広島大学学位請求論文

Current-density functional theory for bosonic superfluids

(ボゾン超流動体のための流れ密度汎関数理論)

D210219
藍沢　友也

広島大学

先進理工系科学研究科

先進理工系科学専攻

量子物質科学プログラム

主指導教員：樋口　克彦

2024年2月19日

目次

1. 主論文

Current-density functional theory for bosonic superfluids
(ボゾン超流動体のための流れ密度汎関数理論)
藍沢　友也

2. 公表論文

Current-density functional theory for bosonic superfluids
T. Aizawa, M. Higuchi and K. Higuchi, J. Phys. Commun. **7, 075003 (2023)**

主論文

Doctoral Thesis

Current-density functional theory for bosonic superfluids

(ボソン超流動体のための流れ密度汎関数理論)

D210219
Tomoya Aizawa

Hiroshima University

Graduate School of Advanced Science and Engineering

Division of Advanced Science and Engineering

Quantum Matter Program

supervisor：Katsuhiko Higuchi

February 19, 2024

Abstract

As for the conventional theory for superfluids, the macroscopic theory and the microscopic one are raised mainly. The former corresponds to the two-fluid model[15,16] which regards superfluids as the system consisting of the superfluid and normal fluid components. The latter corresponds to the Gross-Pitaevskii(GP) theory[17-19], which gives physical quantities of the superfluid component by the order parameter of the Bose-Einstein Condensation(BEC), and then, the Bogoliubov theory[20,21], which gives physical quantities of the normal fluid component by using the quasiparticle description. Although there are theories such as the above ones approaching in terms of the microscopic surface, there are also some problems to be solved. As one of these problems, the GP and Bogoliubov theories cannot calculate physical quantities such as the density and current-density of the superfluid and normal fluid simultaneously within just one theory.

To solve these problems, we have developed the current-density functional theory for bosonic superfluids(sf-CDFT) in the thermal equilibrium state. In sf-CDFT, we have chosen the particle number density, current-density of superfluids, and also, the order parameter of the BEC as basic variables reproduced in sf-CDFT. It is shown that sf-CDFT can reproduce the particle number density and current-density of the superfluid and normal fluid components simultaneously while incorporating the effect of the interaction between these two fluids. Physical quantities such as the particle number density and current-density of these two fluids are determined by solutions of two crucial equations called the Gross-Pitaevskii-Kohn-Sham(GPKS) and Kohn-Sham(KS) equations. Moreover, in the discussion, we propose some interesting comparisons of sf-CDFT with conventional theories for superfluids, and in addition to this, the sum rule for the exchange-correlation(xc) energy functional defined in sf-CDFT is derived and would be useful for the development of its approximate form.

Contents

Chapter 1

Introduction

1.1 Approach of conventional theories for superfluids

The liquid helium-4 and the dilute Bose gases, what are called superfluids generally, have been studied actively, and research for superfluids has been one of the well-known study fields in modern condensed matter physics nowadays[1-8]. At the beginning of the history of research for superfluids, F. London[11] pointed out the relation between superfluidity and BEC[9,10] after the discovery of superfluidity[1,2]. Specifically, this relation can be explained by the concept of the off-diagonal-long-range-order(ODLRO) introduced by O. Penrose[12], L. Onsager[13], and C.N. Yang[14].

In terms of conventional approaches for superfluids, we can raise the macroscopic and microscopic theories for superfluids, respectively. As the macroscopic theory for superfluids, the two-fluid model[15,16], which is externalism and known as the theory that regards superfluids as the system consisting of the superfluid (non-viscosity) and normal fluid (viscosity) components, is used for the description of the macroscopic behavior of superfluids. On the other hand, as for the microscopic theory for superfluids, the Gross-Pitaevskii(GP)[17-19] and Bogoliubov[20,21] theories have been used for the research of superfluids in terms of the microscopic surface. The GP theory is the approach that considers the delta function model as the weakly boson-boson interaction potential,

$$u(\mathbf{r}, \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}'), \tag{1.1}$$

where $u(\mathbf{r}, \mathbf{r}')$ is the boson-boson interaction potential and g is the positive factor which denotes the strength of their interaction[17,18]. Since the GP theory describes and gives the behavior of the order parameter of the BEC by solving the GP equation[17-19], and since the order parameter of the BEC corresponds to the single-particle state which is occupied by a lot of particles described as the order of the total particle number $O(N)$, we can calculate the density and current-density described by the order parameter of the BEC in the GP theory, which are related to a fluid component that the BEC is caused, i.e, the superfluid component. On the other hand, in general, the many-body wave function of the system in the ground state is approximately described by the multiplication of N set of the order parameter of the BEC(it is generally called the Hartree approximation[62]), so the GP theory, which deals with the order parameter of the BEC, is the theory concerning the ground state of the system. Then, the Bogoliubov theory deals with superfluids in the excited states, which consist of bosons interacting weakly. The Bogoliubov theory applies the quasiparticle description to the excited states of superfluids, specifically, this theory considers that the properties concerning the excited states are given from the excited energy spectrum of the quasiparticle while the properties concerning the ground state are given by solving the GP equation. In this way, the Bogoliubov theory is the approach that we can calculate the density and current-density concerning the excited states by using the excited energy spectrum of the quasiparticle. Also, since the density and current-density concerning the excited states correspond to the remaining component except for the superfluid component concerning the ground state, from the point of view of the two-fluid model, these physical quantities concerning the excited states correspond to those of the normal fluid component. Thus, the Bogoliubov theory enables the calculation of the density and current-density of the normal fluid component.

Although we mention some conventional theories for superfluids in the above, there are also some problems to be solved. In the GP and Bogoliubov theories, as mentioned in equation (1.1), the boson-boson interaction is assumed as the delta function model, and it leaves room for improvement. The real system as superfluids, for example, the liquid helium-4, is constituted by bosons interacting strongly. Indeed, some experimental results for the liquid helium-4 cannot be described by using the GP or Bogoliubov theories[22,23]. Moreover, the simultaneous treatment of the superfluid and normal fluid components cannot be done in these conventional theories. Thus, it would be convenient if we could describe physical quantities such as the density and current-density of the superfluid and normal fluid components simultaneously.

On the other hand, concerning the fermion system, the density functional theory(DFT)[24,25] and its extensions[26-35] have been used for the investigation of the electronic and magnetic properties of some materials. DFT deals with many-electrons systems in which they interact. Particularly, DFTs for superconductors, in which $U(1)$ gauge symmetry breaking emerges, have been also developed at present[36-43]. Also, the order parameter for superconductors has been discussed, and there are several types of DFTs developed so far[42,43]. In addition, as for the fermionic superfluids, work like the superfluid local density approximation has been also developed based on DFT[44-47].

1.2 Proposal of the current-density functional theory for bosonic superfluids

In this paper, we propose the current-density functional theory for bosonic superfluids(sf-CDFT) which enables the simultaneous treatment of the superfluid and normal fluid components. In our theory, the particle number density, current-density, and the order parameter of the BEC are chosen as reproduced basic variables. The paper on this theory is organized as follows: In Chapter 2, we first introduce conventional theories for superfluids such as the two-fluid model, the GP and Bogoliubov theories. In Chapter 3, let us explain the finite temperature density functional theory(FTDFT) for the electron system in the thermal equilibrium state, which is supposed to be applied to develop sf-CDFT. In the crucial Chapter 4, we propose sf-CDFT. In this chapter, similar to DFT or FTDFT, we first prove that the extension of the Hohenberg-Kohn(HK) theorem is established. HK theorem can be divided into two theorems, the first one is that basic variables, external potentials, and the density matrix in the thermal equilibrium state are in one-to-one correspondence, and another one is that the variational principle concerning a functional of basic variables can be proved. Next, we introduce the non-interaction reference system similar to DFT or FTDFT, and there we can derive two single-particle equations called the Gross-Pitaevskii-Kohn-Sham(GPKS) and Kohn-Sham(KS) equations using this HK theorem. It is shown that the particle number density and current-density of the superfluid component can be calculated by the solution of the GPKS equation while those of the normal fluid one can be calculated by solutions of the KS equation. After these formulations, in Chapter 5, we discuss sf-CDFT. In the first section, we derive the sum rule for the exchange-correlation(xc) energy functional defined in sf-CDFT, and then from the next section, we start to compare sf-CDFT with conventional theories for superfluids raised in the above. In this discussion, we can find some interesting features, particularly, we can show that sf-CDFT reproduces the particle number density and current-dnsity of the superfluid and normal fluid components simultaneously while incorporating the effect of the interaction between the superfluid and normal fluid components. In the final Chapter 6, we present the conclusion of this paper.

Chapter 2

Conventional theories for superfluids

In this chapter, we briefly summarize several theories for superfluids which are known conventionally. In section 2.1, we first introduce the two-fluid model[15,16] which is externalism describing the macroscopic properties of superfluids, in this model superfluid(non-viscous fluid) and normal fluid(viscous fluid) are introduced as components constituting superfluids. In section 2.2, we summarize the definition of the order parameter of the BEC[12,13], which provides the particle number density and current-density of the superfluid component. Sections 2.3 and 2.4 give two microscopic conventional theories for superfluids respectively. In section 2.3, the Gross-Pitaevskii theory[17-19], which gives the equation the order parameter of the BEC follows, is introduced and this theory describes the behavior of the superfluid. Then, in section 2.4, the Bogoliubov theory[20,21] that describes the excited states of superfluids is introduced and this theory enables us to describe the properties of the normal fluid.

2.1 Two-fluid model

The two-fluid model, which describes the macroscopic behavior of superfluids, was proposed by L. Tisza and L.D. Landau[15,16]. In this model, if we write the phase transition temperature of the BEC like T_c, superfluids under the condition of $T < T_c$ are considered that they consist of two fluid components called the superfluid and the normal fluid, respectively. The superfluid is the non-viscous fluid while the normal fluid is the viscous one, and it is known that each fluid moves independently when its fluid velocity is very small. However, when their fluid velocity become large, it is also known that the quantum vortex is generated in the superfluid and two fluid components interact with each other through the quantum vortex[63]. In this section, we first describe the case of two fluid components moving independently, and after that, we will discuss the case they interact with each other.

First, we consider superfluids in the stationary state. Now let us write the particle number density of the superfluid like $n_{\rm sf}(\mathbf{r})$, and also the one of the normal fluid like $n_{\rm nf}(\mathbf{r})$. In addition, we write the fluid velocity of the superfluid like $\boldsymbol{v}_{\rm sf}(\mathbf{r})$, and also the one of the normal fluid like $\boldsymbol{v}_{\rm nf}(\mathbf{r})$. In this case, the total density $n(\mathbf{r})$ and the total current-density $\boldsymbol{j}(\mathbf{r})$ are described as

$$n(\mathbf{r}) = n_{\rm sf}(\mathbf{r}) + n_{\rm nf}(\mathbf{r}), \tag{2.1}$$

$$\boldsymbol{j}(\mathbf{r}) = n_{\rm sf}(\mathbf{r})\boldsymbol{v}_{\rm sf}(\mathbf{r}) + n_{\rm nf}(\mathbf{r})\boldsymbol{v}_{\rm nf}(\mathbf{r}). \tag{2.2}$$

The particle number density and the current-density of the superfluid $n_{\rm sf}(\mathbf{r})$ and $n_{\rm sf}(\mathbf{r})\boldsymbol{v}_{\rm sf}(\mathbf{r})$ are calculated by using the order parameter of the BEC, which is explained in next section, and concerning the normal fluid, it is known that $n_{\rm nf}(\mathbf{r})$ and $n_{\rm nf}(\mathbf{r})\boldsymbol{v}_{\rm nf}(\mathbf{r})$ are given by the quasiparticle description. As regards this, we will describe in section 2.4. In this section, we next show the continuity equation related to $n(\mathbf{r})$ and $\boldsymbol{j}(\mathbf{r})$ below.

Now we consider superfluids in which the current-density $\boldsymbol{j}(\mathbf{r})$ occurs and in this case, a vector potential $\boldsymbol{A}(\mathbf{r})$, which is considered the fictitious potential that appears when we are in the rotational coordinate system which is related with the current-density $\boldsymbol{j}(\mathbf{r})$, exists. In detail, we will discuss the derivation of this potential in Appendix A, so here we only mention the formula of this potential. Now, we are in the rotational coordinate system which moves with $\boldsymbol{j}(\mathbf{r})$, and when we write the position vector of this coordinate system $\mathbf{r}$, and the angular velocity vector concerning $\boldsymbol{j}(\mathbf{r})$ like $\boldsymbol{\omega}$, then we can describe the formula of a vector potential $\boldsymbol{A}(\mathbf{r})$ as

$$\boldsymbol{A}(\mathbf{r}) = -m\boldsymbol{\omega} \times \mathbf{r}, \tag{2.3}$$

where m is the mass of a particle constituting superfluids, and here $\boldsymbol{\omega}$ is the vector in the direction of the z-axis like (0, 0, ω). Therefore, due to the addition of the term that is proportional to $\boldsymbol{A}(\mathbf{r})$, the total density $n(\mathbf{r})$ and the total current-density $\boldsymbol{j}(\mathbf{r})$ follow the continuity equation as

$$\nabla \cdot (\boldsymbol{j}(\mathbf{r}) + n(\mathbf{r})\boldsymbol{A}(\mathbf{r})/m) = 0, \tag{2.4}$$

Next, we discuss the case that two fluid components interact with each other. As the history of the experimental research for hydrodynamic properties of superfluids such as the liquid helium-4, research for the thermal counterflow in superfluids is one of the most attractive studies[64]. The thermal counterflow is the flow that the superfluid and normal fluid components flow in the opposite direction respectively, and this flow is caused by the inflow of the heat. The experimental situation is described in Fig.2.1.

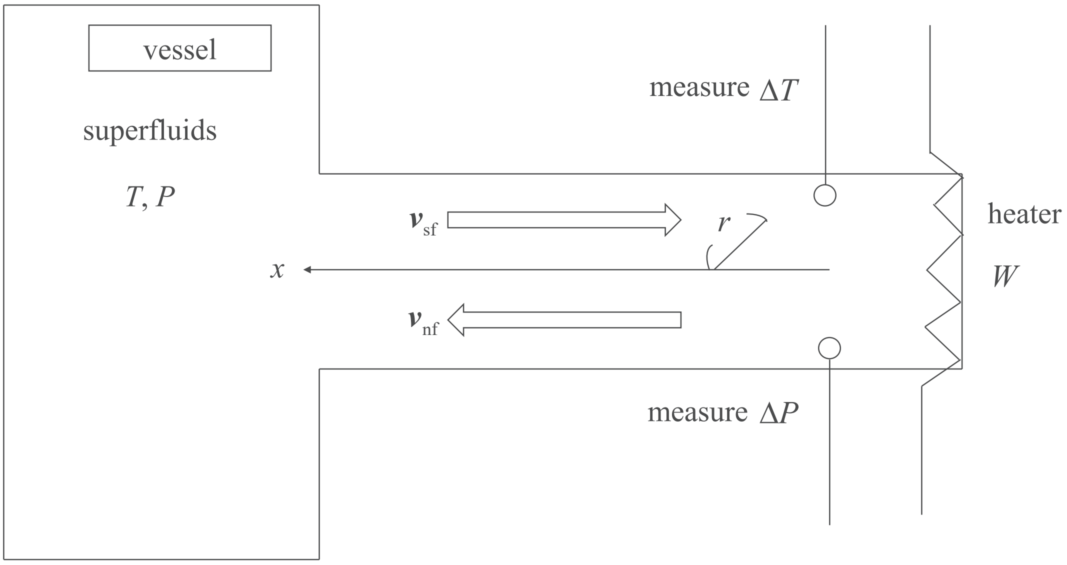

Fig. 2.1: The experiment of the thermal counterflow

Now, we consider superfluids such as the liquid helium(its temperature and pressure are T, P) in the thermal equilibrium state in the above vessel(the axis of the center of the vessel is x, and the radius of the vessel is a), and here we add the heat per unit of time W from the heater. This heat makes the changes of temperature and pressure like ΔT, ΔP from initial values, and the flow velocities of the superfluid and normal fluid components $\boldsymbol{v}_{\mathrm{sf}}(\mathbf{r}, t)$ and $\boldsymbol{v}_{\mathrm{nf}}(\mathbf{r}, t)$, also the gradients of temperature and pressure ∇T and ∇P are produced along the axis-x. In this way, the non-equilibrium state that the superfluid and normal fluid flow respectively realizes in superfluids, and after enough time passes, the state of the system becomes the thermal equilibrium state again(its temperature and pressure are $T + \Delta T$ and $P + \Delta P$). Under this process, the hydrodynamic equations of motion concerning the superfluid and normal fluid flow velocities $\boldsymbol{v}_{\mathrm{sf}}(\mathbf{r}, t)$ and $\boldsymbol{v}_{\mathrm{nf}}(\mathbf{r}, t)$ are described respectively,

$$n_{\rm sf}[\frac{\partial}{\partial t}\boldsymbol{v}_{\rm sf} + (\boldsymbol{v}_{\rm sf}\cdot\nabla)\boldsymbol{v}_{\rm sf}] = -\frac{n_{\rm sf}}{n}\nabla P + sn_{\rm sf}\nabla T, \tag{2.5}$$

$$n_{\rm nf}[\frac{\partial}{\partial t}\boldsymbol{v}_{\rm nf} + (\boldsymbol{v}_{\rm nf}\cdot\nabla)\boldsymbol{v}_{\rm nf}] = -\frac{n_{\rm nf}}{n}\nabla P - sn_{\rm sf}\nabla T + \eta_{\rm nf}\nabla^2\boldsymbol{v}_{\rm nf}, \tag{2.6}$$

where in equations (2.5) and (2.6), we omitted arguments of $\mathbf{r}$ and t to make these equations simple, and s is the entropy density per unit of mass of superfluids, and the coefficient $\eta_{\rm nf}$ denotes the viscosity of the normal fluid component. As seen in terms described by the gradient of T in (2.5) and (2.6), the normal fluid flows in the direction from a high-temperature area to a low-temperature area, while the superfluid component flows in the opposite direction. Since this vessel is closed and there is no additional source or sink in superfluids, the thermal counterflow that the total current-density $\boldsymbol{j}(\mathbf{r}, t)$ is zero occurs in superfluids. In the process of the state change of the system, we first focus on the superfluid component. In the thermal equilibrium state after the non-equilibrium state that the thermal counterflow occurs, the superfluid flows stationarily and the relation between the gradient of temperature and that of pressure written as

$$\nabla P = sn\nabla T \tag{2.7}$$

is derived from the equation (2.5). Since we are considering the flow and gradient in the direction of the x-axis, from now on let us write the dependence of x in the above equations. In short, the equation (2.7) is rewritten as

$$\frac{dP}{dx} = sn\frac{dT}{dx}. \tag{2.8}$$

On the other hand, next, we consider the normal fluid component. When the heat W is small and the relative velocity between the superfluid and normal fluid components is small, we can consider the Hagen-Poiseuille(or Poiseuille) flow as the normal fluid flow. In this case, the flow velocity of the normal fluid $\boldsymbol{v}_{\rm nf}$ is the velocity of the Hagen-Poiseuille flow which depends on the distance r from the central axis-x and the solution of equation (2.6) can be obtained as

$$v_{\rm nf}(r) = -\frac{a^2}{4\eta_{\rm nf}}(1 - \frac{r^2}{a^2})\frac{dP}{dx}. \tag{2.9}$$

Thus, the mean flow velocity at the cross-section of the vessel $\bar{v}_{\rm nf}$ is calculated as

$$\bar{v}_{\rm nf} = \frac{1}{\pi a^2}\int_0^a v_{\rm nf}(r)2\pi r dr = -\frac{a^2}{8\eta_{\rm nf}}\frac{dP}{dx} = -\frac{a^2 sn}{8\eta_{\rm nf}}\frac{dT}{dx}, \tag{2.10}$$

here in the last term, we used the equation (2.8). On the other hand, the heat added from the heater is carried by the normal fluid and it flows as the heat energy flow per unit of time and space given by

$$\frac{W}{\pi a^2} = sn\bar{v}_{\mathrm{nf}}T. \tag{2.11}$$

Thus, by equations (2.10) and (2.11), we can derive the following relation,

$$\frac{W}{\pi a^2} = snT\bar{v}_{\mathrm{nf}} = -\frac{(asn)^2 T}{8\eta_{\mathrm{nf}}}\frac{dT}{dx}, \tag{2.12}$$

therefore, the gradient of temperature, i.e., the amount of change concerning temperature ΔT is proportional to the heat energy from the heater W. By the way, in the actual experiment, this amount of change ΔT(or ΔP) is measured. The above relation between ΔT(or ΔP) and W described by (2.12) has been verified in experiments under the condition that the heat W is small[64].

However, in the case that W becomes large, it has been observed that ΔT(or ΔP) does not follow the above relation and the additional term for (2.12) which is proportional to W^3 instead of W occurs[65]. To explain this, C.J. Gorter and J.H. Mellink, scientists who observed this had introduced the mutual friction between the superfluid and normal fluid like $\boldsymbol{F}_{\mathrm{sf-nf}}$ into equations (2.5) and (2.6)[65],

$$n_{\mathrm{sf}}[\frac{\partial}{\partial t}\boldsymbol{v}_{\mathrm{sf}} + (\boldsymbol{v}_{\mathrm{sf}}\cdot\nabla)\boldsymbol{v}_{\mathrm{sf}}] = -\frac{n_{\mathrm{sf}}}{n}\nabla P + sn_{\mathrm{sf}}\nabla T - \boldsymbol{F}_{\mathrm{sf-nf}}, \tag{2.13}$$

$$n_{\mathrm{nf}}[\frac{\partial}{\partial t}\boldsymbol{v}_{\mathrm{nf}} + (\boldsymbol{v}_{\mathrm{nf}}\cdot\nabla)\boldsymbol{v}_{\mathrm{nf}}] = -\frac{n_{\mathrm{nf}}}{n}\nabla P - sn_{\mathrm{sf}}\nabla T + \eta_{\mathrm{nf}}\nabla^2\boldsymbol{v}_{\mathrm{nf}} + \boldsymbol{F}_{\mathrm{sf-nf}}. \tag{2.14}$$

The mutual friction $\boldsymbol{F}_{\mathrm{sf-nf}}$ can be written as the below by the comparison with results of experiments[65],

$$F_{\mathrm{sf-nf}} \simeq An_{\mathrm{sf}}n_{\mathrm{nf}}(v_{\mathrm{sf}} - v_{\mathrm{nf}})^3, \tag{2.15}$$

where A is the function of temperature(When we consider (2.15) as the form of the mutual friction and follow the similar way mentioned above using equations (2.13) and (2.14), we can indicate that the additional term mentioned above is proportional to W^3). Besides, H.E. Hall and W.F. Vinen have shown that this mutual friction is related to the interaction between the normal fluid and the quantum vortex caused in the superfluid[63]. In their discussion, the concept of the motion of the vortex filament has been used to explain the mutual friction.

2.2 Order parameter of the BEC

In this section, we briefly describe the definition of the order parameter of the BEC when bosons interact with each other, proposed by O. Penrose[12] and L. Onsager[13]. BEC, which is the phase transition phenomenon caused in the boson system, is essential to understand the superfluidity, and it is well known that we can define the BEC by using the single-particle state description described by wave functions of plane waves when bosons do not interact. However, when bosons interact with each other, we cannot simply use this description for the definition of the BEC. Therefore, as explained below, the definition of the BEC when bosons interact was proposed by using the concept of the one-particle reduced density matrix.

First, we consider the one-particle reduced density matrix $\rho_1(\mathbf{r}, \mathbf{r}')$ defined as

$$\rho_1(\mathbf{r}, \mathbf{r}') \triangleq \left\langle \Psi \middle| \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') \middle| \Psi \right\rangle, \tag{2.16}$$

where $\hat{\psi}^\dagger(\mathbf{r})$, $\hat{\psi}(\mathbf{r})$ are field operators for bosons, and $|\Psi\rangle$ is the state vector of the N particles system. As the above definition, $\rho_1(\mathbf{r}, \mathbf{r}')$ is the probability amplitude that the state of the system $|\Psi\rangle$ stays as it was when a particle at $\mathbf{r}'$ is deleted and a particle at $\mathbf{r}$ is created. Here $\rho_1(\mathbf{r}, \mathbf{r}')$ is obviously the Hermite matrix, and this matrix can conduct the spectral decomposition by using its eigenvalues and eigenfunctions as

$$\rho_1(\mathbf{r}, \mathbf{r}') = \sum_i N_i u_i^*(\mathbf{r}) u_i(\mathbf{r}'), \tag{2.17}$$

where N_i is the eigenvalue of $\rho_1(\mathbf{r}, \mathbf{r}')$ for the single-particle state i, and $u_i(\mathbf{r})$ is the eigenfunction of $\rho_1(\mathbf{r}, \mathbf{r}')$ for i. Concerning the derivation of the equation (2.6), we proved this in Appendix B. Here, let us show that the eigenvalue N_i of $\rho_1(\mathbf{r}, \mathbf{r}')$ is the occupation number for the single-particle state i below.

First, taking into consideration the definition of $\rho_1(\mathbf{r}, \mathbf{r}')$ given by the equation (2.16), when $\mathbf{r}$ equals $\mathbf{r}'$, the one-particle reduced density matrix equals the particle number density which is the expectation value of the particle number density operator given by

$$\hat{n}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}), \tag{2.18}$$

then we write the particle number density like $n(\mathbf{r})$, and describe

$$\rho_1(\mathbf{r}, \mathbf{r}) = \left\langle \Psi \middle| \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \middle| \Psi \right\rangle \equiv n(\mathbf{r}). \tag{2.19}$$

On the other hand, by the equation (2.17),

$$\rho_1(\mathbf{r},\mathbf{r}) = \sum_i N_i |u_i(\mathbf{r})|^2, \tag{2.20}$$

so compare equations (2.19) and (2.20),

$$n(\mathbf{r}) = \sum_i N_i |u_i(\mathbf{r})|^2, \tag{2.21}$$

here integrate both hand sides of equation (2.21) concerning $\mathbf{r}$, and consider

$$N = \int n(\mathbf{r}) d\mathbf{r}, \tag{2.22}$$

therefore,

$$N = \sum_i N_i \int |u_i(\mathbf{r})|^2 d\mathbf{r} = \sum_i N_i, \tag{2.23}$$

where we considered that eigenfunctions of $\rho_1(\mathbf{r},\mathbf{r}')$ were normalized. As equation (2.23), the eigenvalue N_i of $\rho_1(\mathbf{r},\mathbf{r}')$ is the occupation number for the single-particle state i.

Now we define the BEC in the system consisting of interacting bosons that the BEC is caused when the eigenvalue of $\rho_1(\mathbf{r},\mathbf{r}')$ for the one single-particle state (here we write it as $i = 0$) is $O(N)$, and the others($i \neq 0$) are $O(1)$. At this time, let us rewrite the equation (2.17) as

$$\rho_1(\mathbf{r},\mathbf{r}') = \sum_i N_i u_i^*(\mathbf{r}) u_i(\mathbf{r}') = N_0 u_0^*(\mathbf{r}) u_0(\mathbf{r}') + \sum_{i\neq 0} N_i u_i^*(\mathbf{r}) u_i(\mathbf{r}'), \tag{2.24}$$

where in equation (2.24), we divided the term of the sum for i into two terms which are the term of $i = 0$ and the others $i \neq 0$. Here eigenfunctions $u_0(\mathbf{r})$ and $u_i(\mathbf{r})$ are about the order of $V^{-1/2}$(V is the volume of the system) due to the normalization of the wave function, and when the BEC is caused, eigenvalues N_0 and N_i are written as

$$N_0 = O(N), N_i = O(1) (i \neq 0), \tag{2.25}$$

at this time, we take the limit $|\mathbf{r} - \mathbf{r}'| \to \infty$ which is equivalent to the thermodynamic limit $N \to \infty, V \to \infty$ keeping N/V constantly concerning both hand sides of equation (2.24), then we obtain

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho_1(\mathbf{r},\mathbf{r}') = N_0 u_0^*(\mathbf{r}) u_0(\mathbf{r}'). \tag{2.26}$$

Eq. (2.26) is the formula representing the condition that the BEC is caused, and it is said that the system has the off-diagonal long-range order (ODLRO). Here, we rewrite the right-hand side of equation (2.26) by using

$$\psi(\mathbf{r}) \triangleq \sqrt{N_0} u_0(\mathbf{r}), \tag{2.27}$$

then the equation (2.26) is

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho_1(\mathbf{r},\mathbf{r}') = \psi^*(\mathbf{r}) \psi(\mathbf{r}'). \tag{2.28}$$

On the other hand, about the equation (2.16), we apply the cluster decomposition principle,

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho_1(\mathbf{r},\mathbf{r}') = \left\langle \Psi \middle| \hat{\psi}^\dagger(\mathbf{r}) \middle| \Psi \right\rangle \left\langle \Psi \middle| \hat{\psi}(\mathbf{r}') \middle| \Psi \right\rangle, \tag{2.29}$$

therefore, we obtain

$$\psi(\mathbf{r}) = \sqrt{N_0} u_0(\mathbf{r}) = \left\langle \Psi \middle| \hat{\psi}(\mathbf{r}) \middle| \Psi \right\rangle \tag{2.30}$$

$$\psi^*(\mathbf{r}) = \sqrt{N_0} u_0^*(\mathbf{r}) = \left\langle \Psi \middle| \hat{\psi}^\dagger(\mathbf{r}) \middle| \Psi \right\rangle. \tag{2.31}$$

$\psi(\mathbf{r})$ is the order parameter of the BEC, also known as the macroscopic wave function, and the space integral of $|\psi(\mathbf{r})|^2$ gives the total particle number for the single-particle state $i = 0$, which is the state the BEC is caused. When the BEC is caused in the system, bosons whose particle number is macroscopic as $O(N)$ occupy the same single-particle state $i = 0$ described by $\psi(\mathbf{r})$, and therefore these bosons behave like following the same wave function $\psi(\mathbf{r})$.

The order parameter $\psi(\mathbf{r})$ is the crucial parameter that features the BEC, and generally the complex classical field, so we can write $\psi(\mathbf{r})$ by using the amplitude and the phase as

$$\psi(\mathbf{r}) = A(\mathbf{r}) e^{i\theta(\mathbf{r})}, \tag{2.32}$$

where $A(\mathbf{r})$ is the complex amplitude and $\theta(\mathbf{r})$ is the phase of the real number.

Now considering that the space integral of $|\psi(\mathbf{r})|^2$ gives the particle number of bosons occupying the single-particle state $i = 0$,

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = N_0 \int |u_0(\mathbf{r})|^2 d\mathbf{r} = N_0, \tag{2.33}$$

so, as the equation (2.33), we can interpret $|\psi(\mathbf{r})|^2$ as the particle number density concerning the single-particle state that the BEC is caused, therefore, we write this density as $n_0(\mathbf{r})$,

$$|\psi(\mathbf{r})|^2 \triangleq n_0(\mathbf{r}), \tag{2.34}$$

then, from equations (2.21) and (2.23), we obtain

$$\psi(\mathbf{r}) = \sqrt{n_0(\mathbf{r})} e^{i\theta(\mathbf{r})}. \tag{2.35}$$

Where we contained the term of the phase factor into $e^{i\theta(\mathbf{r})}$. In this way, the particle number density concerning the single-particle state that the BEC is caused $n_0(\mathbf{r})$ is the density concerning the state that the superfluidity is caused, therefore, equals the particle number density of the superfluid component $n_{\mathrm{sf}}(\mathbf{r})$. On the other hand, concerning the phase $\theta(\mathbf{r})$ in equation (2.35), it is shown that this phase gives the fluid velocity of the superfluid in a later section.

2.3 Gross-Pitaevskii theory

In this section, we derive the equation that the order parameter of the BEC $\psi(\mathbf{r})$ follows. It is necessary to understand the behavior of the order parameter of the BEC for investigating the properties of the superfluid. Therefore, in this section, we start to discuss the Heisenberg equation of motion that the field operator for bosons follows and aim to derive the equation of motion that the order parameter of the BEC satisfies when bosons weakly interact with each other.

At first, we consider the boson system in which the external field corresponding to the external potential $V_{\mathrm{ext}}(\mathbf{r})$ is applied, and the Hamiltonian of this system $\hat{H}$ is given by

$$\hat{H} = \hat{T} + \hat{V} + \hat{W}, \tag{2.36}$$

where $\hat{T}$, $\hat{V}$ and $\hat{W}$ are the kinetic energy, external potential, and boson-boson interaction operators, respectively, given by

$$\hat{T} = \int \hat{\psi}^\dagger(\mathbf{r})(-\frac{\hbar^2\nabla^2}{2m})\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{2.37}$$

$$\hat{V} = \int \hat{\psi}^\dagger(\mathbf{r})V_{\text{ext}}(\mathbf{r})\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{2.38}$$

$$\hat{W} = \frac{1}{2}\iint \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')u(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})d\mathbf{r}d\mathbf{r}'. \tag{2.39}$$

Here, m is the mass of the boson, $u(\mathbf{r},\mathbf{r}')$ denotes the boson-boson interaction potential.
Then, we consider the grand canonical Hamiltonian which is used in the method of the grand canonical ensemble given by

$$\hat{K} \triangleq \hat{H} - \mu\hat{N}, \tag{2.40}$$

where μ is the chemical potential and $\hat{N}$ is the total particle number operator given by

$$\hat{N} = \int \hat{n}(\mathbf{r})d\mathbf{r}. \tag{2.41}$$

To deal with the case that bosons weakly interact, here we consider the potential which is described by the delta function as $u(\mathbf{r},\mathbf{r}')$,

$$u(\mathbf{r},\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}'), \tag{2.42}$$

where g is the positive constant that denotes the strength of the boson-boson interaction. It is known that this description does not function well concerning the liquid helium, but not the dilute Bose gas.

Under this description, the operator $\hat{K}$ is described as

$$\hat{K} = \int \hat{\psi}^\dagger(\mathbf{r})(-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) - \mu)\hat{\psi}(\mathbf{r})d\mathbf{r} + \frac{g}{2}\int \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})d\mathbf{r}. \tag{2.43}$$

Next, concerning $\hat{K}$, we consider the Heisenberg equation of motion below,

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) = [\hat{\psi}(\mathbf{r},t),\hat{K}], \tag{2.44}$$

where $\hat{\psi}(\mathbf{r},t)$ is the field operator for bosons which is described by the Heisenberg picture as,

$$\hat{\psi}(\mathbf{r},t) = e^{i\frac{\hat{K}}{\hbar}t}\hat{\psi}(\mathbf{r})e^{-i\frac{\hat{K}}{\hbar}t}. \tag{2.45}$$

Substitute equation (2.43) into (2.44), and proceed the calculation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) &= [\hat{\psi}(\mathbf{r},t), \int \hat{\psi}^\dagger(\mathbf{r}')(-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}') - \mu)\hat{\psi}(\mathbf{r}')d\mathbf{r}'] \\ &+ [\hat{\psi}(\mathbf{r},t), \frac{g}{2}\int \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}')d\mathbf{r}'] \end{aligned} \tag{2.46}$$

here we use the following formula of the commutation relation,

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}], \tag{2.47}$$

moreover, we consider the commutation relation of field operators for bosons as,

$$[\hat{\psi}(\mathbf{r},t), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}'), \tag{2.48}$$

$$[\hat{\psi}(\mathbf{r},t), \hat{\psi}(\mathbf{r}')] = 0, \tag{2.49}$$

$$[\hat{\psi}^\dagger(\mathbf{r},t), \hat{\psi}^\dagger(\mathbf{r}')] = 0. \tag{2.50}$$

Then, by using equations from (2.47) to (2.50), we can derive the following equation,

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) = (-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\mathbf{r}) - \mu)\hat{\psi}(\mathbf{r},t) + g\hat{\psi}^\dagger(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t). \tag{2.51}$$

Here, we consider that we expand the field operator (2.45) by using eigenfunctions of the one-particle reduced density matrix as

$$\hat{\psi}(\mathbf{r},t) = \sum_i u_i(\mathbf{r})\hat{a}_i(t), \tag{2.52}$$

where, $\hat{a}_i(t)$ is the annihilation operator of bosons for the eigenfunction of the one-particle reduced density matrix $u_i(\mathbf{r})$, which is described by the Heisenberg picture. This operator of bosons satisfies the following commutation relation,

$$[\hat{a}_i(t), \hat{a}_j^\dagger(t)] = \delta_{i,j}, \tag{2.53}$$

$$[\hat{a}_i(t), \hat{a}_j(t)] = 0, \tag{2.54}$$

$$[\hat{a}_i^\dagger(t), \hat{a}_j^\dagger(t)] = 0. \tag{2.55}$$

Now, we divide the right-hand side of equation (2.52) into two terms which are respectively the term that the BEC is caused and others like

$$\hat{\psi}(\mathbf{r}, t) = u_0(\mathbf{r})\hat{a}_0(t) + \sum_{i\neq 0} u_i(\mathbf{r})\hat{a}_i(t). \tag{2.56}$$

Here, we consider the commutation relation of the annihilation and creation operators $\hat{a}_0(t)$ and $\hat{a}_0^\dagger(t)$ as

$$[\hat{a}_0(t), \hat{a}_0^\dagger(t)] = \hat{a}_0(t)\hat{a}_0^\dagger(t) - \hat{a}_0^\dagger(t)\hat{a}_0(t) = 1, \tag{2.57}$$

therefore,

$$\hat{a}_0(t)\hat{a}_0^\dagger(t) = \hat{a}_0^\dagger(t)\hat{a}_0(t) + 1, \tag{2.58}$$

here, concerning both hand sides of equation (2.58), we calculate the expectation by using eigenfunctions of the one-particle reduced density matrix as bases for the trace,

$$\langle \hat{a}_0(t)\hat{a}_0^\dagger(t)\rangle = \langle \hat{a}_0^\dagger(t)\hat{a}_0(t)\rangle + 1 = N_0(t) + 1, \tag{2.59}$$

where, the notation $\langle \cdots \rangle$ means the expectation by using eigenfunctions of the one-particle reduced density matrix as bases for the trace, and $N_0(t)$ is the expectation of the occupation particle number concerning the state that the BEC is caused. When the BEC is caused, $N_0(t)$ is macroscopic like $O(N)$, and 1 is too small compared with $N_0(t)$, therefore, we rewrite the equation (2.59) as

$$\langle \hat{a}_0(t)\hat{a}_0^\dagger(t)\rangle = \langle \hat{a}_0^\dagger(t)\hat{a}_0(t)\rangle + 1 \approx N_0(t) = \langle \hat{a}_0^\dagger(t)\hat{a}_0(t)\rangle, \tag{2.60}$$

then,

$$\langle \hat{a}_0(t)\hat{a}_0^\dagger(t)\rangle = \langle \hat{a}_0^\dagger(t)\hat{a}_0(t)\rangle = N_0(t). \tag{2.61}$$

Eq. (2.61) means that we ignore the non-commutativity of $\hat{a}_0(t)$ and $\hat{a}_0^\dagger(t)$ and in this case, it follows that we consider these operators as the classical number,

$$\hat{a}_0(t) = \hat{a}_0^\dagger(t) = \sqrt{N_0(t)}. \tag{2.62}$$

Here, we omitted the phase factor of $\hat{a}_0(t)$ and $\hat{a}_0^\dagger(t)$ in equation (2.62).
Therefore, we apply this approximation that the first term in the right-hand side of equation (2.56) becomes the classical field, equation (2.56) is

$$\hat{\psi}(\mathbf{r}, t) = \sqrt{N_0(t)}u_0(\mathbf{r}) + \sum_{i\neq 0} u_i(\mathbf{r})\hat{a}_i(t). \tag{2.63}$$

Here, we consider equations (2.27) and (2.30), and we can describe equation (2.63) as

$$\hat{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) + \sum_{i\neq 0} u_i(\mathbf{r})\hat{a}_i(t). \tag{2.64}$$

Eq. (2.64) means the description that we represent the field operator for bosons by the sum of the term of the order parameter of the BEC, which is the expectation of the field operator, and another term of the fluctuation around the order parameter, which is described by the difference between the field operator and the order parameter. Here, when we ignore this fluctuation term, the field operator equals the order parameter of the BEC, and then we can derive the following equation from equations (2.51) and (2.64),

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = (-\frac{\hbar^2\nabla^2}{2m} + V_{\mathrm{ext}}(\mathbf{r}) - \mu)\psi(\mathbf{r}, t) + g|\psi(\mathbf{r}, t)|^2\psi(\mathbf{r}, t). \tag{2.65}$$

This equation (2.65) is called the Gross-Pitaevskii(GP) equation[17-19]. When the temperature $T = 0$, i.e, the state of superfluids is the ground state, it is theoretically considered that all particles occupy one single-particle state described by $\psi(\mathbf{r}, t)$ due to without the Pauli exclusion principle, so in this case, the ground state of superfluids is the state of the system that the BEC is caused, and its state is given by the order parameter of the BEC $\psi(\mathbf{r}, t)$. So, the GP theory describes the ground state of superfluids.

The stationary solution of the equation (2.65) $\psi(\mathbf{r})$ is also given by the same calculation procedure,

$$(-\frac{\hbar^2\nabla^2}{2m}+V_{\mathrm{ext}}(\mathbf{r})-\mu)\psi(\mathbf{r})+g|\psi(\mathbf{r})|^2\psi(\mathbf{r})=0. \tag{2.66}$$

The time-dependent GP equation describes the time evolution of the order parameter of the BEC $\psi(\mathbf{r},t)$, and it is known that this GP equation is useful for dealing with the dilute Bose gas although it is not appropriate for the liquid helium because particles constituting the liquid helium interact strongly.

Next, we derive the continuity equation which the particle number density of the superfluid component satisfies. First, we take the complex conjugate of the equation which is the multiplication of the GP equation (2.65) and the order parameter of the BEC and subtract its original one from the conjugate equation, then we can get

$$\frac{\partial}{\partial t}|\psi(\mathbf{r},t)|^2+\frac{\hbar}{2mi}\nabla\cdot(\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t)-\psi(\mathbf{r},t)\nabla\psi^*(\mathbf{r},t))=0, \tag{2.67}$$

here, we use equation (2.34) and define as

$$\boldsymbol{j}_0(\mathbf{r},t)\triangleq\frac{\hbar}{2mi}(\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t)-\psi(\mathbf{r},t)\nabla\psi^*(\mathbf{r},t)), \tag{2.68}$$

therefore, we can describe equation (2.67) as

$$\frac{\partial}{\partial t}n_0(\mathbf{r},t)+\nabla\cdot\boldsymbol{j}_0(\mathbf{r},t)=0, \tag{2.69}$$

this equation (2.69) is the continuity equation concerning $n_0(\mathbf{r},t)$ and $\boldsymbol{j}_0(\mathbf{r},t)$, and we can interpret that $\boldsymbol{j}_0(\mathbf{r},t)$ is the particle number current-density by equation (2.68).

Next, we substitute equation (2.35) into equation (2.68), and then we can describe the current-density as

$$\boldsymbol{j}_0(\mathbf{r},t)=n_0(\mathbf{r},t)\frac{\hbar}{m}\nabla\theta(\mathbf{r},t), \tag{2.70}$$

in this way, we define the fluid velocity of the superfluid component $\boldsymbol{v}_0(\mathbf{r},t)$ as

$$\boldsymbol{v}_0(\mathbf{r},t)=\frac{\hbar}{m}\nabla\theta(\mathbf{r},t). \tag{2.71}$$

The velocity $\boldsymbol{v}_0(\mathbf{r}, t)$ is described by the phase of the order parameter of the BEC.

On the other hand, we substitute the equation (2.35) into the GP equation (2.65), and then focus on the real part of this equation, we can get the following equation as a result,

$$m\frac{\partial}{\partial t}\boldsymbol{v}_0(\mathbf{r}, t) = -\nabla(gn_0(\mathbf{r}, t) + V_{\mathrm{ext}}(\mathbf{r}) - \mu + P_0(\mathbf{r}, t) + \frac{1}{2}m(\boldsymbol{v}_0(\mathbf{r}, t))^2), \tag{2.72}$$

where, $P_0(\mathbf{r}, t)$ is defined as

$$P_0(\mathbf{r}, t) \triangleq -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n_0(\mathbf{r}, t)}}{\sqrt{n_0(\mathbf{r}, t)}}. \tag{2.73}$$

This equation (2.72) is called the Euler equation concerning the superfluid component, and the fourth term on the right-hand side of the equation (2.72) is called the quantum pressure term, which contains the effect of the quantum mechanical correction. In general, if the spatial change of $n_0(\mathbf{r}, t)$ is mild, we can ignore this quantum pressure term.

2.4 Bogoliubov theory

The GP equation, which was discussed in the former section, is derived from the way that in equation (2.64) we approximate the field operator for bosons as the classical field, i.e., the order parameter of the BEC $\psi(\mathbf{r}, t)$. Additional to this theory which uses the GP equation, i.e., the theory of the ground state of superfluids, the theory that it describes the excited states of superfluids by the quasiparticle description was developed by N.N. Bogoliubov[20]. His method starts from the step in which we describe the field operator for bosons as the sum of the order parameter of the BEC $\psi(\mathbf{r}, t)$ and its fluctuation term $\tilde{\hat{\psi}}(\mathbf{r}, t)$, and substitutes it into the Hamiltonian of the system given by equation (2.36), then ignores higher terms than $O(\tilde{\hat{\psi}}^2)$. After that, we can get the formula of the Hamiltonian, which is described by the zeroth, first and second-order terms of $\tilde{\hat{\psi}}(\mathbf{r}, t)$, but actually, we can drop the first-order term of $\tilde{\hat{\psi}}(\mathbf{r}, t)$ due to the GP equation. Therefore, after this, we apply the Bogoliubov transformation to $\tilde{\hat{\psi}}(\mathbf{r}, t)$ and describe the excited states of superfluids by the quasiparticle description. In this section, we explain this procedure below.

To make the discussion simple, first we consider the situation that the superfluid component flows by the fluid velocity $\boldsymbol{v}_0$, i.e., its velocity does not depend on the time and position vector. In addition, in terms of the particle number density of the superfluid, we also consider the case that n_0 does not depend on the time and position vector(Namely, we here consider the homogeneous superfluid system). These situations correspond with the case that the order parameter of the BEC is written as

$$\psi(\mathbf{r}) = \sqrt{n_0} e^{i\theta(\mathbf{r})}, \tag{2.74}$$

therefore, it follows that we consider the stationary state and the case that the stationary current occurs in superfluids.
The solution of the GP equation under the above situation is given by

$$\mu = gn_0 + \frac{1}{2} m \boldsymbol{v}_0^2, \tag{2.75}$$

$$\psi(\mathbf{r}) = \sqrt{n_0} e^{i \frac{m}{\hbar} \boldsymbol{v}_0 \cdot \mathbf{r}}. \tag{2.76}$$

Where we considered $V_{\text{ext}}(\mathbf{r}) = 0$. Next, we consider the fluctuation operators $\tilde{\hat{\psi}}(\mathbf{r}, t)$ and $\tilde{\hat{\psi}}^{\dagger}(\mathbf{r}, t)$. Now we expand these operators by the plane wave function as the bases like

$$\tilde{\hat{\psi}}(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k} \neq \mathbf{0}} e^{i(\frac{m}{\hbar} \boldsymbol{v}_0 + \mathbf{k}) \cdot \mathbf{r}} \hat{a}_{\mathbf{k}}(t). \tag{2.77}$$

Where concerning the wave number index of the sum **k**, we eliminated the term $\mathbf{k} = \mathbf{0}$ which corresponds with the order parameter of the BEC (2.76) to avoid the double count of this term when we consider the field operator for bosons. And here, we considered the annihilation operator which deletes one boson having the wave number **k** as $\hat{a}_{\mathbf{k}}(t)$.(V is the volume of the system.)

Now, let us consider that we can write the grand canonical Hamiltonian as equation (2.43) in the system constituting bosons interacting weakly like equation (2.42), and substitute

$$\hat{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}) + \tilde{\hat{\psi}}(\mathbf{r}, t) \tag{2.78}$$

into this Hamiltonian, then we can get

$$
\begin{aligned}
\hat{K} &= K_0 + \hat{K}_1 + \hat{K}_2, && (2.79)\\
K_0 &= \int \psi^*(\mathbf{r})\hat{h}\psi(\mathbf{r})d\mathbf{r} + \frac{g}{2}\int |\psi(\mathbf{r})|^4 d\mathbf{r}, && (2.80)\\
\hat{K}_1 &= \int (\hat{h} + g|\psi(\mathbf{r})|^2)\psi^*(\mathbf{r})\tilde{\hat{\psi}}(\mathbf{r},t)d\mathbf{r} + \int (\hat{h} + g|\psi(\mathbf{r})|^2)\psi(\mathbf{r})\tilde{\hat{\psi}}^\dagger(\mathbf{r},t)d\mathbf{r}, \\
& && (2.81)\\
\hat{K}_2 &= \int (2g|\psi(\mathbf{r})|^2\tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\tilde{\hat{\psi}}(\mathbf{r},t) + \tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\hat{h}\tilde{\hat{\psi}}(\mathbf{r},t) + \frac{g}{2}\psi^*(\mathbf{r})^2\tilde{\hat{\psi}}(\mathbf{r},t)\tilde{\hat{\psi}}(\mathbf{r},t) \\
&\quad + \frac{g}{2}\psi(\mathbf{r})^2\tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\tilde{\hat{\psi}}^\dagger(\mathbf{r},t))d\mathbf{r}, && (2.82)\\
\hat{h} &= -\frac{\hbar^2\nabla^2}{2m} - \mu, && (2.83)
\end{aligned}
$$

where we ignored higher terms than $O(\tilde{\hat{\psi}}^2)$. Then, we focus on the first-order term and find that we can drop this first-order term due to the GP equation like

$$
(\hat{h} + g|\psi(\mathbf{r})|^2)\psi(\mathbf{r}) = 0, \tag{2.84}
$$

therefore, we can get the following result.

$$
\begin{aligned}
\hat{K} &= K_0 + \hat{K}_2, && (2.85)\\
K_0 &= \int \psi^*(\mathbf{r})\hat{h}\psi(\mathbf{r})d\mathbf{r} + \frac{g}{2}\int |\psi(\mathbf{r})|^4 d\mathbf{r}, && (2.86)\\
\hat{K}_2 &= \int (2g|\psi(\mathbf{r})|^2\tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\tilde{\hat{\psi}}(\mathbf{r},t) + \tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\hat{h}\tilde{\hat{\psi}}(\mathbf{r},t) + \frac{g}{2}\psi^*(\mathbf{r})^2\tilde{\hat{\psi}}(\mathbf{r},t)\tilde{\hat{\psi}}(\mathbf{r},t) \\
&\quad + \frac{g}{2}\psi(\mathbf{r})^2\tilde{\hat{\psi}}^\dagger(\mathbf{r},t)\tilde{\hat{\psi}}^\dagger(\mathbf{r},t))d\mathbf{r}. && (2.87)
\end{aligned}
$$

Next, we substitute (2.77) into $\hat{K}_2$ and rewrite this by the creation and annihilation operators $\hat{a}^\dagger_{\mathbf{k}}(t)$, $\hat{a}_{\mathbf{k}}(t)$ like

$$
\hat{K}_2 = \sum_{\mathbf{k}\neq\mathbf{0}}(\epsilon^0_{\mathbf{k}} + \hbar\mathbf{k}\cdot\boldsymbol{v}_0 + gn_0)\hat{a}^\dagger_{\mathbf{k}}(t)\hat{a}_{\mathbf{k}}(t) + \frac{gn_0}{2}\sum_{\mathbf{k}\neq\mathbf{0}}(\hat{a}^\dagger_{\mathbf{k}}(t)\hat{a}^\dagger_{\mathbf{-k}}(t) + \hat{a}_{\mathbf{k}}(t)\hat{a}_{\mathbf{-k}}(t)), \tag{2.88}
$$

where,

$$\epsilon^0_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}. \tag{2.89}$$

Then, next, we introduce the Bogoliubov transformation below to diagonalize the operator $\hat{K}_2$,

$$\hat{A}_{\mathbf{k}} = u_{\mathbf{k}} \hat{a}_{\mathbf{k}} + v_{\mathbf{k}} \hat{a}^{\dagger}_{\text{-}\mathbf{k}} \tag{2.90}$$

$$\hat{A}^{\dagger}_{\text{-}\mathbf{k}} = u_{\mathbf{k}} \hat{a}^{\dagger}_{\text{-}\mathbf{k}} + v_{\mathbf{k}} \hat{a}_{\mathbf{k}}. \tag{2.91}$$

However, we omitted the symbol of the time to avoid making the discussion complex, and we will follow this rule in the below discussion. And here, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the classical numbers that we will determine from now on.

This Bogoliubov transformation is used to diagonalize the Hamiltonian and this is made by using the creation and annihilation operators concerning the quasiparticle $\hat{A}^{\dagger}_{\mathbf{k}}, \hat{A}_{\mathbf{k}}$. First, we can derive the following relational expression by the definition (2.90) and (2.91),

$$u_{\mathbf{k}} = u^*_{\text{-}\mathbf{k}}, v_{\mathbf{k}} = v^*_{\text{-}\mathbf{k}}, \tag{2.92}$$

therefore, as the classical numbers that satisfy (2.92), we opt $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ which are real and even functions of **k**.

Next, we consider the quasiparticle of the excited states of superfluids which describes the Landau energy spectrum[16], then we require the commutation relation for bosons concerning the creation and annihilation operators of quasiparticle,

$$[\hat{A}_{\mathbf{k}}, \hat{A}^{\dagger}_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}, \tag{2.93}$$

$$[\hat{A}_{\mathbf{k}}, \hat{A}_{\mathbf{k}'}] = 0, \tag{2.94}$$

$$[\hat{A}^{\dagger}_{\mathbf{k}}, \hat{A}^{\dagger}_{\mathbf{k}'}] = 0. \tag{2.95}$$

As the appropriate values for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ which satisfy equations from (2.90) to (2.95), we can derive the following relational expression,

$$u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1. \tag{2.96}$$

In this way, let us rewrite equation (2.88) by using $\hat{A}^{\dagger}_{\mathbf{k}}, \hat{A}_{\mathbf{k}}$. By using the relations of (2.90) and (2.91) and calculating carefully, we can derive the following result,

$$\hat{K}_2 = \sum_{\mathbf{k}\neq\mathbf{0}}[(\epsilon^0_{\mathbf{k}} + gn_0)(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) - 2gn_0u_{\mathbf{k}}v_{\mathbf{k}} + \hbar\mathbf{k}\cdot\boldsymbol{v}_0]\hat{A}^\dagger_{\mathbf{k}}\hat{A}_{\mathbf{k}}$$
$$+ \sum_{\mathbf{k}\neq\mathbf{0}}[\frac{gn_0}{2}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) - u_{\mathbf{k}}v_{\mathbf{k}}(\epsilon^0_{\mathbf{k}} + gn_0)](\hat{A}_{\mathbf{k}}\hat{A}_{\text{-}\mathbf{k}} + \hat{A}^\dagger_{\mathbf{k}}\hat{A}^\dagger_{\text{-}\mathbf{k}}) + \tilde{K}_0. \quad (2.97)$$

Where,

$$\tilde{K}_0 = \sum_{\mathbf{k}\neq\mathbf{0}}(\epsilon^0_{\mathbf{k}} + gn_0 + \hbar\mathbf{k}\cdot\boldsymbol{v}_0)v^2_{\mathbf{k}} - gn_0\sum_{\mathbf{k}\neq\mathbf{0}}u_{\mathbf{k}}v_{\mathbf{k}}. \quad (2.98)$$

Then, we summarize such like,

$$\epsilon_{\mathbf{k}} \triangleq (\epsilon^0_{\mathbf{k}} + gn_0)(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) - 2gn_0u_{\mathbf{k}}v_{\mathbf{k}}, \quad (2.99)$$

therefore,

$$\hat{K}_2 = \sum_{\mathbf{k}\neq\mathbf{0}}[\epsilon_{\mathbf{k}} + \hbar\mathbf{k}\cdot\boldsymbol{v}_0]\hat{A}^\dagger_{\mathbf{k}}\hat{A}_{\mathbf{k}}$$
$$+ \sum_{\mathbf{k}\neq\mathbf{0}}[\frac{gn_0}{2}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) - u_{\mathbf{k}}v_{\mathbf{k}}(\epsilon^0_{\mathbf{k}} + gn_0)](\hat{A}_{\mathbf{k}}\hat{A}_{\text{-}\mathbf{k}} + \hat{A}^\dagger_{\mathbf{k}}\hat{A}^\dagger_{\text{-}\mathbf{k}}) + \tilde{K}_0. \quad (2.100)$$

Therefore, as the values for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ which enable us to drop non-diagonal terms, we find that they should satisfy,

$$\frac{gn_0}{2}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) - u_{\mathbf{k}}v_{\mathbf{k}}(\epsilon^0_{\mathbf{k}} + gn_0) = 0. \quad (2.101)$$

In this way, we can derive formulas of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ specifically by (2.96) and (2.101),

$$u^2_{\mathbf{k}} = \frac{1}{2}(\frac{\epsilon^0_{\mathbf{k}} + gn_0}{E_{\mathbf{k}}} + 1), \quad (2.102)$$
$$v^2_{\mathbf{k}} = \frac{1}{2}(\frac{\epsilon^0_{\mathbf{k}} + gn_0}{E_{\mathbf{k}}} - 1), \quad (2.103)$$
$$E_{\mathbf{k}} \triangleq \sqrt{\epsilon^0_{\mathbf{k}}(\epsilon^0_{\mathbf{k}} + 2gn_0)}. \quad (2.104)$$

Then, substitute from (2.101) to (2.104) into (2.99),

$$\epsilon_{\mathbf{k}} = E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^0(\epsilon_{\mathbf{k}}^0 + 2gn_0)}. \tag{2.105}$$

Therefore, we finally summarize the equation (2.100) as

$$\hat{K}_2 = \sum_{\mathbf{k}\neq\mathbf{0}} [E_{\mathbf{k}} + \hbar\mathbf{k}\cdot\boldsymbol{v}_0]\hat{A}_{\mathbf{k}}^\dagger\hat{A}_{\mathbf{k}} + \tilde{K}_0. \tag{2.106}$$

This equation (2.106) is the energy term given by the excited states of superfluids, and it is described by the creation and annihilation operators of the quasiparticle. And then, we can also derive formulas of the particle number density and current-density in the excited states by using the above results. First, we should remember the formula of the particle number density operator given by (2.18), and moreover we consider the current-density operator given by,

$$\hat{\boldsymbol{j}}(\mathbf{r}) = \frac{\hbar}{2mi}(\hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) - \hat{\psi}(\mathbf{r})\nabla\hat{\psi}^\dagger(\mathbf{r})). \tag{2.107}$$

By substituting (2.76), (2.77), (2.78), (2.90), and (2.91) into (2.18) and (2.107) respectively, and calculating carefully, we can derive the following result,

$$n = n_0 + \frac{1}{V}\sum_{\mathbf{k}\neq\mathbf{0}}[(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)f_B(\tilde{E}_{\mathbf{k}}) + v_{\mathbf{k}}^2], \tag{2.108}$$

$$\boldsymbol{j} = n\boldsymbol{v}_0 + \frac{1}{V}\sum_{\mathbf{k}\neq\mathbf{0}}\frac{\hbar\mathbf{k}}{m}[(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)f_B(\tilde{E}_{\mathbf{k}}) + v_{\mathbf{k}}^2], \tag{2.109}$$

where,

$$\tilde{E}_{\mathbf{k}} = E_{\mathbf{k}} + \hbar\mathbf{k}\cdot\boldsymbol{v}_0, \tag{2.110}$$

$$f_B(E) = \frac{1}{e^{\beta E} - 1}. \tag{2.111}$$

However, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are values given by (2.102) and (2.103), respectively. In this way, the particle number density and current-density concerning the excited states of superfluids are given by the excited energy spectrum of the quasiparticle, respectively.

Chapter 3

Finite temperature density functional theory(FTDFT)

In this chapter, we will explain Density functional theory (DFT) for the electron system which is applied to sf-CDFT. DFT is one of the theories for dealing with the electron system, and this theory was formulated by P.C. Hohenberg, W. Kohn in 1964[24], and W. Kohn, L.J. Sham in 1965[25]. In this theory, we can calculate the electron number density and the energy of the real system in the ground state, and also the excited states, instead of solving the Schrödinger equation of the many-body system. Therefore, although the original DFT is the theory related to the ground state, here we explain the Finite temperature density functional theory (FTDFT) which is applied to the system at a finite temperature in the thermal equilibrium state.

3.1 Hohenberg-Kohn theorem

The expansion of DFT to the system at the finite temperature was done by N.D. Mermin[26]. The theory is called Finite temperature density functional theory (FTDFT), and this theory enables us to deal with the electron system at the finite temperature in the thermal equilibrium state while the original DFT is applied to the ground state. In this section, we will explain the Hohenberg-Kohn (HK) theorem, which is proved in FTDFT.

First, we consider the electron system in the thermal equilibrium state, which touches the reserver whose temperature and chemical potential are θ and μ, respectively. In this system, under the external potential $v(\mathbf{r})$, we describe the Hamiltonian as

$$\hat{H} = \hat{T} + \hat{V} + \hat{W}, \tag{3.1}$$

$$\hat{T} = \int \hat{\psi}^\dagger(\mathbf{r})(-\frac{\hbar^2\nabla^2}{2m})\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{3.2}$$

$$\hat{V} = \int \hat{\psi}^\dagger(\mathbf{r})v(\mathbf{r})\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{3.3}$$

$$\hat{W} = \frac{1}{2}\iint \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})d\mathbf{r}d\mathbf{r}'. \tag{3.4}$$

Eq. (3.3) can be rewritten below by using (2.18),

$$\hat{V} = \int v(\mathbf{r})\hat{n}(\mathbf{r})d\mathbf{r}. \tag{3.5}$$

In this way, the operator $\hat{n}(\mathbf{r})$ is coupled with the external potential $v(\mathbf{r})$ so that the electron number density can be chosen as the basic variable, which is explained later. For this system, we can prove two crucial theorems as below. In short, HK theorem I insist that the potential $v(\mathbf{r})$, density matrix of the system $\hat{\rho}_{eq}$, and electron number density in the thermal equilibrium state $n_{eq}(\mathbf{r})$ are in one-to-one correspondence. Here, $n_{eq}(\mathbf{r})$ is

$$n_{eq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{eq}\hat{n}(\mathbf{r})]. \tag{3.6}$$

First, we prove this theorem I.

Since the Hamiltonian given by (3.1) is uniquely determined by the potential $v(\mathbf{r})$, the density matrix is also uniquely determined by it,

$$\hat{\rho}_{eq} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]}. \tag{3.7}$$

Then, we can calculate $n_{eq}(\mathbf{r})$ by using this $\hat{\rho}_{eq}$ like (3.6). Therefore, the electron number density $n_{eq}(\mathbf{r})$ is determined if the potential is given.

Next, we prove that the potential is uniquely determined if $\hat{\rho}_{eq}$ is given. We assume that the density matrix is obtained from two different potentials $v(\mathbf{r})$ and $v'(\mathbf{r})$, i.e,

$$\hat{\rho}_{eq} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]} = \frac{e^{-\beta(\hat{H}'-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}'-\mu\hat{N})}]}, \tag{3.8}$$

here, $\hat{H}$ and $\hat{H}'$ are the Hamiltonian under the potential $v(\mathbf{r})$ and $v'(\mathbf{r})$, respectively. (3.8) can be rewritten as

$$e^{-\beta(\hat{H}-\hat{H}')} = \frac{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]}{\mathrm{Tr}[e^{-\beta(\hat{H}'-\mu\hat{N})}]}, \tag{3.9}$$

Since the right-hand side of (3.9) is the classical number, $\hat{H} - \hat{H}'$ in the left-hand side must be the classical number. In short, it follows that $v(\mathbf{r})$ differs from $v'(\mathbf{r})$ by more than a constant. This contradicts our assumption, and therefore, the potential is uniquely determined if $\hat{\rho}_{eq}$ is given. Thus, $v(\mathbf{r})$ and $\hat{\rho}_{eq}$ are in one-to-one correspondence.

Next, we prove that $n_{eq}(\mathbf{r})$ and $\hat{\rho}_{eq}$ are in one-to-one correspondence by using Gibbs's variational principle[66,67] below. According to this principle, the functional of the density matrix $\hat{\rho}'$ as

$$\Omega_v[\hat{\rho}'] \triangleq \mathrm{Tr}[\hat{\rho}'(\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}')], \tag{3.10}$$

becomes minimum and equals the grand potential when $\hat{\rho}'$ equals the density matrix in the thermal equilibrium state $\hat{\rho}_{eq}$. Then, we assume that $n_{eq}(\mathbf{r})$ is obtained from two different density matrices $\hat{\rho}_{eq}$ and $\hat{\rho}'_{eq}$. Under this,

$$\begin{aligned}
\Omega_{v'}[\hat{\rho}'_{eq}] &= \mathrm{Tr}[\hat{\rho}'_{eq}(\hat{H}' - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}'_{eq})] \\
&< \mathrm{Tr}[\hat{\rho}_{eq}(\hat{H}' - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}_{eq})] \\
&= \Omega_v[\hat{\rho}_{eq}] + \mathrm{Tr}[\hat{\rho}_{eq}(\hat{V}' - \hat{V})] \\
&= \Omega_v[\hat{\rho}_{eq}] + \int d\mathbf{r}(v'(\mathbf{r}) - v(\mathbf{r}))n_{eq}(\mathbf{r}).
\end{aligned} \tag{3.11}$$

As well as the above,

$$\begin{aligned}
\Omega_v[\hat{\rho}_{eq}] &= \mathrm{Tr}[\hat{\rho}_{eq}(\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}_{eq})] \\
&< \mathrm{Tr}[\hat{\rho}'_{eq}(\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}'_{eq})] \\
&= \Omega_{v'}[\hat{\rho}'_{eq}] + \mathrm{Tr}[\hat{\rho}'_{eq}(\hat{V} - \hat{V}')] \\
&= \Omega_{v'}[\hat{\rho}'_{eq}] + \int d\mathbf{r}(v(\mathbf{r}) - v'(\mathbf{r}))n_{eq}(\mathbf{r}).
\end{aligned} \tag{3.12}$$

However, equations (3.11) and (3.12) lead to an inconsistent inequality as

$$\Omega_v[\hat{\rho}_{eq}] + \Omega_{v'}[\hat{\rho}'_{eq}] < \Omega_v[\hat{\rho}_{eq}] + \Omega_{v'}[\hat{\rho}'_{eq}], \tag{3.13}$$

therefore, $\hat{\rho}_{eq}$ is determined uniquely if $n_{eq}(\mathbf{r})$ is determined. Thus, the potential $v(\mathbf{r})$, density matrix of the system $\hat{\rho}_{eq}$, and the electron number density in the thermal equilibrium state $n_{eq}(\mathbf{r})$ are in one-to-one correspondence. In short, the HK theorem I was proved. The density $n_{eq}(\mathbf{r})$ is regarded as the basic variable because it determines the thermal equilibrium properties of the system. Finally, we indicate the figure of this relation in Fig. 3.1.

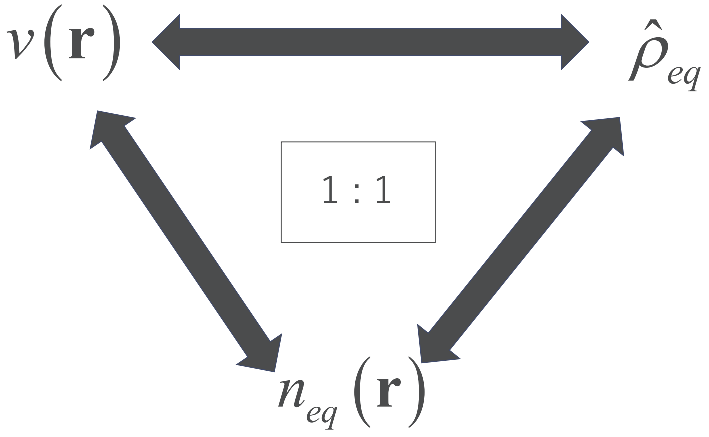

Fig. 3.1: Relation in the HK theorem I

Next, HK theorem II insists that the functional of the basic variable $\Omega_v[n]$ takes a minimum value at the thermal equilibrium value of the basic variable $n_{eq}(\mathbf{r})$. This theorem concerning the basic variable is obtained by rewriting Gibbs's variational principle with the aid of HK theorem I. Here, the functional of the basic variable $\Omega_v[n]$ is defined by

$$\Omega_v[n] = F[n] + \int d\mathbf{r} v(\mathbf{r}) n(\mathbf{r}), \tag{3.14}$$

$$F[n] \triangleq \mathrm{Tr}[\hat{\rho}[n](\hat{T} + \hat{W} + \beta^{-1} \ln \hat{\rho}[n])]. \tag{3.15}$$

Here, $F[n]$ is the universal functional defined by (3.15). In equation (3.15), $\hat{\rho}[n]$ is the density matrix which is uniquely determined by the basic variable $n(\mathbf{r})$ via

HK theorem I. Then, the above variational principle concerning the basic variable is given by

$$\min_n \Omega_v[n] = \Omega_v[n_{eq}]. \tag{3.16}$$

We prove this theorem below.
Consider HK theorem I, and we can describe $\hat{\rho}$ as the functional of the basic variable like $\hat{\rho} = \hat{\rho}[n]$. Therefore, the functional $\Omega_v[\hat{\rho}]$ can be rewritten as $\Omega_v[n]$. Thus, we have

$$\begin{aligned}\Omega_v[\hat{\rho}] &= \Omega_v[\hat{\rho}[n]] \\ &= \Omega_v[n] \\ &= \mathrm{Tr}[\hat{\rho}[n](\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}[n])] \\ &= F[n] + \int d\mathbf{r} v(\mathbf{r}) n(\mathbf{r}),\end{aligned} \tag{3.17}$$

on the other hand, we also have

$$\begin{aligned}\Omega_v[\hat{\rho}_{eq}] &= \Omega_v[\hat{\rho}[n_{eq}]] \\ &= \Omega_v[n_{eq}] \\ &= \mathrm{Tr}[\hat{\rho}[n_{eq}](\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}[n_{eq}])] \\ &= F[n_{eq}] + \int d\mathbf{r} v(\mathbf{r}) n_{eq}(\mathbf{r}).\end{aligned} \tag{3.18}$$

According to Gibbs's variational principle, the right-hand side of equation (3.17) becomes minimum when $\hat{\rho}[n]$ coincides with $\hat{\rho}[n_{eq}]$, therefore, we have

$$\min_n \Omega_v[n] = \Omega_v[n_{eq}]. \tag{3.19}$$

Thus, $\Omega_v[n]$ takes a minimum value at the thermal equilibrium value of the basic variable $n_{eq}(\mathbf{r})$.

3.2 Kohn-Sham equation

In this section, we explain how to calculate the basic variable in FTDFT. We first introduce the noninteracting reference system which touches the reservers whose temperature and chemical potential are θ, μ, respectively, and in which the basic variable of the real system in the thermal equilibrium state is reproduced. The Hamiltonian of this reference system $\hat{H}_S$ is given by

$$\hat{H}_S = \hat{T} + \hat{V}_S, \tag{3.20}$$

$$\hat{V}_S = \int v_S(\mathbf{r})\hat{n}(\mathbf{r})d\mathbf{r}, \tag{3.21}$$

where $v_S(\mathbf{r})$ is the effective potential which is determined later so that the thermal equilibrium value of the basic variable in the reference system coincides with one in the real system. As well as the case of the real system, we can prove the HK theorem for the reference system(see Fig.3.2). In short, the effective potential $v_S(\mathbf{r})$, the density matrix of the reference system $\hat{\rho}_{Seq}$, and variable $n_{Seq}(\mathbf{r})$ in the thermal equilibrium state are in one-to-one correspondence.

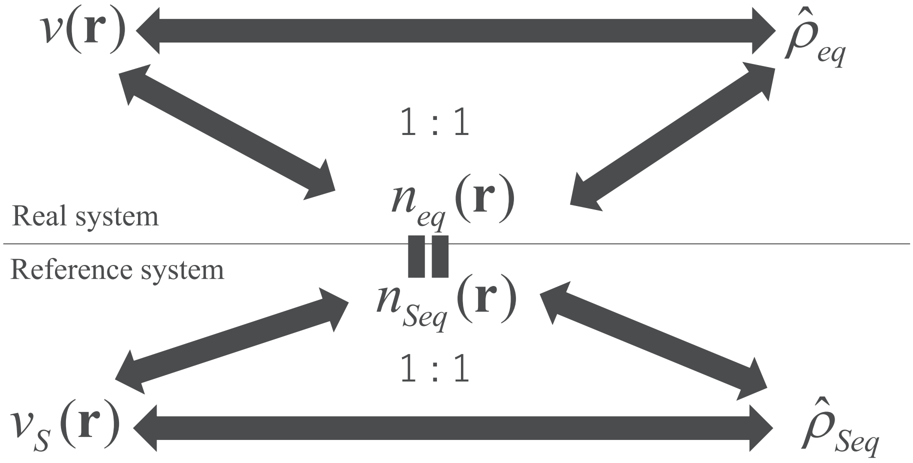

Fig. 3.2: Relation of the real and reference system

In addition, the functional $\Omega_{v_S}[n_S]$ given by

$$\Omega_{v_S}[n_S] = T_S[n_S] - \theta S_S[n_S] + \int (v_S(\mathbf{r}) - \mu) n_S d\mathbf{r}, \tag{3.22}$$

$$T_S[n_S] = \mathrm{Tr}[\hat{\rho}_S[n_S]\hat{T}], \tag{3.23}$$

$$S_S[n_S] = -k_B \mathrm{Tr}[\hat{\rho}_S[n_S] \ln \hat{\rho}_S[n_S]], \tag{3.24}$$

becomes minimum at the thermal equilibrium value of the basic variable. In other words,

$$\min_{n_S} \Omega_{v_S}[n_S] = \Omega_{v_S}[n_{Seq}] = \Omega_{v_S}[n_{eq}]. \tag{3.25}$$

Here, $n_{Seq}(\mathbf{r})$ denotes the thermal equilibrium value of the basic variable in the reference system given by

$$\hat{\rho}_{Seq} = \frac{e^{-\beta(\hat{H}_S - \mu\hat{N})}}{\Xi}, \tag{3.26}$$

$$\Xi = \mathrm{Tr}[e^{-\beta(\hat{H}_S - \mu\hat{N})}], \tag{3.27}$$

$$n_{Seq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{Seq}\hat{n}(\mathbf{r})]. \tag{3.28}$$

Then, let us derive the formula of the effective potential $v_S(\mathbf{r})$. First, the universal functional defined by the equation (3.15) can be rewritten as

$$F[n] = T[n] + W[n] - \theta S[n], \tag{3.29}$$

where we use the notation as

$$T[n] = \mathrm{Tr}[\hat{\rho}[n]\hat{T}], \tag{3.30}$$

$$W[n] = \mathrm{Tr}[\hat{\rho}[n]\hat{W}], \tag{3.31}$$

$$S[n] = -k_B \mathrm{Tr}[\hat{\rho}[n] \ln \hat{\rho}[n]]. \tag{3.32}$$

Here, we formally rewrite the equation (3.29) by $T_S[n]$, $S_S[n]$, and the Coulomb interaction of electrons $U[n]$ as

$$F[n] = T_S[n] + U[n] - \theta S_S[n] + F_{xc}[n], \tag{3.33}$$

where, $U[n]$ is

$$U[n] = \frac{1}{2} \iint \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'. \tag{3.34}$$

In equation (3.33), the functional $F_{xc}[n]$ is the xc energy functional of FTDFT and is defined as the functional described by the difference between functionals of the real and reference system,

$$F_{xc}[n] = (T[n] - T_S[n]) + (W[n] - U[n]) - \theta(S[n] - S_S[n]). \tag{3.35}$$

Substituting (3.33) into $\Omega_v[n]$ and using this for HK theorem II in the real system, we have

$$\left.\frac{\delta T_S[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} + \left.\frac{\delta U[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} - \theta\left.\frac{\delta S_S[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} + \left.\frac{\delta F_{xc}[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} + v(\mathbf{r}) - \mu = 0. \tag{3.36}$$

Similarly, we can derive below from HK theorem II in the reference system,

$$\left.\frac{\delta T_S[n_S]}{\delta n_S(\mathbf{r})}\right|_{n_S=n_{Seq}} - \theta\left.\frac{\delta S_S[n_S]}{\delta n_S(\mathbf{r})}\right|_{n_S=n_{Seq}} + v_S(\mathbf{r}) - \mu = 0. \tag{3.37}$$

We can recognize that (3.36) is the equation for the thermal equilibrium value of the basic variable $n_{eq}(\mathbf{r})$ of the real system while (3.37) is for $n_{Seq}(\mathbf{r})$ of the reference system. When (3.36) coincides with (3.37), the effective potential $v_S(\mathbf{r})$ is considered the potential that enables us to reproduce $n_{eq}(\mathbf{r})$ in the reference system. In short, we can derive the formula of the effective potential which reproduces the same basic variable as one in the real system:

$$\begin{aligned} v_S(\mathbf{r}) &= v(\mathbf{r}) + \left.\frac{\delta U[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} + \left.\frac{\delta F_{xc}[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}} \\ &= v(\mathbf{r}) + \int \frac{e^2 n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \left.\frac{\delta F_{xc}[n]}{\delta n(\mathbf{r})}\right|_{n=n_{eq}}. \end{aligned} \tag{3.38}$$

In this way, we could get the formula of the effective potential $v_S(\mathbf{r})$.

Next, we derive the single-particle equation for calculating the basic variable. First, we focus on the grand canonical Hamiltonian $\hat{H}_S - \mu\hat{N}$ to calculate the expectation of the particle number density operator $\hat{n}(\mathbf{r})$,

$$\hat{K}_S = \hat{H}_S - \mu\hat{N} = \int \hat{\psi}^\dagger(\mathbf{r})(-\frac{\hbar^2\nabla^2}{2m} + v_S(\mathbf{r}) - \mu)\hat{\psi}(\mathbf{r})d\mathbf{r} \equiv \int \hat{\psi}^\dagger(\mathbf{r})(\hat{h}_S - \mu)\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{3.39}$$

where,

$$\hat{h}_S = -\frac{\hbar^2\nabla^2}{2m} + v_S(\mathbf{r}). \tag{3.40}$$

In equation (3.39), $\hat{K}_S$ is the quadratic form concerning the field operator, therefore, we here expand $\hat{\psi}^\dagger(\mathbf{r})$, $\hat{\psi}(\mathbf{r})$ by the eigenfunction of the single-particle Hamiltonian $\hat{h}_S$. Suppose the eigenfunction and eigenvalue of $\hat{h}_S$ are denoted by $\phi_i(\mathbf{r})$, ϵ_i,

$$\hat{h}_S\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r}), \tag{3.41}$$

then, we expand $\hat{\psi}^\dagger(\mathbf{r})$, $\hat{\psi}(\mathbf{r})$ as

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r})\hat{c}_i^\dagger, \tag{3.42}$$

$$\hat{\psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})\hat{c}_i, \tag{3.43}$$

where $\hat{c}_i^\dagger, \hat{c}_i$ are the creation and annihilation operator of fermions with the state of $\phi_i(\mathbf{r})$. By using (3.42) and (3.43), we rewrite (3.39) as

$$\hat{K}_S = \int d\mathbf{r} \sum_i \phi_i^*(\mathbf{r})(\hat{h}_S - \mu)\sum_j \phi_j(\mathbf{r})\hat{c}_i^\dagger\hat{c}_j = \sum_i(\epsilon_i - \mu)\hat{c}_i^\dagger\hat{c}_i, \tag{3.44}$$

in equation (3.44), we considered the orthonormality of $\phi_i(\mathbf{r})$. Hereafter, we will refer to the single-particle equation (3.41) as the Kohn-Sham (KS) equation in FTDFT.

In this way, let us formulate the basic variable, i.e., the electron number density $n(\mathbf{r})$ reproduced in the thermal equilibrium state by using (3.44).

$$\begin{aligned} n(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_S\hat{n}(\mathbf{r})] = \mathrm{Tr}[\hat{\rho}_S\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})] \\ &= \sum_m \left\langle \Phi_m \middle| \frac{e^{-\beta\hat{K}_S}}{\Xi} \sum_{i,j}\phi_i^*(\mathbf{r})\phi_j(\mathbf{r})\hat{c}_i^\dagger\hat{c}_j \middle| \Phi_m \right\rangle \\ &= \sum_{i,j}\phi_i^*(\mathbf{r})\phi_j(\mathbf{r})\sum_m \left\langle \Phi_m \middle| \frac{e^{-\beta\hat{K}_S}}{\Xi}\hat{c}_i^\dagger\hat{c}_j \middle| \Phi_m \right\rangle, \end{aligned} \tag{3.45}$$

here, as the one electron state label i, we consider not only the single-particle state α such as the wave number vector $\mathbf{k}$, but also the spin σ, and in this case we can rewrite (3.45) as

$$\begin{aligned}
&\sum_{i,j} \phi_i^*(\mathbf{r})\phi_j(\mathbf{r}) \sum_m \left\langle \Phi_m \middle| \frac{e^{-\beta \hat{K}_S}}{\Xi} \hat{c}_i^\dagger \hat{c}_j \middle| \Phi_m \right\rangle \\
&= \sum_{\alpha,\alpha',\sigma,\sigma'} \phi_{\alpha,\sigma}^*(\mathbf{r})\phi_{\alpha',\sigma'}(\mathbf{r}) \sum_m \left\langle \Phi_m \middle| \frac{e^{-\beta \hat{K}_S}}{\Xi} \hat{c}_{\alpha,\sigma}^\dagger \hat{c}_{\alpha',\sigma'} \middle| \Phi_m \right\rangle \\
&= \sum_{\alpha,\alpha',\sigma,\sigma'} \phi_{\alpha,\sigma}^*(\mathbf{r})\phi_{\alpha',\sigma'}(\mathbf{r}) \sum_{\{n_{\alpha'',\sigma''}\}} \left\langle \{n_{\alpha'',\sigma''}\} \middle| \frac{e^{-\beta \hat{K}_S}}{\Xi} \hat{c}_{\alpha,\sigma}^\dagger \hat{c}_{\alpha',\sigma'} \middle| \{n_{\alpha'',\sigma''}\} \right\rangle \\
&= \sum_{\alpha,\sigma} |\phi_{\alpha,\sigma}(\mathbf{r})|^2 \sum_{\{n_{\alpha'',\sigma''}\}} \frac{e^{\sum_{\alpha''',\sigma'''}(\epsilon_{\alpha''',\sigma'''}-\mu)n_{\alpha''',\sigma'''}}}{\Xi} n_{\alpha,\sigma} \\
&= \sum_{\alpha,\sigma} |\phi_{\alpha,\sigma}(\mathbf{r})|^2 \frac{e^{-\beta(\epsilon_{\alpha,\sigma}-\mu)}}{e^{-\beta(\epsilon_{\alpha,\sigma}-\mu)}+1} \\
&= \sum_{\alpha,\sigma} |\phi_{\alpha,\sigma}(\mathbf{r})|^2 \frac{1}{e^{\beta(\epsilon_{\alpha,\sigma}-\mu)}+1} \\
&\equiv \sum_{\alpha,\sigma} |\phi_{\alpha,\sigma}(\mathbf{r})|^2 f(\epsilon_{\alpha,\sigma}),
\end{aligned} \tag{3.46}$$

however, in equation (3.46), first we used the eigenstate vector $|\{n_{\alpha,\sigma}\}\rangle$ of the operator $\hat{K}_S$ as bases of the trace(note that the operators $\hat{H}_S$ and $\hat{N}$ are commutative operators as seeing (3.20) and we can consider the simultaneous eigenstate of them), and $n_{\alpha,\sigma}$ is the occupation number with respect to the state (α, σ). Moreover, we used the notation of the Fermi-Dirac distribution function given as

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1}. \tag{3.47}$$

In this way, we could get the formula of the basic variable $n(\mathbf{r})$ given by the equation (3.46). Concerning the KS equation given by (3.41), if we provide the equation (3.41), i.e, the effective potential $v_S(\mathbf{r})$ with the approximate form of the xc energy functional F_{xc}, and we conduct the self-consistent calculation by using (3.38), (3.41) and (3.46), then we can get the electron number density in the thermal equilibrium state $n(\mathbf{r})$.

Chapter 4

Current-density functional theory for bosonic superfluids(sf-CDFT)

In this chapter, we will propose the finite temperature current-density functional theory for bosonic superfluids in the thermal equilibrium state, which is named sf-CDFT. In this theory, we chose the particle number density, current-density of superfluids, and the order parameter of the BEC as the basic variables reproduced in sf-CDFT. It is shown that the sf-CDFT enables us to reproduce the particle number density and current-density of the superfluid and normal fluid components simultaneously while incorporating the effect of their interaction. We can show that these hydrodynamic physical quantities of two fluid components are determined by solving two single-particle equations named the Gross-Pitaevskii-Kohn-Sham and Kohn-Sham equations. As the crucial things, we can discuss some advantage points by the comparison of this sf-CDFT with the conventional theories for superfluids proposed in Chapter 2.

4.1 Hamiltonian

In this section, we first mention the Hamiltonian of the real system which will be used in the after formulation of sf-CDFT. we consider the boson system under the external potentials, and its Hamiltonian given by

$$\begin{aligned}\hat{H}_0 = &\int \hat{\psi}^\dagger(\mathbf{r})[\frac{1}{2m}(\hat{\boldsymbol{p}} + \boldsymbol{A}(\mathbf{r}))^2 + v(\mathbf{r})]\hat{\psi}(\mathbf{r})d\mathbf{r} \\ &+ \frac{1}{2}\iint \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')u(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})d\mathbf{r}d\mathbf{r}', \qquad (4.1)\end{aligned}$$

where the function $u(\mathbf{r},\mathbf{r}')$ denotes the interaction potential of bosons, $\hat{\boldsymbol{p}}$ is the momentum operator, $v(\mathbf{r})$ is the external potential, for example, it is considered the potential which is made by the vessel, and $\boldsymbol{A}(\mathbf{r})$ denotes one vector potential, for example caused by rotating the vessel[48], which is proposed in Chapter 2. The Hamiltonian (4.1) is similar to one in the current-density functional theory for fermion systems[29]. For later discussion, let us rewrite the equation (4.1) as

$$\hat{H}_0 = \hat{T} + \hat{W} + \int d\mathbf{r}[v(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2]\hat{n}(\mathbf{r}) + \int d\mathbf{r}\hat{\boldsymbol{j}}(\mathbf{r}) \cdot \boldsymbol{A}(\mathbf{r}), \tag{4.2}$$

$$\hat{T} = \int \hat{\psi}^\dagger(\mathbf{r})(-\frac{\hbar^2\nabla^2}{2m})\hat{\psi}(\mathbf{r})d\mathbf{r}, \tag{4.3}$$

$$\hat{W} = \frac{1}{2}\iint \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')u(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})d\mathbf{r}d\mathbf{r}', \tag{4.4}$$

$$\hat{n}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}), \tag{4.5}$$

$$\hat{\boldsymbol{j}}(\mathbf{r}) = \frac{\hbar}{2mi}(\hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) - \hat{\psi}(\mathbf{r})\nabla\hat{\psi}^\dagger(\mathbf{r})), \tag{4.6}$$

where operators in equations (4.3) to (4.6) have been already proposed in Chapter 2. While formulating the current-density functional theory(CDFT) for fermion systems[29], as well as the original DFT[24,25], physical quantities coupled with external potentials can be chosen as the basic variables. For the Hamiltonian (4.2), $\hat{n}(\mathbf{r})$ and $\hat{\boldsymbol{j}}(\mathbf{r})$ are coupled with external potentials $v(\mathbf{r})$ and $\boldsymbol{A}(\mathbf{r})$ so that the particle number density and current-density can be chosen as the basic variables. Here, it would be useful to reproduce not only these physical quantities but also the order parameter of the BEC which is given by the expectation of the field operator in describing the properties of the superfluid component. So in this theory, we chose the order parameter of the BEC, in addition to the particle number density and current-density as the basic variables. For this aim, instead of applying the extended constrained-search theory[30,31] to this system, one artificial fields $D(\mathbf{r})$ and $D^*(\mathbf{r})$ are introduced as the mathematical device[39] to deal with the order parameter of the BEC $\psi(\mathbf{r})$ and $\psi^*(\mathbf{r})$ as the basic variables. These artificial fields are coupled with the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ in the Hamiltonian and we will finally make them zero. The Hamiltonian with these artificial field terms is given by

$$\hat{H} = \hat{H}_0 + \hat{D}, \tag{4.7}$$

$$\hat{D} = \int d\mathbf{r}\hat{\psi}(\mathbf{r})D^*(\mathbf{r}) + \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})D(\mathbf{r}). \tag{4.8}$$

Note that these artificial fields have sometimes been introduced to deal with the basic variables that are not coupled with external potentials. For example, artificial pair fields are introduced to deal with the order parameter of the superconducting state as a basic variable in the DFT for superconductors[36,39].

4.2 Hohenberg-Kohn theorem

Similar to the original DFT, in sf-CDFT, the HK theorem consists of two theorems. HK theorem I insists that the class of potentials $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$, the density matrix of the system $\hat{\rho}_{eq}$, and the class of variables $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ in the thermal equilibrium state are in one-to-one correspondence. Here the variables $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ are calculated by using $\hat{\rho}_{eq}$ as

$$n_{eq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{eq}\hat{n}(\mathbf{r})], \tag{4.9}$$

$$\boldsymbol{j}_{eq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{eq}\hat{\boldsymbol{j}}(\mathbf{r})], \tag{4.10}$$

$$\psi_{eq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{eq}\hat{\psi}(\mathbf{r})], \tag{4.11}$$

$$\psi^*_{eq}(\mathbf{r}) = \mathrm{Tr}[\hat{\rho}_{eq}\hat{\psi}^\dagger(\mathbf{r})]. \tag{4.12}$$

HK theorem I can be proven similarly to that in FTDFT[26]. We show this below.

The Hamiltonian (4.7) is uniquely determined by the class of potentials, so the density matrix of the system $\hat{\rho}_{eq}$ is also uniquely determined by them and it is given by

$$\hat{\rho}_{eq} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]}. \tag{4.13}$$

Subsequently, we can calculate the class of variables $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ by using $\hat{\rho}_{eq}$ as seeing equations (4.9) to (4.12), therefore, the class of variables $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ is determined if the class of potentials is given.

Next, let us prove that the class of potentials is uniquely determined if the density matrix of the system is given. We assume that $\hat{\rho}_{eq}$ is obtained from two different classes of potentials $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$ and $[v'(\mathbf{r}), \boldsymbol{A}'(\mathbf{r}), D'(\mathbf{r}), D^{*'}(\mathbf{r})]$,

$$\hat{\rho}_{eq} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]} = \frac{e^{-\beta(\hat{H}'-\mu\hat{N})}}{\mathrm{Tr}[e^{-\beta(\hat{H}'-\mu\hat{N})}]}, \tag{4.14}$$

here, $\hat{H}$ and $\hat{H}'$ are the Hamiltonian under the potentials $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$ and $[v'(\mathbf{r}), \boldsymbol{A}'(\mathbf{r}), D'(\mathbf{r}), D^{*'}(\mathbf{r})]$, respectively. Eq.(4.14) can be rewritten as

$$e^{-\beta(\hat{H}-\hat{H}')} = \frac{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}]}{\mathrm{Tr}[e^{-\beta(\hat{H}'-\mu\hat{N})}]}, \tag{4.15}$$

Since the right-hand side of (4.15) is the classical number, $\hat{H}-\hat{H}'$ in the left-hand side must be the classical number. In short, it follows that $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$ differ from $[v'(\mathbf{r}), \boldsymbol{A}'(\mathbf{r}), D'(\mathbf{r}), D^{*'}(\mathbf{r})]$ by more than a constant. This contradicts our assumption, and therefore, the potential is uniquely determined if $\hat{\rho}_{eq}$ is given. Thus, $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$ and $\hat{\rho}_{eq}$ are in one-to-one correspondence.

Next, we prove that $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ and $\hat{\rho}_{eq}$ are in one-to-one correspondence by using the Gibbs's variational principle below. According to this principle, the functional of the density matrix $\hat{\rho}'$ as

$$\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}'] \triangleq \mathrm{Tr}[\hat{\rho}'(\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}')], \tag{4.16}$$

becomes minimum and equals the grand potential when $\hat{\rho}'$ equals the density matrix in the thermal equilibrium state $\hat{\rho}_{eq}$. Then, we assume that the class of variables is obtained from two different density matrices $\hat{\rho}_{eq}$ and $\hat{\rho}'_{eq}$. Under this,

$$\begin{aligned}
\Omega_{v',\boldsymbol{A}',D',D^{*'}}[\hat{\rho}'_{eq}] &= \mathrm{Tr}[\hat{\rho}'_{eq}(\hat{H}'-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}'_{eq})] \\
&< \mathrm{Tr}[\hat{\rho}_{eq}(\hat{H}'-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}_{eq})] \\
&= \Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}_{eq}] + \int d\mathbf{r}[v'(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}'(\mathbf{r})^2 - v(\mathbf{r}) - \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2]n_{eq}(\mathbf{r}) \\
&+ \int d\mathbf{r}\boldsymbol{j}_{eq}(\mathbf{r})\cdot[\boldsymbol{A}'(\mathbf{r}) - \boldsymbol{A}(\mathbf{r})] + \int d\mathbf{r}\psi_{eq}(\mathbf{r})[D^{*'}(\mathbf{r}) - D^*(\mathbf{r})] \\
&+ \int d\mathbf{r}\psi^*_{eq}(\mathbf{r})[D'(\mathbf{r}) - D(\mathbf{r})].
\end{aligned} \tag{4.17}$$

As well as the above,

$$\begin{aligned}
\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}_{eq}] &= \mathrm{Tr}[\hat{\rho}_{eq}(\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}_{eq})] \\
&< \mathrm{Tr}[\hat{\rho}'_{eq}(\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}'_{eq})] \\
&= \Omega_{v',\boldsymbol{A}',D',D^{*'}}[\hat{\rho}'_{eq}] + \int d\mathbf{r}[v(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2 - v'(\mathbf{r}) - \frac{1}{2m}\boldsymbol{A}'(\mathbf{r})^2]n_{eq}(\mathbf{r}) \\
&+ \int d\mathbf{r}\boldsymbol{j}_{eq}(\mathbf{r})\cdot[\boldsymbol{A}(\mathbf{r}) - \boldsymbol{A}'(\mathbf{r})] + \int d\mathbf{r}\psi_{eq}(\mathbf{r})[D^*(\mathbf{r}) - D^{*'}(\mathbf{r})] \\
&+ \int d\mathbf{r}\psi^*_{eq}(\mathbf{r})[D(\mathbf{r}) - D'(\mathbf{r})].
\end{aligned} \tag{4.18}$$

However, equations (4.17) and (4.18) lead to an inconsistent inequality as

$$\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}_{eq}] + \Omega_{v',\boldsymbol{A}',D',D^{*\prime}}[\hat{\rho}'_{eq}] < \Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}_{eq}] + \Omega_{v',\boldsymbol{A}',D',D^{*\prime}}[\hat{\rho}'_{eq}], \quad (4.19)$$

therefore, $\hat{\rho}_{eq}$ is determined uniquely if $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ is determined. Thus, the potentials $[v(\mathbf{r}), \boldsymbol{A}(\mathbf{r}), D(\mathbf{r}), D^*(\mathbf{r})]$, density matrix of the system $\hat{\rho}_{eq}$, and variables in the thermal equilibrium state $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ are in one-to-one correspondence. In short, the HK theorem I was proved. The class of variables $[n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi^*_{eq}(\mathbf{r})]$ is regarded as basic variables because it determines the thermal equilibrium properties of the system. We indicate the figure of this relation in Fig. 4.1.

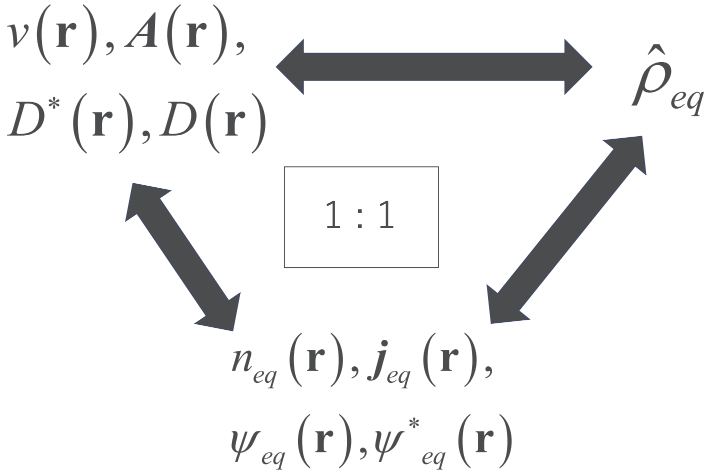

Fig. 4.1: Relation in the HK theorem I

Next, HK theorem Ⅱ insists that the functional of the basic variable described as $\Omega_{v,\boldsymbol{A},D,D^*}[n, \boldsymbol{j}, \psi, \psi^*]$ takes a minimum value at the thermal equilibrium value of basic variables. This theorem concerning basic variables is obtained by rewriting Gibbs's variational principle with the aid of HK theorem I. Here, the functional of the basic variable $\Omega_{v,\boldsymbol{A},D,D^*}[n, \boldsymbol{j}, \psi, \psi^*]$ is defined by

$$\begin{aligned}\Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*] &= F[n,\boldsymbol{j},\psi,\psi^*] + \int d\mathbf{r}(v(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2 - \mu)n(\mathbf{r}) \\ &\quad + \int d\mathbf{r}\boldsymbol{j}(\mathbf{r})\cdot\boldsymbol{A}(\mathbf{r}) + \int d\mathbf{r}\psi(\mathbf{r})D^*(\mathbf{r}) + \int d\mathbf{r}\psi^*(\mathbf{r})D(\mathbf{r}),\end{aligned} \tag{4.20}$$

$$F[n,\boldsymbol{j},\psi,\psi^*] \triangleq \mathrm{Tr}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*](\hat{T} + \hat{W} + \beta^{-1}\ln\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*])]. \tag{4.21}$$

Here, $F[n,\boldsymbol{j},\psi,\psi^*]$ is the universal functional defined by (4.21). In equation (4.21), $\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]$ is the density matrix which is uniquely determined by the basic variable $[n(\mathbf{r}),\boldsymbol{j}(\mathbf{r}),\psi(\mathbf{r}),\psi^*(\mathbf{r})]$ via HK theorem I. Then, the above variational principle concerning the basic variable is given by

$$\min_{n,\boldsymbol{j},\psi,\psi^*} \Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*] = \Omega_{v,\boldsymbol{A},D,D^*}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}]. \tag{4.22}$$

We prove this theorem below.
Consider HK theorem I, and we can describe $\hat{\rho}$ as the functional of the basic variable like $\hat{\rho} = \hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]$. Therefore, the functional $\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}]$ can be rewritten as $\Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*]$. Thus, we have

$$\begin{aligned}\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}] &= \Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]] \\ &= \Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*] \\ &= \mathrm{Tr}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*](\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*])] \\ &= F[n,\boldsymbol{j},\psi,\psi^*] + \int d\mathbf{r}(v(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2 - \mu)n(\mathbf{r}) \\ &\quad + \int d\mathbf{r}\boldsymbol{j}(\mathbf{r})\cdot\boldsymbol{A}(\mathbf{r}) + \int d\mathbf{r}\psi(\mathbf{r})D^*(\mathbf{r}) + \int d\mathbf{r}\psi^*(\mathbf{r})D(\mathbf{r}),\end{aligned} \tag{4.23}$$

on the other hand, we also have

$$
\begin{aligned}
\Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}_{eq}] &= \Omega_{v,\boldsymbol{A},D,D^*}[\hat{\rho}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}]] \\
&= \Omega_v[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}] \\
&= \mathrm{Tr}[\hat{\rho}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}](\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\rho}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}])] \\
&= F[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}] + \int d\mathbf{r}(v(\mathbf{r})+\frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2-\mu)n_{eq}(\mathbf{r}) \\
&+ \int d\mathbf{r}\boldsymbol{j}_{eq}(\mathbf{r})\cdot\boldsymbol{A}(\mathbf{r}) + \int d\mathbf{r}\psi_{eq}(\mathbf{r})D^*(\mathbf{r}) + \int d\mathbf{r}\psi^*_{eq}(\mathbf{r})D(\mathbf{r}),
\end{aligned}
\tag{4.24}
$$

According to Gibbs's variational principle, the right-hand side of equation (4.23) becomes minimum when $\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]$ coincides with $\hat{\rho}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}]$, therefore, we have

$$
\min_{n,\boldsymbol{j},\psi,\psi^*}\Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*] = \Omega_{v,\boldsymbol{A},D,D^*}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi^*_{eq}]. \tag{4.25}
$$

Thus, $\Omega_{v,\boldsymbol{A},D,D^*}[n,\boldsymbol{j},\psi,\psi^*]$ takes a minimum value at the thermal equilibrium value of basic variables $[n_{eq}(\mathbf{r}),\boldsymbol{j}_{eq}(\mathbf{r}),\psi_{eq}(\mathbf{r}),\psi^*_{eq}(\mathbf{r})]$.

4.3 Gross-Pitaevskii-Kohn-Sham equation and Kohn-Sham equation

In this section, we explain how to calculate basic variables in sf-CDFT. Similar to the FTDFT[26], we introduce the noninteracting reference system which touches the reservers whose temperature and chemical potential are θ, μ, respectively, and in which basic variables of the real system in the thermal equilibrium state are reproduced. The Hamiltonian of this reference system $\hat{H}_S$ is given by

$$
\hat{H}_S = \hat{T} + \int d\mathbf{r}[v_S(\mathbf{r})+\frac{1}{2m}\boldsymbol{A}_S(\mathbf{r})^2]\hat{n}(\mathbf{r}) + \int d\mathbf{r}\hat{\boldsymbol{j}}(\mathbf{r})\cdot\boldsymbol{A}_S(\mathbf{r}) + \hat{D}_S, \tag{4.26}
$$

$$
\hat{D}_S = \int d\mathbf{r}\hat{\psi}(\mathbf{r})D^*_S(\mathbf{r}) + \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})D_S(\mathbf{r}), \tag{4.27}
$$

where, $v_S(\mathbf{r})$, $\boldsymbol{A}_S(\mathbf{r})$, $D_S(\mathbf{r})$, $D^*_S(\mathbf{r})$ are the effective potentials which are determined later so that the thermal equilibrium value of basic variables in the reference system coincide with those in the real system. As well as the case of the real system, we can prove HK theorem for the reference system(see Fig.4.2). In short, the class of effective potentials $[v_S(\mathbf{r}),\ \boldsymbol{A}_S(\mathbf{r}),\ D_S(\mathbf{r}),\ D_S^*(\mathbf{r})]$, the density matrix of the reference system $\hat{\rho}_{Seq}$, and variables $[n_{Seq}(\mathbf{r}), \boldsymbol{j}_{Seq}(\mathbf{r}), \psi_{Seq}(\mathbf{r}), \psi_{Seq}^*(\mathbf{r})]$ in the thermal equilibrium state are in one-to-one correspondence.

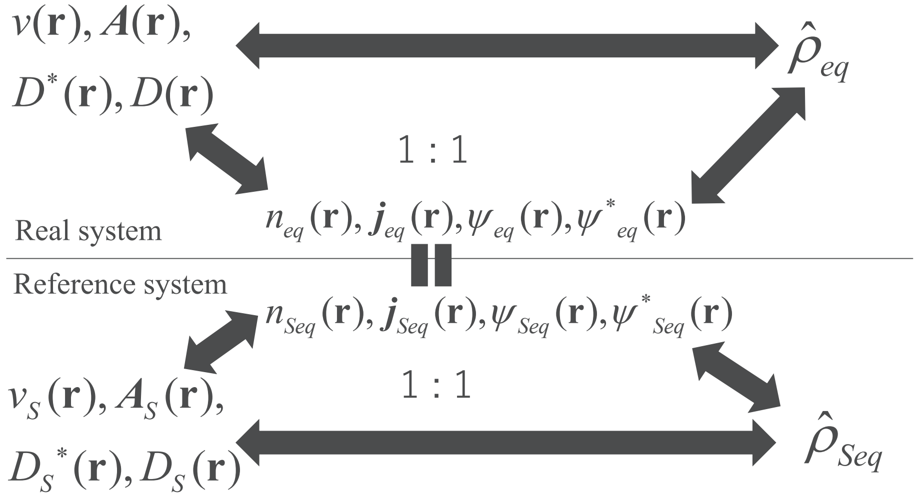

Fig. 4.2: Relation of the real and reference system

In addition, the functional $\Omega_{v_S,\boldsymbol{A}_S,D_S,D_S^*}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]$ given by

$$\begin{aligned}\Omega_{v_S,\boldsymbol{A}_S,D_S,D_S^*}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] &= T_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] - \theta S_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] \\ &\quad + \int (v_S(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}_S(\mathbf{r})^2 - \mu) n_S d\mathbf{r} + \int d\mathbf{r} \boldsymbol{j}_S(\mathbf{r}) \cdot \boldsymbol{A}_S(\mathbf{r}) \\ &\quad + \int d\mathbf{r} \psi_S(\mathbf{r}) D_S^*(\mathbf{r}) + \int d\mathbf{r} \psi_S^*(\mathbf{r}) D_S(\mathbf{r}), \qquad (4.28)\\ T_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] &= \mathrm{Tr}[\hat{\rho}_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]\hat{T}], \qquad (4.29)\\ S_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] &= -k_B \mathrm{Tr}[\hat{\rho}_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] \ln \hat{\rho}_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]], \\ &\qquad (4.30)\end{aligned}$$

becomes minimum at the thermal equilibrium value of basic variables. In other words,

$$\begin{aligned}\min_{n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*} \Omega_{v_S,\boldsymbol{A}_S,D_S,D_S^*}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*] &= \Omega_{v_S,\boldsymbol{A}_S,D_S,D_S^*}[n_{Seq},\boldsymbol{j}_{Seq},\psi_{Seq},\psi_{Seq}^*] \\ &= \Omega_{v_S,\boldsymbol{A}_S,D_S,D_S^*}[n_{eq},\boldsymbol{j}_{eq},\psi_{eq},\psi_{eq}^*]. \\ &\qquad (4.31)\end{aligned}$$

Here, $n_{Seq}(\mathbf{r})$, $\boldsymbol{j}_{Seq}(\mathbf{r})$, $\psi_{Seq}(\mathbf{r})$, $\psi^*_{Seq}(\mathbf{r})$ denote the thermal equilibrium value of basic variables in the reference system given by

$$\begin{aligned}
\hat{\rho}_{Seq} &= \frac{e^{-\beta(\hat{H}_S-\mu\hat{N})}}{\Xi}, && (4.32)\\
\Xi &= \mathrm{Tr}[e^{-\beta(\hat{H}_S-\mu\hat{N})}], && (4.33)\\
n_{Seq}(\mathbf{r}) &= \mathrm{Tr}[\hat{\rho}_{Seq}\hat{n}(\mathbf{r})], && (4.34)\\
\boldsymbol{j}_{Seq}(\mathbf{r}) &= \mathrm{Tr}[\hat{\rho}_{Seq}\hat{\boldsymbol{j}}(\mathbf{r})], && (4.35)\\
\psi_{Seq}(\mathbf{r}) &= \mathrm{Tr}[\hat{\rho}_{Seq}\hat{\psi}(\mathbf{r})], && (4.36)\\
\psi^*_{Seq}(\mathbf{r}) &= \mathrm{Tr}[\hat{\rho}_{Seq}\hat{\psi}^\dagger(\mathbf{r})]. && (4.37)
\end{aligned}$$

Then, let us derive the formula of the effective potentials [$v_S(\mathbf{r})$, $\boldsymbol{A}_S(\mathbf{r})$, $D_S(\mathbf{r})$, $D^*_S(\mathbf{r})$]. First, the universal functional defined by the equation (4.21) can be rewritten as

$$F[n,\boldsymbol{j},\psi,\psi^*] = T[n,\boldsymbol{j},\psi,\psi^*] + W[n,\boldsymbol{j},\psi,\psi^*] - \theta S[n,\boldsymbol{j},\psi,\psi^*], \qquad (4.38)$$

where we use the notation as

$$\begin{aligned}
T[n,\boldsymbol{j},\psi,\psi^*] &= \mathrm{Tr}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]\hat{T}], && (4.39)\\
W[n,\boldsymbol{j},\psi,\psi^*] &= \mathrm{Tr}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]\hat{W}], && (4.40)\\
S[n,\boldsymbol{j},\psi,\psi^*] &= -k_B\mathrm{Tr}[\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]\ln\hat{\rho}[n,\boldsymbol{j},\psi,\psi^*]]. && (4.41)
\end{aligned}$$

Here, we formally rewrite the equation (4.38) by $T_S[n,\boldsymbol{j},\psi,\psi^*]$, $S_S[n,\boldsymbol{j},\psi,\psi^*]$ and the classical boson-boson interaction $U[n]$ as

$$F[n,\boldsymbol{j},\psi,\psi^*] = T_S[n,\boldsymbol{j},\psi,\psi^*] + U[n] - \theta S_S[n,\boldsymbol{j},\psi,\psi^*] + F_{xc}[n,\boldsymbol{j},\psi,\psi^*], \qquad (4.42)$$

where, $U[n]$ is

$$U[n] = \frac{1}{2}\iint u(\mathbf{r},\mathbf{r}')n(\mathbf{r})n(\mathbf{r}')d\mathbf{r}d\mathbf{r}'. \qquad (4.43)$$

In equation (4.42), the functional $F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]$ is the xc energy functional of sf-CDFT and is defined as the functional described by the difference between functionals of the real and reference system,

$$\begin{aligned} F_{xc}[n, \boldsymbol{j}, \psi, \psi^*] = (T[n, \boldsymbol{j}, \psi, \psi^*] - T_S[n, \boldsymbol{j}, \psi, \psi^*]) + (W[n, \boldsymbol{j}, \psi, \psi^*] - U[n]) \\ - \theta(S[n, \boldsymbol{j}, \psi, \psi^*] - S_S[n, \boldsymbol{j}, \psi, \psi^*]). \end{aligned} \tag{4.44}$$

Substituting (4.42) into $\Omega_{v,\boldsymbol{A},D,D^*}[n, \boldsymbol{j}, \psi, \psi^*]$ and using this for HK theorem II in the real system, we have

$$\begin{aligned} &\frac{\delta T_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta n(\mathbf{r})} + \frac{\delta U[n]}{\delta n(\mathbf{r})} - \theta \frac{\delta S_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta n(\mathbf{r})} \\ &\qquad + \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta n(\mathbf{r})} + v(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2 - \mu = 0, \end{aligned} \tag{4.45}$$

$$\frac{\delta T_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \boldsymbol{j}(\mathbf{r})} - \theta \frac{\delta S_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \boldsymbol{j}(\mathbf{r})} + \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \boldsymbol{j}(\mathbf{r})} + \boldsymbol{A}(\mathbf{r}) = \mathbf{0}, \tag{4.46}$$

$$\frac{\delta T_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi(\mathbf{r})} - \theta \frac{\delta S_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi(\mathbf{r})} + \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi(\mathbf{r})} + D^*(\mathbf{r}) = 0, \tag{4.47}$$

$$\frac{\delta T_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi^*(\mathbf{r})} - \theta \frac{\delta S_S[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi^*(\mathbf{r})} + \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi^*(\mathbf{r})} + D(\mathbf{r}) = 0, \tag{4.48}$$

where notations of the functional derivative in equations (4.45) to (4.48) denote the following in detail,

$$\frac{\delta F[n, \boldsymbol{j}, \psi, \psi^*]}{\delta X(\mathbf{r})} = \left. \frac{\delta F[n, \boldsymbol{j}, \psi, \psi^*]}{\delta X(\mathbf{r})} \right|_{n=n_{eq}, \boldsymbol{j}=\boldsymbol{j}_{eq}, \psi=\psi_{eq}, \psi^*=\psi^*_{eq}}. \tag{4.49}$$

Here, F denotes the functional of variables and X deserves variables. Similarly, we can derive below from HK theorem II in the reference system,

$$\begin{aligned} &\frac{\delta T_S[n_S, \boldsymbol{j}_S, \psi_S, \psi_S^*]}{\delta n_S(\mathbf{r})} - \theta \frac{\delta S_S[n_S, \boldsymbol{j}_S, \psi_S, \psi_S^*]}{\delta n_S(\mathbf{r})} \\ &\qquad + \frac{\delta F_{xc}[n_S, \boldsymbol{j}_S, \psi_S, \psi_S^*]}{\delta n_S(\mathbf{r})} + v_S(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}_S(\mathbf{r})^2 - \mu = 0, \end{aligned} \tag{4.50}$$

$$\frac{\delta T_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \boldsymbol{j}_S(\mathbf{r})}-\theta\frac{\delta S_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \boldsymbol{j}_S(\mathbf{r})}+\frac{\delta F_{xc}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \boldsymbol{j}_S(\mathbf{r})}+\boldsymbol{A}_S(\mathbf{r})=\mathbf{0}, \tag{4.51}$$

$$\frac{\delta T_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S(\mathbf{r})}-\theta\frac{\delta S_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S(\mathbf{r})}+\frac{\delta F_{xc}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S(\mathbf{r})}+D_S^*(\mathbf{r})=0, \tag{4.52}$$

$$\frac{\delta T_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S^*(\mathbf{r})}-\theta\frac{\delta S_S[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S^*(\mathbf{r})}+\frac{\delta F_{xc}[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta \psi_S^*(\mathbf{r})}+D_S(\mathbf{r})=0, \tag{4.53}$$

where notations of the functional derivative in equations (4.50) to (4.53) denote the following in detail,

$$\frac{\delta F[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta X(\mathbf{r})}=\left.\frac{\delta F[n_S,\boldsymbol{j}_S,\psi_S,\psi_S^*]}{\delta X(\mathbf{r})}\right|_{n_S=n_{Seq},\boldsymbol{j}_S=\boldsymbol{j}_{Seq},\psi_S=\psi_{Seq},\psi_S^*=\psi_{Seq}^*}. \tag{4.54}$$

We can recognize that equations (4.45) to (4.48) are equations for the thermal equilibrium value of basic variables $n_{eq}(\mathbf{r}),\boldsymbol{j}_{eq}(\mathbf{r}),\psi_{eq}(\mathbf{r}),\psi_{eq}^*(\mathbf{r})$ of the real system while equations (4.50) to (4.53) are for $n_{Seq}(\mathbf{r}),\boldsymbol{j}_{Seq}(\mathbf{r}),\psi_{Seq}(\mathbf{r}),\psi_{Seq}^*(\mathbf{r})$ of the reference system. When (4.45) to (4.48) coincide with (4.50) to (4.53) respectively, the effective potentials $v_S(\mathbf{r})$, $\boldsymbol{A}_S(\mathbf{r})$, $D_S(\mathbf{r})$, $D_S^*(\mathbf{r})$ are considered the potentials that enable us to reproduce $n_{eq}(\mathbf{r}),\boldsymbol{j}_{eq}(\mathbf{r}),\psi_{eq}(\mathbf{r}),\psi_{eq}^*(\mathbf{r})$ in the reference system. In short, we can derive the formulas of the effective potentials which reproduce the same basic variables as those in the real system:

$$v_S(\mathbf{r})=v(\mathbf{r})+\int d\mathbf{r}'u(\mathbf{r},\mathbf{r}')n_{eq}(\mathbf{r}')+\frac{\delta F_{xc}[n,\boldsymbol{j},\psi,\psi^*]}{\delta n(\mathbf{r})}+\frac{1}{2m}\boldsymbol{A}(\mathbf{r})^2-\frac{1}{2m}\boldsymbol{A}_S(\mathbf{r})^2, \tag{4.55}$$

$$\boldsymbol{A}_S(\mathbf{r})=\boldsymbol{A}(\mathbf{r})+\frac{\delta F_{xc}[n,\boldsymbol{j},\psi,\psi^*]}{\delta \boldsymbol{j}(\mathbf{r})}, \tag{4.56}$$

$$D_S(\mathbf{r})=\frac{\delta F_{xc}[n,\boldsymbol{j},\psi,\psi^*]}{\delta \psi^*(\mathbf{r})}, \tag{4.57}$$

$$D_S^*(\mathbf{r})=\frac{\delta F_{xc}[n,\boldsymbol{j},\psi,\psi^*]}{\delta \psi(\mathbf{r})}, \tag{4.58}$$

however, in the derivation of equations (4.55) to (4.58), we made the artificial fields $D(\mathbf{r}), D^*(\mathbf{r})$ zero. In this way, we could get the formulas of the effective potentials.

Taking into consideration that there is an analogy with the vector potential in electromagnetics, the second term of (4.56) may be considered as a sort of vector potential inducing the fluid current consisting of bosons. The vector potential in electromagnetics results from the Coulomb interaction of charged particles, and is coupled with the electric current while the second term of (4.56) results from the boson-boson interaction as (4.56) and is coupled with the current-density $\boldsymbol{j}_{eq}(\mathbf{r})$ as (4.26). On the other hand, as for the effective potential $D_S(\mathbf{r})$, since $D_S(\mathbf{r})$ is coupled with the order parameter of the BEC $\psi_{eq}(\mathbf{r})$, we can recognize that $\psi_{eq}(\mathbf{r})$ is induced by the potential $D_S(\mathbf{r})$ in the reference system. This is similar to the case of superconductors, whose order parameter is induced by the effective pair potential in the reference system in DFT for superconductors.[40,41]

Next, let us derive the single-particle equations for calculating basic variables. First, we focus on the grand canonical Hamiltonian $\hat{H}_S - \mu\hat{N}$ to calculate the expectation of the particle number density operator $\hat{n}(\mathbf{r})$, the current-density operator $\hat{\boldsymbol{j}}(\mathbf{r})$, field operators $\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r})$

$$\hat{K}_S = \hat{H}_S - \mu\hat{N} = \hat{T} + \int d\mathbf{r}[v_S(\mathbf{r}) + \frac{1}{2m}\boldsymbol{A}_S(\mathbf{r})^2 - \mu]\hat{n}(\mathbf{r}) + \int d\mathbf{r}\hat{\boldsymbol{j}}(\mathbf{r})\cdot\boldsymbol{A}_S(\mathbf{r}) + \hat{D}_S, \tag{4.59}$$

here, we can rewrite above (4.59) as

$$\hat{K}_S = \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})(\hat{h}_S - \mu)\hat{\psi}(\mathbf{r}) + \hat{D}_S, \tag{4.60}$$

$$\hat{h}_S = \frac{1}{2m}(\hat{\boldsymbol{p}} + \boldsymbol{A}_S(\mathbf{r}))^2 + v_S(\mathbf{r}). \tag{4.61}$$

As seen in (4.26), the Hamiltonian in the reference system $\hat{H}_S$ and the total particle number operator $\hat{N}$ are not commutative, therefore, the calculation of the trace concerning the expectation of physical quantities such as (4.34) is difficult. However, if $\hat{H}_S$ had been the quadratic form concerning the field operator, it could have been diagonalized simultaneously with $\hat{N}$. On the other hand, $\hat{H}_S$ includes the pair potential term described by $\hat{D}_S$, which is the first-order term of the field operator. Then, with reference to the Bogoliubov theory[20,21], we consider that the field operator for bosons $\hat{\psi}(\mathbf{r})$ is described by the sum of one complex classical field $\Psi(\mathbf{r})$ and the operator of the difference $\hat{\psi}(\mathbf{r})$ and $\Psi(\mathbf{r})$ written as $\hat{\tilde{\psi}}(\mathbf{r})$,

$$\hat{\psi}(\mathbf{r}) = \Psi(\mathbf{r}) + \tilde{\tilde{\hat{\psi}}}(\mathbf{r}). \tag{4.62}$$

As seen in Chapter 2, in the Bogoliubov theory, the solution of the GP equation $\psi_{GP}(\mathbf{r})$ corresponds to this classical field $\Psi(\mathbf{r})$ so that the first-order terms of the fluctuation vanish in its Hamiltonian. On the other hand, in our case, we determine $\Psi(\mathbf{r})$ so that the first order terms of $\tilde{\tilde{\hat{\psi}}}(\mathbf{r})$ vanish in $\hat{K}_S$. Specifically, we substitute (4.62) into (4.60) as

$$\begin{aligned}
\hat{K}_S = &\int d\mathbf{r}\Psi^*(\mathbf{r})[\hat{h}_S - \mu]\Psi(\mathbf{r}) + \int d\mathbf{r}[\Psi(\mathbf{r})D_S^*(\mathbf{r}) + \Psi^*(\mathbf{r})D_S(\mathbf{r})] \\
&+ \int d\mathbf{r}[(\hat{h}_S - \mu)\Psi(\mathbf{r}) + D_S(\mathbf{r})]\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r}) + \int d\mathbf{r}[(\hat{h}_S^\dagger - \mu)\Psi^*(\mathbf{r}) + D_S^*(\mathbf{r})]\tilde{\tilde{\hat{\psi}}}(\mathbf{r}) \\
&+ \int d\mathbf{r}\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})[\hat{h}_S - \mu]\tilde{\tilde{\hat{\psi}}}(\mathbf{r}).
\end{aligned} \tag{4.63}$$

As shown in equation (4.63), the first and second terms on the right-hand side of equation (4.63) deserve the zeroth-order terms of $\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})$ and $\tilde{\tilde{\hat{\psi}}}(\mathbf{r})$. Then, the third and fourth terms are first-order terms, and the last term is the second-order term of $\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})$ and $\tilde{\tilde{\hat{\psi}}}(\mathbf{r})$, respectively. Here, we determine complex classical fields $\Psi(\mathbf{r})$ and $\Psi^*(\mathbf{r})$ as functions that satisfy the below :

$$(\hat{h}_S - \mu)\Psi(\mathbf{r}) = -D_S(\mathbf{r}), \tag{4.64}$$

$$(\hat{h}_S^\dagger - \mu)\Psi^*(\mathbf{r}) = -D_S^*(\mathbf{r}). \tag{4.65}$$

When $\Psi(\mathbf{r})$ and $\Psi^*(\mathbf{r})$ are determined by (4.64) and (4.65), we can eliminate the first-order terms of $\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})$ and $\tilde{\tilde{\hat{\psi}}}(\mathbf{r})(\hat{h}_S$ is the Hermitian operator[51], so note that (4.64) and (4.65) are equivalent). We refer to the equation (4.64) as the Gross-Pitaevskii-Kohn-Sham(GPKS) equation. Thus, using these classical fields, we can rewrite (4.63) as

$$\hat{K}_S = K_0 + \int d\mathbf{r}\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})[\hat{h}_S - \mu]\tilde{\tilde{\hat{\psi}}}(\mathbf{r}), \tag{4.66}$$

here, we described the zeroth-order terms of $\tilde{\tilde{\hat{\psi}}}^\dagger(\mathbf{r})$ and $\tilde{\tilde{\hat{\psi}}}(\mathbf{r})$ as K_0 in the equation (4.66). In this way, we can calculate the trace concerning the expectation of physical quantities by using the grand canonical Hamiltonian given by (4.66).

As a next step, since the operator $\hat{K}_S$ is the quadratic form concerning $\tilde{\hat{\psi}}^\dagger(\mathbf{r})$ and $\tilde{\hat{\psi}}(\mathbf{r})$, we here expand $\tilde{\hat{\psi}}^\dagger(\mathbf{r})$ and $\tilde{\hat{\psi}}(\mathbf{r})$ by using the eigenfunctions of the operator $\hat{h}_S$. We denote the eigenfunctions and eigenvalues of $\hat{h}_S$ as $\phi_i(\mathbf{r})$, ϵ_i, respectively,

$$\hat{h}_S \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}), \tag{4.67}$$

then, we expand as

$$\tilde{\hat{\psi}}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \hat{a}_i, \tag{4.68}$$

$$\tilde{\hat{\psi}}^\dagger(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r}) \hat{a}_i^\dagger, \tag{4.69}$$

where $\hat{a}_i^\dagger$ and $\hat{a}_i$ are the creation and annihilation operators for a certain boson with the state $\phi_i(\mathbf{r})$, respectively. By equations (4.67) to (4.69), we rewrite (4.66) as

$$\hat{K}_S = K_0 + \sum_i (\epsilon_i - \mu) \hat{a}_i^\dagger \hat{a}_i. \tag{4.70}$$

We refer to the equation (4.67) as the Kohn-Sham(KS) equation.

4.4 Formulas of basic variables

Next step, we shall derive formulas of basic variables by using (4.70). Specifically, we substitute (4.70) into (4.32) and (4.33), then by using these results, we calculate the trace such as (4.34) and can get the following results from equations (4.34) to (4.37) by means of the similar calculation procedure with FTDFT,

$$\begin{aligned} n_{eq}(\mathbf{r}) &= |\Psi(\mathbf{r})|^2 + \mathrm{Tr}[\hat{\rho}_{Seq} \tilde{\hat{\psi}}^\dagger(\mathbf{r}) \tilde{\hat{\psi}}(\mathbf{r})] \\ &= |\Psi(\mathbf{r})|^2 + \sum_{i,j} \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}) \mathrm{Tr}[\hat{\rho}_{Seq} \hat{a}_i^\dagger \hat{a}_j] \\ &= |\Psi(\mathbf{r})|^2 + \sum_i |\phi_i(\mathbf{r})|^2 f_B(\epsilon_i), \end{aligned} \tag{4.71}$$

$$
\begin{aligned}
\boldsymbol{j}_{eq}(\mathbf{r}) &= \frac{\hbar}{2mi}(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \Psi(\mathbf{r})\nabla\Psi^*(\mathbf{r})) + \mathrm{Tr}[\hat{\rho}_{Seq} \\
&\times \frac{\hbar}{2mi}(\tilde{\hat{\psi}}^\dagger(\mathbf{r})\nabla\tilde{\hat{\psi}}(\mathbf{r}) - \tilde{\hat{\psi}}(\mathbf{r})\nabla\tilde{\hat{\psi}}^\dagger(\mathbf{r}))] \\
&= \frac{\hbar}{2mi}(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \Psi(\mathbf{r})\nabla\Psi^*(\mathbf{r})) + \sum_{i,j}\mathrm{Tr}[\hat{\rho}_{Seq}\hat{a}_i^\dagger\hat{a}_j] \\
&\times \frac{\hbar}{2mi}(\phi_i^*(\mathbf{r})\nabla\phi_j(\mathbf{r}) - \phi_j(\mathbf{r})\nabla\phi_i^*(\mathbf{r})) \\
&= \frac{\hbar}{2mi}(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \Psi(\mathbf{r})\nabla\Psi^*(\mathbf{r})) \\
&+ \sum_i \frac{\hbar}{2mi}(\phi_i^*(\mathbf{r})\nabla\phi_i(\mathbf{r}) - \phi_i(\mathbf{r})\nabla\phi_i^*(\mathbf{r}))f_B(\epsilon_i),
\end{aligned}
\tag{4.72}
$$

$$
\psi_{eq}(\mathbf{r}) = \Psi(\mathbf{r}) + \mathrm{Tr}[\hat{\rho}_{Seq}\tilde{\hat{\psi}}(\mathbf{r})] = \Psi(\mathbf{r}),
\tag{4.73}
$$

$$
\psi_{eq}^*(\mathbf{r}) = \Psi^*(\mathbf{r}) + \mathrm{Tr}[\hat{\rho}_{Seq}\tilde{\hat{\psi}}^\dagger(\mathbf{r})] = \Psi^*(\mathbf{r}),
\tag{4.74}
$$

where in equations (4.71) and (4.72), $f_B(\epsilon_i)$ denotes the Bose-Einstein distribution function which is the expectation of the occupation number concerning the single-particle state i in the thermal equilibrium state of the reference system. In this way, basic variables $n_{eq}(\mathbf{r}), \boldsymbol{j}_{eq}(\mathbf{r}), \psi_{eq}(\mathbf{r}), \psi_{eq}^*(\mathbf{r})$ can be reproduced in the reference system by solving the GPKS and KS equations.

Here note that the classical field $\Psi(\mathbf{r})$ is just the order parameter of the BEC as shown in equations (4.73) and (4.74). Thus, we can recognize that the GPKS equation is the single-particle equation that the order parameter of the BEC satisfies. As seen in Chapter 2, the order parameter of the BEC is the eigenfunction of the one-particle reduced density matrix whose occupied number, which is its eigenvalue, is $O(N)$. Specifically, $\Psi(\mathbf{r})$ is the function described by the multiplication of the square root of the eigenvalue and the eigenfunction of the one-particle reduced density matrix. Thus, the first term on the right-hand side of (4.71) is regarded as the particle number density of the superfluid component. And more, $n_{eq}(\mathbf{r})$ is the total particle number density of superfluids, so the second term on the right-hand side of (4.71) is regarded as the particle number density of the normal fluid component. Moreover, since we reproduce $n_{eq}(\mathbf{r})$ and $\Psi(\mathbf{r})$ in the reference system, another term, i.e., the term of the normal fluid component can be also reproduced. A similar discussion can be done concerning the current-density $\boldsymbol{j}_{eq}(\mathbf{r})$. The relationship between sf-CDFT and the two-fluid model will be discussed in Chapter 5.

Finally, let us comment on the calculation procedure. This procedure is shown in Fig.4.3. Specifically, we can write it below.
(i)Assume a set of basic variables
(ii)The effective potentials given by (4.55) to (4.58) are prepared.
(iii)By using effective potentials of (ii), solve the GPKS and KS equations.
(iv)Using solutions of the GPKS and KS equations, basic variables are calculated by means of formulas (4.71) to (4.74).
(v)Compare the obtained basic variables with the trial set of those of (i) and verify the self-consistency. If basic variables are inconsistent with some accuracy, this calculation procedure is restarted and the input is changed. We repeat this calculation procedure until the self-consistency is achieved, and when we can verify this self-consistency, it follows that the GPKS and KS equations are solved in conjunction.
(vi)We can calculate the particle number density and current-density of the superfluid component by using the solution of the GPKS equation, while those physical quantities of the normal fluid component by using the solution of the KS equation.

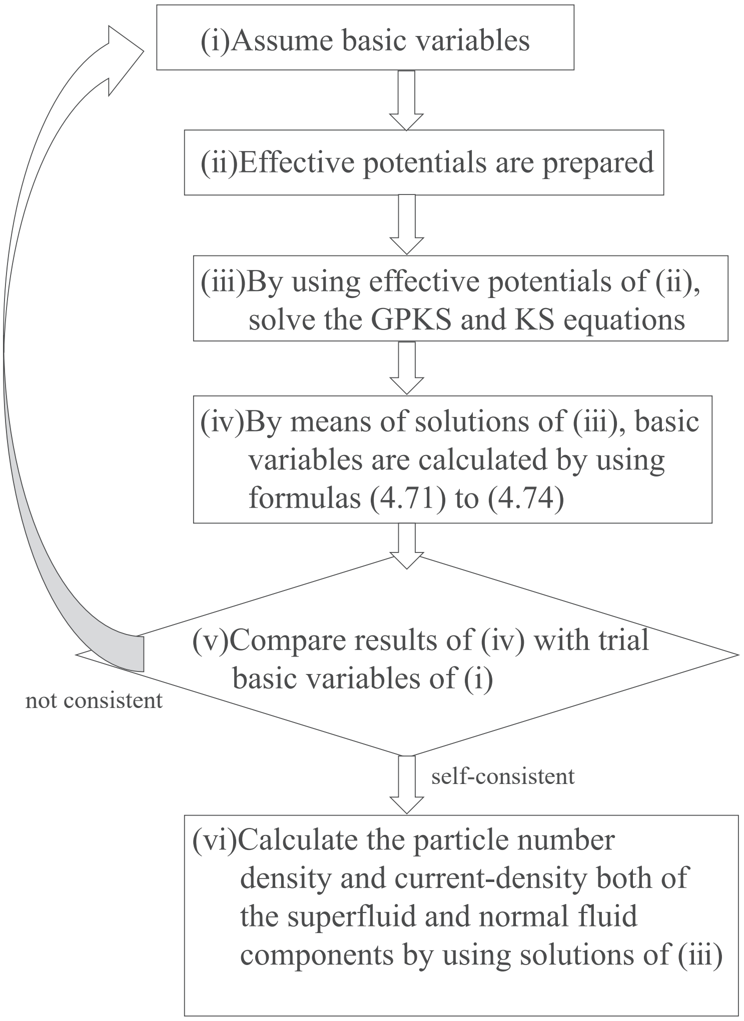

Fig. 4.3: The calculation procedure in sf-CDFT

Chapter 5

Discussion

In this chapter, we will discuss some features and advantages of sf-CDFT. In the first section, we derive the sum rule for the xc energy functional which is expected to be used for developing its approximate form. In the next section, we compare sf-CDFT with conventional theories for superfluids which are introduced in Chapter 2. Specifically, we focus on the comparison with the two-fluid model, the GP theory and the Bogoliubov theory, respectively.

5.1 Sum rule for the exchange-correlation energy functional

Before deriving the sum rule, first, let us show the continuity equation for superfluids. Take the complex conjugate of the equation which is the multiplication of (4.64) and $\Psi^*(\mathbf{r})$, and subtract its original equation from this conjugate one, then we get

$$\nabla \cdot [\boldsymbol{j}_{\mathrm{sf}}(\mathbf{r}) + \frac{1}{m} n_{\mathrm{sf}}(\mathbf{r}) \boldsymbol{A}_S(\mathbf{r})] = -\frac{2}{\hbar} \operatorname{Im}[\Psi(\mathbf{r}) D_S^*(\mathbf{r})]. \tag{5.1}$$

Here, $n_{\mathrm{sf}}(\mathbf{r})$ and $\boldsymbol{j}_{\mathrm{sf}}(\mathbf{r})$ are the particle number density and current-density of the superfluid component shown in a later discussion,

$$n_{\mathrm{sf}}(\mathbf{r}) = |\Psi(\mathbf{r})|^2, \tag{5.2}$$

$$\boldsymbol{j}_{\mathrm{sf}}(\mathbf{r}) = \frac{\hbar}{2mi}(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \nabla\Psi^*(\mathbf{r})\Psi(\mathbf{r})). \tag{5.3}$$

Next, we also follow the same way with the above for the equation (4.67), and we derive

$$\nabla \cdot [\boldsymbol{j}_{\mathrm{nf}}(\mathbf{r}) + \frac{1}{m} n_{\mathrm{nf}}(\mathbf{r}) \boldsymbol{A}_S(\mathbf{r})] = 0, \tag{5.4}$$

where $n_{\mathrm{nf}}(\mathbf{r})$ and $\boldsymbol{j}_{\mathrm{nf}}(\mathbf{r})$ are the particle number density and current-density of the normal fluid component also shown in a later discussion,

$$n_{\mathrm{nf}}(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2 f_B(\epsilon_i), \tag{5.5}$$

$$\boldsymbol{j}_{\mathrm{nf}}(\mathbf{r}) = \sum_i \frac{\hbar}{2mi} (\phi_i^*(\mathbf{r}) \nabla \phi_i(\mathbf{r}) - \phi_i(\mathbf{r}) \nabla \phi_i^*(\mathbf{r})) f_B(\epsilon_i). \tag{5.6}$$

Finally, we add both hand sides of (5.1) and those of (5.4) and use (4.71), (4.72), then we get

$$\nabla \cdot [\boldsymbol{j}_{\mathrm{eq}}(\mathbf{r}) + \frac{1}{m} n_{\mathrm{eq}}(\mathbf{r}) \boldsymbol{A}_S(\mathbf{r})] = -\frac{2}{\hbar} \mathrm{Im}[\Psi(\mathbf{r}) D_S^*(\mathbf{r})]. \tag{5.7}$$

On the other hand, the continuity equation in the real system is given as

$$\nabla \cdot [\boldsymbol{j}_{\mathrm{eq}}(\mathbf{r}) + \frac{1}{m} n_{\mathrm{eq}}(\mathbf{r}) \boldsymbol{A}(\mathbf{r})] = 0. \tag{5.8}$$

Therefore, from equations (4.56), (5.7), and (5.8), we derive the equation of the sum rule for the xc energy functional given as

$$\nabla \cdot \{n_{\mathrm{eq}}(\mathbf{r}) \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \boldsymbol{j}(\mathbf{r})}\} = -\frac{2m}{\hbar} \mathrm{Im}\{\Psi(\mathbf{r}) \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \psi(\mathbf{r})}\}, \tag{5.9}$$

where of course the functional derivative in the equation (5.9) follows the same notation introduced in the equation (4.49).

Eq.(5.9) is the equation of the condition that the xc energy functional should satisfy. The approximate form of the xc energy functional in the original DFT or its extensions has been developed by the equation of the sum rule for the xc energy functional as the restrictive conditions[52-56]. About this, we can suggest some examples which are the generalized gradient approximation[52-54] in DFT, the vorticity expansion approximation in the current-density functional theory(CDFT)[55,56], and so on. Thus, the equation (5.9) is considered to be used for developing the approximate form of the xc energy functional in sf-CDFT.

5.2 Comparison with conventional theories

5.2.1 sf-CDFT and two-fluid model

From this subsection, we shall compare sf-CDFT with conventional theories for superfluids shown in Chapter 2. First, we start to comment on the comparison with the two-fluid model. As shown in Chapter 2, in the two-fluid model, we consider that superfluids consist of two components called the superfluid and normal fluid components respectively, and it is known that they interact through the quantum vortex. In this subsection, we insist that sf-CDFT can reproduce these components simultaneously while incorporating the effect of their interaction.

First, as mentioned in Chapter 4, terms of the particle number density and current-density which are respectively described by the order parameter of the BEC $\Psi(\mathbf{r})$ are physical quantities concerning the superfluid component while the remaining terms which are described by solutions of the KS equation ϵ_i and $\phi_i(\mathbf{r})$ are physical quantities concerning the normal fluid component. Here, we denote the particle number density and current-density of the superfluid component as $n_{\mathrm{sf}}(\mathbf{r})$ and $\boldsymbol{j}_{\mathrm{sf}}(\mathbf{r})$, and also those of the normal fluid component as $n_{\mathrm{nf}}(\mathbf{r})$ and $\boldsymbol{j}_{\mathrm{nf}}(\mathbf{r})$, then at this time, equations (4.71) and (4.72) are rewritten as

$$n_{eq}(\mathbf{r}) = n_{\mathrm{sf}}(\mathbf{r}) + n_{\mathrm{nf}}(\mathbf{r}), \tag{5.10}$$

$$\boldsymbol{j}_{eq}(\mathbf{r}) = \boldsymbol{j}_{\mathrm{sf}}(\mathbf{r}) + \boldsymbol{j}_{\mathrm{nf}}(\mathbf{r}), \tag{5.11}$$

with

$$n_{\mathrm{sf}}(\mathbf{r}) = |\Psi(\mathbf{r})|^2, \tag{5.12}$$

$$\boldsymbol{j}_{\mathrm{sf}}(\mathbf{r}) = \frac{\hbar}{2mi}(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \nabla\Psi^*(\mathbf{r})\Psi(\mathbf{r})), \tag{5.13}$$

$$n_{\mathrm{nf}}(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2 f_B(\epsilon_i), \tag{5.14}$$

$$\boldsymbol{j}_{\mathrm{nf}}(\mathbf{r}) = \sum_i \frac{\hbar}{2mi}(\phi_i^*(\mathbf{r})\nabla\phi_i(\mathbf{r}) - \phi_i(\mathbf{r})\nabla\phi_i^*(\mathbf{r}))f_B(\epsilon_i). \tag{5.15}$$

Also, take the term described by the vector potential $\boldsymbol{A}(\mathbf{r})$ into consideration, and the total current-density in the real system when $\boldsymbol{A}(\mathbf{r})$ occurs is given by

$$\boldsymbol{J}_{eq}(\mathbf{r}) = \boldsymbol{j}_{eq}(\mathbf{r}) + \frac{1}{m}n_{eq}(\mathbf{r})\boldsymbol{A}(\mathbf{r}). \tag{5.16}$$

Here, we can divide this equation (5.16) into two parts concerning the superfluid and the normal fluid components respectively,

$$\boldsymbol{J}_{\rm sf}(\mathbf{r}) = \boldsymbol{j}_{\rm sf}(\mathbf{r}) + \frac{1}{m} n_{\rm sf}(\mathbf{r}) \boldsymbol{A}(\mathbf{r}), \tag{5.17}$$

$$\boldsymbol{J}_{\rm nf}(\mathbf{r}) = \boldsymbol{j}_{\rm nf}(\mathbf{r}) + \frac{1}{m} n_{\rm nf}(\mathbf{r}) \boldsymbol{A}(\mathbf{r}), \tag{5.18}$$

where $\boldsymbol{J}_{\rm sf}(\mathbf{r})$ and $\boldsymbol{J}_{\rm nf}(\mathbf{r})$ are total current-densities concerning the superfluid and normal fluid components respectively. In sf-CDFT, the order parameter of the BEC $\Psi(\mathbf{r})$ is reproduced, and then, physical quantities of the superfluid component such as $n_{\rm sf}(\mathbf{r})$ and $\boldsymbol{j}_{\rm sf}(\mathbf{r})$, which are given by $\Psi(\mathbf{r})$, are also reproduced and also, as shown in (5.17), the total current-density of the superfluid component $\boldsymbol{J}_{\rm sf}(\mathbf{r})$ is reproduced. Similarly, as for the normal fluid component, the particle number density and current-density of superfluids $n_{eq}(\mathbf{r})$ and $\boldsymbol{j}_{eq}(\mathbf{r})$ are reproduced, then physical quantities of the normal fluid component such as $n_{\rm nf}(\mathbf{r})$ and $\boldsymbol{j}_{\rm nf}(\mathbf{r})$, which are given by subtractions between $n_{eq}(\mathbf{r})$ and $n_{\rm sf}(\mathbf{r})$, $\boldsymbol{j}_{eq}(\mathbf{r})$ and $\boldsymbol{j}_{\rm sf}(\mathbf{r})$ respectively, are also reproduced and as shown in (5.18), the total current-density of the normal fluid component $\boldsymbol{J}_{\rm nf}(\mathbf{r})$ is reproduced. Therefore, sf-CDFT can deal with the superfluid and normal fluid components simultaneously. Moreover, as seen in formulas of the effective potentials which are included in the GPKS and KS equations, these potentials include not only the effect of the interaction between the superfluid and normal fluid components described by the classical boson-boson interaction $U[n]$, but also the xc energy functional $F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]$. Thus, sf-CDFT is the theory that it enables the simultaneous reproduction of the superfluid and normal fluid components while incorporating the effect of their interaction. This point is quite different from conventional theories for superfluids like the GP and Bogoliubov theories, as mentioned in the later subsection.

5.2.2 sf-CDFT and Gross-Pitaevskii theory

As mentioned in Chapter 2, the GP theory is related to the superfluid component, and its density and current-density are respectively calculated by using the solution of the Gross-Pitaevskii equation given by

$$(-\frac{\hbar^2\nabla^2}{2m} + v(\mathbf{r}) + g|\Psi_{GP}(\mathbf{r})|^2)\Psi_{GP}(\mathbf{r}) = \mu\Psi_{GP}(\mathbf{r}). \tag{5.19}$$

Here, we can show that the solution of the GPKS equation $\Psi(\mathbf{r})$ given from (4.64) includes some correction terms in addition to the solution of the GP equation given from (5.19). To compare $\Psi(\mathbf{r})$ with $\Psi_{GP}(\mathbf{r})$, first let us rewrite the GPKS equation of (4.64) like,

$$\nabla^2\Psi(\mathbf{r}) = \frac{2m}{\hbar^2} f(\mathbf{r}), \tag{5.20}$$

with

$$\begin{aligned} f(\mathbf{r}) = D_S(\mathbf{r}) + [&\frac{1}{2m}([\hat{\boldsymbol{p}}, \boldsymbol{A}_S(\mathbf{r})] + \boldsymbol{A}_S(\mathbf{r})^2) + v(\mathbf{r}) - \mu \\ &+ v_H(\mathbf{r}) + v_{xc}(\mathbf{r})]\Psi(\mathbf{r}), \end{aligned} \tag{5.21}$$

where $v_H(\mathbf{r})$ and $v_{xc}(\mathbf{r})$ are

$$v_H(\mathbf{r}) = \int d\mathbf{r}' u(\mathbf{r}, \mathbf{r}') n_{eq}(\mathbf{r}'), \tag{5.22}$$

$$v_{xc}(\mathbf{r}) = \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta n(\mathbf{r})}. \tag{5.23}$$

Here, for the comparison with the solution of the GP equation, let us use the delta function model as $u(\mathbf{r}, \mathbf{r}')$ like

$$u(\mathbf{r}, \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}'), \tag{5.24}$$

where g is a positive factor[17,18], and by (5.24) we get

$$v_H(\mathbf{r}) = g n_{eq}(\mathbf{r}). \tag{5.25}$$

Eq.(5.25) is the interaction term which is shown in the GP equation. Eq. (5.20) is similar to the Poisson equation, so we get the general solution for (5.20) from the addition of the general solution of the Laplace equation and the particular solution of (5.20), which is given by using the Green function for the free particle. From this discussion, we can get the general solution of (5.20) as

$$\Psi(\mathbf{r}) = \Psi_{GP}(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int d\mathbf{r}' \frac{D_S(\mathbf{r}') + [\hat{a}_{xc}(\mathbf{r}') + v_{H,\mathrm{nf}}(\mathbf{r}') + v_{xc}(\mathbf{r}')]\Psi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \tag{5.26}$$

where

$$\hat{a}_{xc}(\mathbf{r}) = \frac{[\hat{\boldsymbol{p}}, \boldsymbol{A}_{xc}(\mathbf{r})] + 2\boldsymbol{A}(\mathbf{r}) \cdot \boldsymbol{A}_{xc}(\mathbf{r}) + \boldsymbol{A}_{xc}(\mathbf{r})^2}{2m}, \tag{5.27}$$

$$\boldsymbol{A}_{xc}(\mathbf{r}) = \frac{\delta F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]}{\delta \boldsymbol{j}(\mathbf{r})}, \tag{5.28}$$

$$v_{H,\mathrm{sf}}(\mathbf{r}) = \int d\mathbf{r}' u(\mathbf{r}, \mathbf{r}') n_{\mathrm{sf}}(\mathbf{r}'), \tag{5.29}$$

$$v_{H,\mathrm{nf}}(\mathbf{r}) = \int d\mathbf{r}' u(\mathbf{r}, \mathbf{r}') n_{\mathrm{nf}}(\mathbf{r}'). \tag{5.30}$$

Here, if the xc energy functional is ignored and we take $v_{H,\mathrm{sf}}(\mathbf{r})$, which is the potential concerning the superfluid component, into consideration as $v_H(\mathbf{r})$, our GPKS equation is reduced to the GP equation. Concomitantly with this reduction, the equation (5.26) becomes like $\Psi(\mathbf{r}) = \Psi_{GP}(\mathbf{r})$. On the other hand, we can consider that the second term on the right-hand side of the equation (5.26) is the correction term resulting from the effect of the xc energy functional and classical interaction potential between the superfluid and normal fluid components. Therefore, the order parameter reproduced in sf-CDFT is determined by the interaction term between the superfluid and normal fluid components via $v_{H,\mathrm{nf}}(\mathbf{r})$, while the order parameter of the GP theory is determined by only the interaction in the superfluid component. Moreover, as shown in the equation (5.26), our order parameter in sf-CDFT includes effects concerning the xc energy functional via $v_{xc}(\mathbf{r})$, $\boldsymbol{A}_{xc}(\mathbf{r})$, and $D_S(\mathbf{r})$ which are described as the functional derivative of the xc energy functional, and also about the KS equation, these effects are included in the KS equation as effective potentials, and of course, this KS equation includes the effect of the interaction between the superfluid and normal fluid components. Thus, the physical quantities of these components are considered to be interrelated, and these physical quantities can be determined by solving the GPKS and KS equations in conjunction.

5.2.3 sf-CDFT and Bogoliubov theory

As seen in Chapter 2, the Bogoliubov theory is the theory that the normal fluid component is considered in addition to the superfluid component given by the solution of the GP equation. In this theory, physical quantities such as the density and current-density of the superfluid component are calculated from the GP theory, however, we should calculate them separately with the Bogoliubov theory, and as for physical quantities of the normal fluid component, they can be calculated by the excited energy spectrum of the quasiparticle in the Bogoliubov theory. In other words, about these conventional theories, we cannot calculate these physical quantities of the superfluid and normal fluid components simultaneously within just one theory.

In contrast, in our sf-CDFT, the particle number density and current-density reproduced in this theory can be expressed by two crucial terms, which are described by the order parameter of the BEC given from the GPKS equation and are described by solutions of the KS equation. The former corresponds to the superfluid component, and the latter corresponds to the normal fluid component. In this way, in our sf-CDFT, we can calculate physical quantities such as the particle number density and current-density of the superfluid and normal fluid components simultaneously within just one theory.

In addition, the Bogoliubov theory does not include the term of the effect concerning the interaction between the superfluid and normal fluid components as shown in Chapter 2, on the other hand, as mentioned above, our theory can incorporate this effect in terms concerning not only the classical boson-boson interaction about two-fluids but also the xc energy functional $F_{xc}[n, \boldsymbol{j}, \psi, \psi^*]$. We can insist on this crucial point as the difference between our sf-CDFT and the Bogoliubov theory.

Chapter 6

Conclusion

We have proposed sf-CDFT, which is applied to superfluids consisting of bosons interacting with each other. In our theory, basic variables such as the particle number density and current-density of superfluids, and also the order parameter of the BEC are reproduced if we solve the GPKS and KS equations in conjunction and self-consistently. One of the noteworthiest points in our theory is that physical quantities such as the particle number density and current-density of the superfluid and normal fluid components can be calculated simultaneously. Moreover, sf-CDFT is the theory incorporating the effect of the interaction between the superfluid and normal fluid components, in other words, our theory can consider the effect of the interaction of two fluids. Thus, we may be able to insist that sf-CDFT gives the microscopic foundation of the two-fluid model for superfluids. As for the application to the real system, we can mention that sf-CDFT can be applied to not only superfluids consisting of bosons interacting weakly but also one consisting of bosons interacting strongly such as the liquid helium-4.

In sf-CDFT, the physical quantities of the superfluid component are calculated by using the solution of the GPKS equation while those of the normal fluid component are calculated by using solutions of the KS equation. These two equations are interrelated via the classical boson-boson interaction potential and effective potentials described by the xc energy functional. In other words, the superfluid and normal fluid components move with mutual interaction. Therefore, it is insisted that our theory incorporates the mutual friction of the superfluid and normal fluid components in terms of not only the classical boson-boson interaction but also the xc energy functional. In addition, the backflow effect[57-59] may be incorporated via the developed xc energy functional. It is known that this backflow occurs when bosons constituting superfluids push others out of the way as they move, and that's why the backflow effect is caused by the boson-boson interaction. Thus, this backflow effect may be incorporated when we develop the approximate form of the xc energy functional. This topic is our future study.

We also mention the calculation method in our theory. To carry out the calculation, we need to develop the approximate form of the xc energy functional. About this, we have already prepared the condition formula that the xc energy functional should satisfy and we can utilize this when developing the approximate form of the xc energy functional. In addition to this, we need to develop the numerical calculation method for the differential equation including the vector potential. As for this, we have also developed a method for the case where a uniform magnetic field is applied[60,61]. While referring to this, we can develop the numerical calculation method for the GPKS and KS equations in sf-CDFT.

Appendix

A.A vector potential in the rotational coordinate system

Now, consider that we stand in the rotational coordinate system moving with the current-density $\boldsymbol{j}(\mathbf{r})$, and let us write $\mathbf{r}'$ as the position vector in this rotational coordinate system. Furthermore, we write a constant vector $\boldsymbol{\omega}$ as the angular velocity vector related to $\boldsymbol{j}(\mathbf{r})$, which is in the direction of the z'-axis like

$$\boldsymbol{\omega} = (0, 0, \omega). \tag{A.1}$$

First, we consider the following situation.

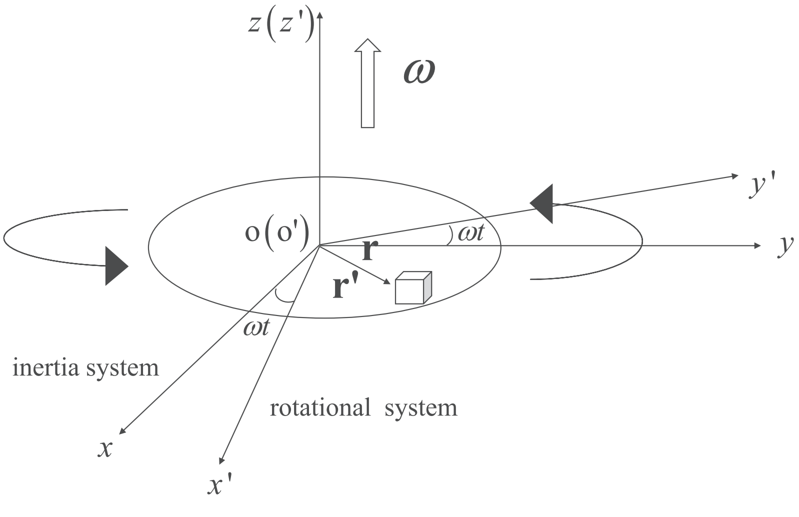

Fig. A.1: The rotational coordinate system

Where the system whose original point is o is the inertia system while the system whose original point is o' is the rotational coordinate system, and $\mathbf{r}$ is the position vector in the inertia system. In this case, the relation of coordinates between the inertia system and the rotational system is described as

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\omega t & \sin\omega t & 0 \\ -\sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{A.2}$$

Next, let us rewrite (A.2) as

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\omega t & -\sin\omega t & 0 \\ \sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}, \tag{A.3}$$

then, differentiate x, y, z with respect to time,

$$\dot{x} = \dot{x}' \cos\omega t - \omega x' \sin\omega t - \dot{y}' \sin\omega t - \omega y' \cos\omega t, \tag{A.4}$$
$$\dot{y} = \dot{x}' \sin\omega t + \omega x' \cos\omega t + \dot{y}' \cos\omega t - \omega y' \sin\omega t, \tag{A.5}$$
$$\dot{z} = \dot{z}'. \tag{A.6}$$

Now, we consider the Lagrangian of the inertia system given by

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - U(x, y, z), \tag{A.7}$$

where m is the mass of a particle constituting the system, and U is the potential energy including the external potential and interaction potential depending on x, y, z. Let us substitute (A.4) to (A.6) into (A.7), and rewrite the Lagrangian as the formula described by coordinates (x', y', z') and $(\dot{x}', \dot{y}', \dot{z}')$,

$$L = \frac{m}{2}\{(\dot{x}' - \omega y')^2 + (\dot{y}' + \omega x')^2 + \dot{z}'^2\} - V(x', y', z'), \tag{A.8}$$

where $V(\mathbf{r}')$ is the potential term rewritten by using (A.3). Then we can calculate the canonical momentum in the rotational coordinate system by using

$$p'_i = \frac{\partial L}{\partial \dot{q}'_i}, \tag{A.9}$$

therefore, a careful calculation by using (A.8) and (A.9) leads us to the following results,

$$
\begin{aligned}
p'_x &= m\dot{x}' - m\omega y', &\text{(A.10)}\\
p'_y &= m\dot{y}' + m\omega x', &\text{(A.11)}\\
p'_z &= m\dot{z}'. &\text{(A.12)}
\end{aligned}
$$

In equations (A.10) to (A.12), we can also rewrite them as the vector notation,

$$\boldsymbol{p'} = m\dot{\boldsymbol{r'}} + m\boldsymbol{\omega} \times \boldsymbol{r'}, \tag{A.13}$$

where $\boldsymbol{p'} = (p'_x, p'_y p'_z)$ is the canonical momentum vector in the rotational coordinate system. Thus, we can calculate the classical Hamiltonian of a particle constituting superfluids in the rotational coordinate system H by using (A.13) and the Legendre transformation given by

$$H = \sum_i p'_i \dot{q'}_i - L, \tag{A.14}$$

therefore, by using (A.8) and (A.14), we finally get the following result,

$$H = \frac{\boldsymbol{p'}^2}{2m} - \boldsymbol{p'} \cdot (\boldsymbol{\omega} \times \mathbf{r}') + \frac{1}{2m}(m\boldsymbol{\omega} \times \mathbf{r}')^2 - \frac{m\omega^2}{2}(x'^2 + y'^2) + V(\mathbf{r}'). \tag{A.15}$$

Here, we can rewrite the equation (A.15) as

$$H = \frac{\boldsymbol{p'}^2}{2m} + \frac{\boldsymbol{p'}}{m} \cdot \boldsymbol{A}(\mathbf{r}') + \frac{1}{2m}\boldsymbol{A}(\mathbf{r}')^2 - \frac{m\omega^2}{2}(x'^2 + y'^2) + V(\mathbf{r}'), \tag{A.16}$$

with

$$\boldsymbol{A}(\mathbf{r}') \equiv -m\boldsymbol{\omega} \times \mathbf{r}'. \tag{A.17}$$

In this way, the fictitious vector potential $\boldsymbol{A}(\mathbf{r}')$ appears in the rotational coordinate system moving with $\boldsymbol{j}(\mathbf{r}')$. Of course, although the above derivation is related to the Hamiltonian of a particle, we can also extend this derivation to the whole system consisting of many particles, and the fictitious vector potential $\boldsymbol{A}(\mathbf{r}')$ also appears in the rotational system as well as (A.16).

B.Spectral decomposition of the one-particle reduced density matrix

Now, we denote the eigenvalues and eigenfunctions of the one-particle reduced density matrix $\rho_1(\mathbf{r},\mathbf{r}')$ as n_i and $u_i(\mathbf{r}')$, respectively, and the eigen equation concerning $\rho_1(\mathbf{r},\mathbf{r}')$ is described for each i,

$$\int d\mathbf{r}'\rho_1(\mathbf{r},\mathbf{r}')u_i(\mathbf{r}') = n_i u_i(\mathbf{r}). \tag{B.1}$$

Here, multiply $u_i^*(\mathbf{r}'')$ to both hand sides of (B.1), and calculate the sum for i concerning both hand sides,

$$\sum_i u_i^*(\mathbf{r}'')\int d\mathbf{r}'\rho_1(\mathbf{r},\mathbf{r}')u_i(\mathbf{r}') = \sum_i n_i u_i^*(\mathbf{r}'')u_i(\mathbf{r}), \tag{B.2}$$

concerning the left-hand side of the equation (B.2),

$$\begin{aligned}\sum_i u_i^*(\mathbf{r}'')\int d\mathbf{r}'\rho_1(\mathbf{r},\mathbf{r}')u_i(\mathbf{r}') &= \int d\mathbf{r}'\rho_1(\mathbf{r},\mathbf{r}')\sum_i u_i^*(\mathbf{r}'')u_i(\mathbf{r}') \\ &= \int d\mathbf{r}'\rho_1(\mathbf{r},\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}'') \\ &= \rho_1(\mathbf{r},\mathbf{r}''), \end{aligned} \tag{B.3}$$

where in the equation (B.3), we considered the property of the complete set concerning the eigenfunctions $u_i(\mathbf{r})$. Thus, we derive the formula of the spectral decomposition of the one-particle reduced density matrix by equations (B.2) and (B.3),

$$\rho_1(\mathbf{r},\mathbf{r}') = \sum_i n_i u_i^*(\mathbf{r}')u_i(\mathbf{r}). \tag{B.4}$$

Acknowledgments

Finally, I really would like to thank Higuchi K professor for the great assistance to my doctoral research.

This work was partially supported by Grant-in-Aid for Scientific Research (No. 18K03510, and No. 18K03461 and No. 23K03250) of the Japan Society for the Promotion of Science.

References

[1] Kapitza P 1938 Viscosity of Liquid Helium below the λ-Point *Nature* **141** 74
[2] Allen J F and Misener A D 1938 Flow of Liquid Helium II *Nature* **141** 75
[3] Anderson M H, Ensher J R, Metthews M R, Wieman C E and Cornell E A 1995 Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor *Science* **269** 198
[4] Khalatnikov I M 1989 *An Introduction to the Theory of Superfluidity,* (New York: Addison-Wesley)
[5] Pethick C J and Smith H 2008 *Bose-Einstein Condensation in Dilute Gases second edition,* (Cambridge: Cambridge University Press)
[6] Pitaevski L and Stringari S 2003 *Bose-Einstein Condensation,* (Oxford: Oxford University Press)
[7] Leggett A J 2006 *Quantum Liquids* (Oxford: Oxford University Press)
[8] Ueda M 2010 *Fundamentals and New Frontiers of Bose-Einstein Condensation* (Singapore: World Scientific)
[9] Bose S N 1924 Planck ' s Law and Light Quantum Hypothesis Z. *Phys.* **26** 178
[10] Einstein A 1924 Quantentheorie des einatomigen idealen Gases *Ber. Berl. Akad.* **22** 261; Einstein A 2005 Quantentheorie des einatomigen idealen Gases II ibid. **23** 3
[11] London F 1938 The λ-Phenomenon of Liquid Helium and the Bose-Einstein Degeneracy *Nature* **141** 643; London F 1938 On the Bose-Einstein Condensation *Phys. Rev.* **54** 947
[12] Penrose O 1951 On the Quantum Mechanics of Helium II *Philos. Mag.* **42** 1373
[13] Penrose O and Onsager L 1956 Bose-Einstein Condensation and Liquid Helium *Phys. Rev.* **104** 576
[14] Yang C N 1962 Concept of Off-Diagonal Long-Range Order and the Quantum Phases of Liquid He and of Superconductors *Rev. Mod. Phys.* **34** 694
[15] Tisza L 1938 Transport Phenomena in Helium II *Nature* **141** 913
[16] Landau L D 1941 The theory of superfluidity of helium II *J. Phys. USSR* **5** 71

[17] Gross E P 1961 Structure of a quantized vortex in boson systems *Nuovo Cimento* **20** 454

[18] Pitaevskii L P 1961 Voetex lines in an imperfect Bose gas *Soviet Physics JETP* **13** 451

[19] Gross E P 1963 Hydrodynamics of a Superfluid Condensate *J. Math. Phys.* **4** 195

[20] Bogoliubov N N 1947 On the theory of superfluidity *J. Phys. (USSR)* **11** 23

[21] de Gennes P G 1989 *Superconductivity of Metals and Alloys* (Reading, MA: Addison Wesley)

[22] Vinen W F 1961 The detection of a single quantum of circulation in liquid helium II *Proc. Roy. Soc. London A* **260** 218

[23] Davis J C, Amar A, Pekola J P and Packard R E 1988 Superfluidity of 3He Films *Phys. Rev. Lett.* **60** 302

[24] Hohenberg P and Kohn W 1964 Inhomogeneous Electron Gas *Phys. Rev.* **136** B864

[25] Kohn W and Sham L J 1965 Self-Consistent Equations Including Exchange and Correlation Effects *Phys. Rev.* **140** A1133

[26] Mermin N D 1965 Thermal Properties of the Inhomogeneous Electron Gas *Phys. Rev. A* **5** 137

[27] von Barth U and Hedin L 1972 A local exchange-correlation potential for the spin polarized case. I *J. Phys. C* **5** 1629

[28] M. M. Pant and A. K. Rajagopal, Theory of inhomogeneous magnetic electron gas, Solid State Commun. **10** 1157 (1972).

[29] Vignale G and Rasolt M 1988 Current- and spin-density-functional theory for inhomogeneous electronic systems in strong magnetic fields *Phys. Rev. B* **37** 10685

[30] Higuchi M and Higuchi K 2004 Arbitrary choice of basic variables in density functional theory: Formalism *Phys. Rev. B* **69** 035113

[31] Higuchi K and Higuchi M 2004 Density functional theory with arbitrary basic variables *J. Magn. Mag. Mater.* **272-276** 659

[32] Higuchi K and Higuchi M 2007 Density functional scheme for calculating the ground-state pair density *J. Mag. Mag. Mater.* **310** 990

[33] Higuchi K and Higuchi M 2009 Kinetic energy contribution to the exchange-correlation energy functional of the extended-constrained search theory *Phys. Rev. A* **79** 022113

[34] Higuchi M and Higuchi K 2013 Pair density functional theory *Comput. Theor. Chem.* **1003** 91

[35] Higuchi K, Fujie Y, Shimizu H and Higuchi M 2019 Time-dependent current-density-functional theory taking into consideration the effect of energy dissipation *Phys. Rev. A* **100** 062503

[36] Oliveira L N, Gross E K U and Koh W 1988 Density-Functional Theory for

Superconductors *Phys. Rev. Lett* **60** 2430
[37] Lüders M, Marques M A L, Lathiotakis N N, Floris A, Profeta G, Fast L, Continenza A, Massidda S and Gross E K U 2005 *Ab initio* theory of superconductivity. I. Density functional formalism and approximate functionals *Phys. Rev. B* **72** 024545
[38] Marques M A L, Lüders M, Lathiotakis N N, Profeta G, Floris A, Fast L, Continenza A, Gross E. K. U and Massidda S 2005 *Ab initio* theory of superconductivity. II. Application to elemental metals *Phys. Rev. B* **72** 024546
[39] Kohn W, Gross E K U and Oliveira L N 1989 *Orbital Magnetism in the Density Functional Theory of Superconductors J. de Phyique (Paris)* **50** 2601
[40] Higuchi K, Niwa H and Higuchi M 2017 Current–Density Functional Theory for the Superconductor and Its Exchange–Correlation Energy Functional *J. Phys. Soc. Jpn.* **86** 104705
[41] Higuchi K and Higuchi M 2022 First-order normal-to-superconductor phase transition of aluminum in magnetic field by current-density functional theory for superconductors *Phys. Rev. B* **106** 184504
[42] Higuchi K, Miki E and Higuchi M 2017 Basic Variables to Be Reproduced in the First-Principles Theory for Superconductors: Fluctuation of the Particle Number *J. Phys. Soc. Jpn.* **86** 064704
[43] Higuchi K and Higuchi M 2021 Cluster decomposition principle and two-electron wave function of the Cooper pair in the BCS superconducting state *J. Phys. Commun.* **5** 095003
[44] Bulgac A and Yu Y 2004 Superfluid LDA (SLDA): Local Density Approximation for Systems with Superfluid Correlations *Int. J. Mod. Phys. E* **13** 147
[45] Bulgac A 2007 Local-density-functional theory for superfluid fermionic systems: The unitary gas *Phys. Rev. A* **76** 040502(R)
[46] Bulgac A, Forbes M M and Magierski P 2012 The Unitary Fermi Gas: From Monte Carlo to Density Functionals 305 *The BCS-BEC Crossover and the Unitary Fermi Gas* ed W Zwerger (Heidelberg: Springer)
[47] Bulgac A 2013 Time-Dependent Density Functional Theory and Real-Time Dynamics of Fermi Superfluids *Ann. Rev. Nucl. Part. Sci.* **63** 97
[48] For example, see, Fetter A L and Svidzinsky A A 2001 Vortices in a trapped dilute Bose-Einstein condensate *J. Phys. : Condens. Matter* **13** R135
[49] Bogoliubov N N 1958 On a new method in the theory of superconductivity *Nuovo Cimento* **7** 794
[50] Valatin J G 1958 Comments on the theory of superconductivity *Nuovo Cimento* **7** 843
[51] The single-particle Hamiltonian $\hat{h}_S$ is a Hermitian operator, since both $v_S(\mathbf{r})$ and $\boldsymbol{A}_S(\mathbf{r})$ are given by equations (4.55) and (4.56), respectively, and are therefore real functions.
[52] Levy M and Perdew J P 1985 Hellmann-Feynman, virial, and scaling requi-

sites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms *Phys. Rev. A* **32** 2010
[53] Perdew J P 1991 *Electronic Structure of Solids '91* (Berlin : Akademie Verlag)
[54] Perdew J P, Burke K and Ernzerhof M 1996 Generalized Gradient Approximation Made Simple *Phys. Rev. Lett.* **77** 3865
[55] Higuchi K and Higuchi M 2007 Comparison between the vorticity expansion approximation and the local density approximation of the current-density functional theory from the viewpoint of sum rules *J. Phys. Cond. Matter* **19** 365216
[56] Higuchi M and Higuchi K 2010 Sum rules for the exchange-correlation energy functional of the extended constrained-search theory: Application to checking the validity of the vorticity expansion approximation of the current-density functional theory *Phys. Rev. A* **81** 042505
[57] Feynman R P and Cohen M 1956 Energy Spectrum of the Excitations in Liquid Helium *Phys. Rev.* **102** 1189
[58] Cohen M and Feynman R P 1957 Theory of Inelastic Scattering of Cold Neutrons from Liquid Helium *Phys. Rev.* **107** 13
[59] Price D L 1978 The *Physics of Liquid and Solid Helium Part II* (New York: Wiley) 675
[60] Higuchi K, Hamal D B and Higuchi M 2015 Relativistic tight-binding approximation method for materials immersed in a uniform magnetic field: Application to crystalline silicon *Phys. Rev. B* **91** 075122
[61] Higuchi K, Hamal D B and Higuchi M 2018 Nonperturbative description of the butterfly diagram of energy spectra for materials immersed in a magnetic field *Phys. Rev. B* **97** 195135
[62] Hartree, D. R., *Proc. Camb. Phil. Soc.* XXIV, pp. 89–132 (1928)
[63] H. E. Hall and W. F. Vinen: *Proc. Roy. Soc. A* **238** (1956) 204, 215.
[64] D. R. Ladner, R. K. Childers, and J. T. Tough: *Phys. Rev.* **B13** (1976) 2918.
[65] C. J. Gorter and J. H. Mellink: *Physica* **15** (1949) 285.
[66] D.Ruelle, A variational formulation of equilibrium statistical mechanics and the Gibbs phase rule. *Comm. Math. Phys.* **5**(1967), 324-329.
[67] D.W.Robinson, Statistical Mechanics of Quantum Spin Systems. II *Comm. Math. Phys.* **7**(1968), 337-348.