{\varphi}(\boldsymbol{r})]^2[\overline{\varphi}(\boldsymbol{r}')]^2\rangle\rangle = 2\int\limits_{\Lambda/u<k<\Lambda} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{T^2}{(\tau+k^2)^2} = 2\frac{S_d\Lambda^d}{(2\pi)^d} \frac{T^2}{(\tau+\Lambda^2)^2}l,$$

$$(3.67)$$

where S_d denotes the area of the unit sphere in the d-dimensional space. It is convenient to introduce the dimensionless variables: $\tilde{\tau} = \tau/\Lambda^2$ and $\tilde{\lambda} = \lambda\Lambda^{d-4}S_d T/(2\pi)^d$. Then expanding to the lowest order in l, we find the following relations:

$$\tilde{\tau}(l) = \tilde{\tau} + \left(2\tilde{\tau} + \frac{3\tilde{\lambda}}{1+\tilde{\tau}}\right)l, \quad \tilde{\lambda}(l) = \tilde{\lambda} + \left((4-d)\tilde{\lambda} - \frac{9\tilde{\lambda}^2}{(1+\tilde{\tau})^2}\right)l. \quad (3.68)$$

These results obtained in the limit $l \to 0$ can be recast in the form of the differential equations:

$$\frac{d\tilde{\tau}}{dl} = 2\tilde{\tau} + \frac{3\tilde{\lambda}}{1+\tilde{\tau}},$$
$$\frac{d\tilde{\lambda}}{dl} = \epsilon\tilde{\lambda} - \frac{9\tilde{\lambda}^2}{(1+\tilde{\tau})^2}, \quad (3.69)$$

where $\epsilon = 4-d$. For $\epsilon < 0$, the only fixed point is at $\tilde{\lambda} = \tilde{\tau} = 0$ which is stable in the infra-red (at $l \to \infty$). This fixed point corresponds to the Ginzburg-Landau theory. For $\epsilon > 0$, the fixed point at $\tilde{\lambda} = \tilde{\tau} = 0$ becomes unstable in the infra-red. There is a partially unstable fixed point at $\tilde{\tau}_* = -\epsilon/6$ and $\tilde{\lambda}_* = \epsilon/9$. The smallness of values $\tilde{\lambda}_*$ and $\tilde{\tau}_*$ for $\epsilon \ll 1$ justifies the expansion in λ which we have performed. Expanding the right hand side of Eq. (3.69) near this fixed point, we obtain ($\delta\tilde{\tau} = \tilde{\tau} - \tilde{\tau}_*$ and $\delta\tilde{\lambda} = \tilde{\lambda} - \tilde{\lambda}_*$):

$$\frac{dt}{dl} = \mathrm{x}_+ t, \qquad \frac{d\delta\tilde{\lambda}}{dl} = \mathrm{x}_- \delta\tilde{\lambda}, \quad (3.70)$$

where $\mathrm{x}_+ = 2 - \epsilon/3$, $\mathrm{x}_- = -\epsilon$, and $t = \delta\tilde{\tau} + (3/2 - \epsilon/4)\delta\tilde{\lambda}$. The above equations imply that variable t corresponds to the relevant direction and measures the distance from the critical line. Then we find that Eq. (3.61) acquires the following form: $\chi = u^2\chi(tu^{\mathrm{x}_+})$. This implies that the correlation length exponent is $\nu = 1/\mathrm{x}_+ = 1/2 + \epsilon/12$. Choosing $u = t^{-\nu}$, we find $\chi \sim t^{-2\nu}$, i.e. $\zeta = O(\epsilon^2)$. Using the relations between the critical exponents, we can determine all the other exponents.

Problem for the seminar 33: Derive the scaling form of the thermodynamic potential and the relations between critical exponents.

Problem for the seminar 34: Derive RG equations for τ and λ in the case of n-component field φ.

Exercise 53: Find behavior of $G_\chi(\boldsymbol{k})$ at $k \to 0$ for $T = T_c$ and $h = 0$.

Exercise 54: Derive the relations $\mu(\beta + \gamma) = \nu$ and $\varepsilon(\beta + \gamma) = \alpha$.

Exercise 55: Derive the scaling form of the specific heat, the correlation length, and the spin-spin correlation function.

Exercise 56: Using the relations between critical exponents, compute the critical exponents α, ε, μ, γ, β, and δ to first order in ϵ.

Exercise 57: Plot the RG flow for Eqs. (3.69).

3.4   The Berezinskii-Kosterlitz-Thouless transition

3.4.1   Transitions beyond the Landau paradigm

As is discussed in the previous lectures, the paradigm of the Landau expansion assumes an existence of the order parameter in the phase of lower symmetry (at $T < T_c$). In particular, this implies the following relations for the correlation function of the order parameter field:

$$\lim_{|\boldsymbol{r}-\boldsymbol{r'}|\to\infty} \langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r'})\rangle \sim \begin{cases} \exp(-|\boldsymbol{r}-\boldsymbol{r'}|/\xi), & T > T_c \\ \langle\varphi(\boldsymbol{r})\rangle^2, & T < T_c. \end{cases} \tag{3.71}$$

The presence of nonzero $\langle\varphi(\boldsymbol{r})\rangle$ at $T < T_c$ breaks the corresponding symmetry down, e.g. $SU(2)$ symmetry in the case of the paramagnet–to–ferromagnet transition. However, this is not the only possible scenario. The alternative paradigm reads

$$\lim_{|\boldsymbol{r}-\boldsymbol{r'}|\to\infty} \langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r'})\rangle \sim \begin{cases} \exp(-|\boldsymbol{r}-\boldsymbol{r'}|/\xi), & T > T_{\mathrm{BKT}}, \\ |\boldsymbol{r}-\boldsymbol{r'}|^{-\eta}, & T < T_{\mathrm{BKT}}, \end{cases} \tag{3.72}$$

without changing the symmetry. Although $\langle\varphi(\boldsymbol{r})\rangle$ vanishes above and below T_{BKT}, i.e., the long-range order is absent, the phases are different due to various behavior of the correlation functions. The corresponding transition is referred to as Berezinskii-Kosterlitz-Thouless transition.

3.4.2   Classical 2D XY model

Let us consider classical 2D XY model described by the Hamiltonian

$$\mathscr{H} = J \sum_{<jk>} \left(1 - \boldsymbol{n}_j \boldsymbol{n}_k\right) \tag{3.73}$$

where $\boldsymbol{n}_j$ is the unit 2D vector associated with the site j at the 2D square lattice. The symbol $<jk>$ denotes summation over all neighboring sites. It is convenient to parameterize the unit vector as $\boldsymbol{n} = \{\cos\theta, \sin\theta\}$. Then the Hamiltonian reads

$$\mathscr{H} = J \sum_{<jk>} \left[1 - \cos(\theta_j - \theta_k)\right]. \tag{3.74}$$

The correlation function which behavior reveals the BKT transition can be chosen as follows

$$\langle\cos(\theta_j - \theta_k)\rangle = \left(\prod_l \int_0^{2\pi} \frac{d\theta_l}{2\pi}\right) \cos(\theta_j - \theta_k) e^{-\beta\mathscr{H}} \bigg/ \left(\prod_l \int_0^{2\pi} \frac{d\theta_l}{2\pi}\right) e^{-\beta\mathscr{H}}. \tag{3.75}$$
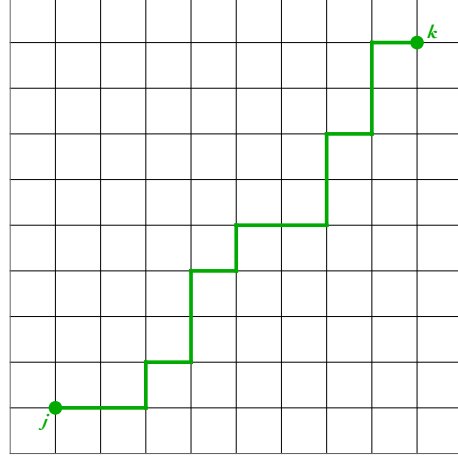
Figure 3.2: Example of the shortest path between sites j and k on the square lattice.

From the above definition we see directly that there is a single parameter governing the physics of the model, namely, J/T. At high temperatures the correlation function (3.75) can be computed perturbatively, by expanding $\exp(-\beta\mathscr{H})$ in a series in powers J/T. Since $\int_0^{2\pi} d\theta_l \exp(i\theta_l) = 0$, one should first find the minimal power n such that the term $(\beta\mathscr{H})^n$ contains the angles θ_j and θ_k one time, as well as the minimal number of angles on the sites belonging to the path connecting the sites j and k (see Fig. 3.2). Then in the continuous limit we find the following result for $T \gg J$

$$\langle\cos(\theta_j - \theta_k)\rangle \sim e^{-|\boldsymbol{r}_j - \boldsymbol{r}_k|/\xi}, \qquad \xi = \frac{a}{\ln(2T/J)}, \qquad (3.76)$$

where a is the lattice constant.

In the opposite case of low temperatures, $T \ll J$, we can assume that directions of unit vectors $\boldsymbol{n}_j$ on the neighboring sites are close to each other (similar to the case of the ferromagnetic state). Then, we can expand the difference $\theta_j - \theta_k$ to lowest order in the lattice constant and find the following continuous version of the Hamiltonian (3.74):

$$\mathscr{H} = (J/2) \int d^2\boldsymbol{r}(\nabla\theta)^2. \qquad (3.77)$$

The correlation function (3.75) can be written as

$$\langle \cos(\theta_j - \theta_k) \rangle = \frac{1}{Z} \int D[\theta] e^{i\theta(\boldsymbol{r}_j) - i\theta(\boldsymbol{r}_k)} e^{-(\beta J/2) \int d^2\boldsymbol{r}(\nabla\theta)^2},$$

$$Z = \int D[\theta] e^{-(\beta J/2) \int d^2\boldsymbol{r}(\nabla\theta)^2}. \tag{3.78}$$

In order to find the correlation function, it is convenient to introduce the Fourier transform $\theta_{\boldsymbol{q}} = \int d^2\boldsymbol{r}\,\theta(\boldsymbol{r})\exp(-i\boldsymbol{q}\boldsymbol{r})$ and rewrite the exponent in the right hand side of the above equation as

$$-\frac{\beta J}{2} \int d^2\boldsymbol{r}(\nabla\theta)^2 + i\theta(\boldsymbol{r}_j) - i\theta(\boldsymbol{r}_k) = -\frac{\beta J}{2} \int \frac{d^2\boldsymbol{q}}{(2\pi)^2} q^2 (\theta_{\boldsymbol{q}} + \gamma_{\boldsymbol{q}})(\theta_{-\boldsymbol{q}} + \gamma_{-\boldsymbol{q}})$$

$$+\frac{\beta J}{2} \int \frac{d^2\boldsymbol{q}}{(2\pi)^2} q^2 \gamma_{\boldsymbol{q}}\gamma_{-\boldsymbol{q}}, \tag{3.79}$$

where $\gamma_{\boldsymbol{q}} = (e^{-i\boldsymbol{q}\boldsymbol{r}_k} - e^{-i\boldsymbol{q}\boldsymbol{r}_j})/(i\beta J q^2)$. Introducing new variable $\tilde{\theta}_{\boldsymbol{q}} = \theta_{\boldsymbol{q}} + \gamma_{\boldsymbol{q}}$, we find

$$\langle \cos(\theta_j - \theta_k) \rangle = \exp\left(-\frac{T}{2J} \int \frac{d^2\boldsymbol{q}}{(2\pi)^2} \frac{|1 - e^{i\boldsymbol{q}(\boldsymbol{r}_j - \boldsymbol{r}_k)}|^2}{q^2}\right)$$

$$\times \frac{1}{Z} \int D[\tilde{\theta}] e^{-(\beta J/2) \int d^2\boldsymbol{r}(\nabla\tilde{\theta})^2} \tag{3.80}$$

The factors in the second line of the above equation cancel each other, and after integration over $\boldsymbol{q}$ we obtain for $T \ll J$:

$$\langle \cos(\theta_j - \theta_k) \rangle \sim |\boldsymbol{r}_j - \boldsymbol{r}_k|^{-T/(2\pi J)}. \tag{3.81}$$

The different asymptotic behavior of the correlation function, $\langle \cos(\theta_j - \theta_k) \rangle$, at low and high temperatures suggests an existence of the transition at $T \sim J$.

3.4.3   The Villain model on the dual lattice

In the low temperature analysis above we have ignored the 2π-periodicity of the Hamiltonian with substituting angle θ_j with $\theta_j + 2\pi$. As we will see below, this periodicity is crucial for an accurate description of the BKT transition.

Let us introduce the function $\tilde{V}(s)$ defined as follows

$$e^{-\beta J(1 - \cos\theta)} = \sum_{s=-\infty}^{\infty} e^{is\theta + \tilde{V}(s)}, \quad e^{\tilde{V}(s)} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-\beta J(1 - \cos\theta) - is\theta} = e^{-\beta J} I_s(\beta J)$$

$$\tag{3.82}$$

where $I_s(z)$ denotes the modified Bessel function. Introducing variable s for each link of a square lattice and using the Fourier representation (3.82), we can integrate over angles θ_l, cf. Eq. (3.75), in the partition function. Such integration for a given site l induces the constraint $s_x + s_y = s_{-x} + s_{-y}$, see Fig. 3.3. From physical point of view an existence of such constraints is related with the following. The number of initial variables (angles) equals the number of sites M. The number of variables s is the same as the number of links, i.e., it equals $2M$. The M constraints conserve the number of degrees of freedom in new representation. In order to resolve this constraint, it is useful to introduce new set of integers associated with the center of each square $\{\tilde{s}\}$. They are related with the initial ones as follows (see Fig. 3.3), $s_x = \tilde{s}_A - \tilde{s}_B$, $s_y = \tilde{s}_D - \tilde{s}_A$, $s_{-x} = \tilde{s}_D - \tilde{s}_C$, and $s_{-y} = \tilde{s}_C - \tilde{s}_B$. We note that the center of squares composes the *dual lattice* with respect to the original one. Finally, the partition function on the dual lattice can be written as

$$Z = \sum_{\{\tilde{s}_l\}} \exp\Big[\sum_{<ll'>} \tilde{V}(\tilde{s}_l - \tilde{s}_{l'})\Big]. \tag{3.83}$$

Using the Poisson resummation formula

$$\sum_{s=-\infty}^{\infty} g(s) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} d\phi\, g(\phi) e^{2\pi i m\phi}, \tag{3.84}$$

we express the partition function as

$$Z = \sum_{\{m_l\}} \prod_l \left(\int_{-\infty}^{\infty} d\phi_l\right) \exp\Big[\sum_{<ll'>} \tilde{V}(\phi_l - \phi_{l'}) + 2\pi i \sum_l m_l \phi_l\Big]. \tag{3.85}$$

Here ϕ_l is a variable that corresponds to s_l in the Poisson formula (3.84).

Using the asymptotic expression of $\tilde{V}(\phi)$ at low temperatures $T \ll J$,

$$\exp\Big[\tilde{V}(\phi)\Big] \approx \exp[-\phi^2/(2\beta J)]/\sqrt{2\pi\beta J}, \tag{3.86}$$

we have obtained the partition function of the so-called the *Villain model* on the dual lattice:

$$Z = \sum_{\{m_l\}} \prod_l \left(\int_{-\infty}^{\infty} d\tilde{\theta}_l\right) \exp\Big[-\frac{\beta J}{2}\sum_{<ll'>} (\tilde{\theta}_l - \tilde{\theta}_{l'})^2 + 2\pi i \beta J \sum_l m_l \tilde{\theta}_l\Big]. \tag{3.87}$$

Here we have introduced $\tilde{\theta}_l = \phi_l/(\beta J)$ and omitted the insignificant constant factor.
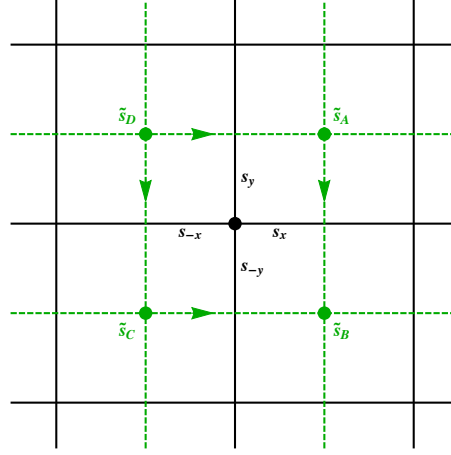
Figure 3.3: Sketch of the original square lattice with variables s_x, s_y associated with links and of the dual lattice with variables $\tilde{s}_{A,B,C,D}$ associated with its sites.

3.4.4   The renormalization group analysis

Let us now consider the partition function of the so-called generalized Villain model:

$$Z = \sum_{\{m_l\}} \prod_l \left(\int\limits_{-\infty}^{\infty} d\theta_l \, y^{m_l^2} e^{2\pi i \beta J \theta_l m_l} \right) \exp\left[-\frac{\beta J}{2} \sum_{<ll'>} (\theta_l - \theta_{l'})^2 \right]. \qquad (3.88)$$

Here we have omitted the tilde sign in θ_l and introduced the so-called *fugacity y*. The fugacity appears due to logarithmic interaction between the integer numbers m_l that represent vortices. This logarithmic interaction is ill-defined at small scales of the order of the lattice spacing. Therefore, it is necessary to introduce the term with the fugacity including the information about microscopics of the model. One can estimate the magnitude of the fugacity as $\ln y \sim -\beta J$.

In what follows, we assume that fugacity is small, $y \ll 1$. Then, summing over integers m_l, we arrive at

$$Z = \prod_l \left(\int\limits_{-\infty}^{\infty} d\theta_l \, \vartheta_3\big(\pi \beta J \theta_l, y\big) \right) \exp\left[-\frac{\beta J}{2} \sum_{<ll'>} (\theta_l - \theta_{l'})^2 \right] \qquad (3.89)$$

where $\vartheta_3(u, y)$ denotes the elliptic theta-function. Using the asymptotic result $\ln \vartheta_3(u, y) = 2y \cos(2u)$ at $y \to 0$, we obtain the following partition function in

the continuum limit (lattice spacing a $\to$ 0):

$$Z = \int D[\theta] \exp(-\beta \mathcal{H}_{\text{eff}}[\theta]) \tag{3.90}$$

where

$$\mathcal{H}_{\text{eff}} = \frac{J}{2} \int d^2 \boldsymbol{r} (\nabla \theta)^2 - 2\tilde{y} \int d^2 \boldsymbol{r} \cos\left[2\pi\beta J\theta\right] \tag{3.91}$$

and $\tilde{y} = y/a^2$. Comparing this equation with Eq. (3.78), one can see that the presence of vortices results in appearing an additional term in the effective Hamiltonian. Since $\mathcal{H}_{\text{eff}}[\theta]$ is non-linear in θ, we can apply the renormalization group method to analyze it. Under assumption of $y \ll 1$, one can derive the following renormalization group equations:

$$\frac{d\bar{y}}{dl} = -\bar{y}x, \qquad \frac{dx}{dl} = -\bar{y}^2. \tag{3.92}$$

Here we introduce $x = \pi\beta J - 2$ and $\bar{y} = 16\sqrt{2}y/(a\Lambda)$ where $\Lambda \sim 1/a$ denotes the ultra-violet cutoff. These renormalization group equations are valid at $|x| \ll 1$ and $\bar{y} \ll 1$ and demonstrate an interesting behavior.

At $x > 0$ there is a line of fixed points $\bar{y} = 0$ (since $\bar{y} > 0$ by definition) stable in the infra-red. At $x < 0$ there is a line of fixed points $\bar{y} = 0$ unstable in the infra-red. The fixed point ($x = 0$, $\bar{y} = 0$) separates lines of stable and unstable fixed points. There are two separatrices $x = \pm\bar{y}$. The renormalization group flow is shown in Fig. 3.4. Since large x corresponds to low temperatures, the line of stable fixed points corresponds to the low temperature phase of the 2D XY model. The existence of the line of fixed points explains the power law behavior of the correlation functions typical for the fixed points. The transition temperature is determined by the position of separatrix $x = y$ or in terms of the temperature: $T_{BKT} = (2 + \bar{y}_0)J/\pi$, where $\bar{y}_0$ is the initial magnitude of the fugacity. The appearance of the correction due to fugacity corresponds physically to the interaction of the spin waves.

For $T > T_{BKT}$ and $y > x$, the fugacity finally flows in the direction of large magnitudes. The condition $\bar{y}(l \sim \ln\xi) \sim 1$ determines the correlation length. The solution of Eqs. (3.92) leads to very unusual behavior of the correlation length: $\ln\xi \sim \sqrt{T_{BKT}/(T - T_{BKT})}$.

> *Problem for the seminar 35:* Integrate over $\tilde{\theta}$ and demonstrate that the integer numbers $m_{\boldsymbol{l}}$ satisfy the constraint $\sum_{\boldsymbol{l}} m_{\boldsymbol{l}} = 0$. In addition, demonstrate the logarithmic interaction between the integer numbers $m_{\boldsymbol{l}}$.

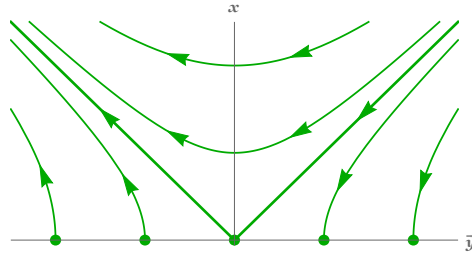> *Problem for the seminar 36:* Derive Eq. (3.76).

Figure 3.4: Renormalization group flow corresponding to Eqs. (3.92). Arrows indicate flow towards infrared.

Problem for the seminar 37: Derive the renormalization group equations for the BKT transition, cf. Eqs. (3.92).

Exercise 58: Compute the correlation function $\langle \cos^3(\theta_j - \theta_k) \rangle$ within exponential accuracy at $T \gg J$.

Exercise 59: Compute the integral

$$\int \frac{d^2\boldsymbol{q}}{(2\pi)^2} \frac{|1 - \exp(i\boldsymbol{q}\boldsymbol{R})|^2}{q^2}.$$

Exercise 60: Find the correlation function $\langle \cos(3(\theta_j - \theta_k)) \rangle$ at low temperatures $T \ll J$.

Exercise 61: Estimate the fugacity $\ln y \sim -\beta J$ from the logarithmic interaction between vortices.

Exercise 62: Find the temperature behavior of correlation length for $T - T_{BKT} \ll T_{BKT}$.

Chapter 4

Statistical mechanics of open systems

In this chapter we discuss how to probe the system in equilibrium and describe the system coupled to thermal reservoir or thermostat.

4.1 Fluctuation-dissipation theorem and the Kubo formula

4.1.1 The generalized susceptibility

Let us consider time-dependent perturbation $\mathscr{V} = -\mathscr{X} f(t)$. Here $f(t)$ is some given classical time-dependent force and $\mathscr{X}$ denotes a certain (many-body) operator. The total Hamiltonian becomes $\mathscr{H} = \mathscr{H}_0 + \mathscr{V}$. Then the quantum mechanical and thermal average of $\mathscr{X}(t)$ are determined as follows

$$\langle \mathscr{X}(t) \rangle = \mathrm{Tr} \left[U^{-1}(t) \mathscr{X} U(t) e^{-\beta \mathscr{H}_0} \right] \bigg/ \mathrm{Tr}\, e^{-\beta \mathscr{H}_0} , \qquad (4.1)$$

the evolution operator being

$$U(t) = \mathcal{T} \exp \left[-i \int\limits_{-\infty}^{t} dt'\, \mathscr{H}(t') \right] . \qquad (4.2)$$

We note that the operator $\mathscr{X}$ couples directly to the external classical force f. This implies that the operator should obey the bosonic commutation relations. As an example, the force can be an external electric field coupling the product of creation and annihilation fermionic operators.

For simplicity, we assume that the average $\langle \mathscr{X}(t) \rangle$ vanishes, $\langle \mathscr{X}(t) \rangle_{f=0} = 0$, in the absence of perturbation, $f = 0$. Then in the limit of $f \to 0$, i.e., in the *linear response* regime, the average $\langle \mathscr{X}(t) \rangle$ should be proportional to f:

$$\langle \mathscr{X}(t) \rangle = \int\limits_{-\infty}^{t} d\tau\, f(\tau) \alpha_{\mathscr{X}}(t - \tau). \tag{4.3}$$

The function $\alpha_{\mathscr{X}}(t)$ is termed as the *generalized susceptibility*.

Let us consider the harmonic force $f(t) = (f_\omega e^{-i\omega t} + f_{-\omega} e^{i\omega t})/2$ with $f_{-\omega} = f_\omega^*$ to ensure that $f(t)$ is a real function. Then we find

$$\langle \mathscr{X}(t) \rangle = \frac{1}{2} \langle \mathscr{X}(t) \rangle_\omega e^{-i\omega t} + \frac{1}{2} \langle \mathscr{X}(t) \rangle_{-\omega} e^{i\omega t},$$

$$\langle \mathscr{X}(t) \rangle_\omega = \alpha_{\mathscr{X}}(\omega) f_\omega, \quad \alpha_{\mathscr{X}}(\omega) = \int\limits_{0}^{\infty} dt\, \alpha_{\mathscr{X}}(t) e^{i\omega t}. \tag{4.4}$$

The imaginary part of the generalized susceptibility determines the energy dissipation rate averaged in time

$$Q = \frac{dE}{dt} = \overline{\left\langle \frac{\partial \mathscr{H}}{\partial t} \right\rangle} = -\overline{\langle \mathscr{X}(t) \rangle \frac{df}{dt}} = \frac{\omega}{2} \operatorname{Im} \alpha_{\mathscr{X}}(\omega) |f_\omega|^2. \tag{4.5}$$

The condition $Q > 0$ implies that $\operatorname{Im} \alpha_{\mathscr{X}}(\omega) \propto \operatorname{sgn} \omega$.

4.1.2　The fluctuation dissipation theorem

Let us compute the energy dissipation rate Q within the framework of quantum mechanics. The Hamiltonian $\mathscr{H}_0$ has eigen energies E_a and eigenstates $|a\rangle$. The time-dependent perturbation results in the transitions between the unperturbed states. The transition probability from a state $|a\rangle$ to a state $|b\rangle$ is given by the Fermi golden rule as

$$w_{a \to b} = \frac{\pi |f_\omega|^2}{2} \big| \langle a | \mathscr{X} | b \rangle \big|^2 \Big[\delta(\omega + E_b - E_a) + \delta(\omega + E_a - E_b) \Big]. \tag{4.6}$$

Then energy dissipation rate Q becomes

$$Q = \sum_{ab} \rho_a w_{a \to b}(E_b - E_a) = \frac{\pi \omega |f_\omega|^2}{2} \sum_{ab} \big| \langle a | \mathscr{X} | b \rangle \big|^2 \delta(\omega + E_a - E_b)$$

$$\times \Big[\rho_b - \rho_a \Big] \tag{4.7}$$

where $\rho_a = \exp(-\beta E_a)/Z$ is the density matrix in the energy representation. Comparing Eqs. (4.5) and (4.7), we find the following result for the imaginary part of the generalized susceptibility:

$$\operatorname{Im} \alpha_{\mathscr{X}}(\omega) = \pi \left(1 - e^{-\beta\omega}\right) \sum_{ab} \rho_a \left|\langle a|\mathscr{X}|b\rangle\right|^2 \delta(\omega + E_a - E_b). \qquad (4.8)$$

Let us turn now to variance for $\mathscr{X}$ which is a different quantity on the first sight:

$$\langle \mathscr{X}^2 \rangle = \operatorname{Tr} \rho \mathscr{X}^2 = \sum_a \rho_a \langle a|\mathscr{X}^2|a\rangle = \sum_{ab} \rho_a \left|\langle a|\mathscr{X}|b\rangle\right|^2. \qquad (4.9)$$

It is convenient to rewrite $\langle \mathscr{X}^2 \rangle$ formally as follows

$$\langle \mathscr{X}^2 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \langle \mathscr{X}^2 \rangle_\omega \qquad (4.10)$$

where

$$\langle \mathscr{X}^2 \rangle_\omega = \pi \left(1 + e^{-\beta\omega}\right) \sum_{ab} \rho_a \left|\langle a|\mathscr{X}|b\rangle\right|^2 \delta(\omega + E_a - E_b). \qquad (4.11)$$

Comparing Eqs. (4.11) and (4.8), we obtain the fluctuation dissipation theorem derived originally by H. Callen and T. Welton [11] ,

$$\langle \mathscr{X}^2 \rangle_\omega = \operatorname{Im} \alpha_{\mathscr{X}}(\omega) \coth \frac{\omega}{2T}, \qquad \langle \mathscr{X}^2 \rangle = \int_0^{\infty} \frac{d\omega}{\pi} \operatorname{Im} \alpha_{\mathscr{X}}(\omega) \coth \frac{\omega}{2T}. \quad (4.12)$$

In conclusion, we draw attention to this remarkable relation connecting the fluctuations in the thermally equilibrium system with the linear response to some time-dependent perturbation and, as a consequence, to energy dissipation.

4.1.3 The Kramers-Kronig relations

Let us consider the generalized susceptibility $\alpha_{\mathscr{X}}(\omega)$ as a function of the frequency ω in the complex plane, $\omega = \omega' + i\omega''$. Since $\alpha_{\mathscr{X}}(t)$ is finite, the generalized susceptibility $\alpha_{\mathscr{X}}(\omega)$ is also finite for $\omega'' > 0$. This implies that $\alpha_{\mathscr{X}}(\omega)$ is analytic function in the upper half-plane of ω, i.e., it has no poles. Such functions in physics are referred as *retarded* functions. Taking Eq. (4.8) into account, we can construct the expression for the retarded function $\alpha_{\mathscr{X}}(\omega)$ in the following form:

$$\alpha_{\mathscr{X}}(\omega) = \sum_{ab} \left(\rho_b - \rho_a\right) \frac{\left|\langle a|\mathscr{X}|b\rangle\right|^2}{\omega + E_a - E_b + i0}. \qquad (4.13)$$

Here we have used the relation $(x+i0)^{-1} = \text{p.v.}\ x^{-1} - \pi\delta(x)$, where p.v. denotes the Cauchy principal value.

Using Eq. (4.8), we find the following relation

$$\text{p.v.} \int\limits_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\text{Im}\,\alpha_{\mathscr{X}}(\Omega)}{\Omega - \omega} = \text{Re}\,\alpha_{\mathscr{X}}(\omega). \tag{4.14}$$

Similarly, we obtain with the help of Eq. (4.13),

$$\text{p.v.} \int\limits_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\text{Re}\,\alpha_{\mathscr{X}}(\Omega)}{\Omega - \omega} = -\,\text{Im}\,\alpha_{\mathscr{X}}(\omega). \tag{4.15}$$

The relations (4.14) and (4.15) are known as the *Kramers-Kronig relations*. In mathematics they are known as the Sokhotski—Plemelj theorem and Hilbert transform.

We note that, using Eq. (4.14), we can reproduce the result (1.33) from the fluctuation-dissipation relation. Provided that the characteristic frequencies in the generalized susceptibility are much smaller than the temperature, we find

$$\langle \mathscr{X}^2 \rangle \approx 2T \int\limits_{0}^{\infty} \frac{d\omega}{\pi} \frac{\text{Im}\,\alpha_{\mathscr{X}}(\omega)}{\omega} = T\,\text{Re}\,\alpha_{\mathscr{X}}(0). \tag{4.16}$$

4.1.4   The Kubo formula

Let us consider the two–time correlation function

$$\langle \mathscr{X}(t)\mathscr{X}(t') \rangle = \text{Tr}\left[\rho\,e^{-i\mathscr{H}_0 t}\,\mathscr{X}\,e^{i\mathscr{H}_0(t-t')}\,\mathscr{X}\,e^{i\mathscr{H}_0 t'}\right]$$

$$= \sum_{ab} \rho_a \big|\langle a|\mathscr{X}|b\rangle\big|^2 e^{i(E_b - E_a)(t-t')}. \tag{4.17}$$

Then one can check that

$$\alpha_{\mathscr{X}}(\omega) = \alpha_{\mathscr{X}}^{R}(\omega) = i \int\limits_{0}^{\infty} dt\,e^{i(\omega+i0)t}\,\text{Tr}\Big(\big[\mathscr{X}(t), \mathscr{X}(0)\big]\rho\Big). \tag{4.18}$$

This relation is referred to as the *Kubo formula*. It is a practical tool of calculating the generalized susceptibilities.

In the similar way one can check that the following relation holds for

$$\langle \mathscr{X}^2 \rangle_\omega = \frac{1}{2i}\alpha_{\mathscr{X}}^{K}(\omega), \quad \alpha_{\mathscr{X}}^{K}(\omega) = i \int\limits_{-\infty}^{\infty} dt\,e^{i\omega t}\,\text{Tr}\Big(\big\{\mathscr{X}(t), \mathscr{X}(0)\big\}\rho\Big). \tag{4.19}$$

The function $\alpha_{\mathscr{X}}^K(\omega)$ is termed as the *Keldysh function*. The fluctuation dissipation theorem relates the Keldysh and retarded response functions as

$$\alpha_{\mathscr{X}}^K(\omega) = 2i \operatorname{Im} \alpha_{\mathscr{X}}^R(\omega) \coth \frac{\omega}{2T}. \tag{4.20}$$

We note that there is analogous expression for the operators obeying the fermionic anti-commutation relations.

Problem for the seminar 38: Consider the Hamiltonian $H = \sum_\alpha \varepsilon_\alpha b_\alpha^\dagger b_\alpha$ where $b_\alpha^\dagger$ and b_α are the creation and annihilation bosonic operators. Find $i \int\limits_0^\infty dt e^{i(\omega+i0)t} \operatorname{Tr}\big([b_\alpha(t), b_\alpha^\dagger]\rho\big)$ and $i \int\limits_0^\infty dt e^{i\omega t} \operatorname{Tr}\big(\{b_\alpha(t), b_\alpha^\dagger\}\rho\big)$.

Problem for the seminar 39: Discuss the fluctuation-dissipation relation for the case of spatially dependent force.

Exercise 63: Prove the relation

$$\alpha(i\omega) = \int\limits_{-\infty}^\infty \frac{d\Omega}{\pi} \frac{\operatorname{Im} \alpha_{\mathscr{X}}(\Omega)}{\Omega - i\omega}.$$

Exercise 64: Let us define the correlation function $R_{\mathscr{X}}(\omega) = \int dt \, \langle \mathscr{X}(t)\mathscr{X}(0)\rangle e^{i\omega t}$. Demonstrate that it satisfies the detailed balance condition: $R_{\mathscr{X}}(-\omega) = e^{-\beta\omega} R_{\mathscr{X}}(\omega)$.

Exercise 65: To derive expression (4.18) by solving the equation for the density matrix to first order in perturbation $V = -\mathscr{X} f(t)$.

Exercise 66: The Hamiltonian is affected by the force $f(t) = ut$. Determine the time dependence of $\langle [\mathscr{H}(t) - \mathscr{H}(0)]^2 \rangle$. Express the result in terms of the generalized susceptibility $\alpha_{\mathscr{X}}$.

4.2 The Gorini-Kossakowski-Sudarshan-Lindblad equation

In this lecture we will derive the equation governing the dynamics of quantum system coupled to the thermal reservoir.

4.2.1 Helical 1D electrons coupled to a magnetic impurity

For definiteness, we consider magnetic impurity of spin S coupled by an exchange interaction to helical 1D electrons. This system is described by the following Hamiltonian

$$H = H_e + H_i + H_{e-i}. \tag{4.21}$$

Here

$$H_e = iv \int dy \Psi^\dagger(y) \sigma_z \partial_y \Psi(y) \tag{4.22}$$

is the Hamiltonian for helical 1D electrons moving along the y axis at velocity v. Here $\Psi(y) = \{\Psi_\uparrow(y), \Psi_\downarrow(y)\}$ and $\Psi^\dagger(y) = \{\Psi^\dagger_\uparrow(y), \Psi^\dagger_\downarrow(y)\}$ denote the spinor annihilation and creation operators of a helical electron at point y. They satisfy the following commutation relation

$$\Psi_\sigma(y)\Psi^\dagger_{\sigma'}(y') + \Psi^\dagger_{\sigma'}(y')\Psi_\sigma(y) = \delta_{\sigma\sigma'}\delta(y - y'). \tag{4.23}$$

The Hamiltonian H_{e-i} describes the exchange interaction between spin S at the point y_0 and helical electrons,

$$H_{e-i} = \frac{\mathcal{J}_{jk}}{\nu} S_j : s_k :, \qquad s_k = \frac{1}{2}\Psi^\dagger(y_0)\sigma_k\Psi(y_0), \qquad : s_k := s_k - \langle s_k \rangle, \tag{4.24}$$

where $\langle s_k \rangle$ is the average value of the spin density of helical electrons and $\nu = 1/(2\pi v)$ stands for the density of states. Finally, the Hamiltonian H_i describes the dynamics of an isolated spin. In the simplest case it is given as

$$H_i = h_j S_j, \qquad h_j = \mathcal{J}_{jk}\langle s_k \rangle/\nu. \tag{4.25}$$

4.2.2 Perturbation theory for the reduced density matrix

The density matrix ρ of the total system is described by the *Liouville equation* with the Hamiltonian H, i.e., $d\rho(t)/dt = -i[H, \rho(t)]$. Our aim is to derive the equation governing the time dynamics for the reduced density matrix of magnetic impurity. The latter is formally defined as $\rho_S = \text{Tr}_e \rho$, where Tr_e denotes the trace over the electronic degrees of freedom. In order to derive the equation for $\rho_S(t)$, we employ second-order perturbation theory in the exchange

interaction $\mathcal{J}_{ij} \ll 1$. At first, we change the representation to the interaction one, $\rho(t) = U^{-1}(t)\rho_I(t)U(t)$, where

$$U(t) = U_\mathrm{i}(t)U_\mathrm{e}(t) = U_\mathrm{e}(t)U_\mathrm{i}(t), \qquad U_\mathrm{e}(t) = e^{-iH_\mathrm{e}t}, \quad U_\mathrm{i}(t) = e^{-iH_\mathrm{i}t}. \quad (4.26)$$

The density matrix $\rho_I(t)$ satisfies the following equation

$$\frac{d\rho_I(t)}{dt} = -i[\mathcal{V}_I(t), \rho_I(t)], \quad \mathcal{V}_I(t) = U^{-1}(t)H_{\mathrm{e-i}}U(t). \qquad (4.27)$$

In order to make the perturbative treatment possible, we formally solve the evolution equation (4.27) and substitute the result back into (4.27):

$$\frac{d\rho_I}{dt} = -i[\mathcal{V}_I(t), \rho_I(-\infty)] + \int_{-\infty}^{t} dt' \left[\mathcal{V}_I(t), [\rho_I(t'), \mathcal{V}_I(t')]\right]. \qquad (4.28)$$

Tracing out electrons, we obtain

$$\frac{d\rho_{S,I}(t)}{dt} = -i\mathrm{Tr}_\mathrm{e}\left[\mathcal{V}_I(t), \rho_I(-\infty)\right] + \int_{-\infty}^{t} dt'\mathrm{Tr}_\mathrm{e}\left([\mathcal{V}_I(t), [\rho_I(t'), \mathcal{V}_I(t')]]\right) \quad (4.29)$$

where $\rho_{S,I}(t)$ is the reduced density matrix in the interacting representation, $\rho_{S,I}(t) = U_\mathrm{i}(t)\rho_S(t)U_\mathrm{i}^{-1}(t)$. We assume that the electron-impurity interaction is switched on adiabatically, so that the distribution of the edge electrons is unperturbed at $t = -\infty$. Therefore, $\mathrm{Tr}_\mathrm{e}\left[\mathcal{V}_I(t), \rho_I(-\infty)\right] = 0$, as $\mathcal{V}_I$ contains the electron operators with zero average alone. Moreover, in the weak coupling regime, $\mathcal{J}_{ij} \ll 1$, it is possible to write approximately $\rho_I(t) \approx \rho_{S,I} \otimes \rho_e^{(0)}$ on the right-hand side of the master equation. Here $\rho_e^{(0)} \propto \exp[-\beta H_\mathrm{e} - (e\beta V/2)\int dy \Psi^\dagger(y)\sigma_z\Psi(y)]$ denotes the initial density matrix for helical 1D electrons with bias voltage V applied. We note that matrix $\rho_e^{(0)}$ is the Gibbs distribution with the chemical potential $\pm eV/2$ for the spin-up/down electrons. Finally, substituting the explicit form of the perturbation $\mathcal{V}_I$, we find

$$\frac{d\rho_{S,I}}{dt} = \mathcal{J}_{rj}\mathcal{J}_{lk} \int_{-\infty}^{t} dt'\left(\chi_{jk}(t-t')\left[S_r^I(t')\rho_{S,I}(t'), S_l^I(t)\right] + \mathrm{h.c.}\right)$$

where $s_k^I(y_0, \tau) = U_\mathrm{e}^{-1}(\tau)s_k(y_0)U_\mathrm{e}(\tau)$, $S_l^I(t) = U_\mathrm{i}^{-1}(t)S_lU_\mathrm{i}(t)$, and

$$\chi_{jk}(\tau) = \frac{1}{\nu^2}\mathrm{Tr}_\mathrm{e}\left[: s_k^I(y_0, \tau) :: s_j^I(y_0, 0) : \rho_0\right]. \qquad (4.30)$$

We note that $\chi_{jk}(\tau)$ is the spin susceptibility of helical 1D electrons.

4.2.3　The Markov approximation and final form of the master equation

Next we employ the *Markov approximation*, i.e., we substitute $\rho_{S,I}(t')$ to $\rho_{S,I}(t)$. This approximation is justified since the correlators χ_{jk} decay typically over the time proportional to either $1/|eV|$ or $1/T$, while the relaxation time of matrix $\rho_{S,I}$ is determined by the scale of the order of $1/[\mathcal{J}^2 \max\{T, |eV|\}]$. Switching back to the Heisenberg picture, we obtain

$$\frac{d\rho_S(t)}{dt} = -i\,[H_{\mathrm{i}}, \rho_S(t)] + \mathcal{J}_{rj}\mathcal{J}_{lk} \int\limits_0^{+\infty} d\tau \Big(\chi_{jk}(\tau)\,\big[S_r^I(-\tau)\rho_S(t), S_l\big] + \mathrm{h.c.}\Big).$$

(4.31)

In order to write down the final form of this master equation, we should compute $\chi_{jk}(\omega) = \int_0^{+\infty} d\tau e^{i\omega\tau} \chi_{jk}(\tau)$. Evaluating the trace in Eq. (4.30) yields

$$\chi_{jk}(\omega) = \frac{i}{4} \sum_{\sigma_1,\sigma_2} \int d\xi_1 d\xi_2\, \sigma_k^{\sigma_1\sigma_2}\sigma_j^{\sigma_2\sigma_1} \frac{1 - f_F(\xi_2 - \sigma_2 V/2)}{\omega + \xi_1 - \xi_2 + i0} f_F(\xi_1 - \sigma_1 V/2)$$

(4.32)

where $f_F(\varepsilon) = 1/[e^{\varepsilon/T} + 1]$.

　　The spin susceptibility can be split into the Hermitian and anti-Hermitian parts:

$$\chi_{jk}(\omega) = \frac{1}{2}\chi_{jk}^{(1)}(\omega) + i\chi_{jk}^{(2)}(\omega), \qquad \chi^{(1)} = \chi^{(1)\dagger}, \quad \chi^{(2)} = \chi^{(2)\dagger}.$$

(4.33)

Here we introduce

$$\chi_{jk}^{(1)}(\omega) = \frac{\pi}{2} \sum_{\sigma_1,\sigma_2} \int d\xi_1 d\xi_2\, \sigma_k^{\sigma_1\sigma_2}\sigma_j^{\sigma_2\sigma_1}\delta(\omega + \xi_1 - \xi_2)(1 - f_F(\xi_2 - \sigma_2 V/2))$$

$$\times f_F(\xi_1 - \sigma_1 V/2)$$

(4.34)

and

$$\chi_{jk}^{(2)}(\omega) = \frac{1}{4} \sum_{\sigma_1,\sigma_2} \mathrm{p.v.} \int d\xi_1 d\xi_2\, \sigma_k^{\sigma_1\sigma_2}\sigma_j^{\sigma_2\sigma_1} f_F\Big(\xi_1 - \frac{\sigma_1 V}{2}\Big)$$

$$\times \frac{(1 - f_F(\xi_2 - \sigma_2 V/2))}{\omega + \xi_1 - \xi_2}$$

(4.35)

where p.v. denotes the Cauchy principal value. The part $\chi_{jk}^{(2)}$ contains the logarithmically diverging contributions. The corresponding terms in the master

equation (4.31) can be cast in the form of unitary dynamics, i.e., they provide us the renormalization of H_i — the so-called Lamb shift. These logarithmically divergent contributions describe the Kondo renormalization of the coupling constants $\mathcal{J}_{jk}$.

Omitting $\chi^{(2)}_{jk}$, we finally obtain the quantum master equation in the following form

$$\frac{d\rho_S}{dt} = i\left[\rho_S, H_\mathrm{i}\right] + \eta_{jk}\left[S_j\rho_S S_k - \rho_S S_k S_j/2 - S_k S_j \rho_S/2\right]. \qquad (4.36)$$

Here the 3×3 matrix $\eta_{jk} = \pi T(\mathcal{J}\Pi_V \mathcal{J}^T)_{jk}$ governs the non-unitary evolution of the reduced generalized density matrix. Here we have introduced

$$\Pi_V = \begin{pmatrix} \frac{V}{2T}\coth\frac{V}{2T} & -\frac{iV}{2T} & 0 \\ \frac{iV}{2T} & \frac{V}{2T}\coth\frac{V}{2T} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (4.37)$$

We note that the eigenvalues of the matrix Π_V are equal to 1 and $(V/2T)[\coth(V/2T) \pm 1] \geqslant 0$. Therefore, the matrix η is positive semidefinite and the master equation (4.36) has the Gorini-Kossakowski-Sudarshan-Lindblad form, ensuring the positivity of ρ_S.

4.2.4 The Gibbs distribution for the reduced density matrix

Applying the corresponding rotation of the spin basis, an arbitrary exchange matrix $\mathcal{J}$ can be reduced to the lower triangular form

$$\mathcal{J} = \begin{pmatrix} \mathcal{J}_{xx} & 0 & 0 \\ \mathcal{J}_{yx} & \mathcal{J}_{yy} & 0 \\ \mathcal{J}_{zx} & \mathcal{J}_{zy} & \mathcal{J}_{zz} \end{pmatrix}. \qquad (4.38)$$

Then the Hamiltonian H_i becomes proportional to spin S_z. Therefore, the stationary density matrix of the spin should be diagonal in the eigen basis of spin S_z, i.e.,

$$\langle m|\rho_S|m'\rangle = \delta_{m,m'}\rho_{S,m}, \qquad S_z|m\rangle = m|m\rangle, \qquad m = -S, \ldots, S. \qquad (4.39)$$

Substituting this diagonal anzats into Eq. (4.36), we find that $\rho_{S,m}$ should satisfy the following equation

$$\eta_{jk}\rho_{S,m+1}\langle m|S_j|m+1\rangle\langle m+1|S_k|m\rangle + \eta_{jk}\rho_{S,m-1}\langle m|S_j|m-1\rangle\langle m-1|S_k|m\rangle$$
$$= \eta_{jk}\rho_{S,m}\langle m|S_k|m+1\rangle\langle m+1|S_j|m\rangle + \eta_{jk}\rho_{S,m}\langle m|S_k|m-1\rangle\langle m-1|S_j|m\rangle. \qquad (4.40)$$

Let us demonstrate that the solution of this equation has the form $\rho_{S,m} \propto \exp(\beta_{\text{eff}} m)$. Using the matrix elements of the spin operators,

$$\langle m|S_x|m+1\rangle = \langle m+1|S_x|m\rangle = \frac{1}{2}\sqrt{(S+m+1)(S-m)},$$

$$\langle m|S_y|m+1\rangle = -\langle m+1|S_y|m\rangle = \frac{i}{2}\sqrt{(S+m+1)(S-m)}, \qquad (4.41)$$

we find

$$\left(e^{\beta_{\text{eff}}}\eta_+ - \eta_-\right)(S+m+1)(S-m) + \left(e^{-\beta_{\text{eff}}}\eta_- - \eta_+\right)$$
$$\times (S+m)(S-m+1) = 0 \qquad (4.42)$$

where $\eta_\pm = \eta_{xx} + \eta_{yy} \pm i\eta_{xy} \mp i\eta_{yx}$. Hence, we obtain that

$$e^{\beta_{\text{eff}}} = \frac{\eta_-}{\eta_+}. \qquad (4.43)$$

At $V = 0$ the parameter β_{eff} vanishes, i.e., the impurity spin is equally distributed over the states with all possible spin projections. At $V \gg T$, the parameter β_{eff} tends to the V-independent constant. Therefore, at large voltage the impurity spin is still not fully polarized.

Problem for the seminar 40: Derive Eq. (4.32).

Problem for the seminar 41: Analyse $\chi_{jk}^{(2)}(\omega)$ and derive the Kondo renormalization of $\mathcal{J}_{jk}$.

Exercise 67: Prove commutation relation (4.23).

Exercise 68: Compute the density of states of 1D helical electrons governed by the Hamiltonian H_{e}.

Exercise 69: Demonstrate that $\chi_{jk}^{(2)}(\omega)$ results in the unitary dynamics for $\rho_S(t)$.

Exercise 70: Compute $\text{Tr}\,\rho_S(t)$.

Chapter 5

Thermalization of an isolated quantum system

5.1   The eigenstate thermalization hypothesis

In the present course we have postulated the Gibbs distribution for the density matrix of quantum system. One way of how such distribution could occur we discussed in the previous lecture. For a quantum system weakly coupled to large quantum system (reservoir), the Gibbs distribution for the reduced density matrix can be induced as a result of the interaction. However, one can ask what happens if the quantum system is completely isolated. In this lecture we discuss this point, following recent review by Deutsch [12].

5.1.1   Ergodicity and chaos in classical mechanics

Let us consider classical system described by a set of N canonically conjugated coordinates $\Gamma = \{q_1, p_1, \ldots, q_N, p_N\}$. During its time evolution the system moves in the 2^N dimensional phase space $\mathscr{S}$. The system is called *ergodic* if the time average of observable O is equivalent to microcanonical average,

$$\lim_{\mathcal{T} \to \infty} \frac{1}{\mathcal{T}} \int\limits_0^{\mathcal{T}} dt \, O(\Gamma(t)) \equiv \frac{\int_{\Gamma_E} d\Gamma \, O(\Gamma)}{\int_{\Gamma_E} d\Gamma}. \tag{5.1}$$

Here Γ_E denotes the subspace of $\mathscr{S}$ in which the constants of motion, e.g. energy, remain fixed. Although the ergodicity exists in many systems, there is a class of systems in which ergodicity breaks down. They are so-called the integrable models. The phonon modes in the perfect harmonic crystal are an example of such system. For the system close to integrable one, the ergodicity occurs in the limit $N \to \infty$ as follows from the Kolmogorov–Arnold–Moser theorem.

Another important concept related to the classical systems is *chaos*. A chaotic system is such that, if one starts to evolve it from two close initial conditions, after sufficiently long time these two states will be in very different places of the phase space. This implies a divergence of the neighboring trajectories in the phase space. This divergence is characterized by the Lyapunov exponents. We underline that ergodicity and chaos are not interchangeable notions. However, in the limit $N \to \infty$ the majority of classical systems are ergodic and chaotic. Ergodicity and chaos of classical system allow its thermalization.

5.1.2   Chaos in an isolated quantum system

The concept of chaos comes across difficulties to define in the case of quantum dynamics. The problem lies in linearity of the Schrödinger equation. However, quantum chaotic system can be formulated in terms of statistics of its energy levels. There is the Bohigas–Giannoni–Schmit conjecture. The energy levels

of a quantum system, which the classical analogue is chaotic, have the statistics described by the random matrix theory. The chaotic behavior in the quantum systems is active field of research at present.

5.1.3 Eigenstate thermalization hypothesis

An idea of how the quantum system thermalizes is based on the *eigenstate thermalization hypothesis*. It can be formulated in the following form. The matrix element of some operator A can be written as

$$\langle a|A|b \rangle = \mathcal{A}(E)\delta_{ab} + e^{-S(E)/2}g_{ab}(E,\omega) \tag{5.2}$$

where $E = (E_a + E_b)/2$ and $\omega = E_a - E_b$, and $g_{ab}(E,\omega)$ is a bounded smooth function. The entropy is defined as

$$e^{-S(E)} = E\sum_a \delta_\Gamma(E - E_a) = \frac{E}{\pi}\sum_a \frac{\Gamma}{(E - E_a)^2 + \Gamma^2}. \tag{5.3}$$

Here Γ is a small broadening of the many-particle levels E_a, making function $S(E)$ smeared and monotonous,

$$dS/dE \equiv 1/T > 0. \tag{5.4}$$

The entropy $S(E)$ is an extensive quantity proportional to the number of degrees of freedom in the quantum system. We assume that the energy E changes slowly on the energy scale of the order of temperature T. We note that the statistical properties of $g_{ab}(E,\omega)$ resemble the random independent quantities from the Gaussian distribution.

Let us demonstrate that, if Eq. (5.2) holds for, then the function $\mathcal{A}(E)$ coincides with the proper Gibbs average,

$$\mathcal{A}_G = \frac{\mathrm{Tr}\, Ae^{-H/T}}{\mathrm{Tr}\, e^{-H/T}} \tag{5.5}$$

where temperature T is defined in Eq. (5.4). Let us consider

$$\mathrm{Tr}\, Ae^{-H/T} = \sum_a \langle a|A|a \rangle e^{-E_a/T} = \int d\varepsilon e^{-\varepsilon/T}\sum_a \delta(\varepsilon - E_a)\langle a|A|a \rangle. \tag{5.6}$$

Now using Eq. (5.2), we find

$$\mathrm{Tr}\, A\, e^{-H/T} \approx \int d\varepsilon\, e^{-\varepsilon/T}\mathcal{A}(\varepsilon)\sum_a \delta(\varepsilon - E_a) = \int d\varepsilon\, e^{S(\varepsilon)-\varepsilon/T}\mathcal{A}(\varepsilon)/\varepsilon \tag{5.7}$$

Since $S(\varepsilon)$ is an extensive quantity, we can take the integral over ε by the saddle–point method. The saddle–point magnitude of $\varepsilon = E$ is determined by Eq. (5.4). Then we find

$$\mathrm{Tr}\, A\, e^{-H/T} \approx e^{S(E)-E/T} \mathcal{A}(E)/E. \tag{5.8}$$

Hence, we obtain

$$\mathcal{A}_G \approx \mathcal{A}(E) + O(1/S). \tag{5.9}$$

We note that this relation implies that in essence, the matrix element of an operator behaves as a thermal (Gibbs) average with the proper temperature.

Now we consider time average of operator. Let us introduce the state $|\psi_t\rangle = \sum_a c_a e^{-iE_a t}|a\rangle$ and define the average $A_t = \langle\psi_t|A|\psi_t\rangle$. Then we can define the time average as

$$\overline{A} = \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} dt\, A_t. \tag{5.10}$$

Under assumption that Eq. (5.2) holds for, we demonstrate that the time average $\overline{A}$ coincides with the thermal or Gibbs average for the temperature corresponding to the energy $E = \sum_a |c_a|^2 E_a$. We can write

$$\overline{A} = \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} dt \left[\sum_a |c_a|^2 \langle a|A|a\rangle + \sum_{b\neq a} c_a^* c_b\, e^{i(E_a-E_b)t} \langle a|A|b\rangle \right]$$
$$= \sum_a |c_a|^2 \langle a|A|a\rangle, \tag{5.11}$$

since for the non-degenerate levels the oscillating terms vanish in the limit $\mathcal{T} \to \infty$. Next using Eq. (5.2), we find

$$\overline{A} \approx \sum_a |c_a|^2 \left[\mathcal{A}(E) + \mathcal{A}'(E)(E_a - E) + \frac{1}{2}\mathcal{A}''(E)(E - E_a)^2 + \dots \right] \approx \mathcal{A}(E). \tag{5.12}$$

Since we have demonstrated above that $\mathcal{A}(E)$ is equivalent to the Gibbs average $\mathcal{A}_G$, we show that the ETH hypothesis implies the ergodicity.

Exercise 71: Show that $\overline{(A_t - \overline{A})^2} \propto \exp(-S(E))$.

Chapter 6

Solution of problems for seminars

6.1 Seminar I

In this section, we present solutions for the problems Nos. 1, 2 and 3.

6.1.1 Problems 1 and 2

We consider simplest system in statistical physics. The system obeys the following assumptions:

- all particles are identical;

- particles are non-interacting;

- each particle can occupy two energy levels (the ground state and the excited state).

The above assumptions lead to the following Hamiltonian:

$$\mathcal{H} = \sum_{j=1}^{N} H_j, \qquad H_j = -\frac{B}{2}\sigma_j^z. \tag{6.1}$$

All information about the system could be obtained from the statistical sum which can be calculated in two ways.

The first one is applicable for the non-interacting systems. In this case the system can be split into two independent parts, A and B, such that $H = H_A + H_B$. Then the partition function becomes $Z = Z_A \times Z_B$ where $Z_i =$

$\text{tr}_i[\exp{(-\beta H_i)}]$. Applying this result to our system, we arrive at

$$\text{Partition function:} \quad Z = \text{tr}\left\{\exp\left(\frac{\beta B}{2}\sigma^z\right)\right\}^N = 2^N \cosh^N\left(\frac{\beta B}{2}\right) \quad (6.2)$$

$$\text{Free energy:} \quad F = -T\ln(Z) = -TN\ln\left[2\cosh\left(\frac{B}{2T}\right)\right] \quad (6.3)$$

$$\text{Entropy:} \quad S = -\frac{\partial F}{\partial T} = N\left[\ln\left[2\cosh\left(\frac{B}{2T}\right)\right] - \frac{B}{2T}\tanh\left(\frac{B}{2T}\right)\right] \quad (6.4)$$

$$\text{Energy:} \quad E = F + TS = -N\frac{B}{2}\tanh\left(\frac{B}{2T}\right) \quad (6.5)$$

$$\text{Specific heat:} \quad C_V = T\frac{\partial S}{\partial T} = \frac{\partial E}{\partial T} = \frac{N}{4\cosh^2\left(\frac{B}{2T}\right)}\left(\frac{B}{T}\right)^2 \quad (6.6)$$

$$\text{Chemical potential:} \quad \mu = \frac{\partial F}{\partial N} = -TN\ln\left[2\cosh\left(\frac{B}{2T}\right)\right] \quad (6.7)$$

The second interesting approach is the following. Instead of summation over all independent states, we perform it over all possible eigen energies $\mathcal{E}_\lambda$ of the many-body Hamiltonian $\mathcal{H}$. Then, the partition function becomes

$$Z = \sum_\lambda \exp(-\beta\mathcal{E}_\lambda) = \sum_{\mathcal{E}_\lambda} g(\mathcal{E}_\lambda)\exp(-\beta\mathcal{E}_\lambda). \quad (6.8)$$

On the right hand side one should take the sum over all possible eigen energies and the quantity $g(\mathcal{E}_\lambda)$ is termed as the density of states. It characterizes the degeneracy of the eigenstates. In our case, the eigenstates can be described by a number of spins k anti-parallel to the direction of the magnetic field B. Then, one can find $\mathcal{E}_k = -BN/2 + Bk$. Since we can choose arbitrary k spins among N, such eigenstate has the degeneracy $g(\mathcal{E}_k) = C_N^k$, where C_N^k denotes the binomial coefficients. Finally, using Newton's binomial theorem, we obtain the same result as in the first approach.

6.1.2   Problem 3

One of most powerful techniques to prove the thermodynamics identities is a method of Jacobians. Let us suppose that we have a pair of independent thermodynamics variables X and Y, for example, V, T or P, S but not conjugated, e.g. P, V. Then, the Jacobian of transformation from variables X, Y to A, B reads

$$\frac{\partial(A, B)}{\partial(X, Y)} = \det\begin{pmatrix} \frac{\partial A}{\partial X} & \frac{\partial B}{\partial X} \\ \frac{\partial A}{\partial Y} & \frac{\partial B}{\partial Y} \end{pmatrix}. \quad (6.9)$$

The definition of the Jacobian leads to several useful identities:

$$\frac{\partial(A,Y)}{\partial(X,Y)} = \left(\frac{\partial A}{\partial X}\right)_Y, \qquad \frac{\partial(A,B)}{\partial(X,Y)} = \frac{\partial(A,B)}{\partial(C,D)}\frac{\partial(C,D)}{\partial(X,Y)}. \qquad (6.10)$$

Using this identities, we obtain

$$C_P - C_V = T\left(\frac{\partial S}{\partial T}\right)_P - T\left(\frac{\partial S}{\partial T}\right)_V = T\frac{\partial(S,P)}{\partial(T,P)} - T\frac{\partial(S,V)}{\partial(T,V)}$$

$$= T\frac{\partial(S,P)}{\partial(T,V)}\frac{\partial(T,V)}{\partial(T,P)} - T\frac{\partial(S,V)}{\partial(T,V)},$$

$$T\left[\left(\frac{\partial S}{\partial T}\right)_V\left(\frac{\partial P}{\partial V}\right)_T - \left(\frac{\partial P}{\partial T}\right)_V\left(\frac{\partial S}{\partial V}\right)_T\right]\frac{1}{\left(\frac{\partial P}{\partial V}\right)_T} - C_V$$

$$= -T\left(\frac{\partial P}{\partial T}\right)_V\frac{\partial^2 F}{\partial V\partial T}\frac{1}{\left(\frac{\partial P}{\partial V}\right)_T} = -T\left(\frac{\partial P}{\partial T}\right)_V^2\frac{1}{\left(\frac{\partial P}{\partial V}\right)_T}. \qquad (6.11)$$

6.2 Seminar II

In this section, we consider the solutions of problems Nos. 4, 5, and 6.

6.2.1 Problem 4

In the previous seminar we have found several thermodynamic quantities of the spin system in the magnetic field. One can calculate the fluctuation of energy, using the expression from the second lecture. However, it is instructive to calculate fluctuations from the first principles. We will use the second approach for calculating the partition function from the previous seminar. This leads to

$$\langle\langle E^2\rangle\rangle = \langle E^2\rangle - \langle E\rangle^2 = \frac{1}{Z}\sum_E E^2 g(E)e^{-\beta E} - \left[\frac{1}{Z}\sum_E Eg(E)e^{-\beta E}\right]^2. \qquad (6.12)$$

As is mentioned in the previous seminar, we can parametrize E by the number k of the "flipped" spins, $E = -\frac{NB}{2} + kB$. It is worthwhile to note that the fluctuations similar to the other measured thermodynamic characteristics are independ of the ground state energy. Therefore, we can use the expression $E = Bk$ for the energy of the spin configuration with k "flipped" spins. We start our calculation from the last term on the right hand side of Eq. (6.12) ($p = e^{-\beta B}$),

$$\frac{1}{Z}\sum_E Eg(E)e^{-\beta E} = \frac{1}{Z}\sum_{k=0}^N BkC_N^k e^{-\beta Bk} = \frac{B}{Z}\sum_{k=0}^N kC_N^k p^k = \frac{B}{Z}Np(1+p)^{N-1}. \qquad (6.13)$$

Since the partition function is given as $Z = (1+p)^N$, we find $\langle E \rangle = NBp/(1+p)$. The same technique yields,

$$\langle \langle E^2 \rangle \rangle = B^2 \left(\frac{pN}{1+p} + \frac{p^2 N(N-1)}{(1+p)^2} \right) = \frac{B^2 Np}{(1+p)^2} = \frac{B^2 N}{4 \cosh(\frac{B}{2T})}. \qquad (6.14)$$

6.2.2   Problem 5

The free energy is calculated in Problems 1 and 2. Using these results, we can obtain the following expressions,

$$\text{Magnetization:} \quad M = -\frac{\partial F}{\partial B} = \frac{N}{2} \tanh \left(\frac{B}{2T} \right) \ ,$$

$$\text{Spin susceptibility:} \quad \chi = \frac{\partial M}{\partial B} = \frac{N}{4T} \frac{1}{\cosh^2 \left(\frac{B}{2T} \right)}. \qquad (6.15)$$

For the fluctuation of magnetization, we find

$$\langle \langle M^2 \rangle \rangle = \frac{\langle \langle E^2 \rangle \rangle}{B^2} = \frac{N}{4 \cosh(\frac{B}{2T})} \qquad (6.16)$$

as is expected.

6.2.3   Problem 6

At first, we express ΔP and ΔS via ΔP and ΔV,

$$\begin{pmatrix} \Delta P \\ \Delta S \end{pmatrix} = M \begin{pmatrix} \Delta V \\ \Delta T \end{pmatrix}, \qquad M = \begin{pmatrix} \left(\frac{\partial P}{\partial V} \right)_T & \left(\frac{\partial P}{\partial T} \right)_V \\ \left(\frac{\partial S}{\partial V} \right)_T & \left(\frac{\partial S}{\partial T} \right)_V \end{pmatrix}. \qquad (6.17)$$

We note that $M^T = M$. Using this expression, we obtain the following result for $U_{\min}$,

$$U_{\min} = \frac{1}{2} \left[\left(\frac{\partial S}{\partial T} \right)_V (\Delta T)^2 - \left(\frac{\partial P}{\partial V} \right)_T (\Delta V)^2 \right]. \qquad (6.18)$$

Hence we derive the following expression for the correlation functions (the standard answer for the Gaussian distribution),

$$G = \left\langle \begin{pmatrix} \Delta V \\ \Delta T \end{pmatrix} \begin{pmatrix} \Delta V \\ \Delta T \end{pmatrix}^T \right\rangle = \begin{pmatrix} \langle \Delta V \Delta V \rangle & \langle \Delta T \Delta V \rangle \\ \langle \Delta V \Delta T \rangle & \langle \Delta T \Delta T \rangle \end{pmatrix}$$

$$= T \begin{pmatrix} - \left(\frac{\partial V}{\partial P} \right)_T & 0 \\ 0 & \left(\frac{\partial T}{\partial S} \right)_V \end{pmatrix}. \qquad (6.19)$$

Both matrices G and M are necessary to calculate the other fluctuations. This can be done in the following way,

$$\left\langle \begin{pmatrix} \Delta P \\ \Delta S \end{pmatrix} \begin{pmatrix} \Delta V \\ \Delta T \end{pmatrix}^T \right\rangle = \begin{pmatrix} \langle \Delta P \Delta V \rangle & \langle \Delta P \Delta T \rangle \\ \langle \Delta S \Delta V \rangle & \langle \Delta S \Delta T \rangle \end{pmatrix} = MG$$

$$= T \begin{pmatrix} -1 & \left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial T}{\partial S}\right)_V \\ -\left(\frac{\partial S}{\partial V}\right)_T \left(\frac{\partial V}{\partial P}\right)_T & 1 \end{pmatrix}. \tag{6.20}$$

Finally, we find

$$\left\langle \begin{pmatrix} \Delta P \\ \Delta S \end{pmatrix} \begin{pmatrix} \Delta P \\ \Delta S \end{pmatrix}^T \right\rangle = \begin{pmatrix} \langle \Delta P \Delta P \rangle & \langle \Delta P \Delta S \rangle \\ \langle \Delta S \Delta P \rangle & \langle \Delta S \Delta S \rangle \end{pmatrix} = MGM^T$$

$$= T \begin{pmatrix} -\left(\frac{\partial P}{\partial V}\right)_T + \left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial T}{\partial S}\right)_V \left(\frac{\partial S}{\partial V}\right)_T & 0 \\ 0 & \left(\frac{\partial S}{\partial T}\right)_V - \left(\frac{\partial S}{\partial V}\right)_T \left(\frac{\partial V}{\partial P}\right)_T \left(\frac{\partial P}{\partial T}\right)_V \end{pmatrix}. \tag{6.21}$$

In order to calculate the last expression, one can use the Jacobian method,

$$\left(\frac{\partial P}{\partial T}\right)_V \left(\frac{\partial S}{\partial V}\right)_T = \frac{\partial(PS)}{\partial(TV)} + \left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial P}{\partial V}\right)_T. \tag{6.22}$$

Using the above relation, we find the following result,

$$\begin{pmatrix} \langle \Delta P \Delta P \rangle & \langle \Delta P \Delta S \rangle \\ \langle \Delta S \Delta P \rangle & \langle \Delta S \Delta S \rangle \end{pmatrix} = T \begin{pmatrix} \left(\frac{\partial P}{\partial V}\right)_S & 0 \\ 0 & \left(\frac{\partial S}{\partial T}\right)_P \end{pmatrix}. \tag{6.23}$$

6.3 Seminar III

In this section, we discuss solutions of Problems 7, 8, 9, 10, and 11.

6.3.1 Problem 7

In this problem we will find the density of state for free quantum particle in an arbitrary spatial dimension. To solve this problem, we must write the integral for the density of states and use the spherical coordinate system,

$$g(\varepsilon) = \int \frac{d^d \boldsymbol{p}}{(2\pi\hbar)^d} \delta\left(\varepsilon - \frac{p^2}{2m}\right) = \int_0^\infty \frac{\sigma_d p^{d-1} dp}{(2\pi\hbar)^d} \delta\left(\varepsilon - \frac{p^2}{2m}\right)$$

$$= \frac{\sigma_d m}{(2\pi\hbar)^d} (\sqrt{2m\varepsilon})^{d-2}. \tag{6.24}$$

Here $\sigma_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ denotes the area of d-dimensional sphere, S_d.

6.3.2   Problem 8

In this problem, we will find the density of states of ideal two-dimensional electron gas in the perpendicular magnetic field. Let vector potential be $\boldsymbol{A} = \{0, Bx, 0\}$. Then Hamiltonian is $H = \frac{\hat{p}_x^2}{2m} + \frac{(p_y - \frac{eB}{c}x)^2}{2m} \pm \mu_B B$. Here μ_B denotes the Bohr magneton. We note that the momentum along y-axis and the spin are conserved. Then the eigen energies are given as $\varepsilon_n = \omega_c(n + \frac{1}{2} \pm \frac{1}{2})$ where $\omega_c = \frac{eB}{mc}$ is the cyclotron frequency (the Landau level problem is treated in the course of the quantum mechanics). Then, we obtain

$$g(\varepsilon) = \frac{1}{S}\frac{S}{2\pi l_H^2}\left[\delta(\varepsilon) + 2\sum_{n=1}^{\infty}\delta(\varepsilon - \omega_c n)\right] = \frac{m\omega_c}{2\pi}\left[\delta(\varepsilon) + 2\sum_{n=1}^{\infty}\delta(\varepsilon - \omega_c n)\right].$$
(6.25)

Here $l_H = \sqrt{\hbar/(eB)}$ denotes the magnetic length and $S/(2\pi l_H^2)$ stands for the Landau level degeneracy.

6.3.3   Problem 9

This problem is important in the Fermi gas theory. We will calculate the temperature correction to the chemical potential at $T \ll E_F$ for an ideal Fermi gas. We note that for all normal metals in $d = 3$, the Fermi energy is of the order of $E_F \approx 1\,\text{eV} \approx 1.1 \times 10^5$ K.

The temperature behavior of the chemical potential is related with conserving the number of particles at a given volume, cf. Eq. (1.48). Let $\beta = \beta_0 + \delta\beta$, then we find

$$0 = \frac{\partial N}{\partial T} = \int\limits_0^{\infty} \frac{e^{\beta_0(\varepsilon - \mu)}}{\left(1 + e^{\beta_0(\varepsilon - \mu)}\right)^2}\left(\frac{\varepsilon - \mu}{T^2} + \frac{1}{T}\frac{\partial\mu}{\partial T}\right)g(\varepsilon)d\varepsilon. \qquad (6.26)$$

The main technique to calculate such integrals with the Fermi distribution is integration over variable $\xi = \varepsilon - \mu$. The advantage of using such variable is that the fermions only in the vicinity of the Fermi surface take part in perturbing the ground state, i.e., $\xi \sim T$ provides the dominant contribution to the integrals. Using condition, $E_F \gg T$, we obtain

$$0 = \frac{\partial N}{\partial T} = \int\limits_{-\infty}^{\infty} \frac{1}{4\cosh^2(\beta\xi/2)}\left(\frac{\xi}{T^2} + \frac{1}{T}\frac{\partial\mu}{\partial T}\right)(g(\mu) + g'(\mu)\xi)d\xi$$

$$= \int\limits_{-\infty}^{\infty} \frac{1}{4\cosh^2(\beta\xi/2)}\left(g'(\mu)\frac{\xi^2}{T^2} + \frac{g(\mu)}{T}\frac{\partial\mu}{\partial T}\right)d\xi = \frac{\pi^2}{3}Tg'(\mu) + g\frac{\partial\mu}{\partial T}. \quad (6.27)$$

Hence, we find $\partial\mu/\partial T = -\pi^2 g'(\mu)T/(3g(\mu))$ and, consequently, $\mu = E_F - \pi^2 g'(\mu)T^2/[6g(\mu)]$.

6.3.4 Problem 10

In this problem we find the specific heat of ideal degenerate Fermi gas in an arbitrary spatial dimension. We use integration over ξ to find an answer. Then, we obtain, cf. Eq. (1.50),

$$
C_V = \frac{\partial}{\partial T}\int_0^\infty d\varepsilon\, g(\varepsilon)\varepsilon f_F(\varepsilon) = \int_{-\infty}^\infty d\xi \frac{1}{4\cosh^2(\beta\xi/2)}\left(\frac{g(\mu)\mu}{T}\frac{\partial\mu}{\partial T}\right.
$$

$$
\left. +(g(\mu)+g'(\mu)\mu)\frac{\xi^2}{T^2}\right) = g(\mu)\mu\frac{\partial\mu}{\partial T} + (g(\mu)+g'(\mu)\mu)\frac{\pi^2}{3}T = \frac{\pi^2}{3}g(\mu)T.
$$

$$(6.28)$$

6.3.5 Problem 11

We find the zero-field spin susceptibility of ideal two-dimensional electron gas. The weak fields do not change "trajectories" of electrons. Thus we can use the density of states for a Fermi gas in the absence of the magnetic field. This problem could also be solved by taking the derivative of integral over the chemical potential (For $d = 2$, the density of states is constant, $g(\varepsilon) = m/(2\pi)$.),

$$
\chi = -\frac{\partial^2\Omega}{\partial B^2} = -\frac{\partial^2}{\partial B^2}\frac{\Omega_0(\mu+\mu_B B)+\Omega_0(\mu-\mu_B B)}{2} = \frac{\mu_B}{2}\frac{\partial}{\partial B}\int_0^\infty d\varepsilon\, g(\varepsilon)
$$

$$
\times\left[f_F(\varepsilon-\mu_B B)-f_F(\varepsilon+\mu_B B)\right] = \mu_B^2\int_0^\infty d\varepsilon\, g(\varepsilon)\left(-\frac{\partial f_F(\varepsilon)}{\partial\varepsilon}\right) = \mu_B^2 g(\mu).
$$

$$(6.29)$$

Here $\Omega_0(\mu)$ stands for the thermodynamic potential of ideal Fermi gas at $B = 0$.

6.4 Seminar IV

In this section, we consider the solutions for Problems 12 and 13.

6.4.1 Problem 12

The problem is to find the magnetization of ideal two-dimensional electron gas in the presence of a relatively strong perpendicular magnetic field $T \ll \mu_B B \ll$

E_F. It is more complicated problem compared with the previous one. In this case we should use the expression for the density of states, obtained in the Problem 8. Then the energy can be written as

$$E = \int\limits_0^\infty \varepsilon g(\varepsilon) f_F(\varepsilon - \mu) d\varepsilon = \frac{m\omega_c}{\pi} \sum_{n=1}^\infty \omega_c n f_F(\omega_c n - \mu). \tag{6.30}$$

In the limit $\mu_B B = 2\omega_c \gg T$ we can approximate the Fermi distribution function by the Heaviside step function. In this case the energy becomes

$$E = \frac{m\omega_c^2}{\pi} \sum_{n=1}^N n = \frac{m\omega_c^2 N(N+1)}{2\pi}. \tag{6.31}$$

Here $N = [\mu/\omega_c]$ is the number of filled states. As a result, the magnetization reads,

$$M = -\frac{\partial E}{\partial B} = -\frac{2\mu_B m\omega_c N^2}{\pi}. \tag{6.32}$$

In order to find the magnetization at $T \sim \omega_c$, we use the Poisson summation formula,

$$\sum_{n=-\infty}^\infty \delta(n - x) = \sum_{k=-\infty}^\infty e^{2\pi i k x}. \tag{6.33}$$

Using this formula to simplify the expression for the energy, we obtain

$$E = \frac{m\omega_c^2}{2\pi} \sum_{n=-\infty}^\infty \int\limits_{-\infty}^\infty dx \delta(x - n) |x| f_F(\omega_c |x| - \mu)$$

$$= \frac{m\omega_c^2}{\pi} \sum_{k=-\infty}^\infty \mathrm{Re} \int\limits_0^\infty dx e^{i2\pi k x} x f_F(\omega_c x - \mu). \tag{6.34}$$

The term $k = 0$ in the sum is an energy of the Fermi gas at temperature T in zero magnetic field. Since it is independent of the magnetic field, we can study the difference ΔE between the energy energy in the finite and zero magnetic fields,

$$\Delta E = \frac{2m\omega_c^2}{\pi} \sum_{k=1}^\infty \mathrm{Re} \int_0^\infty dx e^{i2\pi k x} x f_F(\omega_c x - \mu) = \frac{2m\omega_c^2}{\pi} \sum_{k=1}^\infty \frac{1}{4\pi^2 k^2}$$

$$\times \mathrm{Re} \left(1 - \int_0^\infty dx e^{i2\pi k x} (1 - i2\pi k x) \partial_x f_F(\omega_c x - \mu) \right). \tag{6.35}$$

The last formula is obtained using integration by parts. This expression is suitable for the integration over variable $\xi = \omega_c x - \mu$ at $\mu \gg T$. This leads to the following integral,

$$\Delta E = \sum_{k=1}^{\infty} \frac{m\omega_c^2}{2\pi^3 k^2} \operatorname{Re} \left[1 + \left(i2\pi k \frac{\mu}{\omega_c} - 1 \right) e^{i2\pi k\mu/\omega_c} \beta \int_{-\infty}^{\infty} d\xi \frac{e^{i2\pi k\xi/\omega_c}}{4\cosh^2(\beta\xi/2)} \right].$$
(6.36)

The last integral can be calculated and finally:

$$\Delta E = \frac{2m\omega_c^2}{\pi} \sum_{k=1}^{\infty} \frac{1}{4\pi^2 k^2} \operatorname{Re} \left(1 + \left(i2\pi k \frac{\mu}{\omega_c} - 1 \right) e^{i2\pi k\mu/\omega_c} \frac{2\pi^2 kT}{\omega_c \sinh\left(\frac{2\pi^2 kT}{\omega_c}\right)} \right)$$

$$= \frac{2m\omega_c^2}{\pi} \sum_{k=1}^{\infty} \frac{1}{4\pi^2 k^2} \left[1 - \left(\sin(2\pi k\mu/\omega_c) 2\pi k \frac{\mu}{\omega_c} + \cos(2\pi k\mu/\omega_c) \right) \right.$$

$$\left. \times \frac{2\pi^2 kT}{\omega_c \sinh\left(\frac{2\pi^2 kT}{\omega_c}\right)} \right].$$
(6.37)

To find the expression for the magnetization per unit area, it is enough to take the derivative of "fast" terms with respect to magnetic field alone,

$$M = -\frac{\partial \Delta E}{\partial B} = -\frac{2m\mu^2}{B\pi} \sum_{k=1}^{\infty} \frac{2\pi^2 kT}{\omega_c \sinh\left(\frac{2\pi^2 kT}{\omega_c}\right)} \cos(2\pi k\mu/\omega_c).$$
(6.38)

6.4.2 Problem 13

The study of the Bose-Einstein condensate starts from calculating the number of non-condensed particles. For $T > T_{\text{BEC}}$, all particles are non-condensed and this number conserves,

$$N = \int_{0}^{\infty} \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} g(\varepsilon) d\varepsilon.$$
(6.39)

For $d = 3$, the density of states is given as $g(\varepsilon) = \frac{m^{3/2}}{\sqrt{2}\pi^2} \sqrt{\varepsilon}$. Substituting the expression for the density of states into the integral, we arrive at,

$$N = \frac{m^{3/2}}{\sqrt{2}\pi^2} \int_{0}^{\infty} \frac{\sqrt{\varepsilon}}{e^{\beta(\varepsilon-\mu)} - 1} d\varepsilon = \frac{m^{3/2}}{\sqrt{2}\pi^2} \int_{0}^{\infty} \frac{\sqrt{\varepsilon} e^{-\beta(\varepsilon-\mu)}}{1 - e^{-\beta(\varepsilon-\mu)}} d\varepsilon$$

$$= \frac{m^{3/2}}{\sqrt{2}\pi^2} \sum_{n=1}^{\infty} \int_{0}^{\infty} \sqrt{\varepsilon} e^{-\beta(\varepsilon-\mu)n} d\varepsilon \approx \left(\frac{mT}{2\pi} \right)^{3/2} \sum_{n=1}^{\infty} \frac{1}{(n)^{3/2}} e^{\beta\mu n}$$
(6.40)

One can take the derivative with respect to the temperature for small μ:

$$\frac{\partial N}{\partial T} = \left(\frac{m}{2\pi}\right)^{3/2} \frac{3}{2} T^{1/2} \sum_{n=1}^{\infty} \frac{e^{-|\beta\mu|n}}{n^{3/2}} + \left(\frac{mT}{2\pi}\right)^{3/2} \sum_{n=1}^{\infty} \frac{e^{-|\beta\mu|n}}{n^{1/2}} \left(-\frac{\mu}{T^2} + \frac{1}{T}\frac{\partial\mu}{\partial T}\right)$$
$$= 0. \tag{6.41}$$

The main contribution to the first term can be calculated for $\mu = 0$. To calculate the second term, we can replace the sum with the integral. Also we note that we can neglect the term proportional to μ. Then we obtain,

$$0 = \frac{3N}{2} T_{\text{BEC}}^{-3/2} T^{1/2} + \left(\frac{mT}{2\pi}\right)^{3/2} \int_0^{\infty} dn \frac{1}{n^{1/2}} e^{-|\beta\mu|n} \frac{1}{T}\frac{\partial\mu}{\partial T}$$
$$= \frac{3N}{2} T_{\text{BEC}}^{-3/2} T^{1/2} + N\left(\frac{T}{T_{\text{BEC}}}\right)^{3/2} \frac{1}{\zeta(3/2)} \frac{\sqrt{\pi T}}{\sqrt{|\mu|}} \frac{1}{T}\frac{\partial\mu}{\partial T}. \tag{6.42}$$

Eventually, this leads to the following equation for μ,

$$0 = \frac{3}{2\sqrt{\pi}} \zeta(3/2) + \frac{T_{\text{BEC}}^{1/2}}{\sqrt{|\mu|}} \frac{\partial\mu}{\partial T}. \tag{6.43}$$

Hence, we obtain,

$$\mu = -\left(\frac{3\zeta(3/2)}{4\sqrt{\pi}}\right)^2 \frac{(T - T_{\text{BEC}})^2}{T_{\text{BEC}}}. \tag{6.44}$$

6.5   Seminar V

In this section, we present the solution of Problem 14.

6.5.1   Problem 14

Using expression (2.9) for the first-order correction to the thermodynamic potential, we find

$$\Omega = \frac{\Omega_0(\mu_+) + \Omega_0(\mu_-)}{2} + \frac{U}{V}\left[\int \frac{d^3\boldsymbol{p}}{(2\pi)^3}\langle a_{\boldsymbol{p}\uparrow}^{\dagger} a_{\boldsymbol{p}\uparrow}\rangle\right]\left[\int \frac{d^3\boldsymbol{q}}{(2\pi)^3}\langle a_{\boldsymbol{q}\downarrow}^{\dagger} a_{\boldsymbol{q}\downarrow}\rangle\right]$$
$$= \frac{\Omega_0(\mu_+) + \Omega_0(\mu_-)}{2} + \frac{U}{4V} N_0(\mu_+) N_0(\mu_-). \tag{6.45}$$

Here $\mu_{\pm} = \mu \pm \mu_B B$, $\Omega_0(\mu)$ is the thermodynamic potential of noninteracting electrons in zero magnetic field, and $N_0(\mu)$ is the number of particles as a function of the chemical potential in the absence of interaction.

As in the lecture, we determine the chemical potential from the condition of the fixed number of particles,

$$N = \frac{N_0(\mu_+) + N_0(\mu_-)}{2} - \frac{U}{4V}\frac{\partial}{\partial \mu}\left[N_0(\mu_+)N_0(\mu_-)\right]. \qquad (6.46)$$

Hence, we find that the chemical potential is given as

$$\mu = \mu_0 + \frac{U}{2V}\frac{\frac{\partial}{\partial \mu_0}\left[N_0(\mu_0^+)N_0(\mu_0^-)\right]}{\frac{\partial}{\partial \mu_0}\left[N_0(\mu_0^+) + N_0(\mu_0^-)\right]} \qquad (6.47)$$

where $\mu_0^\pm = \mu_0 \pm \mu_B B$, and

$$N = \left[N_0(\mu_0^+) + N_0(\mu_0^-)\right]/2. \qquad (6.48)$$

Therefore, we can write the thermodynamic potential as

$$\Omega(\mu) = \frac{\Omega_0(\mu_0^+) + \Omega_0(\mu_0^-)}{2} - \frac{UN}{2V}\frac{\frac{\partial}{\partial \mu_0}\left[N_0(\mu_0^+)N_0(\mu_0^-)\right]}{\frac{\partial}{\partial \mu_0}\left[N_0(\mu_0^+) + N_0(\mu_0^-)\right]}$$

$$+ \frac{U}{4V}N_0(\mu_0^+)N_0(\mu_0^-). \qquad (6.49)$$

Next, we find the free energy,

$$F = \Omega + \mu N = F_0(B) + \frac{U}{4V}N_0(\mu_0^+)N_0(\mu_0^-),$$

$$F_0(B) = \frac{\Omega_0(\mu_0^+) + \Omega_0(\mu_0^-)}{2} + \mu_0 N. \qquad (6.50)$$

Here $F_0(B)$ stands for the free energy in the absence of interaction. We note that the chemical potential μ_0 is a function of B in accordance with Eq. (6.48). Using Eq. (6.48), we find in the limit $B \to 0$,

$$\mu_0(B) = \mu_0 - \frac{1}{2}(\mu_B B)^2 \frac{N_0''(\mu_0)}{N_0'(\mu_0)}. \qquad (6.51)$$

We note that $\chi_0 = \mu_B^2 N_0'(\mu_0)$. At low temperatures, $T \ll E_F$, we can write $N_0(\mu_0) \propto \mu_0^{3/2}$. Therefore, we find $\mu_0(B) = \mu_0 - (\mu_B B/2)^2/\mu_0$. Now we can compute the zero-field spin susceptibility (per unit volume) at the fixed number of particles,

$$\chi = -\frac{1}{V}\frac{\partial^2 F}{\partial B^2}\bigg|_{B=0} = \chi_0 - \frac{U}{4V^2}\frac{\partial^2}{\partial B^2}\left[N_0(\mu_0(B) + \mu_B B)N_0(\mu_0(B) - \mu_B B)\right]\bigg|_{B=0}$$

$$= \chi_0 + \frac{\mu_B^2 U}{2V^2}N_0'^2(\mu_0). \qquad (6.52)$$

At low temperatures, $T \ll E_F$, we obtain

$$\chi = \chi_0 + \frac{9}{8} \frac{\mu_B^2 U N^2}{V^2 E_F^2} = \nu_F \mu_B^2 \left[1 + \frac{2}{\pi^3} a p_F \right] \tag{6.53}$$

where $\nu_F = m p_F / \pi^2$ denotes the noninteracting density of states at the Fermi energy. Equation (6.53) provides us the expression for χ as a function of N.

We note that result (6.53) can readily be obtained from Eq. (6.45),

$$\chi = -\frac{\partial^2 \Omega}{\partial B^2} = \chi_0 - \frac{U}{4V} \frac{\partial^2}{\partial B^2} \left[N_0(\mu_+) N_0(\mu_-) \right] = \chi_0 + \frac{\mu_B^2 U}{2V} \left[N_0'^2(\mu) \right.$$
$$\left. - N_0(\mu) N_0''(\mu) \right]. \tag{6.54}$$

This result gives the spin susceptibility as a function of chemical potential. In order to express it as a function of N, we should involve that $\chi_0 = \mu_B^2 N_0'(\mu)$ and the shift of the chemical potential due to interaction, see Eq. (6.53). Then, we obtain

$$\chi = \mu_B^2 N_0'(\mu_0) + \frac{\mu_B^2 U}{2V} N_0(\mu_0) N_0''(\mu_0) + \frac{\mu_B^2 U}{2V} \left[N_0'^2(\mu_0) - N_0(\mu) N_0''(\mu_0) \right]$$
$$= \mu_B^2 N_0'(\mu_0) + \frac{\mu_B^2 U}{2V} N_0'^2(\mu_0). \tag{6.55}$$

6.6 Seminar VI

In this section, we consider Problems 15 and 16.

6.6.1 Problem 15

Let us find variation of chemical potential $\delta\mu$ at zero temperature due to varying the number of particles, δN. Let us use Eq. (2.21) at $p = p_F$ such that $\delta\varepsilon_{\sigma_1\sigma_2}(\boldsymbol{p}) \equiv \delta\mu \, \delta_{\sigma_1\sigma_2}$. Then we obtain

$$\delta\mu \, \delta_{\sigma_1\sigma_2} = \delta\varepsilon_F \, \delta_{\sigma_1\sigma_2} + \sum_{\sigma_3,\sigma_4} \int \frac{d^3\boldsymbol{p}'}{(2\pi\hbar)^3} f_{\sigma_1\sigma_4,\sigma_2\sigma_3}(\boldsymbol{p}, \boldsymbol{p}') \delta n_{\sigma_3\sigma_4}(\boldsymbol{p}'). \tag{6.56}$$

Here $\delta\varepsilon_F$ is the change of the Fermi energy due to varying the Fermi momentum,

$$\delta\varepsilon_F = \frac{\partial\varepsilon_F}{\partial p_F} \delta p_F = v_F \delta p_F = \frac{p_F}{m_*} \delta p_F, \qquad \delta N = \frac{V p_F^2}{\pi^2\hbar^3} \delta p_F. \tag{6.57}$$

Next, at zero temperature we can write

$$\delta n_{\sigma_3\sigma_4}(\boldsymbol{p}') = -\frac{\partial n^{(0)}(p')}{\partial \varepsilon_{\boldsymbol{p}'}} \frac{\pi^2\hbar^3 \delta N}{p_F m_* V} \delta_{\sigma_3,\sigma_4} = \delta(\varepsilon_{\boldsymbol{p}'} - \varepsilon_F) \frac{\pi^2\hbar^3 \delta N}{p_F m_* V} \delta_{\sigma_3,\sigma_4}. \tag{6.58}$$

Substituting Eqs. (6.57) and (6.58) into Eq. (6.56), we find

$$\delta\mu\,\delta_{\sigma_1\sigma_2} = \frac{\pi^2\hbar^3\delta N}{p_F m_* V}\delta_{\sigma_1\sigma_2} + \frac{\pi^2\hbar^3\delta N}{2p_F m_* V}\sum_{\sigma_3,\sigma_4}\int_0^\pi \frac{d\theta\sin\theta}{2}\Big[F^{(0)}(\theta)\delta_{\sigma_1\sigma_2}\delta_{\sigma_4\sigma_3}$$

$$+F^{(\sigma)}(\theta)\boldsymbol{\sigma}_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_4\sigma_3}\Big]\delta_{\sigma_3\sigma_4} \tag{6.59}$$

where $\theta = \angle(\boldsymbol{p}',\boldsymbol{p})$. Hence, we obtain,

$$\delta\mu = \frac{1+F_0^{(0)}}{\nu_F V}\delta N. \tag{6.60}$$

Here $\nu_F = \frac{p_F m_*}{\pi^2\hbar^3}$ denotes the density of states at the Fermi surface. Finally, we find

$$\frac{\partial\mu}{\partial N} = \frac{1+F_0^{(0)}}{\nu_F V}. \tag{6.61}$$

6.6.2 Problem 16

The correction to the quasiparticle energy at $p = p_F$ in the magnetic field and interaction can be written as,

$$\delta\varepsilon(\boldsymbol{p})_{\sigma_1,\sigma_2} = -\mu_B\boldsymbol{B}\boldsymbol{\sigma}_{\sigma_1,\sigma_2} + \sum_{\sigma_3,\sigma_4}\int \frac{d^3\boldsymbol{p}'}{(2\pi\hbar)^3}f_{\sigma_1\sigma_4,\sigma_2\sigma_3}\delta n_{\sigma_3\sigma_4}(\boldsymbol{p}'). \tag{6.62}$$

We are interested in the change $\delta n_{\sigma_3\sigma_4}(\boldsymbol{p}')$ that occurs due to magnetic field. At zero temperature we find

$$\delta n_{\sigma_3\sigma_4}(\boldsymbol{p}') = \frac{\partial n^{(0)}(p')}{\partial\varepsilon_{\boldsymbol{p}'}}\delta\varepsilon(\boldsymbol{p}')_{\sigma_3,\sigma_4} = -\delta(\varepsilon_{\boldsymbol{p}'} - \varepsilon_F)\,\delta\varepsilon(\boldsymbol{p}')_{\sigma_3,\sigma_4}. \tag{6.63}$$

Hence, we obtain

$$\delta\varepsilon(\boldsymbol{p})_{\sigma_1,\sigma_2} = -\mu_B(\boldsymbol{\sigma},\boldsymbol{B})_{\sigma_1,\sigma_2} - \frac{1}{2}\sum_{\sigma_3,\sigma_4}\int_0^\pi \frac{d\theta\sin\theta}{2}\Big[F^{(0)}(\theta)\delta_{\sigma_1\sigma_2}\delta_{\sigma_4\sigma_3}$$

$$+F^{(\sigma)}(\theta)\boldsymbol{\sigma}_{\sigma_1\sigma_2}\boldsymbol{\sigma}_{\sigma_4\sigma_3}\Big]\delta\varepsilon_{\sigma_3\sigma_4}(\boldsymbol{p}') \tag{6.64}$$

where $\theta = \angle(\boldsymbol{p}',\boldsymbol{p})$. Let us seek the solution of Eq. (6.64) in the form of the energy shift in the absence of interaction but with the renormalized g-factor, $\delta\varepsilon(\boldsymbol{p})_{\sigma_1,\sigma_2} = -(g/2)\mu_B\boldsymbol{B}\boldsymbol{\sigma}_{\sigma_1,\sigma_2}$. Then, it leads to the following equation,

$$-\frac{g}{2}\mu_B\boldsymbol{B}\boldsymbol{\sigma}_{\sigma_1,\sigma_2} = -\mu_B\boldsymbol{B}\boldsymbol{\sigma}_{\sigma_1,\sigma_2} + F^{(\sigma)_0}\frac{g}{2}\mu_B\boldsymbol{B}\boldsymbol{\sigma}_{\sigma_1,\sigma_2}. \tag{6.65}$$

Finally, we obtain the renormalized g-factor in the Fermi liquid,

$$g = \frac{2}{1 + F_0^{(\sigma)}}. \tag{6.66}$$

Since the quasiparticle energy shift due to magnetic field is momentum-independent, we can use the expression for the free electron gas, cf. Eq. (6.53), but with the renormalized g-factor. Then, we find the Pauli spin susceptibility of the Fermi liquid,

$$\chi = \frac{g}{2}\mu_B^2 \nu_F. \tag{6.67}$$

6.7   Seminar VII

In this section we present the solutions for Problems 17, 18, and 19.

6.7.1   Problem 17

The ground state energy of the weakly non-ideal Bose gas has the following form (see Eq. (2.41)):

$$E_0 = \frac{UN^2}{2V} + \sum_{\boldsymbol{p}} \left[\varepsilon(p) - \varepsilon^{(0)}(p) - \frac{UV}{N} \right]. \tag{6.68}$$

It is useful to point out that a sum over $\boldsymbol{p}$ diverges. Fortunately, this divergence has a physical origin. At first, we should understand that potential U is a constant in the sum and does not represent some physical measurable quantity. The real physical quantity is the scattering length. This means that we must express all results in terms of the scattering length. In the main approximation, the ground state energy and the scattering length are $E_0 = \frac{UN^2}{2V}$ and $a = \frac{mU}{4\pi}$, respectively. Therefore, we obtain $E_0 = \frac{2\pi a N^2}{mV}$. In order to find next order correction in the ground state energy, we have to write the following expression that relates the scattering length and U,

$$U = \frac{4\pi a}{m} \left[1 - \frac{4\pi a}{mV} \sum_{\boldsymbol{p} \neq \boldsymbol{0}} \frac{1}{p^2} \right]. \tag{6.69}$$

This expression involves a diverging sum. This divergence indicates that one cannot approximate the interaction potential by the constant U at very short scales. However, using the above expression, we find

$$E_0 = \frac{Nmu^2}{2} + \sum_{\boldsymbol{p}} \left[\varepsilon(p) - \varepsilon^{(0)}(p) - mu^2 + \frac{m^3 u^4}{p^2} \right] \tag{6.70}$$

where $u = \sqrt{\frac{4\pi a N}{m^2 V}}$. Surprisingly this integral converges! We see that the divergence has been removed by introducing the proper expression for the scattering length. This effect is called the renormalization. Now we should calculate the following integral,

$$f(X) = \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \left[\sqrt{\varepsilon^{(0)}(p)^2 + \varepsilon^{(0)}(p)X} - \varepsilon^{(0)}(p) - \frac{X}{2} + \frac{X^2}{8\varepsilon^{(0)}(p)} \right]. \quad (6.71)$$

To calculate integral, we should find the magnitude of function $f(X)$ at the point $X = 2mu^2$. To calculate the above integral we should take the third derivative and note that $f(0) = f'(0) = f''(0) = 0$. We have:

$$f'''(X) = V\frac{3\sqrt{2m^3}}{16\pi^2} \int\limits_0^\infty d\varepsilon \frac{\varepsilon}{(X + \varepsilon)^{5/2}} = \frac{\sqrt{2m^3}}{4\pi^2\sqrt{X}}. \quad (6.72)$$

As a result

$$f(X) = V\frac{2\sqrt{2m^3}X^{5/2}}{15\pi^2}, \qquad f(X = 2mu^2) = V\frac{16m^4u^5}{15}. \quad (6.73)$$

Substituting the above expression to E_0 results in Eq. (2.43).

6.7.2 Problem 18

In this problem we should calculate the number of particles in the condensate at temperatures $\mu(0) \ll T \ll T_{\text{BEC}}(an^{1/3})^{1/4}$. The number of particles in the condensate can be calculated as follows, see Eq. (2.48),

$$\begin{aligned}
N_0(T) &= N - V \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \left[u_p^2 f_B(\varepsilon_p) + v_p^2(f_B(\varepsilon_p) + 1) \right] \\
&= N - V \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \left[\frac{\varepsilon_0(p) + mu^2}{\varepsilon_p} f_B(\varepsilon_p) + \frac{\varepsilon_0(p) + mu^2 - \varepsilon(p)}{2} \right] \\
&= N_0(T = 0) - V \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \frac{\varepsilon_0(p) + mu^2}{\varepsilon_p} f_B(\varepsilon_p). \quad (6.74)
\end{aligned}$$

Let us transform integration over p to integration over $\varepsilon_0 = \varepsilon_p^{(0)} = p^2/(2m)$. Then we find

$$N_0(T) = N_0(T = 0) - \frac{V}{\pi^2}\sqrt{\frac{m^3}{2}} \int\limits_0^\infty d\varepsilon_0 \sqrt{\varepsilon_0}\frac{\varepsilon_0 + mu^2}{\varepsilon_p} f_B(\varepsilon_p). \quad (6.75)$$

Next, we change the integration variable ε_0 to the integration over $\varepsilon = \sqrt{(\varepsilon_0 + mu^2)^2 - (mu^2)^2}$. Then we obtain

$$N_0(T) = N_0(T{=}0) - \frac{V}{\pi^2}\sqrt{\frac{m^3}{2}} \int\limits_0^\infty \sqrt{\sqrt{\varepsilon^2 + (mu^2)^2} - mu^2}\, f_B(\varepsilon)d\varepsilon$$

$$= N_0(T{=}0) - N + N_0^{(0)}(T) - \frac{V}{\pi^2}\sqrt{\frac{m^3}{2}} \int\limits_0^\infty \left(\sqrt{\sqrt{\varepsilon^2 + (mu^2)^2} - mu^2} - \sqrt{\varepsilon} \right)$$

$$\times f_B(\varepsilon)d\varepsilon = N_0(T{=}0) - N + N_0^{(0)}(T) - \frac{Vm^3u^3}{\pi^2\sqrt{2}} F(mu^2/T). \qquad (6.76)$$

Here $N_0^{(0)}(T) = N[1 - (T/T_{\text{BEC}}^{(0)})^{3/2}]$ is the number of condensate particles for the noninteracting Bose gas. The function $F(z)$ is given as

$$F(z) = \int_0^\infty dx \frac{\sqrt{\sqrt{1+x^2}-1} - \sqrt{x}}{e^{zx}-1}$$

$$= \begin{cases} z^{-1}\displaystyle\int_0^\infty dx \frac{\sqrt{\sqrt{1+x^2}-1}-\sqrt{x}}{x} = -\dfrac{\pi}{z\sqrt{2}}, & z \ll 1, \\[4mm] \displaystyle\int_0^\infty dy \frac{-\sqrt{y}z^{-3/2}+yz^{-2}}{e^y-1} = -\dfrac{\zeta(3/2)\sqrt{\pi}}{2z^{3/2}} + \dfrac{\pi^2}{6z^2}, & z \gg 1. \end{cases}$$
$$(6.77)$$

Hence we obtain

$$N_0(T) = N_0(T{=}0) - \frac{VmT^2}{6\sqrt{2}u}, \qquad T \ll mu^2, \qquad (6.78)$$

and

$$N_0(T) = N_0(T{=}0) - N \left(\frac{T}{T_{\text{BEC}}^{(0)}} \right)^{3/2}, \qquad mu^2 \ll T \ll T_{\text{BEC}}. \qquad (6.79)$$

6.7.3   Problem 19

The vortex solution of the Gross–Pitaevskii equation (2.53) can be represented as $\Psi_0(\boldsymbol{r}) = e^{i\varphi} A f(r/r_0)$ where $f(0) = 1$ and the scale r_0 describes the vortex size. Substituting the above ansatz into Eq. (2.53) and introducing new variable $\xi = r/r_0$, we find,

$$-\frac{A}{2mr_0^2} \left[\frac{1}{\xi}\partial_\xi\left(\xi\partial_\xi f\right) - \frac{f}{\xi^2} \right] - \mu A f + \frac{4\pi a}{m}A^3 f^3 = 0. \qquad (6.80)$$

If we choose the amplitude $A = \sqrt{\mu m/(4\pi a)}$ and the size $r_0 = \sqrt{2m/\mu}$, we obtain the dimensionless equation which can numerically be solved

$$-\left[\frac{1}{\xi}\partial_\xi\left(\xi\partial_\xi f\right) - \frac{f}{\xi^2}\right] - f + f^3 = 0. \tag{6.81}$$

6.8 Seminar VIII

In this section we consider the solutions for Problems 20, 21, and 22.

6.8.1 Problem 20

The energy of two excitations is given as $\varepsilon(p_1) + \varepsilon(p_2) + (\boldsymbol{p_1} + \boldsymbol{p_2})\boldsymbol{v}$. We expect that this combination should be positive. This equation leads to the following expression for the critical velocity: $v_{\mathrm{cr},2} = \min\left(\frac{\varepsilon(p_1)+\varepsilon(p_2)}{p_1+p_2}\right)$. This expression is symmetric with respect to p_1 and p_2. Let us assume that $p_1 \geqslant p_2$. Then we find $\frac{\varepsilon(p_1)+\varepsilon(p_2)}{p_1+p_2} \geqslant \frac{\varepsilon(p_1)}{p_1}$. Taking the minimum from both sides of this inequality, we find $v_{\mathrm{cr},2} \geqslant v_{\mathrm{cr}}$.

6.8.2 Problem 21

The normal component density in superfluid liquid is given by the following expression, cf. Eq. (2.57),

$$\rho_n = \frac{1}{3}\int\frac{d^3\boldsymbol{p}}{(2\pi)^3}p^2\left(-\frac{\partial f_B}{\partial\varepsilon}\right) = \frac{\beta}{12}\int\frac{d^3\boldsymbol{p}}{(2\pi)^3}\frac{p^2}{\sinh^2\left(\beta\varepsilon(p)/2\right)}. \tag{6.82}$$

The excitation spectrum $\varepsilon(p)$ consists of two segments: phonon and roton ones. We should calculate the contributions from both of them. We start from the phonon contribution

$$\rho_{n,p} = \frac{\beta}{12}\int\frac{d^3\boldsymbol{p}}{(2\pi)^3}\frac{p^2}{\sinh^2\left(\beta up/2\right)} = \frac{4T^4}{3\pi^2 u^5}\int\limits_0^\infty\frac{x^4 dx}{\sinh^2 x} = \frac{2\pi^2 T^4}{45u^5}. \tag{6.83}$$

Let us turn now to the roton contribution. At low temperatures such as $m_r T \ll p_0^2$ and $\Delta \gg T$ we find

$$\rho_{n,r} = \frac{\beta}{12}\int\frac{d^3\boldsymbol{p}}{(2\pi)^3}\frac{p^2}{\sinh^2\left(\beta\varepsilon(p)/2\right)} \simeq \frac{\beta}{6\pi^2}p_0^4 e^{-\Delta/T}\int\limits_{-\infty}^\infty d\delta p\, e^{-\beta\delta p^2/(2m_r)}$$

$$= \frac{p_0^4}{6\pi^2}\sqrt{\frac{2\pi m_r}{T}}e^{-\Delta/T}, \tag{6.84}$$

where $\delta p = p - p_0$. We note that though the roton contribution is exponentially small at $T \ll \Delta$, it predominates over the phonon one at high temperatures $T \gtrsim 0.7$ K.

6.8.3 Problem 22

The roton contribution to the specific heat can similarly be calculated using the same integral from the previous problem. Assuming that $m_r T \ll p_0^2$ and $T \ll \Delta$, we obtain

$$E_{\mathrm{r}} = V \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \frac{\varepsilon(p)}{e^{\beta\varepsilon(p)} - 1} \simeq V \frac{p_0^2 \Delta}{2\pi^2} e^{-\beta\Delta} \int\limits_{-\infty}^{\infty} d\delta p \, e^{-\beta\delta p^2/(2m_r)}$$

$$= V \frac{p_0^2 \Delta}{2\pi^2} e^{-\beta\Delta} \sqrt{2\pi m_{\mathrm{r}} T}. \qquad (6.85)$$

Hence we find

$$C_V = \frac{\partial E_{\mathrm{r}}}{\partial T} = V \frac{p_0^2 \Delta^2 m r^{1/2}}{\sqrt{2\pi^3} T^{3/2}} e^{-\Delta/T}. \qquad (6.86)$$

6.9 Seminar IX

In this section we present the solutions for Problems 23 and 24.

6.9.1 Problem 23

We should find the temperature dependence of the superconducting gap near T_c. It can be found from the self-consistent equation, cf. Eq. (2.73),

$$1 = \frac{\lambda g(E_F)}{2} \int\limits_{0}^{\infty} \frac{d\xi}{\varepsilon_\xi} \tanh\left(\frac{\varepsilon_\xi}{2T}\right) \qquad (6.87)$$

where $\varepsilon_\xi = \sqrt{\xi^2 + \Delta^2}$ is the spectrum of superconducting quasiparticles. Here we again use the trick called "integration over ξ", described above. This integral does not converge and must be regularized at some ultra-violet scale. As it is mentioned in the Lecture, this ultra-violet scale determines the magnitude of the zero-temperature gap. Therefore, it is convenient to rewrite the self-consistent

equation as,

$$\ln\left(\frac{\Delta_0}{\Delta}\right) = \int\limits_0^\infty \frac{d\xi}{\varepsilon_\xi}\left(1 - \tanh\left(\frac{\varepsilon_\xi}{2T}\right)\right) = 2I(u),$$

$$I(u) = \int\limits_0^\infty \frac{dx}{\sqrt{x^2 + u^2}}\frac{1}{\exp[\sqrt{x^2 + u^2}] + 1} \tag{6.88}$$

where $u = \Delta/T$.

In order to evaluate $I(u)$, we consider the technique which helps us to find the asymptotics of integrals. With this method one can find not only the power-law terms but also the logarithmic one. First of all, we choose $y = \sqrt{x^2 + u^2}$ as an integration variable,

$$I(u) = \int\limits_u^\infty \frac{dy}{\sqrt{y^2 - u^2}}\frac{1}{e^y + 1} = \int\limits_0^\infty dy \frac{\Theta(y - u)}{\sqrt{y^2 - u^2}}\frac{1}{e^y + 1}. \tag{6.89}$$

After that we can use the representation for the first function known as the Mellin transform,

$$\frac{\Theta(y - u)}{\sqrt{y^2 - u^2}} = -\int\limits_{a-i\infty}^{a+i\infty} \frac{\sqrt{\pi}u^{\alpha-1}\Gamma(\frac{1-\alpha}{2})}{\alpha\Gamma(-\frac{\alpha}{2})}y^{-\alpha}\frac{d\alpha}{2\pi i} \tag{6.90}$$

where $0 < a < 1$. Substituting this expression into Eq. (6.89), we find,

$$I(u) = -\int\limits_{a-i\infty}^{a+i\infty} \frac{d\alpha}{2\pi i}\frac{\sqrt{\pi}u^{\alpha-1}\Gamma(\frac{1-\alpha}{2})}{\alpha\Gamma(-\frac{\alpha}{2})}\int\limits_0^\infty \frac{dy\,y^{-\alpha}}{e^y + 1}dy = \int\limits_{a-i\infty}^{a+i\infty} \frac{d\alpha}{2\pi i}\frac{\sqrt{\pi}u^{\alpha-1}\Gamma(\frac{1-\alpha}{2})}{\alpha\Gamma(-\frac{\alpha}{2})}$$

$$\times\Gamma(1 - \alpha)\zeta(1 - \alpha)(2^\alpha - 1). \tag{6.91}$$

Here $\zeta(z)$ denotes the Riemann zeta-function. Using the following identity, $\zeta(1 - \alpha) = \frac{2^{-\alpha}\pi^{1-\alpha}\zeta(\alpha)}{\Gamma(1-\alpha)\sin(\pi\alpha/2)}$, we find,

$$I(u) = \int\limits_{a-i\infty}^{a+i\infty} \frac{d\alpha}{2\pi i}\frac{\pi^{3/2-\alpha}u^{\alpha-1}\Gamma(\frac{1-\alpha}{2})}{\alpha\Gamma(-\frac{\alpha}{2})\sin(\pi\alpha/2)}(1 - 2^{-\alpha})\zeta(\alpha) = -\int\limits_{a-i\infty}^{a+i\infty} \frac{d\alpha}{2\pi i}\pi^{1/2-\alpha}u^{\alpha-1}$$

$$\times\Gamma\left(\frac{1-\alpha}{2}\right)\Gamma\left(\frac{\alpha}{2}\right)(1 - 2^{-\alpha})\zeta(\alpha). \tag{6.92}$$

Performing this integral, one should close the contour on the right-hand side of complex plane, resulting in the following expansion in a series in u:

$$I(u) = \frac{1}{2}\left(\ln(\pi/u) - \gamma\right) + \frac{7\zeta(3)}{16\pi^2}u^2 + \dots \tag{6.93}$$

Here $\gamma = 0.577$ denotes the Euler's constant. Substituting the expansion (6.93) into the self-consistent equation, we obtain the following equation for $\Delta \ll T$:

$$\ln\left(\frac{\Delta_0}{\Delta}\right) = \ln\frac{\pi T}{\Delta} - \gamma + \frac{7\zeta(3)}{8\pi^2}\left(\frac{\Delta}{T}\right)^2. \tag{6.94}$$

This expression gives the value for $T_c = \Delta_0 e^\gamma/\pi$ and also leads to the following temperature dependence,

$$\Delta(T) = T_c\left[\frac{8\pi^2}{7\zeta(3)}\left(1 - \frac{T}{T_c}\right)\right]^{1/2}. \tag{6.95}$$

The condensation free energy can be written as follows, cf. Eq. (2.72),

$$F_{\text{cond}} = F[\Delta] - F[0] = \sum_{\boldsymbol{p}}\left(|\xi_{\boldsymbol{p}}| - \varepsilon(p) + \frac{\Delta^2}{2\varepsilon(p)}\right) - \sum_{\boldsymbol{p}}\frac{\Delta^2}{\varepsilon(p)}f_F(\varepsilon(p))$$

$$-2T\sum_{\boldsymbol{p}}\ln\frac{1 + e^{-\beta\varepsilon(p)}}{1 + e^{-\beta|\xi_{\boldsymbol{p}}|}}. \tag{6.96}$$

The first sum over p has been found in the Lecture. The second sum is calculated above. Therefore, we find,

$$F_{\text{cond}} = -\frac{1}{4}Vg(E_F)\Delta^2 - Vg(E_F)\Delta^2 I(\Delta/T) + 2Vg(E_F)T^2 K(\Delta/T),$$

$$K(u) = \int\limits_0^\infty dx\ln\frac{1 + e^{-\sqrt{x^2 + u^2}}}{1 + e^{-x}}. \tag{6.97}$$

It is readily to check that $K'(u) = uI(u)$. Hence, we obtain at $u \ll 1$.

$$K(u) = \frac{u^2}{4}\left(\ln\frac{\pi}{u} - \gamma + \frac{1}{2}\right) + \frac{7\zeta(3)u^4}{64\pi^2} + \dots. \tag{6.98}$$

Summing all contributions, we find

$$F_{\text{cond}} = -\frac{7\zeta(3)}{32\pi^2}\frac{Vg(E_F)\Delta^4}{T^2} = -\frac{2\pi^2}{7\zeta(3)}Vg(E_F)(T_c - T)^2. \tag{6.99}$$

6.9.2 Problem 24

We should find the magnitude of jump-like discontinuity in the specific heat at the superconducting transition point. We use Eq. (2.78) and the expression for $\Delta(T)$ from the previous problem. Then, we find

$$C_V = V g(E_F) \int\limits_0^\infty d\xi \frac{\varepsilon(p)}{2\cosh^2\left(\frac{\varepsilon(p)}{2T}\right)} \left(\frac{\varepsilon(p)}{T^2} - \frac{1}{2\varepsilon(p)T} \frac{d\Delta^2}{dT} \right). \qquad (6.100)$$

Hence, we find for the specific heat jump,

$$\Delta C_V = -V g(E_F) \frac{d\Delta^2}{dT} \int\limits_0^\infty d\xi \frac{1}{4T\cosh^2\left(\frac{\varepsilon(p)}{2T}\right)} = V \frac{4\pi^2}{7\zeta(3)} g(E_F) T_c = V \frac{4mp_F}{7\zeta(3)} T_c.$$

$$(6.101)$$

We note that this result can be obtained as second derivative of F_{cond}, cf. Eq. (6.99).

6.10 Seminar X

In this seminar we consider Problems 25, 26, and 27.

6.10.1 Problem 25

This problem is solved with applying the general method useful in many other problems. Let us consider two operators A and B. They obey the following property: if $C := [A, B]$, then $[C, A] = [C, B] = 0$. In this case, we can simplify the expression $\exp(A + B)$. First of all, let us consider how A 'acts' on some function of B,

$$[A, B^n] = [A, B^{n-1}]B + B^{n-1}[A, B] = nCB^{n-1} \quad \Rightarrow \quad [A, f(B)] = Cf'(B).$$

$$(6.102)$$

The other important identity is a derivative of operator $\exp[A(x)]$ with respect to x. The convenient expression can be derived in the following way,

$$\partial_x e^{A(x)} = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{k=0}^{n-1} A^k(x) A'(x) A^{n-1-k}(x) = \sum_{n=1}^{\infty} \sum_{k=0}^{n-1} \int_0^1 dt \, \frac{t^k(1-t)^{n-1-k}}{k!(n-k-1)!} A^k(x)$$

$$\times A'(x) A^{n-1-k}(x) = \sum_{k=0}^{\infty} \sum_{n=k+1}^{\infty} \int_0^1 dt \, \frac{t^k(1-t)^{n-1-k}}{k!(n-k-1)!} A^k(x) A'(x) A^{n-1-k}(x)$$

$$= \int_0^1 dt \left(\sum_{j=0}^{\infty} \frac{t^k A^k(x)}{k!} \right) A'(x) \sum_{l=0}^{\infty} \frac{(1-t)^l A^l(x)}{l!} = \int_0^1 dt \, e^{tA(x)} A'(x) e^{(1-t)A(x)}.$$

$$(6.103)$$

After the above preliminaries we turn our attention to the problem. We should calculate the following expression

$$f(\alpha_q, \beta_q) = \left\langle \exp[\alpha_q b_q + \beta_q b_q^\dagger] \right\rangle = \mathrm{Tr}\left\{ \exp[\alpha_q b_q + \beta_q b_q^\dagger] e^{-\beta H} \right\} / \mathrm{Tr}\, e^{-\beta H}.$$

$$(6.104)$$

Let us calculate the derivative over α_q (here $A = \alpha_q b_q + \beta_q b_q^\dagger$),

$$\frac{\partial f}{\partial \alpha_q} = \int_0^1 dt \, \mathrm{Tr}\left[e^{tA} b_q \, e^{(1-t)A} e^{-\beta H} \right] / \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}[b_q e^A e^{-\beta H}] / \mathrm{Tr}\, e^{-\beta H}$$

$$- \int_0^1 dt \, \mathrm{Tr}\left\{ [b_q, e^{tA}] e^{(1-t)A} e^{-\beta H} \right\} / \mathrm{Tr}\, e^{-\beta H}. \qquad (6.105)$$

Since $[b_q, A] = \beta_q$, we find $[b_q, e^{tA}] = \beta_q t e^{tA}$. Next, we use the following transformations

$$\mathrm{Tr}[b_q e^A e^{-\beta H}] = \mathrm{Tr}[e^A e^{-\beta H} b_q] = e^{\beta \omega_q} \mathrm{Tr}[e^A b_q e^{-\beta H}] = e^{\beta \omega_q} \int_0^1 dt \, \mathrm{Tr}[e^{tA} e^{(1-t)A}]$$

$$\times b_q e^{-\beta H}] = e^{\beta \omega_q} \int_0^1 dt \left(\mathrm{Tr}[e^{tA} b_q e^{(1-t)A} e^{-\beta H}] - \mathrm{Tr}\left\{ e^{tA} [b_q, e^{(1-t)A}] e^{-\beta H} \right\} \right)$$

$$= e^{\beta \omega_q} \left(\frac{\partial f}{\partial \alpha_q} - \frac{\beta_q}{2} \right) \mathrm{Tr}\, e^{-\beta H}. \qquad (6.106)$$

Hence, we obtain the equation for the function f,

$$\frac{\partial f}{\partial \alpha_q} = \frac{\beta_q}{2} \coth \frac{\omega_q}{2T} f. \tag{6.107}$$

Using the initial condition $f(0, \beta_q) = 1$, we find

$$f(\alpha_q, \beta_q) = \exp\left(\frac{\alpha_q \beta_q}{2} \coth \frac{\omega_q}{2T}\right). \tag{6.108}$$

As $f(0, \alpha_+) = 1$, we have $f = \exp[\frac{\alpha_+ \alpha_-}{2} \coth\left(\frac{\omega_q}{2T}\right)]$ yielding the answer for the problem.

6.10.2 Problem 26

The annihilation operator for the electron traveling to the right side is determined as $\psi_R(x) = \sum_p \exp(-ipx) a_{+,p}^\dagger$ and obeys the commutation relations

$$[b_{+,q}^\dagger, \psi_R(x)] = -\sqrt{\frac{2\pi}{qL}} e^{-iqx} \psi_R(x), \qquad [b_{+,q}, \psi_R(x)] = -\sqrt{\frac{2\pi}{qL}} e^{iqx} \psi_R(x). \tag{6.109}$$

Here we use the representation of the bosonic operators in terms of electron density. Now let us try to represent the fermionic operator $\psi_R(x)$ as the product of fermionic operator $\Psi_R(x)$ and bosonic operators. Using the methods developed in Problem 25, one can check that provided that $[b_{+,q}^\dagger, \Psi_R(x)] = [b_{+,q}, \Psi_R(x)] = 0$, the operator

$$\psi_R(x) = \Psi_R(x) \exp\left[-(2\pi/(qL))^{1/2} \sum_{q>0} \left(e^{-iqx} b_{+,q}^\dagger - e^{iqx} b_{+,q}\right)\right] \tag{6.110}$$

obeys the commutation relations Eq. (6.109).

We note that the operator $\Psi_R(x)$ should change the total number of the right movers N_R by one. Let us consider the operator $\phi_{R,0}$ that satisfies the following commutation relation

$$[\mathcal{N}_R, \phi_{R,0}] = i \quad \Rightarrow \quad [e^{i\phi_{R,0}}, \mathcal{N}_R] = e^{i\phi_{R,0}}. \tag{6.111}$$

As follows from the last commutation relation, operator $e^{i\phi_{R,0}}$ has single nonzero matrix element $\langle N_R - 1|e^{i\phi_{R,0}}|N_R\rangle$. The same matrix element has the fermionic operator $\Psi_R(x)$.

Finally, for the formulation in the real space, it is convenient to have the following relation $\rho_R(x) = \partial\phi_R(x)/\partial x$. Then using the relation

$$\rho_R(x) = \frac{\mathcal{N}_R}{L} + (q/(2\pi L))^{1/2} \sum_{q>0} \left(e^{-iqx} b^\dagger_{+,q} + e^{iqx} b_{+,q} \right), \qquad (6.112)$$

we find finally,

$$\psi_R(x) \sim e^{i\phi_R(x)}, \quad \phi_R(x) = \phi_{R,0} + \frac{\mathcal{N}_R x}{L} + i \sum_{q>0} \sqrt{\frac{2\pi}{qL}} \left(e^{-iqx} b^\dagger_{+,q} - e^{iqx} b_{+,q} \right).$$
$$(6.113)$$

This relation is referred to as the Mattis–Mandelstam formula.

6.10.3   Problem 27

Let us introduce new bosonic operators,

$$a^\dagger_{\eta,q} = \frac{b^\dagger_{\eta,\uparrow,q} + b^\dagger_{\eta,\downarrow,q}}{\sqrt{2}}, \quad a_{\eta,q} = \frac{b_{\eta,\uparrow,q} + b_{\eta,\downarrow,q}}{\sqrt{2}},$$

$$d^\dagger_{\eta,q} = \frac{b^\dagger_{\eta,\uparrow,q} - b^\dagger_{\eta,\downarrow,q}}{\sqrt{2}}, \quad d_{\eta,q} = \frac{b_{\eta,\uparrow,q} - b_{\eta,\downarrow,q}}{\sqrt{2}}. \qquad (6.114)$$

We emphasize that they obey the usual commutation relations,

$$[a^\dagger_{\eta,q}, a_{\eta',q'}] = \delta_{\eta,\eta'}\delta_{q,q'}, \qquad [d^\dagger_{\eta,q}, d_{\eta',q'}] = \delta_{\eta,\eta'}\delta_{q,q'}. \qquad (6.115)$$

The bosonic states for operators $a^\dagger, a$ and $d^\dagger, d$ are independent,

$$[a^\dagger_{\eta,q}, d_{\eta',q'}] = 0, \qquad [d^\dagger_{\eta,q}, a_{\eta',q'}] = 0. \qquad (6.116)$$

We note that the operators $a^\dagger, a$ corresponds to the total density whereas the operators $d^\dagger, d$ describe the spin density. In terms of new operators the Hamiltonian can be rewritten as

$$\mathcal{H}_{LL} = \sum_{\eta,q>0} v_F q d^\dagger_{\eta,q} d_{\eta,q} + \sum_{\eta,q>0} \left[(v_F + 2g_4)q a^\dagger_{\eta,q} a_{\eta,q} + g_2(a^\dagger_{\eta,q} a^\dagger_{-\eta,q} + a_{\eta,q} a_{-\eta,q}) \right].$$
$$(6.117)$$

We apply the canonical transformation to the operators $a^\dagger, a$,

$$a^\dagger_{\eta,q} = \cosh\theta_q \boldsymbol{\beta}^\dagger_{\eta,q} + \sinh\theta_q \boldsymbol{\beta}_{-\eta,q}, \quad a_{\eta,q} = \cosh\theta_q \boldsymbol{\beta}_{\eta,q} + \sinh\theta_q \boldsymbol{\beta}^\dagger_{-\eta,q}, \quad (6.118)$$

where

$$\cosh 2\theta_q = \frac{v_F + 2g_4}{u}, \quad \sinh 2\theta_q = -\frac{2g_2}{u}, \quad u = \sqrt{(v_F + 2g_4)^2 - 4g_2^2}.$$
(6.119)

The Hamiltonian, rewritten in new operators, reads

$$\mathscr{H}_{\mathrm{LL}} = E_{\mathrm{G}} + \sum_{\eta,q>0} v_F q d_{\eta,q}^\dagger d_{\eta,q} + \sum_{\eta,q>0} uq\, \boldsymbol{\beta}_{\eta,q}^\dagger \boldsymbol{\beta}_{\eta,q}, \quad E_{\mathrm{G}} = \frac{1}{2} \sum_{q>0} (u - v_F - 2g_4)q.$$
(6.120)

The disentangling of spin and density channels in the Luttinger liquid Hamiltonian is an example of the spin–charge separation in the strongly correlated systems.

6.11 Seminar XI

In this section we present the solutions for Problems 28 and 29.

6.11.1 Problem 28

Let us consider the ground state of the one-dimensional Ising model in the absence of magnetic field. In the ground state all spins are parallel to each other. One can consider a perturbation of the ground state. The excited state corresponding to such perturbation is called the *domain wall*: some spins are parallel to the initial direction and the others are not. There is only a single site at which neighboring spins are antiparallel to each other. The difference between energy of the ground state and the excited state with the domain wall equals $\Delta E = 2J$. If we have n domain walls, the energy of this configuration will be $\Delta E_n = 2Jn$. The free energy of the model in zero magnetic field becomes

$$F = -LT \ln \left(1 + e^{-2\beta J}\right).$$
(6.121)

This leads to the energy $E = 2LJ \exp(-\beta J)/[\exp(\beta J) + \exp(-\beta J)]$. So, the domain wall density can be written as

$$\rho = \frac{E}{2JL} = \frac{1}{\exp(2\beta J) + 1}.$$
(6.122)

We note that the density of domain walls coincides with the Fermi–Dirac distribution.

6.11.2   Problem 29

The problem for calculating the correlation function is not considered before in this course. We cannot use the free energy to solve it. Fortunately, the transfer matrix can serve for this purpose as well. At first, we calculate the average spin in the one-dimensional Ising model with the periodic boundary conditions,

$$\langle \sigma_i \rangle = \frac{1}{Z} \sum_{\sigma_1 \dots \sigma_N} \sigma_i e^{-\beta E_{\sigma_1,\dots,\sigma_N}} = \frac{1}{Z} \sum_{\sigma_i} \sigma_i (\mathcal{T}^L)_{\sigma_i,\sigma_i}, \quad Z = \mathrm{tr}\, \mathcal{T}^L \quad (6.123)$$

where $L = N - 1$. As in the lecture, we can rewrite the last expression as a trace of matrix product:

$$\langle \sigma_i \rangle = \frac{1}{Z} \mathrm{tr}\left[\tau_z \mathcal{T}^L\right] = \frac{1}{Z} \mathrm{tr}\left[\mathcal{U}^{-1} \tau_z \mathcal{U} \Lambda^L\right] = \cos(2\phi)$$

$$= \frac{\sinh(\beta h)}{\sqrt{e^{-4\beta J} + \sinh^2(\beta h)}}. \qquad (6.124)$$

The matrix τ_z helps us to calculate the correlation function,

$$\langle \sigma_i \sigma_{i+n} \rangle = \frac{1}{Z} \mathrm{tr}\left[\tau_z \mathcal{T}^n \tau_z \mathcal{T}^{L-n}\right] = \frac{1}{Z} \mathrm{tr}\left[\mathcal{U}^{-1} \tau_z \mathcal{U} \Lambda^n \mathcal{U}^{-1} \tau_z \mathcal{U} \Lambda^{L-n}\right]$$

$$= \cos^2(2\phi) + \left(\frac{\lambda_-}{\lambda_+}\right)^n \sin^2(\phi). \qquad (6.125)$$

For the physical applications, the so-called irreducible correlation function is of more interest,

$$\langle\langle \sigma_i \sigma_{i+n} \rangle\rangle = \langle \sigma_i \sigma_{i+n} \rangle - \langle \sigma_i \rangle \langle \sigma_{i+n} \rangle = e^{-n \ln(\lambda_+/\lambda_-)} \sin^2(\phi). \qquad (6.126)$$

The decaying character of this function describes the physical properties inherent in the system.

6.12   Seminar XII

In this section we consider Problems 30, 31, and 32.

6.12.1   Problem 30

The expansion of the thermodynamic potential for the antiferromagnet in the vicinity of the Néel temperature can be written as

$$F = F_0 + AL^2 + BL^4 + D(\boldsymbol{HL})^2 + D'H^2 L^2 - \frac{\chi_P}{2} H^2 + \frac{\beta}{2}(L_x^2 + L_y^2)$$

$$- \frac{\gamma}{2}(H_x^2 + H_y^2) - \frac{H^2}{8\pi}. \qquad (6.127)$$

Here we assume that $A = a(T - T_c)$ and $\beta > 0$ (easy axis). Then at $H = 0$, we find

$$
L_z = \begin{cases} \sqrt{a(T_c - T)/(2B)}, & T < T_c, \\ 0, & T > T_c. \end{cases} \tag{6.128}
$$

The magnetization is given as

$$
M = -\frac{H}{4\pi} - \frac{\partial F}{\partial H}. \tag{6.129}
$$

For $T > T_c$, in the field parallel to the z axis we find

$$
M_z = \chi_z H_z, \qquad \chi_z = \chi_p. \tag{6.130}
$$

For $T < T_c$, we obtain

$$
M_z = \chi_z H_z, \qquad \chi_z = \chi_p - 2(D+D')L^2 = \chi_p - a(D+D')(T_c - T)/B. \tag{6.131}
$$

6.12.2 Problem 31

The effective Hamiltonian that describes fluctuations at $T > T_c$ has the form, cf. Eq. (3.42),

$$
\mathscr{H}_{\text{eff}} \approx \mathscr{H}_{\text{eff}}^{(2)} = \frac{1}{2} \sum_{\boldsymbol{p}} \varphi_{\boldsymbol{p}} \varphi_{-\boldsymbol{p}} \left(bp^2 + T - T_c \right). \tag{6.132}
$$

Here we neglect the quartic term in Eq. (3.42). To calculate the correction to the free energy due to fluctuations, we should evaluate the following integral,

$$
e^{-\beta \delta F} = \int \prod_{\boldsymbol{p}} d\varphi_{\boldsymbol{p}} \, e^{-\beta \mathscr{H}_{\text{eff}}^{(2)}}. \tag{6.133}
$$

It is a product of the Gaussian integrals. We note that $\varphi_{\boldsymbol{p}} = \varphi_{-\boldsymbol{p}}^{\dagger}$. The result of calculation becomes (within accuracy of some constant),

$$
\delta F = \frac{T}{2} \sum_{\boldsymbol{p}} \ln \left(\frac{bp^2 + T - T_c}{T\pi} \right). \tag{6.134}
$$

To calculate the correction to the specific heat, we differentiate with respect to the temperature,

$$
\delta C_P = -T \frac{\partial^2 \delta F}{\partial^2 T} \simeq \frac{T_c^2}{2} \sum_{\boldsymbol{p}} \frac{1}{(bp^2 + T - T_c)^2} = \frac{T_c^2 V}{2} \frac{S_d}{(2\pi)^d} \int_0^{\infty} \frac{dp \, p^{d-1}}{(bp^2 + T - T_c)^2}
$$

$$
= -\frac{T_c^2 V}{2(T - T_c)^2} \frac{S_d}{(2\pi)^d} \frac{(d-2)\pi}{4 \sin\left(\frac{\pi d}{2}\right)} \left(\frac{T - T_c}{b} \right)^{d/2}. \tag{6.135}
$$

Here S_d is the area of unit sphere in the d-dimensional space. We note that, for $d > 4$, δC_P vanishes as $T \to T_c$. For $d < 4$, δC_P diverges as the temperature approaches T_c.

6.12.3   Problems 32

Before calculating the order parameter, we find the following average ($T > T_c$)

$$\langle \varphi_{\boldsymbol{k}} \varphi_{\boldsymbol{q}} \rangle = \frac{\int \prod_{\boldsymbol{p}} d\varphi_{\boldsymbol{p}} \varphi_{\boldsymbol{k}} \varphi_{\boldsymbol{q}} e^{-\beta \mathscr{H}_{\text{eff}}^{(2)}}}{\int \prod_{\boldsymbol{p}} d\varphi_{\boldsymbol{p}} e^{-\beta \mathscr{H}_{\text{eff}}^{(2)}}} = \frac{\delta_{\boldsymbol{k}, -\boldsymbol{q}} T_c}{bq^2 + T - T_c}. \tag{6.136}$$

We note that $G(\boldsymbol{x}) = \langle \varphi((\boldsymbol{x})) \varphi(0) \rangle = \sum_{\boldsymbol{p}} e^{i\boldsymbol{p}\boldsymbol{x}} \langle \varphi_{\boldsymbol{p}} \varphi_{-\boldsymbol{p}} \rangle$. Therefore, we find,

$$\langle \varphi^2 \rangle = G(0) = \frac{S_d V T_c}{(2\pi)^d} \int\limits_0^\infty \frac{dp\, p^{d-1}}{bp^2 + T - T_c} = \frac{S_d}{(2\pi)^d} \frac{\pi V T_c (T - T_c)^{d/2-1}}{2 \sin\left(\frac{\pi d}{2}\right) b^{d/2}}. \tag{6.137}$$

6.13   Seminar XIII

In this section we solve Problems 33 and 34.

6.13.1   Problem 33

The scaling dimension of thermodynamic potential δF is $\Delta_F = d$. Therefore, one can write,

$$\delta F = t^{d/\Delta_t} f\left(ht^{-\Delta_h/\Delta_t}\right). \tag{6.138}$$

Using the relation $\varphi = -\frac{\partial F}{\partial h}$, we have $\Delta_\varphi = d - \Delta_h$. Next, using the relation $C_P = T_c \frac{\partial^2 \delta F}{\partial^2 t}$, one can note that (at zero field) $\alpha = 2 - d/\Delta_t$. This leads to the relation $\nu d = 2 - \alpha$. For $t \to 0$, we should have $F \propto t^{d/\Delta_t}(ht^{-\Delta_h/\Delta_t})^{-\varepsilon}$ since $C_P \propto h^{-\varepsilon}$. Hence we obtain the relation $\alpha\mu = \nu\varepsilon$.

6.13.2   Problem 34

For the n-component field φ, we have the following effective Hamiltonian,

$$\mathcal{H}_{\text{eff}}[\varphi] = \frac{1}{2} \int d^d\boldsymbol{r} \left[\tau\boldsymbol{\varphi}^2 + (\nabla\boldsymbol{\varphi})^2 + \frac{\lambda}{2}(\boldsymbol{\varphi}^2)^2\right]. \tag{6.139}$$

Our aim is to perform an integral over the modes with the momenta between Λ and $\Lambda' = \Lambda/u$. Splitting on the fast and slow components in the same way as in

the lecture, we find the following expression for the effective Hamiltonian,

$$\mathcal{H}_{\text{eff}}[\varphi] \approx \mathcal{H}_{\text{eff}}[\underline{\varphi}] + \mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}] + \mathcal{H}_{\text{eff}}^{\text{int}},$$

$$\mathcal{H}_{\text{eff}}[\underline{\varphi}] = \frac{1}{2} \int d^d \boldsymbol{r} \left[\tau \underline{\boldsymbol{\varphi}}^2 + (\nabla \underline{\boldsymbol{\varphi}})^2 + \frac{\lambda}{2} (\underline{\boldsymbol{\varphi}}^2)^2 \right],$$

$$\mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}] = \frac{1}{2} \int d^d \boldsymbol{r} \left[\tau \overline{\boldsymbol{\varphi}}^2 + (\nabla \overline{\boldsymbol{\varphi}})^2 \right],$$

$$\mathcal{H}_{\text{eff}}^{\text{int}} = \frac{\lambda}{4} \int d^d \boldsymbol{r} \left[2(\underline{\boldsymbol{\varphi}}^2)(\overline{\boldsymbol{\varphi}}^2) + 4(\underline{\boldsymbol{\varphi}}\overline{\boldsymbol{\varphi}})^2 \right]. \tag{6.140}$$

We have neglected the terms vanishing due to fast oscillations after integration over the whole space. Also we assume that the fast component $\overline{\varphi}$ is small. So, the term proportional to λ can be omitted in the effective Hamiltonian for $\overline{\varphi}$, $\mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}]$. Now we should take an average over $\mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}]$. This produces the correction to $\mathcal{H}_{\text{eff}}[\underline{\varphi}]$. The correction can be written as,

$$e^{-\delta\mathcal{H}_{\text{eff}}[\underline{\varphi}]/T} = \int D[\overline{\varphi}] \, e^{-(\mathcal{H}_{\text{eff}}^{\text{int}}+\mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}])/T} \bigg/ \int D[\overline{\varphi}] \, e^{-\mathcal{H}_{\text{eff}}^{(0)}[\overline{\varphi}]/T} \tag{6.141}$$

Hence, to second order in λ, we find

$$\delta\mathcal{H}_{\text{eff}}[\underline{\varphi}] = \langle \mathcal{H}_{\text{eff}}^{\text{int}} \rangle - \frac{\beta}{2} \langle \langle (\mathcal{H}_{\text{eff}}^{\text{int}})^2 \rangle \rangle. \tag{6.142}$$

Here $\langle \langle (\mathcal{H}_{\text{eff}}^{\text{int}})^2 \rangle \rangle = \langle (\mathcal{H}_{\text{eff}}^{\text{int}})^2 \rangle - \langle \mathcal{H}_{\text{eff}}^{\text{int}} \rangle^2$. The average of interaction term is given as

$$\langle \mathcal{H}_{\text{eff}}^{\text{int}} \rangle = \frac{\lambda(n+2)}{2} \int d^d \boldsymbol{r} \underline{\boldsymbol{\varphi}}^2 G_{\overline{\varphi}}(\boldsymbol{0}). \tag{6.143}$$

Here $\langle \overline{\varphi}_i(\boldsymbol{r})\overline{\varphi}_j(\boldsymbol{r}') \rangle = \delta_{ij} G_{\overline{\varphi}}(\boldsymbol{r} - \boldsymbol{r}')$. The other term can be found as

$$\langle \langle (\mathcal{H}_{\text{eff}}^{\text{int}})^2 \rangle \rangle = \frac{\lambda^2(n+8)}{2} \int d^d \boldsymbol{r} \int d^d \boldsymbol{r}' (\underline{\boldsymbol{\varphi}}^2(\boldsymbol{r}))^2 G_{\overline{\varphi}}^2(\boldsymbol{r}'). \tag{6.144}$$

Therefore, we reproduce the same expression for $\mathcal{H}_{\text{eff}}[\underline{\varphi}] + \delta\mathcal{H}_{\text{eff}}[\underline{\varphi}]$ as for $\mathcal{H}_{\text{eff}}[\underline{\varphi}]$ but the coupling constants are different,

$$\tau \to \tau(l) = e^{2l}\tau + (n+2)\lambda e^{2l} G_{\overline{\varphi}}(\boldsymbol{0}),$$

$$\lambda \to \lambda(l) = e^{(4-d)l}\lambda - (n+8)\beta\lambda^2 e^{(4-d)l} \int d^d \boldsymbol{r}' G_{\overline{\varphi}}^2(\boldsymbol{r}'). \tag{6.145}$$

Note here that we have used the same choice of exponent $\rho = (d + 2)/2$ as in the Lecture. We remind that $u = e^l$. Now we calculate the integrals over the Green's functions,

$$G_{\overline{\varphi}}(\mathbf{0}) = \int \frac{d^d \mathbf{k}}{(2\pi)^d} G_{\overline{\varphi}}(\mathbf{k}) = \frac{S_d T}{(2\pi)^d} \int\limits_{\Lambda/u}^{\Lambda} \frac{k^{d-1} dk}{k^2 + \tau} \approx \frac{S_d}{(2\pi)^d} \frac{T\Lambda^d}{\Lambda^2 + \tau} l,$$

$$\int d^d \mathbf{r}' G_{\overline{\varphi}}^2(\mathbf{r}') = \int \frac{d^d \mathbf{k}}{(2\pi)^d} G_{\overline{\varphi}}^2(\mathbf{k}) = \frac{S_d T^2}{(2\pi)^d} \int\limits_{\Lambda/u}^{\Lambda} \frac{k^{d-1} dk}{(k^2 + \tau)^2} \approx \frac{S_d}{(2\pi)^d} \frac{T^2 \Lambda^d}{(\Lambda^2 + \tau)^2} l.$$

$$\text{(6.146)}$$

Then we substitute this expression into the previous equation. Also we will introduce new notations, $\tilde{\tau} = \tau/\Lambda^2$ and $\tilde{\lambda} = \lambda T \Lambda^{d-4} S_d / (2\pi)^d$. Then, expanding to lowest order in l, we find,

$$\tilde{\tau}(l) = \tilde{\tau} + \left(2\tilde{\tau} + \frac{(n+2)\tilde{\lambda}}{1 + \tilde{\tau}}\right) l, \quad \tilde{\lambda}(l) = \tilde{\lambda} + \left((4 - d)\tilde{\lambda} - \frac{(n+8)\tilde{\lambda}^2}{(1 + \tilde{\tau})^2}\right) l.$$

$$\text{(6.147)}$$

These relations can be represented in the form of the renormalization group equations,

$$\frac{d\tilde{\tau}}{dl} = 2 + \frac{(n+2)\tilde{\lambda}}{1 + \tilde{\tau}}, \qquad \frac{d\tilde{\lambda}}{dl} = (4 - d) - \frac{(n+8)\tilde{\lambda}^2}{(1 + \tilde{\tau})^2}. \qquad \text{(6.148)}$$

6.14   Seminar XIV

In this section we consider Problems 35, 36, and 37.

6.14.1   Problem 35

The correlation function $\langle \cos(\theta_0 - \theta_n) \rangle$ is determined as

$$\langle \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{n}}) \rangle = \left(\prod_l \int\limits_0^{2\pi} \frac{d\theta_l}{2\pi}\right) \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{n}}) \exp\left[\beta J \sum_{<jk>} \cos(\theta_j - \theta_k)\right]$$

$$\left/ \left(\prod_l \int\limits_0^{2\pi} \frac{d\theta_l}{2\pi}\right) \exp\left[\beta J \sum_{<jk>} \cos(\theta_j - \theta_k)\right].\right. \qquad \text{(6.149)}$$

Let us rewrite this expression as an expression on the dual lattice in a way analogous to Eq. (3.83). Then, we find

$$\langle \cos(\theta_0 - \theta_n) \rangle = \sum_{\{s_l\}} \prod_{<ll'>} I_{|s_l - s_{l'} + \Delta_{ll'}|}(\beta J) \Big/ \sum_{\{s_l\}} \prod_{<ll'>} I_{|s_l - s_{l'}|}(\beta J). \quad (6.150)$$

Here s_l is an integer number and $\Delta_{<ll'>} = 1$ if the link between the sites l and l' on the dual lattice is crossed by the path from point 0 to point n. Otherwise, $\Delta_{<ll'>} = 0$. We note that this path can be arbitrary. The result is independent of the particular path choice. At high temperatures $T \gg J$, one can use the following expansion for the modified Bessel function, $I_{|s|}(z) = (z/2)^{|s|}/(|s|!)$, at $z \ll 1$. Then, as it follows from Eq. (6.150), the contribution lowest in powers βJ to the correlation function $\langle \cos(\theta_0 - \theta_n) \rangle$ will be determined by the shortest path between points 0 and n. Each link of this path has $\Delta_{<ll'>} = 1$ and, thus, contributes a factor $\beta J/2$. Therefore, we find

$$\langle \cos(\theta_0 - \theta_n) \rangle = (\beta J/2)^{N_{\text{links}}} \quad (6.151)$$

where N_{links} is the number of shortest path links between the points 0 and n.

6.14.2 Problem 36

In this problem we calculate the integral over $\tilde{\theta}_l$ in expression (3.87) from the main part of Lectures. Let us write,

$$Z = \sum_{\{m_l\}} \prod_l \left(\int d\tilde{\theta}_l \right) \exp \left[-\beta F_0(\tilde{\theta}, m) \right],$$

$$F_0(\tilde{\theta}, m) = \frac{J}{2} \sum_{\langle l,l' \rangle} (\tilde{\theta}_l - \tilde{\theta}_{l'})^2 - i2\pi J \sum_l m_l \tilde{\theta}_l. \quad (6.152)$$

In order to calculate this integral, let us consider a shift of integration variables: $\tilde{\theta}_l \mapsto \tilde{\theta}_l + a_l$. We should find such variables a_l which eliminate the terms linearly dependent on $\tilde{\theta}_l$. After such transformation the free energy becomes

$$F_0(\tilde{\theta}, m) \mapsto F(a, \tilde{\theta}, m) = F_0(\tilde{\theta}, 0) + F_0(a, m) + F_1(a, \tilde{\theta}, m),$$

$$F_1(a, \tilde{\theta}, m) = J \sum_{\langle l,l' \rangle} (\tilde{\theta}_l - \tilde{\theta}_{l'})(a_l - a_{l'}) - i2\pi J \sum_l m_l \tilde{\theta}_l$$

$$= 2J \sum_{\langle l,l' \rangle} \tilde{\theta}_l (a_l - a_{l'} - i\pi m_l). \quad (6.153)$$

So, we attempt to find variables a_l nullifying F_1. For the square lattice, we should solve the following set of equations

$$4a_{j,k} - a_{j+1,k} - a_{j-1,k} - a_{j,k-1} - a_{j,k+1} = 4i\pi m_{j,k}. \tag{6.154}$$

In order to solve the above equations, we use the periodic boundary conditions. We introduce the Green's function, determined as

$$4G_{j,k} - G_{j+1,k} - G_{j-1,k} - G_{j,k-1} - G_{j,k+1} = \delta_{j,0}\delta_{k,0}. \tag{6.155}$$

Performing the Fourier transform,

$$G_{j,k} = \int\limits_0^{2\pi} \frac{dq_x dq_y}{(2\pi)^2} e^{iq_x \mathsf{a}j} e^{iq_y \mathsf{a}k} G(q_x, q_y), \tag{6.156}$$

we obtain

$$G(q_x, q_y) = \frac{1}{4 - 2\cos(q_x\mathsf{a}) - 2\cos(q_y\mathsf{a})}. \tag{6.157}$$

The integral over $\boldsymbol{q}$ has logarithmic divergence. The latter is associated with an existence of zero mode (translation) in the operator (6.154). Performing the integral over $\boldsymbol{q}$, we find

$$G_{j,k} = \frac{1}{2\pi} \ln\left(\frac{L}{r_{jk}}\right) \tag{6.158}$$

where L is a typical size of the system and $r_{jk} = \mathsf{a}\sqrt{j^2 + k^2}$ is the distance between the origin $(0,0)$ and the point (j,k). With the help of the Green's function G we can find a_l satisfying Eq. (6.154) as

$$a_l = \sum_{l'} G(|\boldsymbol{l} - \boldsymbol{l}'|)m_{l'}. \tag{6.159}$$

Hence, we obtain

$$Z = \prod_l \left(\int d\tilde{\theta}_l\right) \exp\left[-\beta F_0(\tilde{\theta}, 0)\right] \sum_{\{m_l\}} \exp\left[-2\pi J\beta \sum_{l,l'} m_l m_{l'} \ln\frac{L}{|\boldsymbol{l} - \boldsymbol{l}'|}\right]$$

$$\equiv Z_0 \exp\left[-2\pi J\beta \ln\frac{L}{r_v}\left(\sum_l m_l\right)^2 - 2\pi J\beta \ln\frac{r_v}{\mathsf{a}} \sum_l m_l^2\right.$$

$$\left. -2\pi J\beta \sum_{l\neq l'} m_l m_{l'} \ln\frac{r_v}{|\boldsymbol{l} - \boldsymbol{l}'|}\right]. \tag{6.160}$$

Here the length scales satisify $L \gg r_v \gg \mathsf{a}$, where r_v is a typical distance between vortices. In the limit $\beta J \gg 1$, the first two terms should acquire the minimal possible values so $\sum_l m_l = 0$ and each $m_l = \pm 1$.

6.14.3   Problem 37

The action S is determined as, see Eq. (3.91):

$$S = \beta \mathcal{H}_{\text{eff}} = \frac{\beta J}{2} \int d^2 \boldsymbol{r} (\nabla \theta)^2 - 2\beta \tilde{y} \int d^2 \boldsymbol{r} \cos(2\pi \beta J \theta). \qquad (6.161)$$

In order to derive the RG equations, let us choose the convenient variables. We denote $2\pi \beta J = g$ and $2\tilde{y}\beta = u$. Also we rescale θ: $\theta \to \theta/g$. Then we find

$$S = \frac{1}{2g} \int (\nabla \theta)^2 - u \int d^2 \boldsymbol{r} \cos(\theta). \qquad (6.162)$$

The original field θ is determined as

$$\theta(\boldsymbol{r}) = \sum_{|\boldsymbol{p}|<\Lambda} \theta_{\boldsymbol{p}} e^{i\boldsymbol{p}\boldsymbol{r}}. \qquad (6.163)$$

Let us split it into the slow and fast components, $\theta = \theta' + \Theta$,

$$\theta'(\boldsymbol{r}) = \sum_{|\boldsymbol{p}|<\Lambda'} \theta_{\boldsymbol{p}} e^{i\boldsymbol{p}\boldsymbol{r}}, \qquad \Theta(\boldsymbol{r}) = \sum_{\Lambda>|\boldsymbol{p}|>\Lambda'} \theta_{\boldsymbol{p}} e^{i\boldsymbol{p}\boldsymbol{r}}. \qquad (6.164)$$

Expanding S in the fast component Θ to second order, we derive the following action:

$$S_\Lambda = \frac{1}{2g} \int d^2 \boldsymbol{r} \left[(\nabla \theta)^2 + (\nabla \Theta)^2 \right] - u \int d^2 \boldsymbol{r} \left[\cos \theta - \Theta \sin \theta - \frac{\Theta^2}{2} \cos \theta \right]. \qquad (6.165)$$

The term $-\sin(\theta)\Theta$ is insignificant since it is a product of slow and fast modes. Omitting this term, we find the action for the slow modes,

$$S_{\Lambda'} = \frac{1}{2g_\Lambda} \int d^2 \boldsymbol{r} (\nabla \theta)^2 - u \int d^2 \boldsymbol{r} \cos(\theta) + \delta S_{\Lambda'}, \qquad (6.166)$$

where

$$\delta S_{\Lambda'} \approx \langle S_{\text{int}} \rangle - \frac{1}{2} \langle\langle S_{\text{int}}^2 \rangle\rangle, \qquad S_{\text{int}} = -\frac{u}{2} \int d^2 \boldsymbol{r} \, \Theta^2 \cos \theta,$$

$$\langle A \rangle = \int D[\Theta] \, A[\Theta] \, e^{-\frac{1}{2g_\Lambda} \int d^2 \boldsymbol{r} (\nabla \Theta)^2} \Big/ \int D[\Theta] \, e^{-\frac{1}{2g_\Lambda} \int d^2 \boldsymbol{r} (\nabla \Theta)^2}. \qquad (6.167)$$

Next, we find several averages. At first, we get

$$\langle S_{\text{int}} \rangle = \frac{u}{2} \int d^2 \boldsymbol{r} \, \langle \Theta^2 \rangle \cos \theta = \frac{u}{2} \int d^2 \boldsymbol{r} \, G(0) \cos \theta \frac{gu}{4\pi} \frac{\Lambda - \Lambda'}{\Lambda'} \int d^2 \boldsymbol{r} \, \cos \theta. \qquad (6.168)$$

Here $G(r) = \langle\Theta(\boldsymbol{r})\Theta(0)\rangle$. Thus average $\langle S_{\text{int}}\rangle$ entails the renormalization of the parameter u,

$$u_{\Lambda'} = u_{\Lambda} + \frac{g_{\Lambda}u_{\Lambda}}{4\pi}\frac{\Lambda - \Lambda'}{\Lambda'}. \tag{6.169}$$

The second average is more complicated,

$$\langle\langle S_{\text{int}}^2\rangle\rangle = \frac{u^2}{4}\int d^2\boldsymbol{r_1}d^2\boldsymbol{r_2}\,\cos\theta(\boldsymbol{r_1})\cos\theta(\boldsymbol{r_2})\langle\langle\Theta^2(\boldsymbol{r_1})\Theta^2(\boldsymbol{r_2})\rangle\rangle$$

$$= \frac{u^2}{2}\int d^2\boldsymbol{r}d^2\delta\boldsymbol{r}\,\cos\theta(\boldsymbol{r})\cos(\theta(\boldsymbol{r}+\delta\boldsymbol{r}))G^2(\delta r) = \frac{u^2}{2}\int d^2\boldsymbol{r}d^2\delta\boldsymbol{r}\cos\theta(\boldsymbol{r})$$

$$\times\cos\left(\theta(\boldsymbol{r}) + \delta\boldsymbol{r}^\alpha\partial_\alpha\theta + \frac{1}{2}\delta\boldsymbol{r}^\alpha\delta\boldsymbol{r}^\beta\partial_\alpha\partial_\beta\theta\right)\,G^2(\delta r) = \frac{u^2}{2}\int d^2\boldsymbol{r}d^2\delta\boldsymbol{r}\cos\theta(\boldsymbol{r})$$

$$\times\left[\cos\theta(\boldsymbol{r}) - \sin\theta(\boldsymbol{r})\frac{\delta\boldsymbol{r}^\alpha\delta\boldsymbol{r}^\beta}{2}\partial_\alpha\partial_\beta\theta - \cos\theta(\boldsymbol{r})\frac{\delta\boldsymbol{r}^\alpha\delta\boldsymbol{r}^\beta}{2}\partial_\alpha\theta\partial_\beta\theta\right]G^2(\delta r) \tag{6.170}$$

The term $(u^2/2)\int d^2\boldsymbol{r}d^2\delta\boldsymbol{r}\cos^2\theta G^2(\delta r)$ is unimportant since leads to the fluctuation at small scales. Omitting this term, we obtain

$$\langle\langle S_{\text{int}}^2\rangle\rangle = -\frac{u^2}{4}\int d^2\boldsymbol{r}\cos\theta\left[\sin\theta\partial_\alpha\partial_\beta\theta + \cos\theta\partial_\alpha\theta\partial_\beta\theta\right]\int d^2\delta\boldsymbol{r}G^2(\delta r)\delta\boldsymbol{r}^\alpha\delta\boldsymbol{r}^\beta$$

$$= \frac{u^2g^2}{8}\int d^2\boldsymbol{r}\left[1 - \cos(2\theta)\right](\nabla\theta)^2\frac{\Lambda - \Lambda'}{\pi\Lambda^5}. \tag{6.171}$$

Therefore, $\langle\langle S_{\text{int}}^2\rangle\rangle$ contributes to the kinetic term, $(\nabla\theta)^2$. Thus, we obtain the following two relations,

$$u_{\Lambda'} = u_{\Lambda} + \frac{g_{\Lambda}u_{\Lambda}}{4\pi}\ln\left(\frac{\Lambda}{\Lambda'}\right),\,\frac{1}{g_{\Lambda'}} = \frac{1}{g_{\Lambda}} - \frac{u_{\Lambda}^2g_{\Lambda}^2}{8\pi}\frac{\Lambda - \Lambda'}{\Lambda^5}.$$

In order to represent the above relations as some RG equation, we introduce $\gamma_{\Lambda} = u_{\Lambda}/\Lambda^2$ and $l = -\ln\Lambda$. Then, one can write

$$\frac{\partial\gamma}{\partial l} = \left(2 - \frac{g}{4\pi}\right)\gamma, \qquad \frac{\partial g}{\partial l} = -\frac{\gamma^2g^4}{8\pi}. \tag{6.172}$$

6.15 Seminar XV

In this section we present the solutions for Problems 38 and 39.

6.15.1   Problem 38

Let us start from calculating the function

$$D^R(\omega) = i \int_0^\infty dt\, e^{i(\omega+i0)t} \operatorname{Tr}\Big([b_\alpha(t), b_\alpha^\dagger]\rho\Big). \tag{6.173}$$

The operator $b_\alpha(t)$ satisfies the equation of motion,

$$\frac{db_\alpha(t)}{dt} = i[H, b_\alpha(t)]. \tag{6.174}$$

Using commutation relations $[b_\alpha, b_\beta^\dagger] = \delta_{\alpha\beta}$, we find

$$b_\alpha(t) = e^{-i\varepsilon_\alpha t} b_\alpha. \tag{6.175}$$

Hence, we find

$$D^R(\omega) = i \int_0^\infty dt\, e^{i(\omega-\varepsilon_\alpha+i0)t} \langle[b_\alpha, b_\alpha^\dagger]\rangle = i \int_0^\infty dt\, e^{i(\omega-\varepsilon_\alpha+i0)t} = -\frac{1}{\omega - \varepsilon_\alpha + i0}. \tag{6.176}$$

Next, we compute the function

$$D^K(\omega) = i \int_0^\infty dt\, e^{i\omega t} \operatorname{Tr}\Big(\{b_\alpha(t), b_\alpha^\dagger\}\rho\Big) = i \int_0^\infty dt\, e^{i(\omega-\varepsilon_\alpha)t}\Big[2f_B(\varepsilon_\alpha) + 1\Big]$$

$$= 2\pi i\delta(\omega - \varepsilon_\alpha)\Big[2f_B(\varepsilon_\alpha) + 1\Big]. \tag{6.177}$$

Here we have used the fact that $\langle b_\alpha^\dagger b_\alpha\rangle = f_B(\varepsilon_\alpha)$.

Comparing Eqs. (6.176) and (6.177), we find

$$D^K(\omega) = 2i \operatorname{Im} D^R(\omega) \coth\frac{\omega}{2T}. \tag{6.178}$$

6.15.2   Problem 39

Let us consider the case when the applied force depends on the spatial coordinate r. Then the perturbation has the following form, $\mathscr{V} = -\int d\boldsymbol{r}\, f(r, t)\mathscr{X}(\boldsymbol{r})$. In what follows, we use the interaction representation. This means, in particular, that the density matrix satisfies the following equation,

$$\frac{d\rho(t)}{dt} = -i[\mathscr{V}(t), \rho(t)]. \tag{6.179}$$

Within the linear response one can relate the generalized susceptibility with the average of corresponding operator $\mathscr{Y}(\boldsymbol{r}, t)$ and applied force $\mathscr{X}(\boldsymbol{r}, t)$ by means of the following relation,

$$\langle\mathscr{Y}(\boldsymbol{r}, t)\rangle = \int\limits_{-\infty}^{t} dt' \int d\boldsymbol{r}' f(\boldsymbol{r}', t')\alpha_{\mathscr{Y}\mathscr{X}}(\boldsymbol{r}, t; \boldsymbol{r}', t'). \qquad (6.180)$$

The average $\langle\mathscr{Y}(\boldsymbol{r}, t)\rangle$ is determined in a standard way,

$$\langle\mathscr{Y}(\boldsymbol{r}, t)\rangle = \mathrm{Tr}\big(\mathscr{Y}(\boldsymbol{r}, t)\rho(t)\big). \qquad (6.181)$$

Since we are interested in the linear response, we can approximate the density matrix $\rho(t)$ as

$$\rho(t) \approx \rho_0 - i \int\limits_{-\infty}^{t} dt'[\mathscr{V}(t'), \rho_0] \qquad (6.182)$$

where ρ_0 is the density matrix in the absence of perturbation. Let us introduce the following notation, $\langle\hat{O}\rangle_0 = \mathrm{Tr}(O\rho_0)$. Also we assume that $\langle\mathscr{Y}(\boldsymbol{r}, t)\rangle_0 = 0$. Then, we find

$$\langle\mathscr{Y}(\boldsymbol{r}, t)\rangle \approx -i \int\limits_{-\infty}^{t} dt' \,\mathrm{Tr}\Big(\mathscr{Y}(\boldsymbol{r}, t)[\mathscr{V}(t'), \rho_0]\Big) = -i \int\limits_{-\infty}^{t} dt' \langle[\mathscr{A}(\boldsymbol{r}, t), \mathscr{V}(t')]\rangle_0$$

$$= i \int\limits_{-\infty}^{t} dt' \int d\boldsymbol{r}' f(\boldsymbol{r}', t')\langle[\mathscr{Y}(\boldsymbol{r}, t), \mathscr{X}(\boldsymbol{r}', t')]\rangle_0. \qquad (6.183)$$

Comparing Eqs. (6.180) and (6.183), we obtain our final conclusion:

$$\alpha_{\mathscr{Y}\mathscr{X}}(\boldsymbol{r}, t; \boldsymbol{r}', t') = i\langle[\mathscr{Y}(\boldsymbol{r}, t), \mathscr{X}(\boldsymbol{r}', t')]\rangle_0. \qquad (6.184)$$

We note that the generalized susceptibility depends only on $\boldsymbol{r} - \boldsymbol{r}'$ for the system with the translational invariance.

6.16   Seminar XVI

In this section we consider Problems 40 and 41.

6.16.1 Problem 40

Let us start from the case when the bias voltage is absent, $V = 0$. The spin susceptibility has the following form, see Eq. (4.30),

$$
\chi_{jk}(\tau) = \frac{1}{\nu^2} \operatorname{Tr}_e \left[: s_k^I(y_0, \tau) :: s_j^I(y_0, 0) : \rho_0 \right] = \frac{1}{4\nu^2} \langle : \Psi^\dagger(y_0, \tau) \sigma_k \Psi(y_0, 0) :
$$

$$
\times : \Psi^\dagger(y_0, 0) \sigma_j \Psi(y_0, \tau) : \rangle_0 = \sum_{s_1, s_2} \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_3 s_4}}{4\nu^2} \langle : \Psi_{s_1}^\dagger(y_0, \tau) \Psi_{s_2}(y_0, 0) :
$$

$$
\times : \Psi_{s_3}^\dagger(y_0, 0) \Psi_{s_4}(y_0, 0) : \rangle_0. \tag{6.185}
$$

In order to calculate the above average, we should diagonalize the Hamiltonian,

$$
H_e = iv \int dy \, \Psi^\dagger(y) \sigma^z \partial_y \Psi(y) = -v \sum_s s \int \frac{dk}{2\pi} \Psi_s^\dagger(k) k \Psi_s(k)
$$

$$
= \sum_s \int \frac{dk}{2\pi} \xi_s(k) \Psi_s^\dagger(k) \Psi_s(k), \tag{6.186}
$$

where $\xi_s(k) = -vsk$. Therefore, we can write

$$
\Psi_s(y, \tau) = \int \frac{dk}{2\pi} \Psi_s(k) e^{-i\xi_s(k)\tau}, \qquad \Psi_s^\dagger(y, \tau) = \int \frac{dk}{2\pi} \Psi_s^\dagger(k) e^{i\xi_s(k)\tau}. \tag{6.187}
$$

The commutation relations for the creation and annihilation operators have the standard form,

$$
\Psi_s(k) \Psi_{s'}^\dagger(k') + \Psi_{s'}^\dagger(k') \Psi_s(k) = 2\pi \delta(k - k') \delta_{s,s'}. \tag{6.188}
$$

Using the Fourier representation, we can rewrite the susceptibility as

$$
\chi_{jk}(\tau) = \sum_{s_1, s_2} \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_3 s_4}}{4\nu^2} \int \prod_{i=1}^4 \frac{dk_i}{2\pi} e^{-i(\xi_{s_2}(k_2) - \xi_{s_1}(k_1))\tau} e^{-i(k_2 + k_4 - k_1 - k_3)y_0}
$$

$$
\times \langle : \Psi_{s_1}^\dagger(k_1) \Psi_{s_2}(k_2) :: \Psi_{s_3}^\dagger(k_3) \Psi_{s_4}(k_4) : \rangle_0. \tag{6.189}
$$

Now we treat the average written in the last line. At first, we calculate the simpler expression,

$$
\langle \Psi_{s_1}^\dagger(k_1) \Psi_{s_2}(k_2) \rangle_0 = 2\pi \delta(k_1 - k_2) \delta_{s_1, s_2} - \langle \Psi_{s_2}(k_2) \Psi_{s_1}^\dagger(k_1) \rangle_0
$$

$$
= 2\pi \delta(k_1 - k_2) \delta_{s_1, s_2} - \langle \Psi_{s_1}^\dagger(k_1) \Psi_{s_2}(k_2) \rangle_0 e^{\beta \xi_{s_1}(k_1)}. \tag{6.190}
$$

To obtain the last line in the above equation, we employ the following relation, $\Psi_{s_1}^\dagger(k_1) \rho_0 = \rho_0 \Psi_{s_1}^\dagger(k_1) e^{\beta \xi_{s_1}(k_1)}$, where ρ_0 is the equilibrium density matrix. Finally, we obtain

$$
\langle \Psi_{s_1}^\dagger(k_1) \Psi_{s_2}(k_2) \rangle_0 = 2\pi \delta(k_1 - k_2) \delta_{s_1, s_2} f_F(\xi_{s_1}(k_1)),
$$

$$
\langle \Psi_{s_2}(k_2) \Psi_{s_1}^\dagger(k_1) \rangle_0 = 2\pi \delta(k_1 - k_2) \delta_{s_1, s_2} [1 - f_F(\xi_{s_1}(k_1))] \tag{6.191}
$$

where $f_F(\varepsilon) = 1/[1 + \exp(\varepsilon/T)]$. Now we are ready to calculate the average,

$$\langle \Psi_{s_1}^\dagger(k_1)\Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0 = 2\pi\delta(k_1 - k_2)\langle \Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0\delta_{s_1,s_2}$$
$$-\langle \Psi_{s_2}(k_2)\Psi_{s_1}^\dagger(k_1)\Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0 = 2\pi\delta(k_1 - k_2)\langle \Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0\delta_{s_1,s_2}$$
$$+\langle \Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\Psi_{s_1}^\dagger(k_1)\Psi_{s_4}(k_4)\rangle_0 = 2\pi\delta(k_1 - k_2)\langle \Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0\delta_{s_1,s_2}$$
$$+2\pi\delta(k_1 - k_4)\delta_{s_1,s_4}\langle \Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\rangle_0 - \langle \Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\Psi_{s_1}^\dagger(k_1)\rangle_0$$
$$= 2\pi\delta(k_1 - k_2)\langle \Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0\delta_{s_1,s_2} + 2\pi\delta(k_1 - k_4)\delta_{s_1,s_4}\langle \Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\rangle_0$$
$$-\langle \Psi_{s_1}^\dagger(k_1)\Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0 e^{\beta\xi_{s_1}(k_1)}. \tag{6.192}$$

Hence, we find

$$\langle \Psi_{s_1}^\dagger(k_1)\Psi_{s_2}(k_2)\Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4)\rangle_0 = (2\pi)^2\Big[\delta(k_1 - k_2)\delta(k_3 - k_4)f_F(\xi_{s_3}(k_3))$$
$$\times\delta_{s_1,s_2}\delta_{s_3,s_4} + \delta(k_1 - k_4)\delta(k_2 - k_3)\delta_{s_1,s_4}\delta_{s_2,s_3}[1 - f_F(\xi_{s_2}(k_2))]\Big]f_F(\xi_{s_1}(k_1)). \tag{6.193}$$

Consequently, we obtain

$$\langle : \Psi_{s_1}^\dagger(k_1)\Psi_{s_2}(k_2) :: \Psi_{s_3}^\dagger(k_3)\Psi_{s_4}(k_4) : \rangle_0 = (2\pi)^2\delta(k_1 - k_4)\delta(k_2 - k_3)\delta_{s_1,s_4}\delta_{s_2,s_3}$$
$$\times[1 - f_F(\xi_{s_2}(k_2) - s_2eV/2)]\Big]f_F(\xi_{s_1}(k_1) - s_1eV/2). \tag{6.194}$$

Here we have augmented the chemical potential $seV/2$ to the distribution function of the edge electrons. This chemical potential appears due to the presence of a bias voltage V. Substituting this average in the expression for the susceptibility leads to

$$\chi_{jk}(\tau) = \sum_{s_1,s_2}\frac{\sigma_k^{s_1s_3}\sigma_j^{s_3s_1}}{4\nu^2}\int\frac{dk_1}{2\pi}\frac{dk_3}{2\pi}e^{-i(\xi_{s_3}(k_3)-\xi_{s_1}(k_1))\tau}f_F(\xi_{s_1}(k_1) - s_1eV/2)$$
$$\times[1 - f_F(\xi_{s_3}(k_3) - s_3eV/2)] = \frac{\sigma_k^{s_1s_2}\sigma_j^{s_2s_1}}{4}\int d\xi_1 d\xi_2 e^{-i(\xi_2-\xi_1)\tau}f_F(\xi_1 - s_1eV/2)$$
$$\times[1 - f_F(\xi_2 - s_2eV/2)]. \tag{6.195}$$

Next, we find in the frequency domain,

$$\chi_{jk}(\omega) = \sum_{s_1,s_2}i\frac{\sigma_k^{s_1s_2}\sigma_j^{s_2s_1}}{4}\int d\xi_1 d\xi_2\frac{f_F(\xi_1 - s_1eV/2)(1 - f_F(\xi_2 - s_2eV/2))}{\omega - \xi_2 + \xi_1 + i0}. \tag{6.196}$$

We can simplify the above integral with the aid of shift $\xi_{1,2} \mapsto \xi + s_{1,2}eV/2$. Also we introduce new variable $\omega_{12} = \omega + (s_1 - s_2)eV/2$. As a result, we obtain

$$
\begin{aligned}
\chi_{jk}(\omega) &= \sum_{s_1,s_2} i \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_2 s_1}}{4} \int d\xi_1 d\xi_2 \frac{f_F(\xi_1)(1 - f_F(\xi_2))}{\omega_{12} - \xi_2 + \xi_1 + i0} \\
&= \sum_{s_i} i \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_2 s_1}}{4} \int d\xi_1 d\xi_2 \frac{f_F(\xi_1) f_F(\xi_2)}{\omega_{12} + \xi_2 + \xi_1 + i0}.
\end{aligned} \tag{6.197}
$$

Introducing new variables $\xi_+ = \frac{\xi_1 + \xi_2}{2}$ and $\xi_- = \xi_1 - \xi_2$, we derive the following expression,

$$
\begin{aligned}
\chi_{jk}(\omega) &= \sum_{s_i} i \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_2 s_1}}{4} \int d\xi_+ d\xi_- \frac{f_F(\xi_+ + \frac{\xi_-}{2}) f_F(\xi_+ - \frac{\xi_-}{2})}{\omega_{12} + 2\xi_+ + i0} \\
&= \sum_{s_i} i \frac{\sigma_k^{s_1 s_2} \sigma_j^{s_2 s_1}}{4} \int d\xi \frac{1}{\omega_{12} + \xi + i0} \frac{\xi}{\exp(\xi/T) - 1}.
\end{aligned} \tag{6.198}
$$

Finally, for the real part of $\chi_{jk}(\omega)$, we find

$$
\operatorname{Re} \chi_{jk}(\omega) = -\frac{\pi}{4} \sum_{s_i} \sigma_k^{s_1 s_2} \sigma_j^{s_2 s_1} \frac{\omega_{12}}{e^{-\omega_{12}/T} - 1}. \tag{6.199}
$$

6.16.2 Problem 41

The anti-hermitian part of the spin susceptibility is determined as (for zero frequency), see Eq. (4.35),

$$
\hat{\chi}^{(2)}(0) = \frac{1}{2} \text{p.v.} \int_{-\infty}^{\infty} d\xi \frac{\xi}{e^{\xi/T} - 1}
\begin{pmatrix}
\frac{\xi}{\xi^2 - (eV)^2} & \frac{ieV}{\xi^2 - (eV)^2} & 0 \\
-\frac{ieV}{\xi^2 - (eV)^2} & \frac{\xi}{\xi^2 - (eV)^2} & 0 \\
0 & 0 & \frac{1}{\xi}
\end{pmatrix}. \tag{6.200}
$$

This integral contains linearly divergent term. However, this term is independent of V and T. Therefore, we can omit it. We find to first order in V,

$$
\begin{aligned}
\chi_{jk}^{(2)}(0) &\to \frac{ieV \varepsilon_{jkz}}{2} \text{p.v.} \int_{-\infty}^{\infty} \frac{d\xi}{\xi} \frac{1}{e^{xi/T} - 1} = \frac{ieV \varepsilon_{jkz}}{4} \text{p.v.} \int_{-\infty}^{\infty} \frac{d\xi}{\xi} \tanh \frac{\xi}{2T} \\
&\simeq \frac{ieV}{2} \varepsilon_{jkz} \ln(\Lambda/T).
\end{aligned} \tag{6.201}
$$

Here Λ is the ultra-violet cut-off. As a result, we can write,

$$
\begin{aligned}
\chi_{jk}^{(2)}(0) \mathcal{J}_{rj} \mathcal{J}_{lk} \Big([S_r \rho, S_l] + [S_l, \rho S_r] \Big) = \chi_{jk}^{(2)}(0) \mathcal{J}_{rj} \mathcal{J}_{lk} \Big\{ S_r \rho S_l - S_l S_r \rho \\
+ S_l \rho S_r - \rho S_r S_l \Big\}.
\end{aligned} \tag{6.202}
$$

Since $\chi_{jk}^{(2)}(0)$ is an antisymmetric matrix, we can omit the symmetric part in the above expression. This yields

$$\chi_{jk}^{(2)}(0)\mathcal{J}_{rj}\mathcal{J}_{lk}\left(S_rS_l\rho - \rho S_rS_l\right) = i\chi_{jk}^{(2)}(0)\mathcal{J}_{rj}\mathcal{J}_{lk}\varepsilon_{rlm}[S_m, \rho]. \qquad (6.203)$$

This correction can be interpreted as a correction to the Hamiltonian of impurity,

$$\delta H_{\mathrm{imp}} = \delta h_m S_m \quad \delta h_m = \mathcal{J}_{rj}\mathcal{J}_{lk}\varepsilon_{rlm}\varepsilon_{jkz}\frac{eV}{2}\ln(\Lambda/T). \qquad (6.204)$$

Hence, we obtain

$$\mathcal{J}_{mz} \mapsto \mathcal{J}_{mz} + \nu\mathcal{J}_{rj}\mathcal{J}_{lk}\varepsilon_{rlm}\varepsilon_{jkz}\ln(\Lambda/T). \qquad (6.205)$$

This is nothing but the Kondo renormalization of the exchange coupling.

Bibliography

[1] L. D. Landau and E. M. Lifshitz, *Course in Theoretical Physics*, Vol. 5 (Pergamon Press, Oxford, 1984).

[2] E. Solano-Carrillo, *Quantum theory of entropy production*, PhD Thesis, Columbia University 2018.

[3] Yu. G. Rudoi and A. D. Sukhanov, *Thermodynamic fluctuations within the Gibbs and Einstein approaches*, Physics-Uspekhi 43, 1169 (2000).

[4] L. D. Landau, E. M. Lifshitz, *Course of Theoretical Physics. Vol. 9. Statistical Physics. Part II*, Pergamon Press, Oxford 1981.

[5] L. D. Landau, *The theory of a Fermi liquid*, JETP **3**, 920 (1957).

[6] P. Hohenberg and W. Kohn, *Inhomogeneous electron gas*, Phys. Rev. 136, B864 (1964).

[7] R. W. Richardson, *A restricted class of exact eigenstates of the pairing-force Hamiltonian*, Phys. Lett. **3**, 277, (1963); R. W. Richardson, *Exact eigenstates of pairing-force Hamiltonian*, Nucl. Phys. **52**, 221 (1964).

[8] F. D. M. Haldane, *Luttinger liquid theory of one-dimensional quantum fluids. I. Properties of the Luttinger model and their extension to the general 1D interacting spinless Fermi gas*, J. Phys. C: Solid State Phys. 14, 2585 (1981).

[9] E. Miranda, *Introduction to bosonization*, Braz. J. Phys. 33, 3 (2003).

[10] R. J. Baxter, *Exactly solvable models in statistical mechanics*, Academic Press (1982).

[11] H. B. Callen and T. A. Welton, *Irreversibility and generalized noise*, Phys. Rev. 83, 34 (1951).

[12] J. M. Deutsch, *Eigenstate thermalization hypothesis*, Rep. Prog. Phys. 81 082001 (2018).