

Functional-renormalization-group aided density-functional theory

– ab-initio description of ground and excited states of quantum many-body systems –

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Abstract

The functional renormalization group (FRG) is a fundamental tool in the field theory. One of recent significant developments regarding the FRG is an attempt to employ it for the formulation of the density functional theory (DFT). We call it the functional-renormalization-group aided density-functional theory (FRG-DFT). The FRG-DFT is expected to become a powerful approach for the fundamental problems of the DFT such as the microscopic derivation of the energy density functional and the analyses of excited states involving the large-amplitude collective dynamics.

In this thesis, I present our works with the FRG-DFT toward the unified description of the ground and excited states of realistic models. Together with my collaborators, I formulate the FRG-DFT for infinite matters and apply it to two models. In the first application, we calculate the equation of state (EOS) and the density-density spectral function of the one-dimensional homogeneous matter composed of spinless fermions with a non-local interaction showing a short-range repulsion and a long-range attraction like the nuclear force. We find that the saturation energy extracted from the EOS coincides with that obtained from the Monte Carlo (MC) method within a few percent. Moreover, the spectral function is found to reproduce a notable feature of the non-linear Tomonaga-Luttinger liquid that the spectral function has singularities at the edge of its support in the lower-energy side. This application is the first example in which the ground and excited states are analyzed in a unified manner with the FRG-DFT. The second application is the analysis of the two-dimensional homogeneous electron gas (2DHEG). This is the first example in which a more-than-one-dimensional realistic model is analyzed. The correlation energies are calculated for various Wigner-Seitz radii and found to completely reproduce the exact result at the high-density limit. In the finite density case, we find that the result with the FRG-DFT shows good agreement with the MC results in the high-density case, although the discrepancy between FRG-DFT and MC results becomes larger as the system becomes dilute. Our results suggest that the FRG-DFT is a promising method which is applicable to realistic quantum many-body systems and realizes the unified description of the ground and excited states.

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Chapter 1

Introduction

The renormalization group (RG) is one of the most fundamental concepts in theoretical physics, which has aided the understanding of how macroscopic phenomena emerge from microscopic theories. The modern framework of the RG was based on the work by Wilson [1]. In this framework, fluctuations of a system are gradually integrated out step by step to derive the low-energy effective theory. In such a scheme, the flow equation which describes the RG transformation, i.e. the transformation of effective theory when the fluctuations with some specific momentum scale are integrated out, plays a key role.

The formulations of RG with functional method is called the functional renormalization group (FRG), in which the RG procedure was exactly described by one-parameter differential equations [1–5]. In particular, the FRG with the effective action formalism [4, 5] has been developed as a powerful machinery for the quantum field theory and statistical mechanics; see Refs. [6–11] for reviews.

In the FRG studies, the effective actions of one-particle operators, which are known as the one-particle-irreducible (1PI) effective actions, are often employed. However, the FRG for effective actions of other composite fields $\mathcal{O}$ can also be formulated [7]. Particularly, the effective action for the density fields, which is known as the two-particle-point-irreducible (2PPI) effective action [12], is of great interest since the FRG for this effective action is related to the density functional theory (DFT) [13].

The DFT was developed in a quite different context from the quantum field theory. It is a very successful method for quantum many-body systems used in various fields including the nuclear physics, condensed matter physics, and quantum chemistry; see Refs. [14–19] for recent reviews. In the DFT, the ground-state density plays a central role: The ground-state density can be regarded as a fundamental quantity for the description of the system instead of the many-body wave function, since the ground-state density determines the states of the system as stated in the Hohenberg–Kohn (HK) theorem [13]. The HK theorem also tells us that there exists the energy density functional (EDF), which gives the ground-state density and energy at its minimum point. Particularly, the DFT is known to be a powerful method for the analysis of the ground state thanks to the Kohn–Sham (KS) scheme [20]. In the KS scheme, the

variational equation for the EDF is mapped to a non-interacting Schrödinger equation, which enables one to perform the analysis with relatively small computational efforts. The determination of the EDF is the most important part of analyses with the DFT since it determines the accuracy of the calculation. However, the HK theorem does not provide a recipe for constructing the EDF, and the establishment of way to determine the EDF from microscopic Hamiltonian is a long-standing problem [21].

The DFT was originally developed without relying on the basis of the quantum field theory. It was, however, pointed out that the EDF can be defined as the effective action for the density field [22, 23]. Such a correspondence gives an insight that the EDF can be constructed by use of RG-like flow equations, and powerful schemes developed in the context of the FRG can be employed to attack the aforementioned long-standing problem of the DFT.

The attempt to derive the EDF by use of flow equations in the FRG formalism, which we call the functional-renormalization-group aided density-functional theory (FRG-DFT), was initiated by Polonyi, Sailer, and Schwenk [24–26]. They discussed a flow equation which connects a free system to a fully interacting system. This is conceptually similar to the adiabatic connection [27–31]. However, I emphasize that the FRG-DFT is an attempt in which the EDF are determined by the direct use of the flow equation, while in the most studies with the adiabatic connection, some physical and empirical ansatzes are made for, e.g., the EDF and the density–density response function (or the exchange–correlation kernel) during the evolution rather than the quantities are determined by the flow equation at the FRG-DFT. Moreover, powerful schemes inspired by the FRG are available in the FRG-DFT thanks to the introduction of the effective action formalism.

In addition to the determination of the EDF, there is another advantage of the FRG-DFT regarding the analysis of the excited states. The DFT can be extended to treat the excited states, which is known as the time-dependent density functional theory (TDDFT) [32]; see Refs. [15, 18, 33] for reviews. The TDDFT with the linear response approximation has been successfully applied to the small-amplitude collective modes. In addition, the real-time TDDFT has been developed to describe the non-linear dynamics. The development of a practical method to extract the information of excited states with large-amplitude collective characters is, however, still an open problem. Recently the FRG methods to analyze the excitation states have been devised: Starting from the work by Kamikado et al. [34], the spectral functions were calculated for some fields including the scalar fields in the $O(4)$ model [34], the scalar meson [35–38], vector meson [39], and quark channels [40, 41] in the two-flavor quark–meson model. Together with my collaborators, I used the spectral functions derived with the FRG for the analyses of the soft mode at the QCD critical point [37, 38]. The spectral analysis of the pion superfluid with the FRG was also shown by other authors [42]. In addition, other quantities concerning the real-time dynamics such as the transport coefficients [43] were calculated. A nice point of the FRG is that it is suitable even for the system showing the criticality, i.e., the situation when the system shows large fluctuations. Therefore, the FRG-DFT is expected to provide a method to analyze the large-amplitude collective

excitations.

Although it was the early 2000's that the works by Polonyi, Sailer, and Schwenk were published, the applications of the FRG-DFT to toy models were started in this decade. Until 2017, the FRG-DFT was applied to some models including the zero-dimensional anharmonic oscillator with and without the dimension of time [44, 45], the one-dimensional systems composed of finite number of spinless fermions interacting via an interaction with a short-range repulsion and a long-range attraction like the nuclear force [46], and the one-dimensional systems composed of finite number of spin-1/2 fermions with the contact interaction [47]. However, these applications are limited to the situations of the zero- or one-dimensional finite systems with short-range interactions, and the models are far from those for the realistic quantum many-body systems. Moreover, these works were focused on the analysis of the ground states and there has been no attempts to demonstrate the analyses of the excited states. Thus, it has not been clarified whether the FRG-DFT is a feasible method even for the realistic models and can be utilized for the extraction of the information of the excited states.

In this thesis, I present our works with the FRG-DFT toward the application to realistic models and the unified description of the ground and excited states. I focus on the analyses of homogeneous infinite matters, which were not treated in the previous works. Such a setup is meaningful as the first step to construct the EDF: One of the simple but widely-used approximations for the EDF is the local density approximation (LDA), in which the EDF is constructed from the equation of state of homogeneous matter. Moreover, together with my collaborators, I find that our formalism for the infinite system has large extensibility. In particular, it can be straightforwardly extended to the case of higher dimensions.

For the analyses of infinite matters, we employ the grand canonical formalism, in which the expectation value of the particle number changes during the evolution. We find that the introduction of the flow-parameter-dependent chemical potential is useful to control the expectation value of the particle number during the evolution. In the case when the expectation value of the particle number is fixed, we derive the flow equation which the chemical potential should satisfy.

I show two demonstrations in this thesis. The first one is the application to the one-dimensional homogeneous matter composed of spinless fermions with a non-local interaction showing a short-range repulsion and a long-range attraction like the nuclear force [48]. With the second-order vertex expansion, we calculate the ground-state density dependence of the ground-state energy, i.e., the equation of state (EOS), and derive the saturation energy from the minimum point of the EOS with respect to the density. We find that the saturation energy derived with the FRG-DFT misses only by 2.7 % in comparison with the Monte Carlo (MC) calculation [48], whereas the Hartree-Fock approximation gives 10 % accuracy. Moreover, we calculate the spectral function for the density two-point correlation function, which gives the information of the excited states. We find that the analytic continuation which is needed to derive the spectral function can be performed easily on the level of the flow equation as the FRG studies [34–38]. In the FRG-DFT, more fluctuations are taken into account than in the random phase

approximation (RPA), which is derived on the basis of the linear response approximation. The spectral function derived by the FRG-DFT reproduces the notable feature of the non-linear Tomonaga–Luttinger liquid that the spectral function has singularities at the edge of its support in the lower-energy side, in contrast to the case of the RPA. This demonstration is the first example where the FRG-DFT is applied to an infinite matter, and shows that the FRG-DFT successfully describes the excited states as well as the ground state.

The formalism of the FRG-DFT for infinite matters can be straightforwardly extended to higher-dimensional cases. Our second demonstration is the application to the two-dimensional homogeneous electron gas (2DHEG), which is a system composed of electrons confined in a two-dimensional layer. We focus on the correlation energy of the 2DHEG. We give an expression for the correlation energy by solving the flow equations with the second-order vertex expansion. We analytically prove that our correlation function reproduces the exact result at the high-density limit, which is given by the Gell-Mann–Brueckner resummation [49]. Moreover, we numerically calculate the correlation energies for various Wigner–Seitz radii r_s and compare them with the MC results [50, 51]. We find that our correlation energy coincides with the MC results at high-density case, while the discrepancy between the results with the FRG-DFT and the MC calculations increases as the system becomes dilute. Our demonstration is the first example of the application of the FRG-DFT to a higher-than-one-dimensional system, and state-of-the-art regarding the physical reality. In addition, this demonstration shows that the FRG-DFT successfully works even for long-range interactions for the first time.

In summary, our two applications show that the FRG-DFT formulated for infinite systems is a very promising method in the sense that the FRG-DFT is a feasible way for the analyses of realistic models and gives a unified manner for the description of the ground and excited states.

This thesis is organized as follows: In Chap. 2, the brief review of the formalism of the DFT is presented. The idea and formalism of the conventional FRG is briefly summarized in Chap. 3. In Chap. 4, the formalism of the FRG-DFT is presented, in which it is pointed out that the introduction of the flow-parameter-dependent chemical potential is important when the FRG-DFT is formulated in the grand-canonical formalism. The definition of the EDF in the effective action formalism is explained and the FRG-DFT flow equation is derived. I also explicitly reproduce the expression for the correlation energy found in the adiabatic connection [27–31] from the FRG-DFT from equation for the first time. In Chap. 5, the application to one-dimensional spinless homogeneous matter with a non-local interaction representing the nuclear force is shown. I introduce the flow-parameter-dependent chemical potential and derive the flow equations with the second-order vertex expansion. Our numerical results for the EOS and the spectral function for the density two-point correlation function are also discussed. The application to the 2DHEG is presented in Chap. 6. The flow equation is solved with the second-order vertex expansion and it is proved that the derived correlation energy reproduces the exact result at the high-density limit. The numerical results of

the correlation energy are also discussed. Chapter 7 is devoted to the conclusion and outlook. In Appendix A, the origin of the positive infinitesimal appearing in Chap. 4 is explained. Appendix B is dedicated to the derivation of the expressions for $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$, which appear in the analyses in Chap. 5 and 6.

The thesis is mainly based on Refs. [52–54], in which the present author involved. The correspondence between these references and the contents of this thesis is as follow: The formalism and results regarding the ground state in Chap. 5 are based on Ref. [52]. The formalism and results regarding the excited states in Chap. 5 are based on Ref. [53]. Chapter 6 is based on Ref. [54].

Chapter 2

Density functional theory

The density functional theory (DFT) is one of the most successful methods for the quantum many-body systems, and used in various fields including nuclear physics, condensed matter physics, and quantum chemistry. In this chapter, the formulation of the DFT is briefly shown. The Hohenberg–Kohn theorem, which provides the basis of the DFT, and the Kohn-Sham scheme, which makes the DFT a powerful tool for the analyses of the quantum many-body systems, are explained. After that, a fundamental problem of the DFT is pointed out.

2.1 Hohenberg-Kohn theorem

The Hohenberg-Kohn (HK) theorem [13] provides the basis for the DFT. Here, let us consider a system composed of N -fermions described by the following Hamiltonian:

$$\hat{H} = \hat{T} + \hat{U} + \hat{V}, \quad (2.1)$$

where $\hat{T}$ is the kinetic term

$$\hat{T} = \sum_{i=1}^N \frac{\hat{\mathbf{p}}_i^2}{2m},$$

with the momentum operator of the i -th fermion $\hat{\mathbf{p}}_i$ and the mass of the fermion m , $\hat{U}$ is the two-body interaction

$$\hat{U} = \frac{1}{2} \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N U(\hat{\mathbf{x}}_i, \hat{\mathbf{x}}_j),$$

and $\hat{V}$ is the external field

$$\hat{V} = \sum_{i=1}^N V(\hat{\mathbf{x}}_i).$$

I first show the HK theorem in the case of non-degenerate ground states for simplicity, and after that I present how it is extended to the case of degenerate ground states.

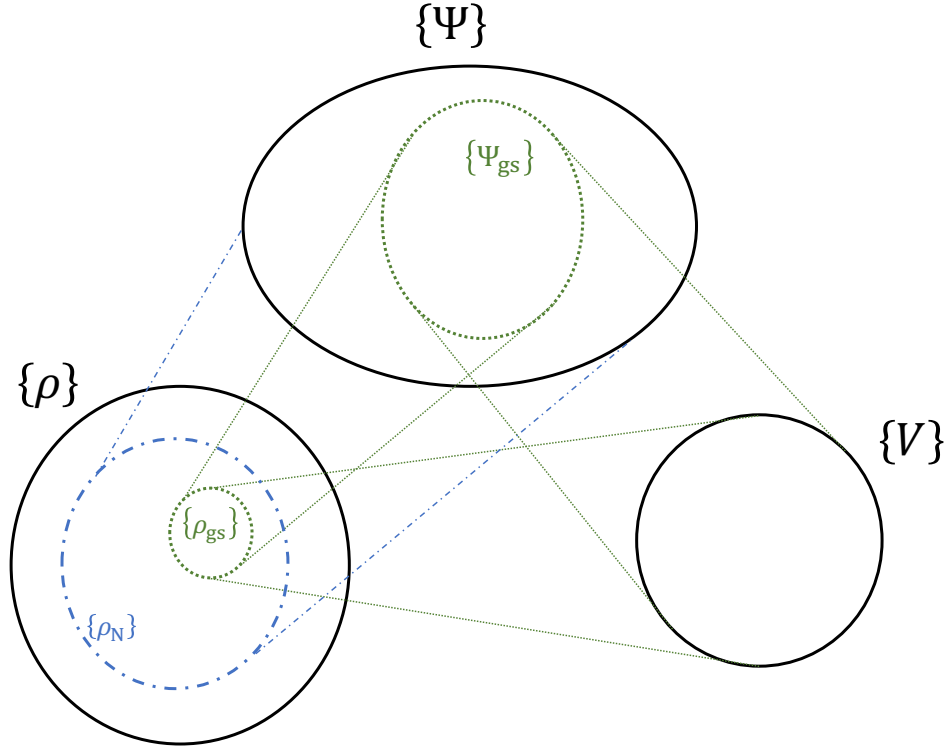


Figure 2.1: Schematic picture for the v - and N -representability. $\{V\}$, $\{\Psi\}$, and $\{\rho\}$ are the sets of the external fields, wave function, and density, respectively. $\{\Psi_{\text{gs}}\}$ and $\{\rho_{\text{gs}}\}$ are the sets of wave functions and the densities which are the ground-state wave functions and densities for at least one external field, respectively. By definition, $\{\rho_{\text{gs}}\}$ is the set of the v -representable densities. $\{\rho_{\text{N}}\}$ is the N -representable densities, i.e., the densities which is reproduced by at least one wave function. $\{\rho_{\text{gs}}\}$ and $\{\rho_{\text{N}}\}$ satisfy $\{\rho_{\text{gs}}\} \subseteq \{\rho_{\text{N}}\}$. Actually $\{\rho_{\text{N}}\} = \{\rho\}$ from the discussion by Harriman [58].

2.1.1 Non-degenerate case

I first assume that the ground state of the system is not degenerate. To discuss the HK theorem, the notion of the v -representability [55–57] is important:

Definition A density ρ satisfies the v -representability if there exists at least one potential V which gives ρ as the ground-state density.

The schematic picture of the v -representability is shown in Fig. 2.1. First, the HK theorem is proved on the assumption that the densities satisfy the v -representability, which was implicitly used in the original proof by Hohenberg and Kohn [13]. After that, I point out the problem of the proof relying on the v -representability and show how it is resolved.

The HK theorem consists of the two statements. The first one is as follows:

Theorem 1 (HK first theorem). *There exists one-to-one correspondence between the ground-state density and the external field up to the constant shift of the energy.*

Proof. First, let us prove there is a one-to-one correspondence between the ground state $|\Psi_{\text{gs}}\rangle$ and the external field $\hat{V}$. Since we consider a non-degenerate ground state, the ground state is uniquely determined if an external field is given. The fact that there is a map from $|\Psi_{\text{gs}}\rangle$ to $\hat{V}$ is proved as follows: Assume that the same ground state $|\Psi_{\text{gs}}\rangle$ is obtained from two different external fields $\hat{V}$ and $\hat{V}'$, the difference of which cannot be absorbed by the constant shift of the energy. Then the following equations are obtained.

$$\begin{aligned}\hat{H} |\Psi_{\text{gs}}\rangle &= E_{\text{gs}} |\Psi_{\text{gs}}\rangle, \\ \hat{H}' |\Psi_{\text{gs}}\rangle &= E'_{\text{gs}} |\Psi_{\text{gs}}\rangle,\end{aligned}$$

where $\hat{H} = \hat{T} + \hat{U} + \hat{V}$, $\hat{H}' = \hat{T} + \hat{U} + \hat{V}'$, and E_{gs} and E'_{gs} are the ground state energies. Subtracting these equations from each other, one has

$$\sum_{i=1}^N (V(\mathbf{x}_i) - V'(\mathbf{x}_i)) \Psi_{\text{gs}}(\mathbf{x}_1, \dots, \mathbf{x}_N) = (E_{\text{gs}} - E'_{\text{gs}}) \Psi_{\text{gs}}(\mathbf{x}_1, \dots, \mathbf{x}_N),$$

where $\Psi_{\text{gs}}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \langle \mathbf{x}_1, \dots, \mathbf{x}_N | \Psi_{\text{gs}} \rangle$. Since this equality is satisfied for all $\mathbf{x}_1, \dots, \mathbf{x}_N$, $V(\mathbf{x}_i) - V'(\mathbf{x}_i)$ is a constant. This is in contradiction with the assumption that the difference $V(\mathbf{x}_i)$ between $V'(\mathbf{x}_i)$ cannot be absorbed by the constant shift of the energy. Therefore, the external field is uniquely determined from $|\Psi_{\text{gs}}\rangle$.

Next, let us prove there is a one-to-one correspondence between the ground state $|\Psi_{\text{gs}}\rangle$ and the density ρ_{gs} . It is trivial that ρ_{gs} is uniquely determined if $|\Psi_{\text{gs}}\rangle$ is given. The fact that there is a map from ρ_{gs} to $|\Psi_{\text{gs}}\rangle$ can be proved. Assume that different ground states $|\Psi_{\text{gs}}\rangle$ corresponding to $\hat{V}$ and $|\Psi'_{\text{gs}}\rangle$ corresponding to $\hat{V}'$ give the same ρ_{gs} . Then one has

$$\begin{aligned}E_{\text{gs}} &= \langle \Psi_{\text{gs}} | (\hat{T} + \hat{U} + \hat{V}) | \Psi_{\text{gs}} \rangle, \\ E'_{\text{gs}} &= \langle \Psi'_{\text{gs}} | (\hat{T} + \hat{U} + \hat{V}') | \Psi'_{\text{gs}} \rangle.\end{aligned}$$

Since $|\Psi_{\text{gs}}\rangle$ is the ground state for $\hat{H} = \hat{T} + \hat{U} + \hat{V}$, one obtains

$$\begin{aligned}E_{\text{gs}} &= \langle \Psi_{\text{gs}} | (\hat{T} + \hat{U}) | \Psi_{\text{gs}} \rangle + \int d\mathbf{x} V(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}) \\ &< \langle \Psi'_{\text{gs}} | (\hat{T} + \hat{U}) | \Psi'_{\text{gs}} \rangle + \int d\mathbf{x} V(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}) \\ &= E'_{\text{gs}} + \int d\mathbf{x} (V(\mathbf{x}) - V'(\mathbf{x})) \rho_{\text{gs}}(\mathbf{x}),\end{aligned}\tag{2.2}$$

where I have used $\rho_{\text{gs}}(\mathbf{x}) = \sum_{i=1}^N \langle \Psi_{\text{gs}} | \delta(\hat{\mathbf{x}}_i - \mathbf{x}) | \Psi_{\text{gs}} \rangle$. In the same manner, one has

$$E'_{\text{gs}} < E_{\text{gs}} + \int d\mathbf{x} (V'(\mathbf{x}) - V(\mathbf{x})) \rho_{\text{gs}}(\mathbf{x}).\tag{2.3}$$

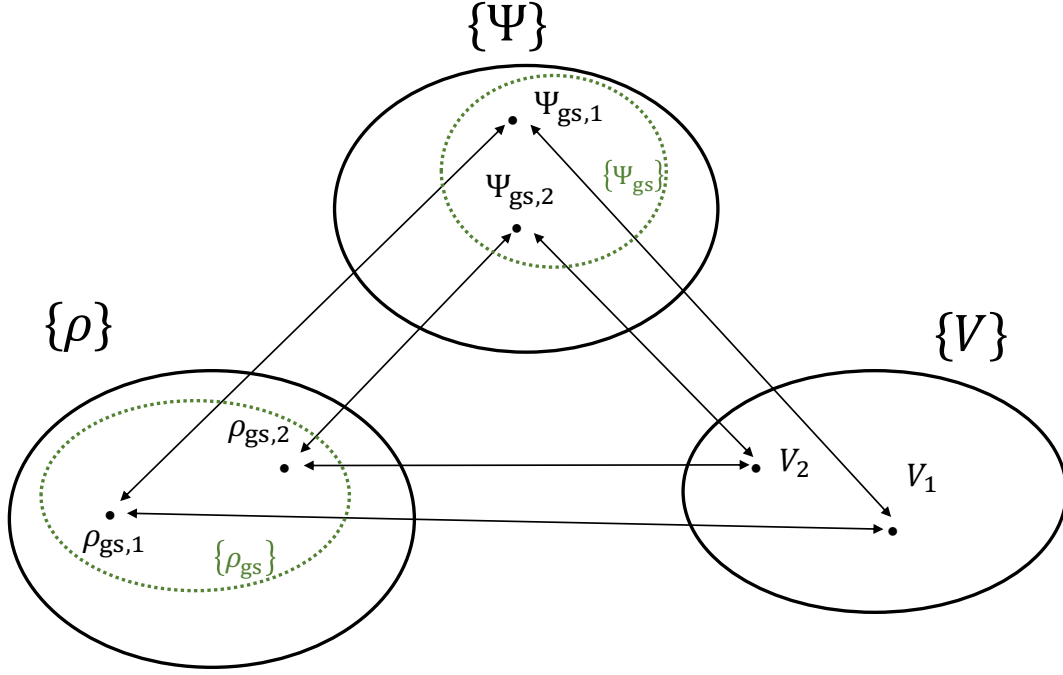


Figure 2.2: Schematic picture for the HK first theorem in the case of non-degenerate ground states. The definitions of $\{\Psi_{\text{gs}}\}$ and $\{\rho_{\text{gs}}\}$ are the same as those in Fig. 2.1. The arrows are representing the one-to-one correspondence. If $\rho_{\text{gs},1} \neq \rho_{\text{gs},2}$, one has $\Psi_{\text{gs},1} \neq \Psi_{\text{gs},2}$ and $V_1 \neq V_2$.

Equations (2.2) and (2.3) are in contradiction with each other since $E_{\text{gs}} + E'_{\text{gs}} < E'_{\text{gs}} + E_{\text{gs}}$ is obtained from these equations. Therefore $|\Psi_{\text{gs}}\rangle$ is uniquely determined by ρ_{gs} .

The fact that there is one-to-one correspondence between $\hat{V}$ and $|\Psi_{\text{gs}}\rangle$, and between $|\Psi_{\text{gs}}\rangle$ and ρ_{gs} leads to the conclusion that there is one-to-one correspondence between $\hat{V}$ and ρ_{gs} . $\square$

The schematic picture of this theorem is shown in Fig. 2.2.

For the second statement of the HK theorem, I define the energy density functional (EDF) as follows:

$$E[\rho] = \langle \Psi_{\text{gs}}[\rho] | (\hat{T} + \hat{U} + \hat{V}) | \Psi_{\text{gs}}[\rho] \rangle. \quad (2.4)$$

Here, $|\Psi_{\text{gs}}[\rho]\rangle$ is defined as the ground state when the ground-state density is ρ . Note that the external field $\hat{V}'$ determined from ρ , or $|\Psi_{\text{gs}}[\rho]\rangle$, is generally not equal to $\hat{V}$ in Eq. (2.4). Equation (2.4) can be rewritten as

$$E[\rho] = F[\rho] + \int d\mathbf{x} V(\mathbf{x}) \rho(\mathbf{x}), \quad (2.5)$$

where $F[\rho]$ is called the universal functional, i.e., a functional determined independently from the external field.

Theorem 2 (HK second theorem). *The EDF $E[\rho]$ defined by Eq. (2.4) satisfies*

$$E[\rho] \geq E_{\text{gs}},$$

where E_{gs} is the ground-state energy. The equality is satisfied only when ρ is equal to the ground-state density ρ_{gs} .

Proof. Since ρ_{gs} is the ground-state density corresponding to $\hat{V}$, $|\Psi_{\text{gs}}[\rho_{\text{gs}}]\rangle$ is the ground state corresponding to $\hat{V}$. Therefore one has $E[\rho_{\text{gs}}] = E_{\text{gs}}$.

When $\rho \neq \rho_{\text{gs}}$, $|\Psi_{\text{gs}}[\rho]\rangle$ is not equal to the ground state corresponding to $\hat{V}$ since there is one-to-one correspondence between ρ and $|\Psi_{\text{gs}}[\rho]\rangle$. Therefore one obtains $E[\rho] > E_{\text{gs}}$. $\square$

From the first theorem, the ground-state density ρ_{gs} determines the external field $\hat{V}$, which means ρ_{gs} determines the Hamiltonian and thus all the states of the system. The second theorem tells us that such a ground-state density is obtained from the minimum point of the EDF. Therefore, the HK theorem suggests that the quantum many-body systems can be analyzed in terms of the ground-state density and the variational equation for the EDF instead of the wave function and the Schrödinger equation.

The assumption of the v -representability, however, causes a serious problem for the variational principle for the EDF. Since I have proved the HK second theorem under the assumption that the densities are v -representable, it is unclear that the variational principle is satisfied for arbitral densities. This forces one to perform the variation of the EDF in the space of v -representable densities. However, whether a given density is v -representable is hard to know and the determination of the v -representable space is almost impossible. Therefore, the HK second theorem should be extended to the case for arbitral densities.

A helpful notion for this problem is the N -representability:

Definition A density ρ satisfies the N -representability if there exists at least one wave function Ψ which gives ρ . Note that Ψ is not needed to be a ground state corresponding to some external field.

The schematic picture of it is shown in Fig. 2.1. By definition, the set of the N -representable densities contains all the v -representable densities. Let us consider whether one can extend the definition of the EDF for the N -representable densities $\{\rho_{\text{N}}\}$. Here, I follow the procedure called the Levy constrained search [59]. I introduce the following functional for the N -representable densities $\rho \in \{\rho_{\text{N}}\}$:

$$E[\rho] = \min_{\Psi \in \{\Psi\}_{\rho}} \langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle = F[\rho] + \int_{\mathbf{x}} V(\mathbf{x})\rho(\mathbf{x}), \quad (2.6)$$

where $\{\Psi\}_{\rho}$ is the set of wave functions giving $\rho \in \{\rho_{\text{N}}\}$ and

$$F[\rho] = \min_{\Psi \in \{\Psi\}_{\rho}} \langle \Psi | (\hat{T} + \hat{U}) | \Psi \rangle. \quad (2.7)$$

$E[\rho]$ gives the ground-state energy E_{gs} and density ρ_{gs} at its minimum point since

$$\begin{aligned} \min_{\rho} E[\rho] &= \min_{\rho} \min_{\Psi \in \{\Psi\}_{\rho}} \langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle \\ &= \min_{\Psi} \langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle \\ &= E_{\text{gs}}, \end{aligned} \tag{2.8}$$

and ρ minimizing $E[\rho]$ corresponds to the density of the ground-state wave function Ψ_{gs} minimizing $\langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle$. In Eq. (2.8), I have used a well-known fact that $\langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle \geq E_{\text{gs}}$, where the equality is satisfied only when $\Psi = \Psi_{\text{gs}}$. Therefore, $E[\rho]$ defined in Eq. (2.6) for the N -representable densities has found to satisfy the variational principle as the EDF defined in Eq. (2.4) for the v -representable densities. Actually, $E[\rho]$ defined in Eq. (2.6) coincides with Eq. (2.4) when ρ is v -representable. Thus $E[\rho]$ defined in Eq. (2.6) can be regarded as the generalization of the EDF to the case of N -representable densities.

Then we should think whether one can know a given density is N -representable. Actually, an arbitral density is known to be N -representable thanks to the discussion by Harriman [58]; see also [60, 61]. Therefore $E[\rho]$ defined in Eq. (2.6) can be regarded as the EDF defined for arbitral densities, and we can extend the variational principle stated in the HK second theorem to the case of arbitral densities.

2.1.2 Degenerate case

We have considered the cases of non-degenerated ground states. Here, I present the extension of the HK theorem to degenerate cases [62]. This extension guarantees that the DFT is in principle applicable to various situation including the cases when some symmetry is broken and degenerate ground states appear, such as non-paramagnetic and superconducting phases.

In the degenerate case, an external field does no longer correspond to a ground-state wave function and density, but it corresponds to the set of the degenerate ground-state wave functions and densities. Therefore there is no one-to-one correspondence between the external field, the ground-state wave function, and the ground-state density as stated in the HK first theorem for the non-degenerate case. However, the essential point of the HK first theorem that the ground-state density, or wave function, uniquely determines the external field is unchanged even for the degenerate case.

In the degenerate case, the HK first theorem is modified as follows:

Theorem 3 (HK first theorem for degenerate ground states). *The ground-state density, and the ground-state wave function, uniquely determines the external field up to the constant shift of the energy. In other words, if there are two different external fields V_1 and V_2 , whose difference cannot be absorbed by the constant shift, and V_i gives the sets of the ground-state wave functions $\{\Psi_{\text{gs},i}\}$ and densities $\{\rho_{\text{gs},i}\}$ for $i = 1, 2$, we have $\{\Psi_{\text{gs},1}\} \cap \{\Psi_{\text{gs},2}\} = \emptyset$, and $\{\rho_{\text{gs},1}\} \cap \{\rho_{\text{gs},2}\} = \emptyset$.*

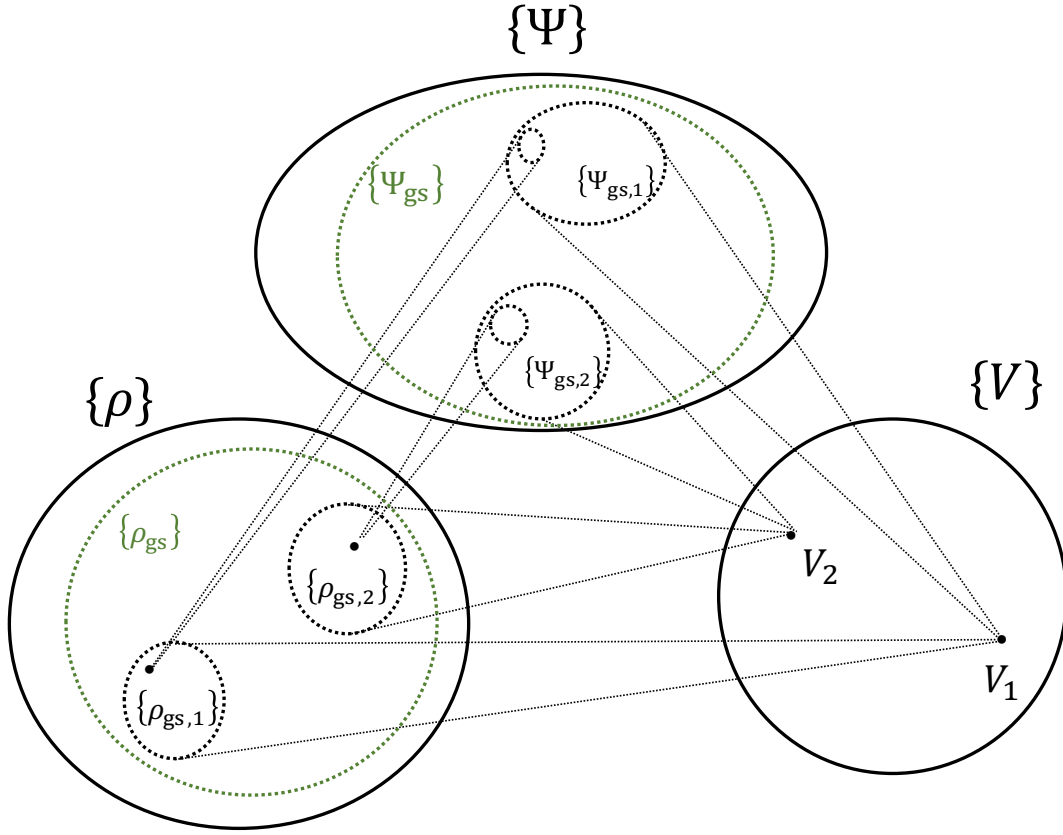


Figure 2.3: Schematic picture for the HK first theorem in the case of degenerate ground states. $\{\Psi_{gs}\}$ and $\{\rho_{gs}\}$ are the same as in Fig. 2.1. An external potential corresponds to a set of degenerate ground-state wave function and a set of degenerate ground-state density. If $V_1 \neq V_2$, there is no intersection between $\{\Psi_{gs,1}\}$ and $\{\Psi_{gs,2}\}$, and $\{\rho_{gs,1}\}$ and $\{\rho_{gs,2}\}$. Degenerate but different wave functions, e.g., $\Psi, \Psi' \in \{\Psi_{gs,1}\}$, can give the same ground-state density $\rho \in \{\rho_{gs,1}\}$.

The proof is in the same manner as that for the non-degenerate case. Figure 2.3 is the schematic picture of the HK first theorem in the degenerate cases.

The HK second theorem can be trivially extended to the degenerate cases. The EDF is defined in the same manner as Eq. (2.6). In that case, there are more-than-one Ψ minimizing $\langle \Psi | (\hat{T} + \hat{U} + \hat{V}) | \Psi \rangle$ in the second line of Eq. (2.8), and there may be more-than-one ρ minimizing the EDF.

In summary, the HK theorem suggests that if the EDF is found, the ground-state density, which determines all the states of the system, is derived. The HK theorem, however, does not provide the scheme to derive the universal part $F[\rho]$ of the EDF. In particular, even the kinetic term in $F[\rho]$ is hard to treat. A successful way to treat the kinetic term is the Kohn-Sham scheme, which will be presented below.

2.2 Kohn-Sham scheme

The Kohn-Sham (KS) scheme gives a nice way to treat the kinetic term. Thanks to the KS scheme [20], the DFT becomes a powerful tool for the analyses of the ground states. The idea of the Kohn-Sham scheme is mapping a system composed of interacting fermions to a fictitious system composed of non-interacting fermions with a fictitious external fields. In this scheme, the universal functional of the EDF is divided into the following terms:

$$F[\rho] = T_s[\rho] + E_H[\rho] + E_{xc}[\rho], \quad (2.9)$$

where $T_s[\rho]$ is the kinetic energy of a non-interacting system with density ρ , $E_H[\rho]$ is the Hartree energy defined by

$$E_H[\rho] = \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' U(\mathbf{x}, \mathbf{x}') \rho(\mathbf{x}) \rho(\mathbf{x}'),$$

and $E_{xc}[\rho]$ is the exchange–correlation term which is defined as the remaining part of $F[\rho]$. Under such a decomposition, let us consider the variational equation for the EDF. The variational equation for the EDF with the constraint $\int d\mathbf{x} \rho(\mathbf{x}) = N$ reads

$$\left. \frac{\delta}{\delta \rho(\mathbf{x})} \left[E[\rho] - \mu \left(\int d\mathbf{x} \rho(\mathbf{x}) - N \right) \right] \right|_{\rho=\rho_{\text{gs}}} = 0, \quad (2.10)$$

where μ is the Lagrangian multiplier. By use of Eq. (2.9), the variational equation is rewritten as follows:

$$\left. \frac{\delta T_s[\rho]}{\delta \rho(\mathbf{x})} \right|_{\rho=\rho_{\text{gs}}} + V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) = \mu, \quad (2.11)$$

where $V_{\text{KS}}[\rho](\mathbf{x})$ is defined as follows:

$$V_{\text{KS}}[\rho](\mathbf{x}) = \int d\mathbf{x}' U(\mathbf{x}, \mathbf{x}') \rho(\mathbf{x}') + \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{x})} + V(\mathbf{x}).$$

A remarkable point for Eq. (2.11) is that it is the same as that obtained from the non-interacting fermions with the external field $V_{\text{KS}}[\rho](\mathbf{x})$. Therefore, $\rho(\mathbf{x})$ satisfying Eq. (2.11) can be obtained from the following Schrödinger equation for the non-interacting system:

$$\left(-\frac{\hbar^2}{2m} \Delta + V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) \right) \phi_i(\mathbf{x}) = \epsilon_i \phi_i(\mathbf{x}), \quad (2.12)$$

where $i \in \mathbb{N}$ is the index for the eigenfunction $\phi_i(\mathbf{x})$ obtained from this equation, and ϵ_i is the eigenvalue corresponding to $\phi_i(\mathbf{x})$. The one-particle state described by $\phi_i(\mathbf{x})$ is called the Kohn-Sham (KS) orbital. We assume that $\epsilon_1 \leq \epsilon_2 \leq \dots$. When the

system is composed of N fermions, the ground state $|\Psi_s[\rho]\rangle$ is described by the Slater determinant of $\phi_1(\mathbf{x}), \dots, \phi_N(\mathbf{x})$:

$$\langle \mathbf{x}_1, \dots, \mathbf{x}_N | \Psi_s[\rho_{\text{gs}}] \rangle = \frac{1}{\sqrt{N!}} \det(\phi_i(\mathbf{x}_j)), \quad (2.13)$$

where i and j run from 1 to N . Then the ground-state density $\rho_{\text{gs}}(\mathbf{x})$ is related to the KS orbitals as follows:

$$\rho_{\text{gs}}(\mathbf{x}) = \langle \Psi_s[\rho_{\text{gs}}] | \sum_{i=1}^N \delta(\mathbf{x} - \hat{\mathbf{x}}_i) | \Psi_s[\rho_{\text{gs}}] \rangle = \sum_{i=1}^N |\phi_i(\mathbf{x})|^2. \quad (2.14)$$

ϵ_i derived from Eq. (2.12) is related to the total ground-state energy. Since $T_s[\rho]$ is defined as the kinetic energy of the non-interacting system, one has

$$T_s[\rho_{\text{gs}}] = \langle \Psi_s[\rho_{\text{gs}}] | \sum_i^N (-1) \frac{\hbar^2 \Delta_i}{2m} | \Psi_s[\rho_{\text{gs}}] \rangle = \sum_{i=1}^N \epsilon_i - \int d\mathbf{x} V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) \rho_{\text{gs}}(\mathbf{x})$$

Therefore, the ground-state energy E_{gs} is derived as

$$\begin{aligned} E_{\text{gs}} &= E[\rho_{\text{gs}}] \\ &= \sum_{i=1}^N \epsilon_i - \int d\mathbf{x} V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}) + E_{\text{H}}[\rho_{\text{gs}}] + E_{\text{xc}}[\rho_{\text{gs}}] + \int d\mathbf{x} V(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}) \\ &= \sum_{i=1}^N \epsilon_i - \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' U(\mathbf{x}, \mathbf{x}') \rho(\mathbf{x}) \rho(\mathbf{x}') - \int d\mathbf{x} \frac{\delta E_{\text{xc}}[\rho_{\text{gs}}]}{\delta \rho(\mathbf{x})} \rho_{\text{gs}}(\mathbf{x}) + E_{\text{xc}}[\rho_{\text{gs}}]. \end{aligned} \quad (2.15)$$

To summarize, the ground-state density and energy are obtained by solving Eq. (2.12). A remark is in order here: Equation (2.12) is needed to be solved consistently with Eq. (2.14) since Eq. (2.12) contains ρ_{gs} in $V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x})$. This is numerically achieved by use of the iteration method. Such a scheme requires relatively small computational resources compared to other methods such as post-Hartree-Fock methods and Monte Carlo calculations, which particularly makes the DFT a powerful tool to investigate the ground state of many-body systems.

A difficult problem, however, still remains. It is the determination of the $E_{\text{xc}}[\rho]$. In most studies, some ansatz is made on $E_{\text{xc}}[\rho]$. One of the most used ansatzes is the local density approximation (LDA):

$$E_{\text{xc}}[\rho] \approx \int d\mathbf{x} E_{\text{xc}}^{\text{LDA}}(\rho(\mathbf{x})) \rho(\mathbf{x}). \quad (2.16)$$

$E_{\text{xc}}^{\text{LDA}}(\rho)$ corresponds to the energy per particle of the homogeneous infinite matter with density ρ . Therefore, by use of the equation of state of the matter composed of

the fermions under consideration, $E_{\text{xc}}[\rho]$ in the LDA is obtained. Another well-known ansatz is the generalized gradient approximation (GGA):

$$E_{\text{xc}}[\rho] \approx \int d\mathbf{x} E_{\text{xc}}^{\text{GGA}}(\rho(\mathbf{x}), |\nabla\rho(\mathbf{x})|) \rho(\mathbf{x}), \quad (2.17)$$

in which the contribution from the gradient of the density $\nabla\rho(\mathbf{x})$ is taken into account. Such an effect of the gradient is particularly important for localized systems such as finite nuclei. Although many functionals for $E_{\text{xc}}[\rho]$, the establishment of the way to construct $E_{\text{xc}}[\rho]$ from microscopic Hamiltonian is still an open problem.

Chapter 3

Functional renormalization group

Before moving on to the FRG-DFT, I briefly review the formulation of the conventional functional renormalization group (FRG) for 1PI effective actions [4]. I introduce the effective average action, which plays a key role in this formalism, and derive the functional flow equation which represents the procedure of the coarse graining. Some non-perturbative approximation methods provided in this formalism are also reviewed.

3.1 Effective average action

The FRG is a formulation for the Wilsonian renormalization group [1] in terms of the functional method. Here, I consider the FRG formulated for the effective action [4]. In this formalism, scale dependent effective actions, which is called the effective average action, play important roles. In this section, we define the effective average action, and discuss its properties.

In the Wilsonian renormalization group, the quantum and thermal fluctuations are gradually integrated out from the higher-momentum scale to the lower-momentum scale. In the FRG, artificial masses are introduced to realize the idea of the renormalization group. If fluctuations with the momentum scale lower than k get massive, these fluctuations become non-effective ones, and then the effective theory at scale k is obtained. Therefore, the renormalization flow from the higher-momentum scale to the lower-momentum scale is realized by changing k from an ultraviolet scale $k = \Lambda$ to an infrared scale $k = 0$.

To implement this procedure, the regulator term is introduced in the FRG. Consider a d -dimensional system composed of field $\Phi_a(X)$, where a is the label of the internal degree of freedom and X is a vector of the time and spacial coordinates, and described by the action $S[\Phi]$. We employ the imaginary-time formalism. The regulator term is defined as the bilinear of the field:

$$\Delta S_k[\Phi] = \frac{1}{2} \int_{X,Y} \Phi_a(X) R_k^{ab}(X-Y) \Phi_b(Y), \quad (3.1)$$

where $\int_X$ is the shorthand of $\int dX$. $R_k^{ab}(X, Y)$ is corresponding to the ‘mass’ introduced by hand, which is called the regulator function. Let us impose some conditions for $R_k^{ab}(X, Y)$ to realize the aforementioned procedure. To see this, the momentum representation is convenient:

$$\Delta S_k[\Phi] = \frac{1}{2} \int_P \tilde{\Phi}_a(P) \tilde{R}_k^{ab}(P) \tilde{\Phi}_b(-P), \quad (3.2)$$

where P is the vector composed of the frequency and spatial momentum, $\int_P := \int dP$, and

$$\begin{aligned} \tilde{R}_k^{ab}(P) &:= \int_X R_k^{ab}(X) e^{-iP \cdot X}, \\ \tilde{\Phi}_a(P) &:= \int_X \Phi_a(X) e^{-iP \cdot X}. \end{aligned}$$

The conditions imposed on $\tilde{R}_k^{ab}(P)$ are as follows:

$$\lim_{P^2/k^2 \rightarrow 0} R_k^{ab}(P) > 0, \quad (3.3)$$

$$\lim_{k^2/P^2 \rightarrow 0} R_k^{ab}(P) = 0, \quad (3.4)$$

$$\lim_{k \rightarrow \Lambda \rightarrow \infty} R_k^{ab}(P) = \infty. \quad (3.5)$$

The first condition makes $R_k^{ab}(P)$ a regulator suppressing infrared fluctuations. All the fluctuations are introduced as k approaches 0 due to the second condition. The third condition is needed to suppress all the fluctuations when k is set to some large ultraviolet scale Λ .

I introduce the effective average action, which plays a key role in the FRG formalism. The effective average action is the extension of the effective action to the case of the presence of the regulator. To define the effective average action, I consider the generating functional for the correlation functions of the fields under the presence of the regulator term:

$$Z_k[J] = \int \mathcal{D}\Phi e^{-S[\Phi] - \Delta S_k[\Phi] + \int_X J^a(X) \Phi_a(X)}. \quad (3.6)$$

The generating functional for the connected correlation function is given by $W_k[J] = \ln Z_k[J]$. The effective average action is given by the Legendre transformation of $W_k[J]$:

$$\begin{aligned} \Gamma_k[\Phi] &:= \sup_J \left(\int_X J^a(X) \Phi_a(X) - W_k[J] \right) - \Delta S_k[\Phi] \\ &= \int_X J_{\text{sup},k}^a[\Phi](X) \Phi_a(X) - W_k[J_{\text{sup},k}[\Phi]] - \Delta S_k[\Phi], \end{aligned} \quad (3.7)$$

where $J_{\text{sup}}^a[\Phi]$ is an external field satisfying

$$\left. \frac{\delta W_k[J]}{\delta J^a(X)} \right|_{J=J_{\text{sup},k}^a[\Phi]} = \Phi_a(X). \quad (3.8)$$

Let me note some properties of the effective average action:

- The effective average action turns into the effective action at $k \rightarrow 0$ since the regulator vanishes at this limit due to Eq. (3.4).
- For large k , the effective average action becomes identical with the bare action $S[\Phi]$ up to the constant as following discussion: The regulator gets large for large k due to Eq. (3.5). In this case, the functional integral in Eq. (3.6) is described by the saddle-point approximation:

$$\int \mathcal{D}\Phi e^{-S[\Phi] - \Delta S_k[\Phi] + \int_X J^a(X) \Phi_a(X)} \approx e^{-S[\bar{\Phi}] - \Delta S_k[\bar{\Phi}] + \int_X J^a(X) \bar{\Phi}_a(X) + \text{const.}},$$

where $\bar{\Phi}[J]$ satisfies

$$\left. \frac{\delta}{\delta \Phi_a(X)} (S[\Phi] + \Delta S_k[\Phi]) \right|_{\Phi=\bar{\Phi}[J]} = J^a(X).$$

By use of this relation, Eq. (3.8) and

$$W_k[J] \approx -S[\bar{\Phi}[J]] - \Delta S_k[\bar{\Phi}[J]] + \int_X J^a(X) \bar{\Phi}_a[J](X) + \text{const.},$$

one has

$$\begin{aligned} \Phi_a(X) &= \left. \frac{\delta W_k[J]}{\delta J^a(X)} \right|_{J=J_{\text{sup},k}^a[\Phi]} \\ &= \left. \frac{\delta}{\delta J^a(X)} \left(-S[\bar{\Phi}[J]] - \Delta S_k[\bar{\Phi}[J]] + \int_Y J^b(Y) \bar{\Phi}_b[J](Y) \right) \right|_{J=J_{\text{sup},k}^a[\Phi]} \\ &= \bar{\Phi}_a[J_{\text{sup},k}[\Phi]](X) \\ &\quad + \left. \int_Y \frac{\delta \bar{\Phi}_b(Y)}{\delta J^a(X)} \left(J^b(Y) - \left. \frac{\delta}{\delta \Phi_b(Y)} (S[\Phi] + \Delta S_k[\Phi]) \right|_{\Phi=\bar{\Phi}[J]} \right) \right|_{J=J_{\text{sup},k}^a[\Phi]} \\ &= \bar{\Phi}_a[J_{\text{sup},k}[\Phi]](X). \end{aligned}$$

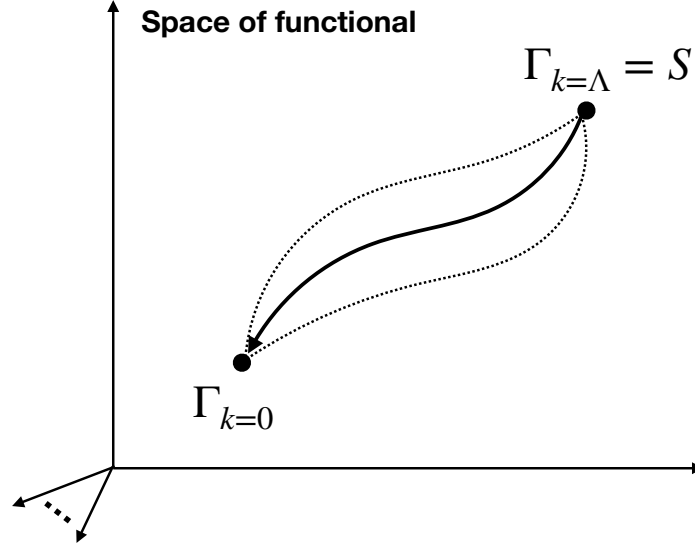


Figure 3.1: Schematic picture of the flow of the effective average action. Although the path from $k = \Lambda$ to $k = 0$ depends on the choice of the regulator, the starting and ending points do not depend on the regulator as far as the conditions Eqs. (3.4) and (3.5) are satisfied.

Therefore,

$$\begin{aligned}
 \Gamma_k[\Phi] &= \int_X J_{\text{sup},k}^a[\Phi](X) \Phi_a(X) - W_k[J_{\text{sup},k}[\Phi]] - \Delta S_k[\Phi] \\
 &\approx \int_X J_{\text{sup}}^a[\Phi](X) \Phi_a(X) - \Delta S_k[\Phi] \\
 &\quad + S[\bar{\Phi}[J_{\text{sup},k}[\Phi]]] + \Delta S_k[\bar{\Phi}[J_{\text{sup},k}[\Phi]]] \\
 &\quad - \int_X J_{\text{sup}}^a[\Phi](X) \bar{\Phi}_a[J_{\text{sup},k}[\Phi]](X) + \text{const.} \\
 &= \int_X J_{\text{sup},k}^a[\Phi](X) \Phi_a(X) - \Delta S_k[\Phi] \\
 &\quad + S[\Phi] + \Delta S_k[\Phi] - \int_X J_{\text{sup},k}^a[\Phi](X) \Phi_a(X) + \text{const.} \\
 &= S[\Phi] + \text{const.}
 \end{aligned}$$

Figure 3.1 shows the schematic picture of the flow of the effective average action. There is an arbitrariness in the choice of the regulator term, and $\Gamma_k[\Phi]$ for intermediate k depends on the choice of the regulator. However, as far as Eqs. (3.3)-(3.5) are satisfied, $\Gamma_\Lambda[\Phi]$ for large Λ becomes the bare action and $\Gamma_0[\Phi]$ becomes the effective action, and the change from $k = \Lambda$ to $k = 0$ can be regarded as the renormalization flow.

3.2 Flow equation

The flow of $\Gamma_k[\Phi]$ is described by the functional differential equation, which is called the Wetterich equation [4]:

$$\partial_k \Gamma_k[\Phi] = \frac{1}{2} \int_{X,Y} \left[\left(\Gamma_k^{(2)}[\Phi] + R_k \right)_{ab}^{-1} (X, Y) \partial_k R_k^{ba}(Y - X) \right], \quad (3.9)$$

Here, $\Gamma_k^{(n)}[\Phi]$ is the n -th derivative of $\Gamma_k[\Phi]$ with respect to the fields. I show the derivation of this equation.

Differentiating Eq. (3.12) with respect to k , one has

$$\begin{aligned} \partial_k \Gamma_k[\Phi] &= -(\partial_k W_k)[J_{\text{sup},k}[\Phi]] - \partial_k \Delta S_k[\Phi] \\ &\quad + \int_X \partial_k J_{\text{sup},k}^a[\Phi](X) \left(\Phi_a(X) - \frac{\delta W_k[J_{\text{sup},k}[\Phi]]}{\delta J^a(X)} \right) \\ &= -(\partial_k W_k)[J_{\text{sup},k}[\Phi]] - \partial_k \Delta S_k[\Phi] \\ &= \frac{1}{Z_k[J_{\text{sup},k}[\Phi]]} \int \mathcal{D}\Phi (\partial_k \Delta S_k[\Phi]) e^{-S[\Phi] - \Delta S_k[\Phi] + \int_X J_{\text{sup},k}^a[\Phi](X) \Phi_a(X)} \\ &\quad - \partial_k \Delta S_k[\Phi] \\ &= \frac{1}{2} \int_{X,Y} \partial_k R_k^{ab}(X - Y) \\ &\quad \times \frac{1}{Z_k[J_{\text{sup},k}[\Phi]]} \int \mathcal{D}\Phi \Phi_a(X) \Phi_b(Y) e^{-S[\Phi] - \Delta S_k[\Phi] + \int_Z J_{\text{sup},k}^c[\Phi](Z) \Phi_c(Z)} \\ &\quad - \frac{1}{2} \int_{X,Y} \partial_k R_k^{ab}(X - Y) \Phi_a(X) \Phi_b(Y) \\ &= \frac{1}{2} \int_{X,Y} \partial_k R_k^{ab}(X - Y) \left. \frac{\delta^2 W_k[J]}{\delta J^a(X) \delta J^b(Y)} \right|_{J=J_{\text{sup},k}[\Phi]}, \end{aligned} \quad (3.10)$$

where Eqs. (3.1) and (3.6)-(3.8) have been used. Differentiating Eq. (3.8) with respect to Φ , one obtains

$$\int_Z \frac{\delta J_{\text{sup},k}^c[\Phi](Z)}{\delta \Phi_b(Y)} \left. \frac{\delta^2 W_k[J]}{\delta J^c(Z) \delta J^a(X)} \right|_{J=J_{\text{sup},k}[\Phi]} = \delta_a^b \delta^{d+1}(X - Y), \quad (3.11)$$

and from the second-order differential of Eq. (3.12) with respect to Φ , one has

$$\frac{\delta^2 \Gamma_k[\Phi]}{\delta \Phi_b(Y) \delta \Phi_c(Z)} = \frac{\delta J_{\text{sup},k}^c[\Phi](Z)}{\delta \Phi_b(Y)} - R_k^{bc}(Y - Z). \quad (3.12)$$

Therefore,

$$\int_Z \left(\frac{\delta^2 \Gamma_k[\Phi]}{\delta \Phi_b(Y) \delta \Phi_c(Z)} + R_k^{bc}(Y - Z) \right) \left. \frac{\delta^2 W_k[J]}{\delta J^c(Z) \delta J^a(X)} \right|_{J=J_{\text{sup},k}[\Phi]} = \delta_a^b \delta^{d+1}(X - Y),$$

which means

$$\left. \frac{\delta^2 W_k[J]}{\delta J^a(X) \delta J^b(Y)} \right|_{J=J_{\text{sup},k}[\Phi]} = \left(\Gamma_k^{(2)}[\Phi] + R_k \right)_{ab}^{-1}(X, Y).$$

With this equation and Eq. (3.10), one has Eq. (3.9).

3.3 Approximation schemes

In principle, the effective action is obtained by solving Eq. (3.9) with the initial condition $\Gamma_\Lambda[\Phi] = S[\Phi]$. The flow equation is, however, a functional differential equation which is hard to solve computationally without any approximation. Therefore some approximation schemes reducing the flow equation to computationally solvable equations are needed for the practical use.

One of such schemes is the Taylor expansion method:

$$\begin{aligned} \Gamma_k[\Phi] = & \Gamma_k[\Phi_{0,k}] + \sum_{n=2}^{\infty} \frac{1}{n!} \int_{X_1, \dots, X_n} \sum_{a_1, \dots, a_n} \frac{\delta^n \Gamma_k[\Phi_{0,k}]}{\delta \Phi_{a_1}(X_1) \cdots \delta \Phi_{a_n}(X_n)} \\ & \times \prod_{i=1}^n (\Phi_{a_i}(X_i) - \Phi_{0,k,a_i}(X_i)). \end{aligned} \quad (3.13)$$

Here, $\Phi_{0,k,a}(X)$ is the average of the field at scale k derived from

$$\frac{\delta \Gamma_k}{\delta \Phi(X)}[\Phi_{0,k}] = 0.$$

By use of this expansion, the flow equation (3.9) is converted to the differential equations for $\{\Gamma_k^{(n)}[\Phi_{0,k}]\}_{n=0}^{\infty}$, where $\Gamma_k^{(n)}[\Phi_{0,k}]$ is the n -th derivative of $\Gamma_k[\Phi]$ with respect to Φ . However, these differential equations form infinite series of coupled equations, in which the flow equation for $\Gamma_k^{(n)}[\Phi_{0,k}]$ depends on $\Gamma_k^{(m \leq n+2)}[\Phi_{0,k}]$, and thus truncation at some order is needed practically. The systematic improvement is possible by including the flow of higher-order derivatives for $\Gamma_k[\Phi]$, which is an advantage of the Taylor expansion scheme.

Another example of the approximation scheme is the derivative expansion scheme, which is the expansion with respect to the time and space derivatives ∂_μ . For instance, the derivative expansion up to second-order for the effective action for the scalar field ϕ reads

$$\Gamma_k[\phi] = \int_X \left[U_k(\phi) + \frac{1}{2} Z_k(\phi) (\partial_\mu \phi)^2 + \mathcal{O}(\partial^4) \right],$$

where $U_k(\phi)$ and $Z_k(\phi)$ are called the effective potential and the wave-function renormalization, respectively. In particular, such a expansion is called the local potential

approximation (LPA) when $Z_k(\phi) = 1$. In contrast to the Taylor expansion scheme, the derivative expansion scheme provides the global information of $\Gamma_k[\Phi]$ on the space of the field. This enables one to investigate first-order phase transitions, which cannot be described in the Taylor expansion scheme.

Chapter 4

Formulation of functional-renormalization-group aided density-functional theory

There are some studies to derive the EDF from the microscopic Hamiltonian. One of those developed recently is the functional-renormalization-group aided density-functional theory (FRG-DFT), which is an attempt to determine the EDFs from microscopic Hamiltonians by borrowing the idea of the FRG [24, 25]. In this chapter, the formal aspect of the functional-renormalization-group aided density-functional theory (FRG-DFT) is reviewed. The formulation of the DFT in terms of the effective action is shown and the flow equation, which plays a key role in the analysis with the FRG-DFT, is derived. At last, I explicitly reproduce the expression for the energy found in the adiabatic connection [27–31] from the FRG-DFT from equation for the first time.

4.1 Definition of EDF in the effective action formalism

A key point of the FRG-DFT is that the EDF can be defined as an effective action [22, 23]. Since the FRG is a formalism based on the effective action formalism, the correspondence between the EDF and the effective action enables one to employ the idea of the FRG. I first show the correspondence between the EDF and the effective action.

Let us consider a system composed of non-relativistic fermions with spin S interacting via a two-body interaction in an external field, whose normal-ordered Hamiltonian

reads:

$$\begin{aligned} \hat{H} = & \sum_s \int_{\mathbf{x}} \hat{\psi}_s^*(\mathbf{x}) \left(\frac{-\hbar^2 \Delta}{2m} + V(\mathbf{x}) \right) \hat{\psi}_s(\mathbf{x}) \\ & + \frac{1}{2} \sum_{s,s'} \int_{\mathbf{x},\mathbf{x}'} \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') U(\mathbf{x},\mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') \hat{\psi}_s(\mathbf{x}), \end{aligned} \quad (4.1)$$

where $\hat{\psi}_s(\mathbf{x})$ and $\hat{\psi}_s^*(\mathbf{x})$ are the fermion fields with spin index s , m is the mass of the fermion, $\int_{\mathbf{x}}$ is the shorthand of $\int d\mathbf{x}$, $U(\mathbf{x},\mathbf{x}')$ is the two-body interaction, and $V(\mathbf{x})$ is the external field. Here, let us assume that $U(\mathbf{x},\mathbf{x}')$ and $V(\mathbf{x})$ are independent of the spin component for simplicity.

The imaginary-time path integral formalism for finite temperature, which makes the relation between the EDF and the effective action clear, is employed below. The action corresponding to the Hamiltonian Eq. (4.1) reads

$$\begin{aligned} S[\psi, \psi^*] = & \sum_s \int_X \psi_s^*(X_\epsilon) \left(\partial_\tau - \frac{\hbar^2 \Delta}{2m} + V(\mathbf{x}) \right) \psi_s(X) \\ & + \frac{1}{2} \sum_{s,s'} \int_{X,X'} \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) U_{2b}(X, X') \psi_{s'}(X') \psi_s(X). \end{aligned} \quad (4.2)$$

Here, $X = (\tau, \mathbf{x})$ is the vector of the imaginary time τ and space coordinate $\mathbf{x}$, and $\int_X$ is the shorthand of $\int_0^\beta d\tau \int d\mathbf{x}$, where β is the inverse temperature. $U_{2b}(X, X')$ is defined as follows:

$$U_{2b}(X, X') = \delta(\tau - \tau') U(\mathbf{x}, \mathbf{x}').$$

X_ϵ is $X_\epsilon = (\tau + \epsilon, \mathbf{x})$, where ϵ is a positive infinitesimal. Such a positive infinitesimal appears from the construction of the path integral formalism based on the normal-ordered Hamiltonian; see Appendix A.

The EDF is defined as the effective action for the density field $\rho_\psi(X) = \sum_s \psi_s^*(X_\epsilon) \psi_s(X)$, which is also known as the two-particle point irreducible effective action. To define the effective action for the density field, the generating functional for the density correlation functions is introduced:

$$Z[J] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{-S[\psi, \psi^*] + \int_X J(X) \rho_\psi(X)}. \quad (4.3)$$

The generating functional for the connected density correlation functions is obtained as

$$W[J] = \ln Z[J]. \quad (4.4)$$

Then the effective action for the density field $\Gamma[\rho]$ is defined as the Legendre transformation of $W[J]$:

$$\Gamma[\rho] = \sup_J \left(\int_X J(X) \rho(X) - W[J] \right). \quad (4.5)$$

By use of $\Gamma[\rho]$, the EDF $E[\rho]$ is defined as follows [22]:

$$E[\rho] = \lim_{\beta \rightarrow \infty} \frac{\Gamma[\rho]}{\beta}. \quad (4.6)$$

Actually, this EDF satisfies the condition claimed in the second statement of the HK theorem, i.e., $E[\rho]$ gives the ground state density ρ_{gs} and energy E_{gs} at its minimum point. Let us consider the variation of $\Gamma[\rho]/\beta$. Here, I consider the τ -averaged particle number $(1/\beta) \int_X \rho(X)$ and impose a constraint that $(1/\beta) \int_X \rho(X)$ is fixed. The variational equation reads

$$\frac{\delta}{\delta \rho(X)} \left(\frac{\Gamma[\rho]}{\beta} - \frac{\mu}{\beta} \int_{X'} \rho(X') \right) = 0, \quad (4.7)$$

where μ is the Lagrangian multiplier, or the chemical potential. This variational equation is rewritten as

$$\Gamma^{(1)}[\rho](X) = J_{\text{sup}}[\rho](X) = \mu, \quad (4.8)$$

where $J_{\text{sup}}[\rho](X)$ is the source maximizing $\int_X J(X)\rho(X) - W[J]$, which satisfies

$$W^{(1)}[J_{\text{sup}}[\rho]](X) = \rho(X). \quad (4.9)$$

Here, the following notations have been introduced:

$$\begin{aligned} \frac{\delta^n \Gamma[\rho]}{\delta \rho(X_1) \cdots \delta \rho(X_n)} &= \Gamma^{(n)}[\rho](X_1, \dots, X_n), \\ \frac{\delta^n W[J]}{\delta J(X_1) \cdots \delta J(X_n)} &= W^{(n)}[J](X_1, \dots, X_n). \end{aligned}$$

Substituting ρ in Eq. (4.9) for the solution of Eq. (4.7) $\rho = \bar{\rho}$, one has

$$\bar{\rho}(X) = W^{(1)}[\mu](X) = \frac{1}{Z[\mu]} \int \mathcal{D}\psi^* \mathcal{D}\psi \rho_\psi(X) e^{-S[\psi, \psi^*] + \mu \int_X \rho_\psi(X')},$$

which is nothing but the average of $\rho_\psi(X)$ for temperature β^{-1} in the presence of the chemical potential μ . Therefore, one has $\bar{\rho} = \rho_{\text{gs}}$ at $\beta \rightarrow \infty$. For $\rho = \bar{\rho}$, $(1/\beta)\Gamma[\rho]$ becomes as follows:

$$\begin{aligned} \frac{1}{\beta} \Gamma[\bar{\rho}] &= \frac{1}{\beta} \left(\int_X J_{\text{sup}}[\bar{\rho}](X) \bar{\rho}(X) - W[J_{\text{sup}}[\bar{\rho}]] \right) \\ &= \frac{\mu}{\beta} \int_X \bar{\rho}(X) - \frac{1}{\beta} W[\mu]. \end{aligned}$$

Here, $-(1/\beta)W[\mu] = -(1/\beta) \ln Z[\mu]$ is the grand potential since $Z[\mu]$ is the grand partition function in the presence of the chemical potential μ , and $(1/\beta) \int_X \bar{\rho}(X)$ is corresponding to the particle number. Therefore, $(1/\beta)\Gamma[\bar{\rho}]$ is identified with the Helmholtz

free energy F_H . The Helmholtz free energy becomes the ground state energy at $\beta \rightarrow \infty$, which follows from the spectral representation of F_H :

$$F_H = -\frac{1}{\beta} \ln \sum_n e^{-\beta E_n},$$

where $\{E_n\}_{n=0}^\infty$ is the eigenenergies of the system satisfying $E_{\text{gs}} = E_0 < E_1 < \dots$. To summarize, the ground state density ρ_{gs} and energy E_{gs} are obtained from the minimum point of $E[\rho]$ given in Eq. (4.14).

I also discuss how the first statement of the HK theorem emerges in the present framework. To discuss the dependence of $\Gamma[\rho]$ on the external field V , let us denote $\Gamma[\rho]$ as $\Gamma[\rho; V]$. From Eq. (4.3), one can see that the change of V can be absorbed by the shift of J . Using this property, one has

$$\Gamma[\rho; V] = \Gamma[\rho; 0] + \int_X V(\mathbf{x})\rho(X). \quad (4.10)$$

Since $\Gamma[\rho; 0]$ does not depend the external field, $(1/\beta)\Gamma[\rho; 0]$ is identified with the universal part of the EDF $F[\rho]$. The fact that the different external fields $V(\mathbf{x})$ and $V'(\mathbf{x})$, the difference of which can not be absorbed by the constant shift, give the different $\rho_{\text{gs}}(X)$ is shown in the present formalism as follows: To prove it, assume that the different external fields $V(\mathbf{x})$ and $V'(\mathbf{x})$ give the same $\rho_{\text{gs}}(X)$. Then the variational equations (4.8) read

$$\begin{aligned} \Gamma^{(1)}[\rho_{\text{gs}}; V](X) &= \Gamma^{(1)}[\rho_{\text{gs}}; 0](X) + V(\mathbf{x}) = \mu, \\ \Gamma^{(1)}[\rho_{\text{gs}}; V'](X) &= \Gamma^{(1)}[\rho_{\text{gs}}; 0](X) + V'(\mathbf{x}) = \mu', \end{aligned}$$

where μ and μ' are the chemical potentials to make $(1/\beta) \int_X \rho_{\text{gs}}(X)$ the same in both cases when the external field is $V(\mathbf{x})$ and $V'(\mathbf{x})$. From these equations, one has

$$V(\mathbf{x}) - V'(\mathbf{x}) = \mu - \mu'.$$

This is in contradict with our assumption that the difference between $V(\mathbf{x})$ and $V'(\mathbf{x})$ cannot be absorbed by the constant shift. Therefore, the fact that the ground-state density uniquely determine the external field is proven in the framework of the effective action.

4.2 FRG-DFT flow equation

The last section has shown that the EDF $E[\rho]$ can be defined as the effective action for the density $\Gamma[\rho]$. Such an effective action formalism enables us to introduce the idea of the FRG to derive $E[\rho]$. In this section, I show the idea of the FRG-DFT and derive the flow equation for the effective action.

In the conventional FRG, regulator terms as Eq. (3.1) are introduced. However, such regulator terms are non-local, and make it difficult to describe the theory in terms of

the density field $\hat{\rho}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$. We will see that the introduction of the regulators for the interaction terms instead of the regulators for particle fields is suitable for constructing a theory based on the density field.

Here, let us consider a system described by the action Eq. (4.2). Following the procedure proposed by Refs. [24, 25], the following regulated action with a flow parameter $\lambda \in [0, 1]$ is introduced:

$$S_\lambda[\psi^*, \psi] = \int_X \psi_s^*(X_\epsilon) \left(\partial_\tau - \frac{\hbar^2 \Delta}{2m} + V(\mathbf{x}) \right) \psi_s(X) + \frac{1}{2} \int_{X, X'} U_{2b, \lambda}(X, X') \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) \psi_{s'}(X') \psi_s(X). \quad (4.11)$$

Here, $U_{2b, \lambda}(X, X') = \delta(\tau - \tau') U_\lambda(\mathbf{x}, \mathbf{x}')$ is the regulated two-body interaction, which satisfies $U_0(\mathbf{x}, \mathbf{x}') = 0$ and $U_1(\mathbf{x}, \mathbf{x}') = U(\mathbf{x}, \mathbf{x}')$. Then $S_{\lambda=0}$ is the action for the free case and $S_{\lambda=1}$ is the action for the fully interacting case.

By use of this regulated action, the λ -dependent effective action can be defined in the same manner as Eq. (4.5):

$$\Gamma_\lambda[\rho] = \sup_J \left(\int_X J(X) \rho(X) - W_\lambda[J] \right), \quad (4.12)$$

where $W_\lambda[J]$ is the λ -dependent generating functional for the connected density correlation functions, which is defined by the λ -dependent generating functional for the density correlation functions $Z_\lambda[J]$ as follows:

$$W_\lambda[J] = \ln Z_\lambda[J] = \ln \int \mathcal{D}\psi^* \mathcal{D}\psi e^{-S_\lambda[\psi, \psi^*] + \int_X J(X) \rho_\psi(X)}. \quad (4.13)$$

The λ -dependent EDF $E_\lambda[\rho]$ is defined as follows:

$$E_\lambda[\rho] = \lim_{\beta \rightarrow \infty} \frac{\Gamma_\lambda[\rho]}{\beta}. \quad (4.14)$$

The variational equation for $\Gamma_\lambda[\rho]$ becomes as follows:

$$\Gamma_\lambda^{(1)}[\rho_{gs, \lambda}](X) = J_{\text{sup}, \lambda}[\rho_{gs, \lambda}](X) = \mu_\lambda, \quad (4.15)$$

where $\rho_{gs, \lambda}$ is the λ -dependent ground-state density and $J_{\text{sup}, \lambda}[\rho](X)$ is the source maximizing $\int_X J(X) \rho(X) - W_\lambda[J]$. Here, I have introduced the λ -dependent chemical potential μ_λ , which is needed to control the expectation value of the number of the particle during the flow in the case of the grand-canonical formulation. In the context of the FRG-DFT, the λ -dependent chemical potential was introduced by the present author and the collaborators [52]. I also remark that the scale dependent chemical potentials were also discussed [63, 64] in the framework of the FRG à la Wetterich [4, 5] and the change of the chemical potential by the interaction was discussed in the context of DFT [19].

The flow equation for the effective action is described as the functional differential equation in the FRG formalism; see Chapter 3.2. Similarly, the evolution for $\Gamma_\lambda[\rho]$ with respect to λ can be described as the functional differential equation. Let us derive such a flow equation. Differentiating Eq. (4.12) with respect to λ , one has

$$\begin{aligned}\partial_\lambda \Gamma_\lambda[\rho] &= -(\partial_\lambda W_\lambda)[J_{\text{sup},\lambda}[\rho]] \\ &\quad + \int_X \partial_\lambda J_{\text{sup},\lambda}[\rho](X) \frac{\delta}{\delta J(X)} \left(\int_X J(X) \rho(X) - W_\lambda[J] \right) \Big|_{J=J_{\text{sup},\lambda}} \\ &= -(\partial_\lambda W_\lambda)[J_{\text{sup},\lambda}[\rho]] \\ &= \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \sum_{s,s'} \langle \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) \psi_{s'}(X') \psi_s(X) \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]},\end{aligned}$$

where $\langle \mathcal{O} \rangle_{\rho,\lambda}$ for an arbitral functional $\mathcal{O}[\psi^*, \psi]$ of ψ^* and ψ is defined as follows:

$$\langle \mathcal{O} \rangle_{\lambda,J} = \frac{1}{Z[J]} \int \mathcal{D}\psi^* \mathcal{D}\psi \mathcal{O}[\psi^*, \psi] e^{-S_\lambda[\psi, \psi^*] + \int_X J(X) \rho_\psi(X)}. \quad (4.16)$$

The right-hand side of the flow equation can be rewritten in terms of $\Gamma_\lambda[\rho]$ by use of the fact that the second derivative of $\Gamma_\lambda[\rho]$ with respect to ρ corresponds to the inverse density–density correlation function: From the second derivative of Eq. (4.13) with respect to J , one has

$$\begin{aligned}W_\lambda^{(2)}[J_{\text{sup},\lambda}[\rho]](X, X') &= \langle \rho_\psi(X) \rho_\psi(X') \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} - \langle \rho_\psi(X) \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} \langle \rho_\psi(X') \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} \\ &= \sum_{s,s'} \langle \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) \psi_{s'}(X') \psi_s(X) \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} - \rho(X) \rho(X'),\end{aligned} \quad (4.17)$$

where the following relation has been used:

$$\langle \rho_\psi(X) \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} = W_\lambda^{(1)}[J_{\text{sup},\lambda}[\rho]](X) = \rho(X), \quad (4.18)$$

which follows from the fact that $J_{\text{sup},\lambda}[\rho]$ is defined so that $J = J_{\text{sup},\lambda}[\rho]$ maximizes $\int_X J(X) \rho(X) - W_\lambda[J]$. Next, I prove the relation

$$\Gamma_\lambda^{(2)-1}[\rho](X, X') = W_\lambda^{(2)}[J_{\text{sup},\lambda}[\rho]](X, X'), \quad (4.19)$$

where $\Gamma_\lambda^{(2)-1}[\rho](X, X')$ is defined as the inverse of $\Gamma_\lambda^{(2)}[\rho](X, X')$:

$$\int_{X'} \Gamma_\lambda^{(2)}[\rho](X, X') \Gamma_\lambda^{(2)-1}[\rho](X', X'') = \delta(X - X'').$$

Differentiating Eq. (4.18) with respect to ρ , one has

$$\int_{X'} \frac{\delta J_{\text{sup},\lambda}[\rho](X')}{\delta \rho(X)} W_\lambda^{(2)}[J_{\text{sup},\lambda}[\rho]](X', X'') = \delta(X - X'').$$

Substituting $J_{\text{sup},\lambda}[\rho](X')$ for $\Gamma_\lambda^{(1)}[\rho](X')$ by use of Eq. (4.15), one gets

$$\int_{X'} \Gamma_\lambda^{(2)}[\rho](X, X') W_\lambda^{(2)}[J_{\text{sup},\lambda}[\rho]](X', X'') = \delta(X - X'').$$

Therefore, one obtains Eq. (4.19). By use of Eqs. (4.17) and (4.19), one has

$$\Gamma_\lambda^{(2)-1}[\rho](X, X') = \sum_{s,s'} \langle \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) \psi_{s'}(X') \psi_s(X) \rangle_{\lambda, J_{\text{sup},\lambda}[\rho]} - \rho(X) \rho(X'),$$

and thus one obtains the flow equation described in terms of $\Gamma_\lambda[\rho]$ as follows:

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \left(\rho(X) \rho(X') + \Gamma_\lambda^{(2)-1}[\rho](X, X') \right). \quad (4.20)$$

Here, it should be noted that $\Gamma_\lambda^{(2)-1}[\rho](X, X')$ does not correspond to the density-density correlation function at $\tau = \tau'$ due to the presence of ϵ : For simplicity, consider the case of $\rho = \rho_{\text{gs},\lambda}$, in which one has

$$\langle \mathcal{O} \rangle_{\lambda, J_{\text{sup},\lambda}[\rho_{\text{gs},\lambda}]} = \frac{1}{Z[J]} \int \mathcal{D}\psi^* \mathcal{D}\psi \mathcal{O}[\psi^*, \psi] e^{-S_\lambda[\psi, \psi^*] + \mu_\lambda \int_X \rho_\psi(X)}, \quad (4.21)$$

for arbitral operator $\mathcal{O}$, since $J_{\text{sup},\lambda}[\rho_{\text{gs},\lambda}] = \mu_\lambda$. This average corresponds to the time-ordered average in the operator formalism as follows:

$$\langle \mathcal{O} \rangle_{\lambda, J_{\text{sup},\lambda}[\rho_{\text{gs},\lambda}]} = \langle T_\tau \hat{\mathcal{O}} \rangle_{\text{op}} := \frac{\text{Tr}[e^{-\beta \hat{K}} T_\tau \hat{\mathcal{O}}]}{\text{Tr} e^{-\beta \hat{K}}},$$

where

$$\begin{aligned} \hat{K} = & \sum_s \int_{\mathbf{x}} \hat{\psi}_s^*(\mathbf{x}) \left(\frac{-\hbar^2 \Delta}{2m} + V(\mathbf{x}) \right) \hat{\psi}_s(\mathbf{x}) \\ & + \frac{1}{2} \sum_{s,s'} \int_{\mathbf{x}, \mathbf{x}'} \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') U_\lambda(\mathbf{x}, \mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') \hat{\psi}_s(\mathbf{x}) \\ & - \mu_\lambda \sum_s \int_{\mathbf{x}} \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_s(\mathbf{x}). \end{aligned}$$

Here, T_τ orders the operators in $\hat{\mathcal{O}}$ according to the value of the imaginary time. Then, $\Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](X, X')$ is written as follows:

$$\begin{aligned} \Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](X, X') = & \sum_{s,s'} \langle T_\tau \hat{\psi}_s^*(\tau + \epsilon, \mathbf{x}) \hat{\psi}_{s'}^*(\tau' + \epsilon, \mathbf{x}') \hat{\psi}_{s'}(\tau', \mathbf{x}') \hat{\psi}_s(\tau, \mathbf{x}) \rangle_{\text{op}} \\ & - \rho_{\text{gs},\lambda}(X) \rho_{\text{gs},\lambda}(X'). \end{aligned} \quad (4.22)$$

In the case of $\tau' > \tau$, Eq. (4.22) corresponds to the density correlation function $\langle \hat{\rho}(\tau', \mathbf{x}') \hat{\rho}(\tau, \mathbf{x}) \rangle_{\text{op}} - \rho_{\text{gs},\lambda}(X) \rho_{\text{gs},\lambda}(X')$, where $\hat{\rho}(\tau, \mathbf{x}) = \sum_s \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_s(\mathbf{x})$. This relation

holds also when $\tau' < \tau$. In the case of $\tau' = \tau$, however, Eq. (4.22) does not correspond to the density correlation function: Equation (4.22) at $\tau = \tau'$ reads

$$\begin{aligned} \Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](\tau, \mathbf{x}, \tau, \mathbf{x}') &= \sum_{s,s'} \langle \hat{\psi}_s^*(\tau, \mathbf{x}) \hat{\psi}_{s'}^*(\tau, \mathbf{x}') \hat{\psi}_{s'}(\tau, \mathbf{x}') \hat{\psi}_s(\tau, \mathbf{x}) \rangle_{\text{op}} \\ &\quad - \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \rho_{\text{gs},\lambda}(\tau, \mathbf{x}'). \end{aligned}$$

The ordering of the field operators in the average in this equation does not correspond to the density correlation function. To construct the theory in terms of the density field and its correlation functions, $\Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](\tau, \mathbf{x}, \tau, \mathbf{x}')$ is rewritten by use of the canonical commutation relation as follows:

$$\begin{aligned} &\Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](\tau, \mathbf{x}, \tau, \mathbf{x}') \\ &= \sum_{s,s'} \langle \hat{\psi}_s^*(\tau, \mathbf{x}) \hat{\psi}_s(\tau, \mathbf{x}) \hat{\psi}_{s'}^*(\tau, \mathbf{x}') \hat{\psi}_{s'}(\tau, \mathbf{x}') \rangle_{\text{op}} \\ &\quad - \sum_{s,s'} \delta_{s,s'} \delta(\mathbf{x} - \mathbf{x}') \langle \hat{\psi}_s^*(\tau, \mathbf{x}) \hat{\psi}_s(\tau, \mathbf{x}) \rangle_{\text{op}} - \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \rho_{\text{gs},\lambda}(\tau, \mathbf{x}') \\ &= \langle \hat{\rho}(\tau, \mathbf{x}) \hat{\rho}(\tau, \mathbf{x}') \rangle_{\text{op}} - \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \rho_{\text{gs},\lambda}(\tau, \mathbf{x}') - \delta(\mathbf{x} - \mathbf{x}') \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \\ &= \sum_{s,s'} \langle T_\tau \hat{\psi}_s^*(\tau + \epsilon' + \epsilon, \mathbf{x}) \hat{\psi}_{s'}^*(\tau + \epsilon, \mathbf{x}') \hat{\psi}_{s'}(\tau, \mathbf{x}') \hat{\psi}_s(\tau + \epsilon', \mathbf{x}) \rangle_{\text{op}} \\ &\quad - \rho_{\text{gs},\lambda}(\tau + \epsilon', \mathbf{x}) \rho_{\text{gs},\lambda}(\tau, \mathbf{x}') - \delta(\mathbf{x} - \mathbf{x}') \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \\ &= \Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}') - \rho_{\text{gs},\lambda}(\tau, \mathbf{x}) \delta(\mathbf{x} - \mathbf{x}'), \end{aligned}$$

where a positive infinitesimal ϵ' satisfying $\epsilon' > \epsilon$ has been introduced. Note that $\Gamma_\lambda^{(2)-1}[\rho_{\text{gs},\lambda}](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}')$ corresponds to the density correlation function. This relation can be extended to the case of other densities. By use of this relation, the right-hand side of Eq. (4.20) is rewritten as follows:

$$\begin{aligned} &\frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \left(\rho(X) \rho(X') + \Gamma_\lambda^{(2)-1}[\rho](X, X') \right) \\ &= \frac{1}{2} \int_{\tau, \mathbf{x}, \mathbf{x}'} \partial_\lambda U_\lambda(\mathbf{x}, \mathbf{x}') \left(\rho(\tau, \mathbf{x}) \rho(\tau, \mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho](\tau, \mathbf{x}, \tau, \mathbf{x}') \right) \\ &= \frac{1}{2} \int_{\tau, \mathbf{x}, \mathbf{x}'} \partial_\lambda U_\lambda(\mathbf{x}, \mathbf{x}') \left(\rho(\tau, \mathbf{x}) \rho(\tau, \mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}') \right. \\ &\quad \left. - \rho(\tau, \mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right) \\ &= \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \left(\rho(X) \rho(X') + \Gamma_\lambda^{(2)-1}[\rho](X_{\epsilon'}, X') - \rho(X) \delta(\mathbf{x} - \mathbf{x}') \right). \end{aligned}$$

Therefore, Eq. (4.20) is rewritten as follows [25, 46]:

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\rho] &= \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \\ &\quad \times \left(\rho(X) \rho(X') + \Gamma_\lambda^{(2)-1}[\rho](X_{\epsilon'}, X') - \rho(X) \delta(\mathbf{x} - \mathbf{x}') \right). \end{aligned} \quad (4.23)$$

I emphasize that $\Gamma_\lambda^{(2)-1}[\rho](X_\epsilon, X')$ can be regarded as the density correlation function in this flow equation thanks to the introduction of ϵ' . The physical meaning of Eq. (4.23) becomes clearer by rewriting it as follows:

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\rho] = & \frac{1}{2} \int_{X, X'} \partial_\lambda U_{2b, \lambda}(X, X') \rho(X) \rho(X') \\ & + \frac{1}{2} \int_{X, X'} \partial_\lambda U_{2b, \lambda}(X, X') \left(\Gamma_0^{(2)-1}[\rho](X_{\epsilon'}, X') - \rho(X) \delta(\mathbf{x} - \mathbf{x}') \right) \\ & + \frac{1}{2} \int_{X, X'} \partial_\lambda U_{2b, \lambda}(X, X') \left(\Gamma_\lambda^{(2)-1}[\rho](X_{\epsilon'}, X') - \Gamma_0^{(2)-1}[\rho](X_{\epsilon'}, X') \right). \end{aligned}$$

The first and second terms is of the first order with respect to $U_{2b, \lambda}$, and can be interpreted as the Hartree and exchange terms, respectively. The third term corresponds to the correlation term.

To summarize, the EDF can be obtained from the microscopic Hamiltonian with solving Eq. (4.23) starting from the effective action for the free case $\Gamma_0[\rho]$. However, the flow equation is the functional differential equation which is difficult to be solved without any approximation as the Wetterich equation (3.9). Some approximation schemes inspired by the FRG, such as the vertex expansion scheme, are available for the practical use of Eq. (4.23).

4.3 Relation to the adiabatic connection

Before closing this chapter, let us discuss the relation between FRG-DFT and the adiabatic connection [27–31]. I explicitly show that the expression for the ground-state energy found in the adiabatic connection scheme is reproduced from Eq. (4.23).

In the adiabatic connection scheme, the change of the system from the free case to the interacting case is considered as the FRG-DFT. The point is that an external field which fixes the ground-state density $\rho_{\text{gs}}(\mathbf{x})$ during the change of the system is introduced. Consider the following λ -dependent normal-ordered Hamiltonian:

$$\hat{H}_\lambda = \hat{T} + \lambda \hat{W} + \hat{V}_\lambda, \quad (4.24)$$

where

$$\hat{T} = \sum_s \int_{\mathbf{x}} \hat{\psi}_s^*(\mathbf{x}) \frac{-\hbar^2 \Delta}{2m} \hat{\psi}_s(\mathbf{x}), \quad (4.25)$$

$$\hat{W} = \frac{1}{2} \sum_{s, s'} \int_{\mathbf{x}, \mathbf{x}'} \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') U(\mathbf{x}, \mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') \hat{\psi}_s(\mathbf{x}), \quad (4.26)$$

$$\hat{V}_\lambda = \sum_s \int_{\mathbf{x}} V_\lambda(\mathbf{x}) \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_s(\mathbf{x}), \quad (4.27)$$

and $V_\lambda(\mathbf{x})$ is the external field fixing the ground-state density. $V_\lambda(\mathbf{x})$ coincides with the KS potential $V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x})$ at $\lambda = 0$, and the external potential applied to the system $V(\mathbf{x})$ at $\lambda = 1$. The ground-state energy of the system $E_\lambda[\rho_{\text{gs}}]$ is obtained as follows:

$$E_\lambda[\rho_{\text{gs}}] = \langle \Psi_\lambda | \hat{H}_\lambda | \Psi_\lambda \rangle, \quad (4.28)$$

where $|\Psi_\lambda\rangle$ is the ground-state wave function. Then the Hellmann-Feynman theorem gives the following relation:

$$\frac{dE_\lambda[\rho_{\text{gs}}]}{d\lambda} = \langle \Psi_\lambda | \frac{d\hat{H}_\lambda}{d\lambda} | \Psi_\lambda \rangle = \langle \Psi_\lambda | \hat{W} | \Psi_\lambda \rangle + \langle \Psi_\lambda | \frac{d\hat{V}_\lambda}{d\lambda} | \Psi_\lambda \rangle. \quad (4.29)$$

Integrating this equation with respect to λ , one has

$$\begin{aligned} E_1[\rho_{\text{gs}}] &= E_0[\rho_{\text{gs}}] + \int_0^1 d\lambda \langle \Psi_\lambda | \hat{W} | \Psi_\lambda \rangle + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) (V(\mathbf{x}) - V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x})) \\ &= E_0[\rho_{\text{gs}}] - \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V(\mathbf{x}) \\ &\quad + \frac{1}{2} \int_0^1 d\lambda \sum_{s,s'} \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x},\mathbf{x}') \langle \Psi_\lambda | \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') \hat{\psi}_s(\mathbf{x}) | \Psi_\lambda \rangle \\ &= E_0[\rho_{\text{gs}}] - \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V(\mathbf{x}) \\ &\quad + \frac{1}{2} \int_0^1 d\lambda \sum_{s,s'} \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x},\mathbf{x}') \left(\langle \Psi_\lambda | \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_s(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') | \Psi_\lambda \rangle \right. \\ &\quad \left. - \delta_{s,s'} \delta(\mathbf{x} - \mathbf{x}') \langle \Psi_\lambda | \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_s(\mathbf{x}) | \Psi_\lambda \rangle \right) \\ &= E_0[\rho_{\text{gs}}] - \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V(\mathbf{x}) \\ &\quad + \frac{1}{2} \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x},\mathbf{x}') \rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') \\ &\quad + \frac{1}{2} \int_0^1 d\lambda \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x},\mathbf{x}') \left(\langle \Psi_\lambda | \hat{\rho}(\mathbf{x}) \hat{\rho}(\mathbf{x}') | \Psi_\lambda \rangle \right. \\ &\quad \left. - \rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right). \end{aligned} \quad (4.30)$$

Here, the canonical commutation relation for $\hat{\psi}_s(\mathbf{x})$ and $\hat{\psi}_s^*(\mathbf{x})$ has been used. $E_0[\rho_{\text{gs}}]$ coincides with $T_s[\rho_{\text{gs}}] + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V_{\text{KS}}[\rho_{\text{gs}}](\mathbf{x}) = \sum_{i=1}^N \epsilon_i$, where ϵ_i is the eigenenergy of the KS orbital appearing in Eq. (2.12) and $N = \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x})$. Then the exchange–correlation energy is extracted by comparing Eq. (4.30) with Eq. (2.15):

$$E_{\text{xc}}[\rho_{\text{gs}}] = \frac{1}{2} \int_0^1 d\lambda \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x},\mathbf{x}') \left(G_\lambda^{(2)}(\mathbf{x},\mathbf{x}') - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right), \quad (4.31)$$

where $G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}')$ is the density–density correlation function:

$$G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}') = \langle \Psi_\lambda | \hat{\rho}(\mathbf{x}) \hat{\rho}(\mathbf{x}') | \Psi_\lambda \rangle - \rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}'). \quad (4.32)$$

An approach in the adiabatic connection is approximating $G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}')$ in Eq. (4.31) by the aid of the fluctuation-dissipation theorem to derive the EDF. $G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}')$ is related to the response function by the fluctuation-dissipation theorem, and then one can employ the Dyson equation-like relation to approximate the response function. Such an approach is called the adiabatic connection fluctuation-dissipation theory [27–31].

Next, I derive the expression for the exchange–correlation energy from Eq. (4.23). Here, $U_{2b,\lambda}(X, X')$ and $\rho(X)$ are set to $\lambda\delta(\tau - \tau')U(\mathbf{x}, \mathbf{x}')$ and τ -independent ground-state density $\rho_{\text{gs}}(\mathbf{x})$, respectively. Under this setup, Eq. (4.23) reads as follows:

$$\begin{aligned} \partial_\lambda \Gamma_\lambda[\rho_{\text{gs}}] = & \frac{1}{2} \int_{\tau, \mathbf{x}, \mathbf{x}'} U(\mathbf{x}, \mathbf{x}') \\ & \times \left(\rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}') - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right). \end{aligned} \quad (4.33)$$

$\Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}')$ corresponds to the density–density correlation function as I have discussed in the previous section. In addition, $\Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\tau + \epsilon', \mathbf{x}, \tau, \mathbf{x}')$ does not depend on τ since the system has time translational symmetry. Therefore, integrating Eq. (4.33) with respect to λ , one has

$$\begin{aligned} \Gamma_1[\rho_{\text{gs}}] = & \Gamma_0[\rho_{\text{gs}}] + \frac{\beta}{2} \int_{\mathbf{x}, \mathbf{x}'} U(\mathbf{x}, \mathbf{x}') \left(\rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\epsilon', \mathbf{x}, 0, \mathbf{x}') \right. \\ & \left. - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right) \\ = & \Gamma_0[\rho_{\text{gs}}; 0] + \beta \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V(\mathbf{x}) \\ & + \frac{\beta}{2} \int_{\mathbf{x}, \mathbf{x}'} U(\mathbf{x}, \mathbf{x}') \left(\rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\epsilon', \mathbf{x}, 0, \mathbf{x}') \right. \\ & \left. - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right), \end{aligned} \quad (4.34)$$

where $\Gamma_0[\rho_{\text{gs}}]$ has been denoted as $\Gamma_0[\rho_{\text{gs}}; V]$ and Eq. (4.10) has been used. Since $\Gamma_0[\rho_{\text{gs}}; 0]/\beta$ at $\beta \rightarrow \infty$ is the kinetic energy of the free system, one has

$$\begin{aligned} E_1[\rho_{\text{gs}}] = & T_s[\rho_{\text{gs}}] + \int_{\mathbf{x}} \rho_{\text{gs}}(\mathbf{x}) V(\mathbf{x}) \\ & + \frac{1}{2} \int_{\mathbf{x}, \mathbf{x}'} U(\mathbf{x}, \mathbf{x}') \left(\rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') + \Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\epsilon', \mathbf{x}, 0, \mathbf{x}') \right. \\ & \left. - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right), \end{aligned} \quad (4.35)$$

where Eq. (4.14) has been used. Therefore, the exchange–correlation energy is extracted as follows:

$$E_{\text{xc}}[\rho_{\text{gs}}] = \frac{1}{2} \int_{\mathbf{x}, \mathbf{x}'} U(\mathbf{x}, \mathbf{x}') \left(\Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\epsilon', \mathbf{x}, 0, \mathbf{x}') - \rho_{\text{gs}}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') \right). \quad (4.36)$$

As seen in

$$\rho_{\text{gs}}(\mathbf{x}) = \frac{1}{Z[J_{\text{sup},\lambda}[\rho_{\text{gs}}]]} \int \mathcal{D}\psi^* \mathcal{D}\psi \rho_\psi(0, \mathbf{x}) e^{-S_\lambda[\psi, \psi^*] + \int_X J_{\text{sup},\lambda}[\rho_{\text{gs}}](\mathbf{x}) \rho_\psi(X)},$$

$J_{\text{sup},\lambda}[\rho_{\text{gs}}]$ plays a role of shifting the external field to fix the ground-state density to $\rho_{\text{gs},\lambda}(\mathbf{x})$. This leads to the following identification: $V_\lambda(\mathbf{x}) = V(\mathbf{x}) - J_{\text{sup},\lambda}[\rho_{\text{gs}}](\mathbf{x})$, where $V_\lambda(\mathbf{x})$ is the external field introduced in Eq. (4.27). Thus, $\Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}]$ coincides with $G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}')$ defined in Eq. (4.32) as explicitly seen in the following expression:

$$\begin{aligned} & \Gamma_\lambda^{(2)-1}[\rho_{\text{gs}}](\epsilon', \mathbf{x}, 0, \mathbf{x}') \\ &= \sum_{s,s'} \langle \psi_s^*(\epsilon' + \epsilon, \mathbf{x}) \psi_s(\epsilon', \mathbf{x}) \psi_{s'}^*(\epsilon, \mathbf{x}') \psi_{s'}(0, \mathbf{x}') \rangle_{\lambda, J_{\text{sup},\lambda}[\rho_{\text{gs}}]} - \rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}') \\ &= \frac{1}{Z[J_{\text{sup},\lambda}[\rho_{\text{gs}}]]} \int \mathcal{D}\psi^* \mathcal{D}\psi \rho_\psi(\epsilon', \mathbf{x}) \rho_\psi(0, \mathbf{x}') e^{-S_\lambda[\psi, \psi^*] + \int_X J_{\text{sup},\lambda}[\rho_{\text{gs}}](\mathbf{x}) \rho_\psi(X)} \\ & \quad - \rho_{\text{gs}}(\mathbf{x}) \rho_{\text{gs}}(\mathbf{x}'). \end{aligned}$$

Therefore, the expression Eq. (4.36) is identical with Eq. (4.31). In summary, the FRG-DFT flow equation reproduces the expression for the energy derived in the adiabatic connection.

Finally, I note that in the FRG-DFT, the effective actions, and all the density correlation functions, are obtained with solving the evolution equation Eq. (4.23) in principle, in contrast to the most studies of the adiabatic connection, in which some ansatz on $W_\lambda = \langle \Psi_\lambda | \hat{W} | \Psi_\lambda \rangle$ or on $G_\lambda^{(2)}(\mathbf{x}, \mathbf{x}')$ are made. Moreover, systematic approximation schemes inspired by the FRG are available in the FRG-DFT.

Chapter 5

FRG-DFT analysis of the one-dimensional spinless nuclear matter

In the last chapter, the formulation of the FRG-DFT has been shown. From now on, I demonstrate how the FRG-DFT works for the analyses of quantum many-body systems using some models. In this chapter, we show the application of the FRG-DFT to a one-dimensional spinless homogeneous nuclear matter. The equation of state (EOS) of this system at zero temperature is derived. The EOS shows the saturation property, i.e., the energy per particle has a minimum point with respect to the density. From this EOS, the saturation point is derived, and the discrepancy between the saturation energy derived with the FRG-DFT and with the extrapolation of the Monte Carlo (MC) results [48] is found to be only 2.7%. The density–density correlation function is also derived in the framework of the FRG-DFT to analyze the excited states of the system. the spectral function is found to reproduce a notable property of the non-linear Tomonaga–Luttinger liquid that the spectral function has singularities at the edge of its support in the lower-energy side. This demonstration shows that the FRG-DFT is a promising way for the analyses of not only ground states but also excited states of infinite matters.

The formalism and results regarding the EOS are based on Ref. [52], and those regarding the spectral function are based on Ref. [53].

5.1 One-dimensional spinless nuclear matter

In this chapter, I employ the (1+1)-dimensional nuclear matter model, which has the two-body interaction proposed by Ref. [48]:

$$U(r) = \frac{g}{\sqrt{\pi}} \left(\frac{1}{\sigma_1} e^{-\frac{r^2}{\sigma_1^2}} - \frac{1}{\sigma_2} e^{-\frac{r^2}{\sigma_2^2}} \right), \quad (5.1)$$

where r is the spatial distance between two particles. This interaction is characterized by short-range repulsion and long-range attraction like the nuclear force. This model has only the central force and does not have the counterpart of the tensor and angular momentum dependent forces since there are no analogs for these forces in one dimension. Here, g , σ_1 , and σ_2 are positive parameters which is determined under the assumption that some relevant dimensionless quantities for (3+1)-dimensional system are also reproduced in the (1+1)-dimensional system. Following Ref. [48], we choose $g = 12$, $\sigma_1 = 0.2$, and $\sigma_2 = 0.8$, where the units in which the mass of the nucleon is 1 are employed. Here, the spinless, or fully spin-polarized, fermions are considered.

This model shows the saturation property for the equation of state. The ground energy near the saturation point in the case of infinite particles was calculated with the extrapolation of the energies of up to 12 nucleons derived by the Monte Carlo calculation [48].

5.2 Flow equation

The unit in which the mass of the nucleon is 1 is used below. The λ -dependent action of the system in the imaginary time formalism reads as follows:

$$S_\lambda[\psi^*, \psi] = \int_X \psi^*(X_\epsilon) \left(\partial_\tau - \frac{\partial_x^2}{2} \right) \psi(X) + \frac{1}{2} \int_{X, X'} U_{2b, \lambda}(X, X') \psi^*(X_\epsilon) \psi^*(X'_\epsilon) \psi(X') \psi(X), \quad (5.2)$$

where X is a vector of the imaginary time τ and spatial coordinate x , $X_\epsilon = (\tau + \epsilon, x)$ with a positive infinitesimal ϵ , $\psi(X)$ and $\psi^*(X)$ are the nucleon fields, and $U_{2b}(X' - X) = \delta(\tau - \tau')U(x - x')$. Since this action has the same form as Eq. (4.11), the flow equation of the λ -dependent effective action for the density field $\rho_\psi(X) = \psi^*(X_\epsilon)\psi(X)$, $\Gamma_\lambda[\rho]$, is given by Eq. (4.23).

The grand canonical formalism is employed, in which the chemical potential μ_λ is used to fix the expectation value of the particle number. The ground-state density $\rho_{\text{gs}, \lambda}(X)$ is related to μ_λ via Eq. (4.15). Consider the homogeneous case, i.e., assume that $\rho_{\text{gs}, \lambda}(X)$ is independent of X . μ_λ is chosen so that $\rho_{\text{gs}, \lambda}(X)$ is fixed to a density n for any λ . For the case of the canonical formalism, see Ref. [46].

The flow equation Eq. (4.23) is a functional differential equation, and is difficult to be numerically solved without any approximation. To convert the flow equation some numerically solvable equations, the vertex expansion scheme is introduced here, in which $\Gamma_\lambda[\rho]$ is expanded as follows:

$$\Gamma_\lambda[\rho] = \Gamma_\lambda[\rho_{\text{gs}, \lambda}] + \mu_\lambda \int_X (\rho(X) - \rho_{\text{gs}, \lambda}(X)) + \sum_{n=2}^{\infty} \frac{1}{n!} \int_{X_1, \dots, X_n} \Gamma_\lambda^{(n)}[\rho_{\text{gs}, \lambda}](X_1, \dots, X_n) \prod_{i=1}^n (\rho(X_i) - \rho_{\text{gs}, \lambda}(X_i)). \quad (5.3)$$

Such an expansion yields infinite series of coupled differential equations for $\{\Gamma_\lambda^{(n)}[\rho_{\text{gs},\lambda}]\}_{n=0}^\infty$. With truncating the series at some order, the equations which can be treated numerically are obtained.

Our aim is to calculate the density dependence of the ground-state energy, and the density–density spectral function. Since the density–density spectral function is defined from the density–density correlation function $G_\lambda^{(2)}$, and the initial conditions for density correlation functions $\{G_\lambda^{(n)}\}_{n=0}^\infty$ are easier to be derived than those for $\{\Gamma_\lambda^{(n)}[\rho_{\text{gs},\lambda}]\}_{n=0}^\infty$, the flow equations for $\{G_\lambda^{(n)}\}_{n=0}^\infty$ are more useful than those for $\{\Gamma_\lambda^{(n)}[\rho_{\text{gs},\lambda}]\}_{n=0}^\infty$. Such flow equations are derived by converting the flow equations for $\{\Gamma_\lambda^{(n)}[\rho_{\text{gs},\lambda}]\}_{n=0}^\infty$ by use of the derivatives of Eq. (4.12) and

$$G_\lambda^{(n)}(X_1, \dots, X_n) = W_\lambda^{(n)}[J_{\text{sup}}[\rho_{\text{gs},\lambda}]](X_1, \dots, X_n) = W_\lambda^{(n)}[\mu_\lambda](X_1, \dots, X_n),$$

where $W_\lambda[J]$ and $J_{\text{sup}}[\rho_{\text{gs},\lambda}]$ are defined in the same manner as in Chap. 4.2. More direct derivation of the flow equations for $\{G_\lambda^{(n)}\}_{n=0}^\infty$ is using the flow equation for $W_\lambda[J_{\text{sup},\lambda}[\rho]]$. By use of

$$\partial_\lambda \Gamma_\lambda[\rho] = -(\partial_\lambda W_\lambda)[J_{\text{sup},\lambda}[\rho]],$$

and Eqs. (4.18) and (4.19), The flow equation (4.20) is rewritten as follows:

$$\begin{aligned} \partial_\lambda W_\lambda[J] = & -\frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \left(W_\lambda^{(1)}[J](X) W_\lambda^{(1)}[J](X') \right. \\ & \left. + W_\lambda^{(2)}[J](X_{\epsilon'}, X') - W_\lambda^{(1)}[J](X) \delta(x - x') \right). \end{aligned} \quad (5.4)$$

From this equation and

$$\begin{aligned} & \partial_\lambda G_\lambda^{(n)}(X_1, \dots, X_n) \\ &= \partial_\lambda W_\lambda^{(n)}[\mu_\lambda](X_1, \dots, X_n) \\ &= \int_X W_\lambda^{(n+1)}[\mu_\lambda](X, X_1, \dots, X_n) \partial_\lambda \mu_\lambda + (\partial_\lambda W_\lambda^{(n)}[\mu_\lambda])(X_1, \dots, X_n), \end{aligned}$$

the flow equation of $G_\lambda^{(n)}$ reads

$$\begin{aligned} & \partial_\lambda G_\lambda^{(n)}(X_1, \dots, X_n) \\ &= \int_X G_\lambda^{(n+1)}(X, X_1, \dots, X_n) \partial_\lambda \mu_\lambda \\ & \quad - \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \\ & \quad \times \left(G_\lambda^{(n+2)}(X_{\epsilon'}, X', X_1, \dots, X_n) - G_\lambda^{(n+1)}(X, X_1, \dots, X_n) \delta(x - x') \right. \\ & \quad \left. + \sum_{k=0}^n \frac{1}{k!(n-k)!} \sum_{\sigma \in S_n} G_\lambda^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) G_\lambda^{(n-k+1)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(n)}) \right). \end{aligned} \quad (5.5)$$

Here, S_n is the symmetric group of order n and

$$\begin{aligned} G_\lambda^{(k+1)}(X, X_{\sigma(1)}, \dots, X_{\sigma(k)}) \Big|_{k=0} &= G_\lambda^{(1)}(X), \\ G_\lambda^{(n-k+1)}(X', X_{\sigma(k+1)}, \dots, X_{\sigma(n)}) \Big|_{k=n} &= G_\lambda^{(1)}(X'). \end{aligned}$$

$G_\lambda^{(0)} = W_\lambda[\mu_\lambda]$ and $G_\lambda^{(1)}(X) = W_\lambda^{(1)}[\mu_\lambda](X)$ are related to the ground-state energy and density, respectively:

$$E_{\text{gs},\lambda} = \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \left(\int_X \mu_\lambda \rho_{\text{gs},\lambda}(X) - G_\lambda^{(0)} \right), \quad (5.6)$$

$$\rho_{\text{gs},\lambda}(X) = G_\lambda^{(1)}(X). \quad (5.7)$$

The flow equation for $G_\lambda^{(n)}$ depends on $G_\lambda^{(m \leq n+2)}$ as seen in Eq. (5.5), which suggests that infinite series of flow equation appears if no approximation is employed.

I have mentioned that μ_λ is chosen so that $\rho_{\text{gs},\lambda}(X) = n$, and $\partial_\lambda \rho_{\text{gs},\lambda}(X) = 0$, is satisfied for any λ . The condition which μ_λ should satisfy is obtained from the flow equation for $G_\lambda^{(1)}(X) = \rho_{\text{gs},\lambda}(X)$:

$$\begin{aligned} 0 &= \int_X G_\lambda^{(2)}(X, X_1) \partial_\lambda \mu_\lambda \\ &\quad - \frac{1}{2} \int_{X, X'} \partial_\lambda U_{2\text{b},\lambda}(X, X') \\ &\quad \times \left(G_\lambda^{(3)}(X_{\epsilon'}, X', X_1) - G_\lambda^{(2)}(X, X_1) \delta(x - x') + 2n G_\lambda^{(2)}(X, X_1) \right). \end{aligned} \quad (5.8)$$

From this equation, the flow equation for $\partial_\lambda \mu_\lambda$ reads

$$\begin{aligned} \partial_\lambda \mu_\lambda &= \frac{1}{2} \int_{X'} \partial_\lambda U_{2\text{b},\lambda}(X_1, X') (2n - \delta(x_1 - x')) \\ &\quad + \frac{1}{2} \int_{X, X', X''} \partial_\lambda U_{2\text{b},\lambda}(X, X') G_\lambda^{(2)-1}(X_1, X'') G_\lambda^{(3)}(X_{\epsilon'}, X', X''), \end{aligned} \quad (5.9)$$

where $G_\lambda^{(2)-1}(X, X')$ is the inverse of $G_\lambda^{(2)}(X, X')$:

$$\int_{X'} G_\lambda^{(2)-1}(X, X') G_\lambda^{(2)}(X', X'') = \delta(X - X'').$$

Under such a choice of μ_λ , the flow equation for $E_{\text{gs},\lambda}$ reads

$$\begin{aligned} \partial_\lambda E_{\text{gs},\lambda} &= \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{X, X'} \partial_\lambda U_{2\text{b},\lambda}(X, X') \left(G_\lambda^{(2)}(X_{\epsilon'}, X') - n\delta(x - x') + n^2 \right) \\ &= \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{X, X'} \partial_\lambda U_{2\text{b},\lambda}(X, X') n^2 \\ &\quad + \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{X, X'} \partial_\lambda U_{2\text{b},\lambda}(X, X') \left(G_0^{(2)}(X_{\epsilon'}, X') - n\delta(x - x') \right) \\ &\quad + \lim_{\beta \rightarrow \infty} \frac{1}{2\beta} \int_{X, X'} \partial_\lambda U_{2\text{b},\lambda}(X, X') \left(G_\lambda^{(2)}(X_{\epsilon'}, X') - G_0^{(2)}(X_{\epsilon'}, X') \right). \end{aligned} \quad (5.10)$$

The first, second, and third terms in the last equality of this equation correspond to the Hartree, exchange, and correlation terms, respectively.

If the flows of $G_\lambda^{(n \geq 2)}$ are ignored, the correlation term in Eq. (5.10) vanishes and only the result of the first-order perturbation, or the Hartree–Fock approximation, is obtained. To include the correlation term, let us take the flow of $G_\lambda^{(2)}$ into account. By use of Eqs. (5.5) and (5.9), the flow equation for $G_\lambda^{(2)}$ reads

$$\begin{aligned} \partial_\lambda G_\lambda^{(2)}(X_1, X_2) = & - \int_{X, X'} \partial_\lambda U_{2b, \lambda}(X, X') G_\lambda^{(2)}(X, X_1) G_\lambda^{(2)}(X', X_2) \\ & - \frac{1}{2} \int_{X, X'} \partial_\lambda U_{2b, \lambda}(X, X') \left(G_\lambda^{(4)}(X_\epsilon, X', X_1, X_2) \right. \\ & \left. - \int_{X'', X'''} G_\lambda^{(3)}(X''', X_1, X_2) G_\lambda^{(2)-1}(X''', X'') G_\lambda^{(3)}(X_\epsilon, X', X'') \right). \end{aligned} \quad (5.11)$$

The terms containing the convolution integrals in the flow equations is easier to treat in the momentum representation in homogeneous systems. The momentum representation for $G_\lambda^{(n)}$ and $U_{2b, \lambda}$ reads as follows:

$$\begin{aligned} \tilde{U}(p) &= \int_X U_{2b}(X) e^{-iP \cdot X} = \int_x U(x) e^{-ipx} = g \left(e^{-\frac{\sigma_1^2 p^2}{4}} - e^{-\frac{\sigma_2^2 p^2}{4}} \right), \quad (5.12) \\ (2\pi)^2 \delta^{(2)} \left(\sum_{k=1}^n P_k \right) \tilde{G}_\lambda^{(n)}(P_1, \dots, P_{n-1}) &= \int_{X_1, \dots, X_n} e^{-i \sum_{k=1}^n P_k \cdot X_k} G_\lambda^{(n)}(X_1, \dots, X_n), \end{aligned} \quad (5.13)$$

respectively, where P is the vector of an imaginary frequency ω_i and spatial momentum p . Equation (5.10) in the momentum representation reads

$$\partial_\lambda \frac{E_{gs, \lambda}}{N} = \frac{n}{2} \tilde{U}(0) + \frac{1}{2n} \int_p \tilde{U}(p) \left(\int_{\omega_i}^{\epsilon'} \tilde{G}_0^{(2)}(P) - n \right) + \frac{1}{2n} \int_P \tilde{U}(p) \left(\tilde{G}_\lambda^{(2)}(P) - \tilde{G}_0^{(2)}(P) \right),$$

where $N = \int_x n$ is the number of particles, $\int_{\omega_i}^{\epsilon'} = \int_{\omega_i} e^{i\omega_i \epsilon'}$, and $\int_P^{\epsilon'} = \int_P e^{i\omega_i \epsilon'}$, and $\int_P = \int_{\omega_i} \int_p = \int d\omega_i / (2\pi) \int dp / (2\pi)$. By integrating this equation with respect to λ , one has

$$\frac{E_{gs, 1}}{N} = \frac{E_{gs, 0}}{N} + \frac{E_H}{N} + \frac{E_{ex}}{N} + \frac{E_{corr}}{N}, \quad (5.14)$$

$$\frac{E_H}{N} = \frac{n}{2} \tilde{U}(0), \quad (5.15)$$

$$\frac{E_{ex}}{N} = \frac{1}{2n} \int_p \tilde{U}(p) \left(\int_{\omega_i}^{\epsilon'} \tilde{G}_0^{(2)}(P) - n \right), \quad (5.16)$$

$$\frac{E_{corr}}{N} = \frac{1}{2n} \int_0^1 d\lambda \int_P \tilde{U}(p) \left(\tilde{G}_\lambda^{(2)}(P) - \tilde{G}_0^{(2)}(P) \right), \quad (5.17)$$

where $E_{\text{gs},0}$ corresponds to the kinetic energy of the free particles and E_{H} , E_{ex} , and E_{corr} are the Hartree, exchange, and correlation energies, respectively. From Eq. (5.12), one immediately finds that $E_{\text{H}}/N = 0$ for our interaction. The flow equation for $\tilde{G}_{\lambda}^{(2)}(P)$ is given as the momentum representation of Eq. (5.11):

$$\partial_{\lambda}\tilde{G}_{\lambda}^{(2)}(P) = -\tilde{U}(p)\tilde{G}_{\lambda}^{(2)}(P)^2 + C_{\lambda}(P), \quad (5.18)$$

where $C_{\lambda}(P)$ is defined as

$$C_{\lambda}(P) = -\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(p') \left(\tilde{G}_{\lambda}^{(4)}(P', -P', P) - \frac{\tilde{G}_{\lambda}^{(3)}(P', -P')\tilde{G}_{\lambda}^{(3)}(P, -P)}{\tilde{G}_{\lambda}^{(2)}(0)} \right), \quad (5.19)$$

I should note that $\tilde{G}_{\lambda}^{(2)}(0)$ should be interpreted as the p limit, i.e., $\tilde{G}_{\lambda}^{(2)}(0) = \lim_{p \rightarrow 0} \tilde{G}_{\lambda}^{(2)}(0, p)$. The p limit of $\tilde{G}_{\lambda}^{(2)}(P)$ corresponds to the static particle-density susceptibility and nonzero in the case of the grand-canonical formulation in general, while $\lim_{p \rightarrow 0} \tilde{G}_{\lambda}^{(2)}(\omega_i, p) = 0$ for finite ω_i [65–67]. The appearance of non-vanishing $\tilde{G}_{\lambda}^{(n)}$ with vanishing ω_i and p is in contrast to the canonical formalism.

$C_{\lambda}(P)$ in Eq. (5.18) contains $\tilde{G}_{\lambda}^{(3,4)}$. Since the flows of $\tilde{G}_{\lambda}^{(3,4)}$ are not taken into account in the vertex expansion scheme up to second order, $C_{\lambda}(P)$ is needed to be approximated. A simple approximation is neglecting the λ dependence of $C_{\lambda}(P)$: $C_{\lambda}(P) \approx C_0(P)$. A concern regarding this approximation is that it breaks a condition imposed by the Pauli blocking effect: The $G_{\lambda}^{(2)}$ can be related to the two-particle distribution function $f_{2,\lambda}(x, x') = \langle \psi^*(\tau + \epsilon, x) \psi^*(\tau + \epsilon, x') \psi^*(\tau, x') \psi^*(\tau, x) \rangle_{\lambda, \mu_{\lambda}}$. As I discussed in the derivation of Eq. (4.23), one has the following relation:

$$\begin{aligned} & \langle \psi^*(\tau + \epsilon, x) \psi^*(\tau + \epsilon, x') \psi^*(\tau, x') \psi^*(\tau, x) \rangle_{\lambda, \mu_{\lambda}} \\ &= \rho_{\text{gs},\lambda}(\tau, x) \rho_{\text{gs},\lambda}(\tau, x') + \Gamma_{\lambda}^{(2)-1}[\rho_{\text{gs},\lambda}](\tau + \epsilon', x, \tau, x) - \rho_{\text{gs},\lambda}(\tau, x) \delta(x - x') \\ &= \rho_{\text{gs},\lambda}(\tau, x) \rho_{\text{gs},\lambda}(\tau, x') + W_{\lambda}^{(2)}[\mu_{\lambda}](\tau + \epsilon', x, \tau, x) - \rho_{\text{gs},\lambda}(\tau, x) \delta(x - x'). \end{aligned}$$

From this relation, one has

$$\begin{aligned} f_{2,\lambda}(x, x') &= n^2 + G_{\lambda}^{(2)}(\tau + \epsilon', x, \tau, x) - n\delta(x - x') \\ &= n^2 + \int_P^{\epsilon'} e^{ip(x-x')} \tilde{G}_{\lambda}^{(2)}(P) - n\delta(x - x'). \end{aligned}$$

The flow equation of $f_{2,\lambda}(x, x')$ is written as follows

$$\partial_{\lambda} f_{2,\lambda}(x, x') = \int_P^{\epsilon'} e^{ip(x-x')} \partial_{\lambda} \tilde{G}_{\lambda}^{(2)}(P).$$

From the Pauli blocking effect, $f_{2,\lambda}(x, x')$ should satisfy $f_{2,\lambda}(x, x) = 0$. Therefore, $\tilde{G}_{\lambda}^{(2)}(P)$ should satisfy the following condition:

$$\int_P^{\epsilon'} \partial_{\lambda} \tilde{G}_{\lambda}^{(2)}(P) = 0.$$

With Eq. (5.18), the condition for $C_\lambda(P)$ is obtained as follows:

$$\int_P^{\epsilon'} C_\lambda(P) = \int_P^{\epsilon'} \tilde{U}(p) \tilde{G}_\lambda^{(2)}(P)^2. \quad (5.20)$$

This condition is broken when $\lambda \neq 0$ if the λ dependence of C_λ is neglected while that of $\tilde{G}_\lambda^{(2)}$ is taken into account. One of the way to restore this condition is approximating $C_\lambda(P)$ with the following form [46]:

$$C_\lambda(P) \approx c_\lambda C_0(P),$$

where c_λ is determined so as to restore Eq. (5.20):

$$c_\lambda = \frac{\int_P^{\epsilon'} \tilde{U}(p) \tilde{G}_\lambda^{(2)}(P)^2}{\int_P^{\epsilon'} C_0(P)}. \quad (5.21)$$

Since the Pauli blocking effect is not broken at $\lambda = 1$, one has $c_0 = 1$. Under the approximation, the flow equation for $\tilde{G}_\lambda^{(2)}(P)$ becomes as follows

$$\partial_\lambda \tilde{G}_\lambda^{(2)}(P) \approx -\tilde{U}(p) \tilde{G}_\lambda^{(2)}(P)^2 + c_\lambda C_0(P). \quad (5.22)$$

Solving this equation and Eq. (5.18), the ground-state energy per particle is obtained.

To derive the spectral function for the density two-point correlation function $\rho_d(\omega, p)$ with real frequency ω , the retarded two-point correlation function $\tilde{G}_{R,\lambda}^{(2)}(\omega, p)$ is needed, since $\rho_d(\omega, p)$ is defined as follows:

$$\rho_d(\omega, p) = -2\text{Im}\tilde{G}_{R,1}^{(2)}(\omega, p). \quad (5.23)$$

$\tilde{G}_{R,\lambda}^{(2)}(\omega, p)$ is obtained from the analytic continuation of $\tilde{G}_\lambda^{(2)}(\omega_i, p)$:

$$\tilde{G}_{R,\lambda}^{(2)}(\omega, p) = -\tilde{G}_{\text{ana},\lambda}^{(2)}(z, p) \Big|_{z \rightarrow \omega + i\delta},$$

where δ is a positive infinitesimal, $\tilde{G}_{\text{ana},\lambda}^{(2)}(z, p)$ is a complex function of $z \in \mathbb{C}$ which is regular in the upper-half plane of z and satisfies $\tilde{G}_{\text{ana},\lambda}^{(2)}(-i\omega_i, p) = \tilde{G}_\lambda^{(2)}(\omega_i, p)$ for $\omega_i \in \mathbb{R}$. In general, the derivation of $\tilde{G}_{R,\lambda}^{(2)}(\omega, p)$ from $\tilde{G}_\lambda^{(2)}(\omega_i, p)$ becomes an obstruction for the numerical analysis. Although there is some numerical procedure to realize such an analytic continuation such as the maximal entropy method and Padé approximation, these scheme requires large computational effort or some prior knowledge for the form of the function. In our case, however, such an analytic continuation can be performed more easily without any ambiguity, as done in the context of the FRG [34–38]. Since $C_0(P)$ is written in terms of the density correlation functions in the free case, one can derive the explicit form of $C_0(P)$ in Eq. (5.22) as a function of ω_i . In this case, the analytic continuation for $C_0(P)$ can be directly performed so that the obtained function

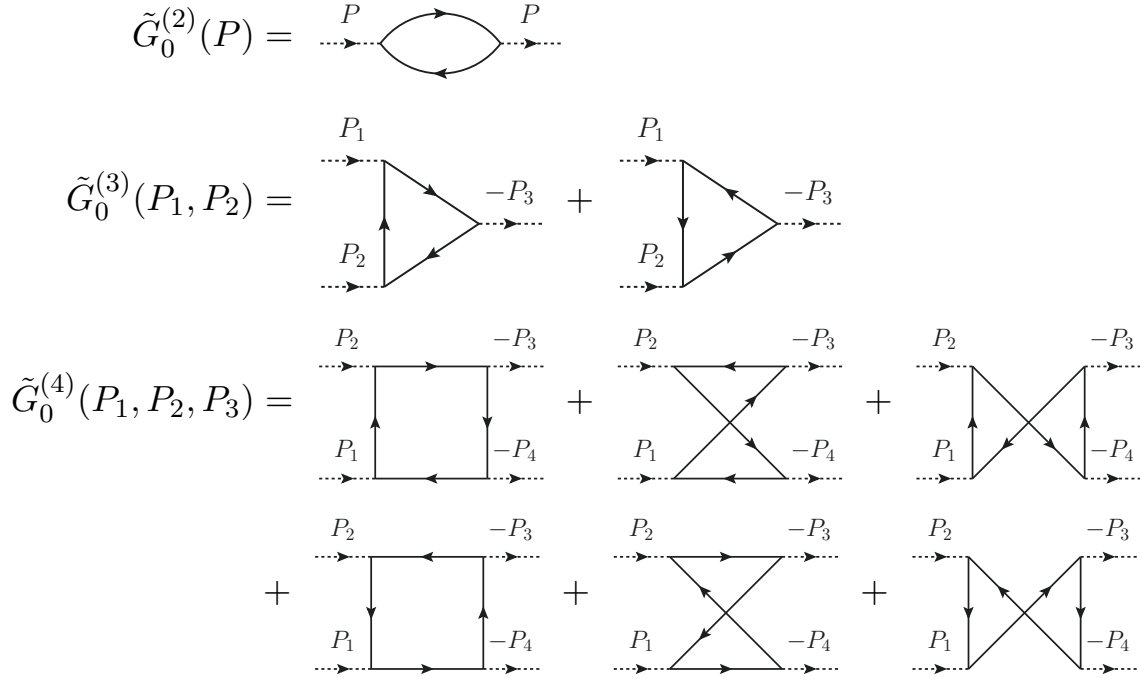


Figure 5.1: The diagrammatic representations of $\tilde{G}_0^{(2,3,4)}$. The solid line is the free fermion propagator $\tilde{G}_{F,0}^{(2)}(P)$. In the diagrams for $\tilde{G}_0^{(3)}$ and $\tilde{G}_0^{(4)}$, $P_3 = -P_1 - P_2$ and $P_4 = -P_1 - P_2 - P_3$, respectively.

$C_{\text{ana},0}(z, p)$ satisfies the regularity at the upper-half plane of z and $C_{\text{ana},0}(-i\omega_i, p) = C_0(\omega_i, p)$ for $\omega_i \in \mathbb{R}$. Therefore the analytic continuation for Eq. (5.22) can be performed directly and the flow equation for $\tilde{G}_{R,\lambda}^{(2)}(\omega, p)$ is derived as follows:

$$\partial_\lambda \tilde{G}_{R,\lambda}^{(2)}(\omega, p) = \tilde{U}(p) \tilde{G}_{R,\lambda}^{(2)}(\omega, p)^2 - c_\lambda C_{R,0}(\omega, p), \quad (5.24)$$

where $C_{R,0}(\omega, p) = C_{\text{ana},0}(\omega + i\delta)$. With solving this flow equation, $\tilde{G}_{R,\lambda}^{(2)}(\omega, p)$ and $\rho_d(\omega, p)$ are calculated without numerical procedures for the analytic continuation.

$\tilde{G}_0^{(2,3,4)}(P)$, $\tilde{G}_{R,0}^{(2)}(\omega, p)$, and $E_{\text{gs},0}/N$ are needed to specify the initial conditions of Eqs. (5.18), (5.22), and (5.24), and to derive $C_0(P)$ and $C_{R,0}(\omega, p)$. Since $E_{\text{gs},0}/N$ is the ground-state energy per particle of non-interacting case, one has

$$\frac{E_{\text{gs},0}}{N} = \frac{p_F^2}{6},$$

where $p_F = \pi n = \sqrt{2\mu_0}$ is the Fermi momentum. The correlation functions at $\lambda = 0$ read

$$\tilde{G}_0^{(n)}(P_1, \dots, P_{n-1}) = - \sum_{\sigma \in S_{n-1}} \int_P \prod_{k=0}^{n-1} \tilde{G}_{F,0}^{(2)} \left(\sum_{i=1}^k P_{\sigma(i)} + P \right). \quad (5.25)$$

Here,

$$\tilde{G}_{\text{F},0}^{(2)} \left(\sum_{i=1}^k P_{\sigma(i)} + P \right) \Big|_{k=0} = \tilde{G}_{\text{F},0}^{(2)}(P),$$

and $\tilde{G}_{\text{F},0}^{(2)}(P)$ is the two-point propagator of free fermions:

$$\tilde{G}_{\text{F},0}^{(2)}(P) = \frac{e^{i\omega_i \epsilon}}{i\omega_i - \xi(p)},$$

where $\xi(p) := p^2/2 - \mu_0$. Equation (5.25) can be represented diagrammatically. The diagrammatic representations for $\tilde{G}_0^{(2,3,4)}$ are shown in Fig. 5.1. As shown in Appendix B, using Eq. (5.25) and performing the frequency integrals, one has the following expressions for $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$, respectively:

$$\tilde{G}_0^{(2)}(P) = 2 \int_{p'} \theta(-\xi(p')) \frac{\xi(p+p') - \xi(p')}{\omega_i^2 + [\xi(p+p') - \xi(p')]^2}, \quad (5.26)$$

$$\begin{aligned} C_0(P) = & 2 \int_{p', p''} U(p') \theta(-\xi(p'')) (\theta(-\xi(p+p'+p'')) - \theta(-\xi(p'+p''))) \\ & \times \left[\frac{(\xi(p''+p) - \xi(p''))^2 - \omega^2}{(\omega^2 + (\xi(p''+p) - \xi(p''))^2)^2} \right. \\ & \left. - \frac{(\xi(p''+p+p') - \xi(p''+p'))(\xi(p''+p) - \xi(p'')) - \omega^2}{(\omega^2 + (\xi(p''+p+p') - \xi(p''+p'))^2)(\omega^2 + (\xi(p''+p) - \xi(p''))^2)} \right]. \quad (5.27) \end{aligned}$$

Those expression actually satisfies $c_0 = 1$; see Appendix B.2.2. The analytic continuation to obtain $\tilde{G}_{\text{R},0}^{(2)}(\omega, p)$ and $C_{\text{R},0}(\omega, p)$ are performed by substituting ω_i to $i\omega$ in Eqs. (5.26) and (5.27). I note that such a procedure for the analytic continuation can be extended to the case of finite temperature as suggested by studies in the FRG [35,36].

5.3 Numerical results

The numerical results of the ground-state energy per particle $E_{\text{gs},1}/N$ and the spectral function for the density two-point function $\rho_{\text{d}}(\omega, p)$ are shown.

5.3.1 Numerical procedure

I briefly describe our numerical procedure. The domains of the ω_i - and p -integrals in E_{ex}/N and E_{corr}/N in Eq. (5.14) are $(-\infty, \infty)$. Since $\tilde{G}_\lambda^{(2)}(P)$ is an even function of ω_i and p , the domains can be reduced to $[0, \infty)$. ω_i has been changed to $\theta_{\omega_i} = (2/\pi) \arctan(\omega/s)$ with an arbitral positive number s to restrict the integral domain to $[0, 1]$. For p -integral, a cutoff $\Lambda = \max(10p_{\text{F}}, 1)$ has been introduced. With discretizing the space with $\theta_{\omega_i} \in [0, 1]$ and $p \in [0, \Lambda]$, $\tilde{G}_\lambda^{(2)}(P)$ for each θ_{ω_i} and p has been calculated. I have checked that the result hardly depends on Λ even if it is set to be larger than $\max(10p_{\text{F}}, 1)$.

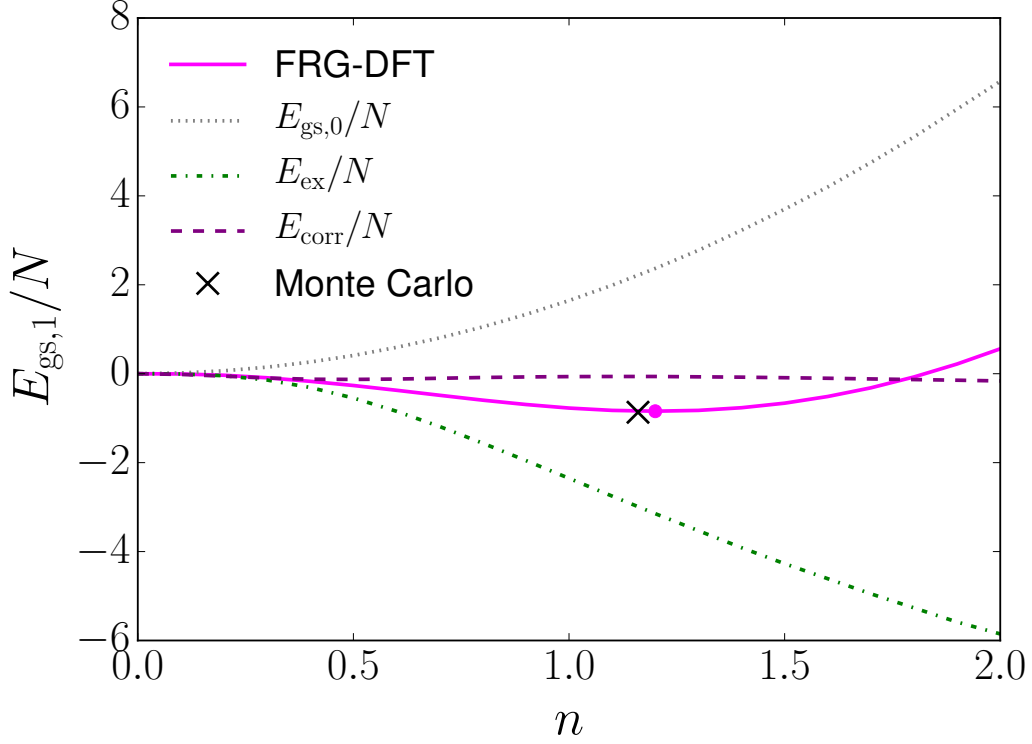


Figure 5.2: The ground-state energy per particle $E_{gs,1}/N$ as a function of density n . The solid magenta line is the result derived by the FRG-DFT. The results of $E_{gs,0}/N$, E_{ex}/N , and E_{corr}/N are also shown as the gray dotted, green dashed–dotted, purple dashed lines, respectively. The black cross is the energy derived by the extrapolation of the MC calculation near the saturation point [48]. The magenta point is the saturation point derived from the FRG-DFT calculation.

5.3.2 Ground state

Figure 5.2 shows the result of the ground-state energy per particle $E_{gs,1}/N$. The energy of free fermions $E_{gs,0}/N$ and the contributions from the exchange term E_{ex}/N and correlation terms E_{corr}/N , and the energy near the saturation point derived by the extrapolation of the MC results [48] are also shown. I again remark that the contribution from the Hartree term vanishes in our case, i.e., the contribution to the mean field from each particle cancels with each other. Since $E_{gs,0}/N$ corresponds to the kinetic energy, it increases as n increases and the Fermi sphere grows. On the other hand, the exchange contribution lowers the ground-state energy since the Pauli exclusion principle tempers the effect of the repulsive core. The contribution from the correlation term is found to show a non-monotonic behavior. Then $E_{gs,1}/N$ shows the saturation point, i.e., has the minimum point with respect to n , due to the competition between $E_{gs,0}/N$ and $E_{ex}/N + E_{corr}/N$.

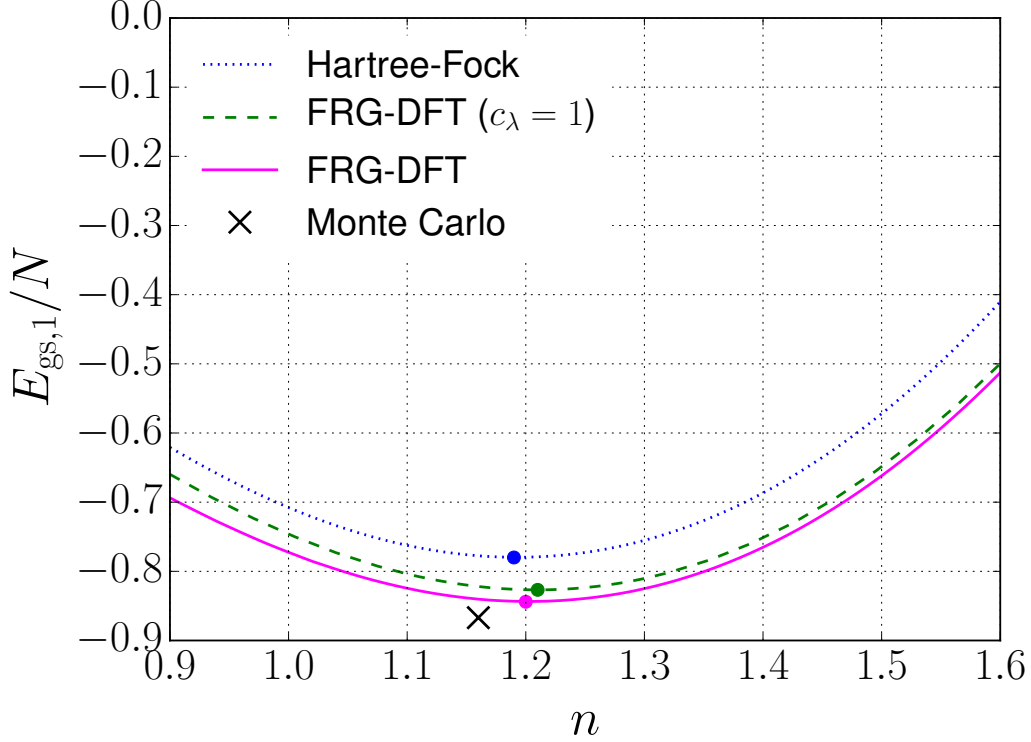


Figure 5.3: The ground-state energy per particle $E_{\text{gs},1}/N$ as a function of density n near the saturation point. The solid magenta and green dashed lines are the results of the FRG-DFT with and without the inclusion of the flow of c_λ , respectively. The result with the Hartree-Fock approximation, which is given as $E_{\text{gs},0}/N + E_{\text{ex}}/N$, is also shown (blue dotted line). The black cross is the energy derived from the extrapolation of the MC results [48]. The density $n = 1.16$ used in the MC simulation is not a calculated but given one, and thus should not be regarded as a derived saturation density. The magenta, green, and blue points shows the saturation points derived from the FRG-DFT, FRG-DFT without the flow of c_λ , and the Hartree-Fock approximation.

Let us discuss the quantitative feature of our results near the saturation point. Figure 5.3 shows the result of the ground-state energy per particle near the saturation point derived by the FRG-DFT. The results derived by the FRG-DFT with fixing $c_\lambda = 1$, the Hartree-Fock approximation which is given as $E_{\text{gs},0}/N + E_{\text{ex}}/N$, and the extrapolation from the MC results [48] are also shown. I again note that the density used in the MC calculation should not be regarded as a derived saturation density since it is not a calculated but given one. Thus only the ground-state energy is used as the benchmark here. One can see that the inclusion of the correlation term with the FRG-DFT makes the energy close to the result by MC calculation in comparison with the Hartree-Fock calculation. Moreover, I find that the inclusion of the flow of c_λ contributes to the approach of the FRG-DFT results to the MC result. Table 5.1

Table 5.1: The saturation energies E_s/N derived from the Hartree–Fock (HF) approximation, FRG-DFT with and without the inclusion of the flow of c_λ , and extrapolation of the MC results [48]. Their relative errors $\Delta E_s/N = |(E_s - E_{s,\text{MC}})/E_{s,\text{MC}}|$ in comparison with the result of the Monte Carlo simulation $E_{s,\text{MC}}/N$ and the saturation densities ρ_s are also shown.

	HF	FRG-DFT ($c_\lambda = 1$)	FRG-DFT	MC [48]
E_s/N	-0.780	-0.827	-0.844	-0.867
$\Delta E_s/N$ (%)	10.0	4.6	2.7	-
ρ_s	1.19	1.21	1.20	-

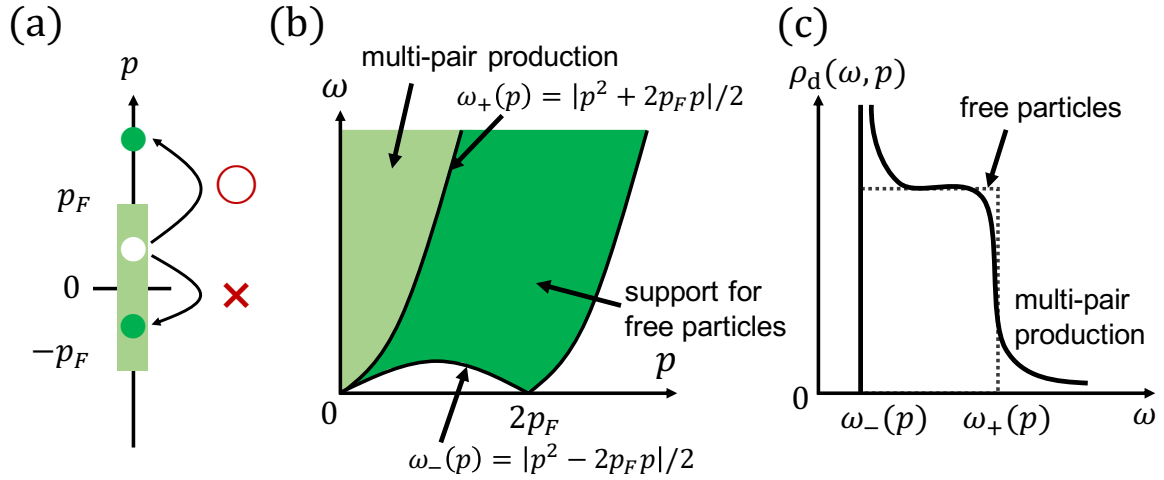


Figure 5.4: (a) Schematic figure of the particle–hole excitation from the Fermi sphere. The Pauli blocking forbid some excitations kinematically, which gives the lower bound of the energy of the support of the density–density spectral function $\omega_-(p)$ in $0 \leq p \leq p_F$. (b) The supports of the spectral functions for the interacting case and free case. The multi-pair productions contribute the emergence of the support in $\omega > \omega_+(p)$. (c) The predicted behavior of $\rho_d(\omega, p)$ at a fixed p in the interacting case (solid line) and free case (dotted line).

show the numerical results of the saturation energy E_s/N and the saturation density ρ_s derived by each method. The discrepancy of E_s/N in comparison with the MC result is only 2.7% in the case of FRG-DFT, which suggests that the inclusion of the correlation term and the flow of c_λ contributes to the improvement of the accuracy. Although there is no benchmark for ρ_s , it seems to converge to a value near 1.20 from the results of the FRG-DFT and Hartree–Fock approximation.

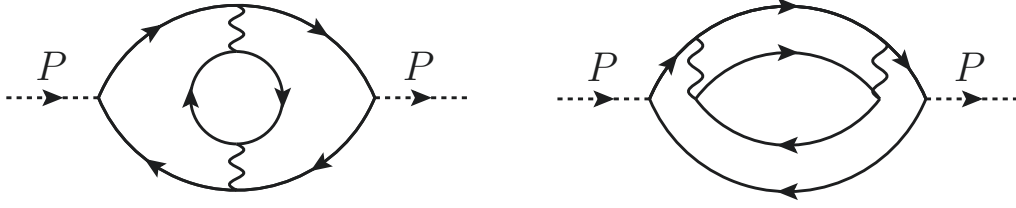


Figure 5.5: Examples of the multi-pair diagrams.

5.3.3 Excited states

Next, I show the result for the spectral function of the density two-point correlation function $\rho_d(\omega, p)$ in (1+1)-dimensional systems. Before presenting our results, we briefly mention the predictions for $\rho_d(\omega, p)$ given in other works. $\rho_d(\omega, p)$ reflects the informations of the particle-hole excitations (Fig. 5.4 (a)). If the particle-hole excitation with a frequency ω and momentum p is allowed, $\rho_d(\omega, p)$ has non-zero value. Figure 5.4 (b) shows the support of $\rho_d(\omega, p)$. The support has the lower bound for ω : $\omega_-(p) = |p^2 - 2p_F p|/2$, which is caused by the kinematic constraint for the particle-hole excitations. In particular, the prevention of the particle-hole excitations by the Fermi sphere gives the lower bound in $0 < p < 2p_F$. In the case of free particles, the support has the upper bound $\omega_+(p) = |p^2 - 2p_F p|/2$, while it broaden out into $\omega > \omega_+(p)$ in the case of interacting particles. The multi-pair productions as in Fig. 5.5 yield such a broadening.

Figure 5.4 (c) shows the strength of $\rho_d(\omega, p)$ at a fixed p . The strength in the presence of the interaction shows remarkable behaviors. One of the powerful tools to analyze one-dimensional interacting fermions is the Tomonaga-Luttinger (TL) model [68, 69]. This model is based on the assumption that the dispersion relation of the fermion is linear. However, this assumption gives rise to a crucial artifact to $\rho_d(\omega, p)$, and the non-linearity of the dispersion relation of one-particle excitation is crucial [70]. The bosonization scheme, which is a powerful method for the analysis of one-dimensional systems, was extended to include the non-linearity [70–72]. With this scheme, it was predicted that the qualitative behavior of $\rho_d(\omega, p)$ drastically deviates from that in the case of free particles: $\rho_d(\omega, p)$ shows a power-law divergence and decrease at $\omega = \omega_-(p)$ and $\omega_+(p)$, respectively. The origin of the divergence is considered to be that the particles near the Fermi surface are scattered by the hole created by the particle-hole excitation, and multiple low-energy particle-hole pairs are created. This mechanism is similar to that for the emergence of the singularity appearing in the X-ray absorption rate of metals [73, 74].

Let us discuss our numerical result for $\rho_d(\omega, p)$. In the discussion below, n is always set to a saturation density derived by the FRG-DFT: $n = \rho_s = 1.20$. Figure 5.6 shows the contour map of $\rho_d(\omega, p)$ on the (ω, p) plane. As shown this figure, we do not have the support of $\rho_d(\omega, p)$ in $\omega > \omega_+(p)$, which reflects that the multi-pair diagrams as Fig. (5.5) are not included in the vertex expansion up to the second order. To include

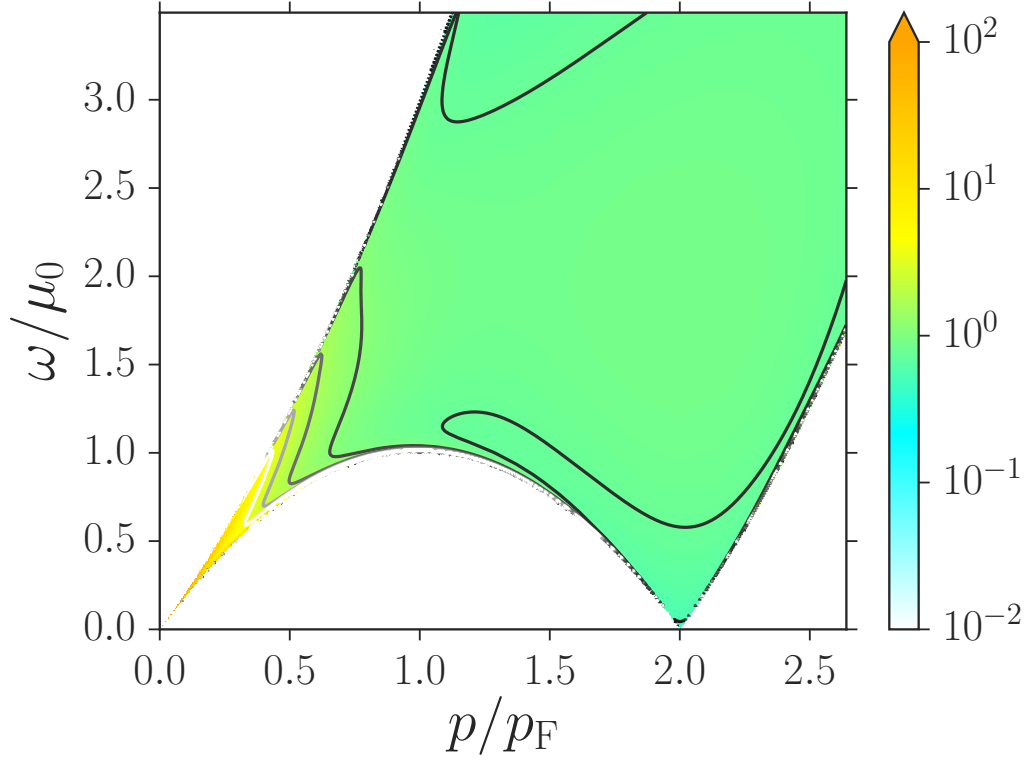


Figure 5.6: The contour map of the density–density spectral function on the (ω, p) -plane.

such contributions, the flow of $\tilde{G}_\lambda^{(4)}(P)$ is needed to be taken into account.

Figure 5.7 is the strength of $\rho_d(\omega, p)$ at $p = p_F$. For comparison, the spectral functions in the case of free fermions and that derived by the random phase approximation (RPA) are also shown. In our formalism, the RPA is reproduced if one ignores $C_{R,0}(P)$ in Eq. (5.24), which corresponds to the exchange contribution. Actually one has the RPA solution

$$\tilde{G}_{R,1}^{(2)}(\omega, p) = \frac{\tilde{G}_{R,0}^{(2)}(\omega, p)}{1 - \tilde{U}(p)\tilde{G}_{R,0}^{(2)}(\omega, p)}, \quad (5.28)$$

if one solves Eq. (5.24) with dropping $C_{R,0}(\omega, p)$. As shown in Fig. 5.7, the singularity at $\omega = \omega_-(p_F) = \mu_0$ is obtained in the case of the FRG-DFT in contrast to the RPA result. The exchange contribution $C_{R,0}(\omega, p)$ is the key ingredient to emerge such a peak, which is included in the FRG-DFT while not in the RPA. The singularity at $\omega = \omega_-(p)$ also appears for other p ; see Fig. 5.8 for the case of $p = 2.5p_F$.

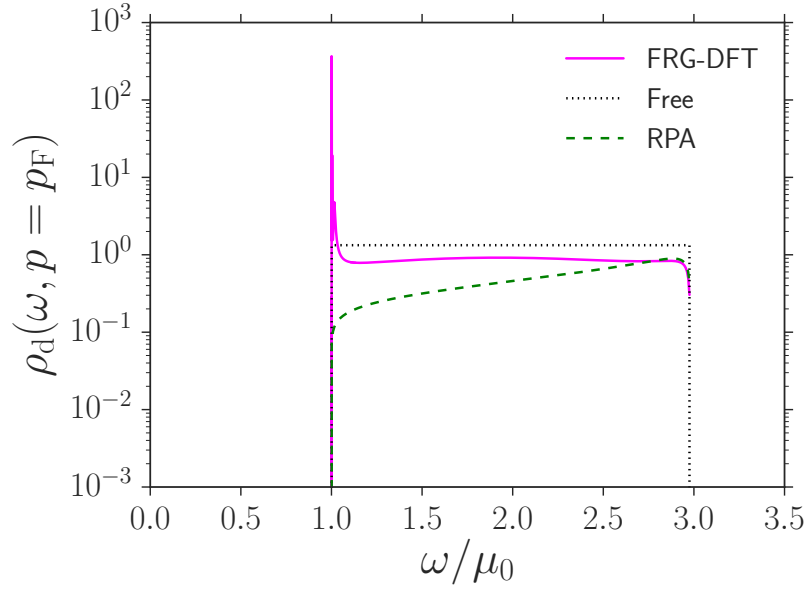


Figure 5.7: The strength of $\rho_d(\omega, p)$ at $p = p_F$. The solid magenta line is the result of the FRG-DFT. $\rho_d(\omega, p)$ in the case of free fermions and that derived by the RPA are also shown as the black dotted and green dashed lines, respectively.

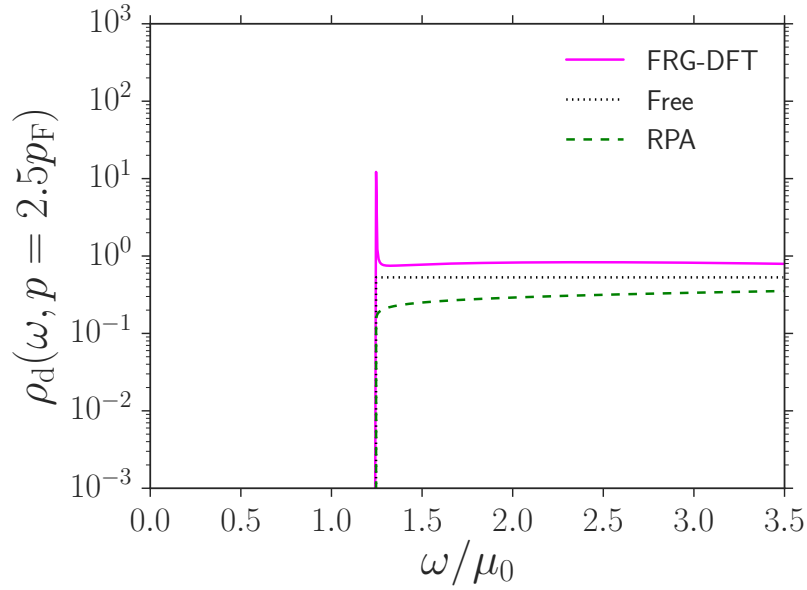


Figure 5.8: The strength of $\rho_d(\omega, p)$ at $p = 2.5p_F$.

5.4 Summary

In this Chapter, I have shown the application of the FRG-DFT to a one-dimensional spinless uniform matter with non-local interaction representing the nuclear force. The equation of state (EOS) and the spectral function for the density two-point function have been calculated with employing the second-order vertex expansion. The saturation energy derived by the EOS has found to miss by only 2.7% in comparison with the Monte Carlo result. In addition, our spectral function has reproduced a notable feature that its support has singularities at the edge in the lower-energy side. Our demonstration suggests that the FRG-DFT is a promising method to analyze the excited states as well as the ground states of uniform matters.

The support of our spectral function has not shown the broadening out into the higher-energy side since the contributions from the multi-pair production are not included. To include such contributions, the flow of the four-point density correlation function is needed to be taken into account.

Our formalism can be extended to the higher-dimensional systems straightforwardly. In the next Chapter, we show our demonstration in the two-dimensional homogeneous electron gas.

Chapter 6

FRG-DFT analysis of the two-dimensional electron gas

The method with the FRG-DFT for infinite matters presented in Chap. 5 can be directly extended to the cases of higher-dimensional systems. One of the next reasonable step is the application to a two-dimensional system, which is expected to be analyzed with lower computational effort than three-dimensional systems. In this chapter, the application of the FRG-DFT to the two-dimensional homogeneous electron gas (2DHEG) is demonstrated.

The homogeneous electron gas is one of the most studied quantum many-body systems [50, 75–82]. In spite of its simplicity, it has played an important role for the study of the physics emerged by the correlation between electrons. Here, we focus on the 2DHEG, which is a homogeneous system composed of electrons confined in a two-dimensional layer. This model has been utilized for the studies of fundamental properties of electrons such as the magnetic phase transition and the Wigner crystallization [75, 83]. The 2DHEG is experimentally realized in, for example, the semiconductor hetero-structures [84] and the atomic-layer materials, and some fascinating phenomena such as the quantum Hall effect [85, 86] have been studied regarding the two-dimensional electrons. There are many theoretical studies for the 2DHEG, and some benchmark results for, e.g. the correlation energy, are available: In the zero-temperature case, the 2DHEG is parametrized by only two parameters: the Wigner–Seitz radius r_s and the spin polarization ζ . In the high-density limit $r_s \rightarrow 0$, the correlation energy is known to be exactly given by the Gell-Mann–Brueckner resummation [49]. The correlation energy has also been calculated by the Monte Carlo (MC) method for some finite r_s and some ξ [50, 51, 75, 77].

Our aim here is to calculate the correlation energy of the 2DHEG by use of the FRG-DFT method and discuss how the FRG-DFT works. I present that the correlation energy derived by the FRG-DFT with the second-order vertex expansion completely reproduces the exact result at the high-density limit given by the Gell-Mann–Brueckner resummation and coincides with the MC results for particularly high-density case.

The contents in this Chapter are based on Ref. [54].

6.1 Two-dimensional homogeneous electron gas

Let us consider the 2DHEG in the spin-unpolarized case. Such a system is parametrized by only one parameter: the Wigner–Seitz radius r_s , which is defined by $r_s = 1/\sqrt{\pi n}$ with the density n . In the following discussion, we employ the Hartree atomic unit.

The 2DHEG describes the electrons in the positive uniform background charge. The Hamiltonian of the 2DHEG reads

$$\begin{aligned}
 \hat{H} &= \hat{H}_{\text{el}} + \hat{H}_{\text{el-i}} + \hat{H}_{\text{i}}, \\
 \hat{H}_{\text{el}} &= \sum_s \int_{\mathbf{x}} \hat{\psi}_s^*(\mathbf{x}) \frac{-\Delta}{2} \hat{\psi}_s(\mathbf{x}) \\
 &\quad + \frac{1}{2} \sum_{s,s'} \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x} - \mathbf{x}') \hat{\psi}_s^*(\mathbf{x}) \hat{\psi}_{s'}^*(\mathbf{x}') \hat{\psi}_{s'}(\mathbf{x}') \hat{\psi}_s(\mathbf{x}), \\
 \hat{H}_{\text{el-i}} &= -n_{\text{i}} \sum_s \int_{\mathbf{x},\mathbf{x}'} \hat{\psi}_s^*(\mathbf{x}) U(\mathbf{x} - \mathbf{x}') \hat{\psi}_s(\mathbf{x}), \\
 \hat{H}_{\text{i}} &= \frac{n_{\text{i}}^2}{2} \int_{\mathbf{x},\mathbf{x}'} U(\mathbf{x} - \mathbf{x}'),
 \end{aligned} \tag{6.1}$$

where $\hat{\psi}_s^*(\mathbf{x})$ and $\hat{\psi}_s(\mathbf{x})$ are the operators for electrons with spin index s , n_{i} is the density of the positive uniform background charge set to be $n_{\text{i}} = n$, and $U(\mathbf{x} - \mathbf{x}')$ is the Coulomb interaction:

$$U(\mathbf{x} - \mathbf{x}') = \frac{1}{|\mathbf{x} - \mathbf{x}'|}.$$

$\hat{H}_{\text{el}}$ contains the kinetic term and the electron–electron interaction term, $\hat{H}_{\text{el-i}}$ is the electron–background interaction term, and $\hat{H}_{\text{i}}$ is the background–background interaction term.

6.2 Flow equation and the solution

Following the procedure presented in Chap. 4.2, the imaginary-time finite-temperature formalism is employed although I focus on the zero-temperature case. the λ -dependent

action is introduced as follows:

$$\begin{aligned}
S_\lambda[\psi^*, \psi] &= S_{\text{el},\lambda}[\psi^*, \psi] + S_{\text{el}-i,\lambda}[\psi^*, \psi] + S_{i,\lambda}, \\
S_{\text{el},\lambda}[\psi^*, \psi] &= \sum_s \int_X \psi_s^*(X_\epsilon) \left(\partial_\tau - \frac{1}{2} \Delta \right) \psi_s(X) \\
&\quad + \frac{1}{2} \sum_{s,s'} \int_{X,X'} U_{2b,\lambda}(X, X') \psi_s^*(X_\epsilon) \psi_{s'}^*(X'_\epsilon) \psi_{s'}(X') \psi_s(X), \\
S_{\text{el}-i,\lambda}[\psi^*, \psi] &= -n_i \sum_s \int_{X,X'} U_{2b,\lambda}(X, X') \psi_s^*(X_\epsilon) \psi_s(X), \\
S_{i,\lambda} &= \frac{n_i^2}{2} \int_{X,X'} U_{2b,\lambda}(X, X'),
\end{aligned} \tag{6.2}$$

where $X = (\tau, \mathbf{x})$ with the imaginary time τ and spatial coordinate $\mathbf{x}$, $\int_X$ is the shorthand of $\int_0^\beta d\tau \int d\mathbf{x}$ with inverse temperature β , and $U_{2b,\lambda}(X, X')$ is defined as follows:

$$U_{2b,\lambda}(X, X') = \frac{\lambda \delta(\tau - \tau')}{|\mathbf{x} - \mathbf{x}'|}.$$

S_0 and S_1 correspond to the action of the free fermions and that for the fully interacting electrons corresponding to the Hamiltonian Eq. (6.1), respectively.

To fix the number of particles to n , we introduce the λ -dependent chemical potential μ_λ . Since we are considering the spin-unpolarized case, we give the same chemical potential to electrons with $s = \uparrow$ and $\downarrow$. At $\lambda = 0$, the chemical potential satisfies $\mu_0 = \pi n = 1/r_s^2$.

The λ -dependent effective action $\Gamma_\lambda[\rho]$ for the density field $\rho_\psi(X) = \sum_s \psi_s^*(X_\epsilon) \psi_s(X)$ is defined in the same manner as Eq. (4.12). A little modification of the flow equation (4.23) is needed since the action Eq. (6.2) has the λ -dependent background terms $S_{\text{el}-i,\lambda}$ and $S_{i,\lambda}$, which did not appear in Eq. (4.11). Even in the present case, the flow equation is derived in the same manner as Chap. 4.2. The flow equation reads

$$\begin{aligned}
\partial_\lambda \Gamma_\lambda[\rho] &= \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') (\rho(X) - n_i) (\rho(X') - n_i) \\
&\quad + \frac{1}{2} \int_{X,X'} \partial_\lambda U_{2b,\lambda}(X, X') \left(\left(\frac{\delta^2 \Gamma_\lambda[\rho]}{\delta \rho(X_\epsilon) \delta \rho(X')} \right)^{-1} - \rho(X) \delta^{(2)}(\mathbf{x} - \mathbf{x}') \right). \tag{6.3}
\end{aligned}$$

The difference in comparison with Eq. (4.23) is that the density $\rho(X)$ in the Hartree term is subtracted by the density of the background charge n_i .

I employ the second order vertex expansion to derive the correlation energy. In the same manner as the derivations of Eq. (5.14), one has the following expression for the

ground-state energy per particle in the momentum representation:

$$\frac{E_{\text{gs},1}}{N} = \frac{E_{\text{gs},0}}{N} + \frac{E_{\text{H}}}{N} + \frac{E_{\text{ex}}}{N} + \frac{E_{\text{corr}}}{N}, \quad (6.4)$$

$$\frac{E_{\text{H}}}{N} = \frac{(n - n_{\text{i}})^2}{2n} \tilde{U}(0), \quad (6.5)$$

$$\frac{E_{\text{ex}}}{N} = \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{\omega_{\text{i}}}^{\epsilon'} \tilde{G}_0^{(2)}(P) - n \right), \quad (6.6)$$

$$\frac{E_{\text{corr}}}{N} = \frac{1}{2n} \int_0^1 d\lambda \int_P \tilde{U}(\mathbf{p}) \left(\tilde{G}_\lambda^{(2)}(P) - \tilde{G}_0^{(2)}(P) \right). \quad (6.7)$$

Here, $N = \int d\mathbf{x} n$, $E_{\text{gs},\lambda} = \lim_{\beta \rightarrow \infty} \Gamma_\lambda[n]/\beta$, $P = (\omega_{\text{i}}, \mathbf{p})$ with the imaginary frequency ω_{i} and momentum $\mathbf{p}$, $\int_{\mathbf{p}} = \int d\mathbf{p}/(2\pi)^2$, $\int_{\omega_{\text{i}}}^{\epsilon'} = \int e^{i\omega_{\text{i}}\epsilon'} d\omega_{\text{i}}/(2\pi)$, $\int_P^{\epsilon'} = \int_{\omega_{\text{i}}}^{\epsilon'} \int_{\mathbf{p}}$, and $\tilde{U}(\mathbf{p})$ and $\tilde{G}_\lambda^{(n)}$ are defined as follows, respectively:

$$\begin{aligned} \tilde{U}(\mathbf{p}) &:= \int_{\mathbf{x}} U(\mathbf{x}) e^{-i\mathbf{p}\cdot\mathbf{x}} = \frac{2\pi}{|\mathbf{p}|}, \\ (2\pi)^3 \delta^{(3)}(P_1 + \dots + P_n) \tilde{G}_\lambda^{(n)}(P_1, \dots, P_{n-1}) \\ &:= \int_{X_1, \dots, X_n} e^{-i(P_1 \cdot X_1 + \dots + P_n \cdot X_n)} G_\lambda^{(n)}(X_1, \dots, X_n), \end{aligned}$$

where $G_\lambda^{(n)}(X_1, \dots, X_n)$ is the n -point density correlation function. $E_{\text{gs},0}$ is the ground-state energy of the free fermions and corresponds to the kinetic energy in the free case. E_{H} , E_{ex} , and E_{corr} correspond to the Hartree, exchange, and correlation energies. One has $E_{\text{H}} = 0$ since $n = n_{\text{i}}$; note that E_{H} diverges if n_{i} is not set to n since $\tilde{U}(0) = \infty$, which means that the system becomes an unphysical one in the case of $n \neq n_{\text{i}}$. The kinetic energy $E_{\text{gs},0}/N$ and the exchange energy E_{ex}/N is known to be [49]

$$\frac{E_{\text{gs},0}}{N} = \frac{1}{2r_{\text{s}}^2}, \quad (6.8)$$

$$\frac{E_{\text{ex}}}{N} = -\frac{4\sqrt{2}}{3\pi r_{\text{s}}}. \quad (6.9)$$

$\tilde{G}_\lambda^{(2)}(P)$ is needed to be derived to calculate E_{corr}/N . The flow equation for $\tilde{G}_\lambda^{(2)}(P)$ can also be derived in the same manner as the derivation of Eq. (5.18):

$$\partial_\lambda \tilde{G}_\lambda^{(2)}(P) = -\tilde{U}(\mathbf{p}) \tilde{G}_\lambda^{(2)}(P)^2 + C_\lambda(P), \quad (6.10)$$

where

$$C_\lambda(P) = -\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \left(\tilde{G}_\lambda^{(4)}(P', -P', P) - \frac{\tilde{G}_\lambda^{(3)}(P', -P') \tilde{G}_\lambda^{(3)}(P, -P)}{\tilde{G}_\lambda^{(2)}(0)} \right). \quad (6.11)$$

Since the flows of $\tilde{G}_\lambda^{(3,4)}(P)$ in $C_\lambda(P)$ are not taken into account in the second-order vertex expansion, $C_\lambda(P)$ is needed to be approximated. Here, its λ dependence is simply ignored: $C_\lambda(P) \approx C_0(P)$. In this case, Eq. (6.10) can be solved analytically. The solution reads

$$\tilde{G}_\lambda^{(2)}(P) = \frac{\tilde{G}_0^{(2)}(P) + \sqrt{\frac{C_0(P)}{\tilde{U}(\mathbf{p})}} \tanh\left(\lambda \sqrt{\tilde{U}(\mathbf{p}) C_0(P)}\right)}{1 + \sqrt{\frac{\tilde{U}(\mathbf{p})}{C_0(P)}} \tilde{G}_0^{(2)}(P) \tanh\left(\lambda \sqrt{\tilde{U}(\mathbf{p}) C_0(P)}\right)}. \quad (6.12)$$

The λ integral of this solution can be performed analytically. Therefore, from Eq. (6.7), the expression for the correlation energy is obtained as follows:

$$\begin{aligned} \frac{E_{\text{corr}}}{N} = & \frac{1}{2n} \int_P^{\epsilon'} \left(\ln \left[\cosh\left(\sqrt{\tilde{U}(\mathbf{p}) C_0(P)}\right) + \sqrt{\frac{\tilde{U}(\mathbf{p})}{C_0(P)}} \tilde{G}_0^{(2)}(P) \sinh\left(\sqrt{\tilde{U}(\mathbf{p}) C_0(P)}\right) \right] \right. \\ & \left. - \tilde{U}(\mathbf{p}) \tilde{G}_0^{(2)}(P) \right). \end{aligned} \quad (6.13)$$

To calculate Eq. (6.13), $\tilde{G}_0^{(2,3,4)}$ should be specified. As Eq. (5.25), we have

$$\tilde{G}_0^{(n)}(P_1, \dots, P_{n-1}) = -N_s \sum_{\sigma \in S_{n-1}} \int_P \prod_{k=0}^{n-1} \tilde{G}_{F,0}^{(2)} \left(\sum_{i=1}^k P_{\sigma(i)} + P \right). \quad (6.14)$$

Here, $N_s = 2$ is the degrees of freedom for the spin, $\tilde{G}_{F,0}^{(2)}(P)$ is the two-point propagator of free fermions:

$$\tilde{G}_{F,0}^{(2)}(P) = \frac{e^{i\omega_i \epsilon}}{i\omega_i - \xi(\mathbf{p})},$$

where $\xi(p) := p^2/2 - \mu_0$. Then one has the following expressions for $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$, respectively:

$$\begin{aligned} \tilde{G}_0^{(2)}(P) = & 2N_s \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \frac{\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')}{\omega_i^2 + [\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')]^2}, \\ C_0(P) = & 2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\ & \times \left[\frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2} \right. \\ & \left. - \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2)(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)} \right], \end{aligned} \quad (6.15)$$

$$(6.16)$$

as shown in Appendix B. I note that the expression Eq. (6.15) yields the correct exchange energy Eq. (6.9) from Eq. (6.6), as shown in Appendix B.1.2.

6.3 Reproduction of the high-density exact result

I show Eq. (6.13) reproduces the exact result at the high-density limit $r_s \rightarrow 0$. To discuss it, let us investigate the behavior of $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$ at $r_s \rightarrow 0$. Instead of r_s , it is convenient to use $p_F = \sqrt{2}/r_s$. Here, $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$ are denoted as $\tilde{G}_0^{(2)}(\omega_i, \mathbf{p}; p_F)$ and $C_0(\omega_i, \mathbf{p}; p_F)$, respectively. From Eqs. (6.15) and (6.16), one finds

$$C_0(\omega_i, \mathbf{p}; p_F) = p_F^{-1} C_0(\bar{\omega}_i, \bar{\mathbf{p}}; 1), \quad (6.17)$$

$$\tilde{G}_0^{(2)}(\omega_i, \mathbf{p}; p_F) = \tilde{G}_0^{(2)}(\bar{\omega}_i, \bar{\mathbf{p}}; 1), \quad (6.18)$$

where $\bar{\mathbf{p}} = \mathbf{p}/p_F$ and $\bar{\omega}_i = \omega_i/p_F^2$. By use of these relations, one has

$$\begin{aligned} \frac{E_{\text{corr}}}{N} = & \frac{2\pi}{r_s^2} \int_{\bar{P}}^{\epsilon'} \left(\ln \left[1 + \sqrt{\frac{\tilde{U}(\bar{\mathbf{p}})}{C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)}} \tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1) \tanh \left(r_s \sqrt{\frac{\tilde{U}(\bar{\mathbf{p}}) C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)}{2}} \right) \right] \right. \\ & \left. - \frac{r_s}{\sqrt{2}} \tilde{U}(\bar{\mathbf{p}}) \tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1) \right) \\ & + \frac{2\pi}{r_s^2} \int_{\bar{P}}^{\epsilon'} \ln \left[\cosh \left(r_s \sqrt{\frac{\tilde{U}(\bar{\mathbf{p}}) C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)}{2}} \right) \right], \end{aligned} \quad (6.19)$$

from Eq. (6.13). Here, $\int_{\bar{P}} = \int e^{ip_F^2 \bar{\omega} \epsilon'} d\bar{\omega} / (2\pi) \int d\bar{\mathbf{p}} / (2\pi)^2$. With expanding Eq. (6.19) with respect to r_s , one has

$$\begin{aligned} \frac{E_{\text{corr}}}{N} = & \frac{2\pi}{r_s^2} \int_{\bar{P}} \left(\ln \left[1 + r_s \frac{\tilde{U}(\bar{\mathbf{p}})}{\sqrt{2}} \tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1) \right] - \frac{r_s}{\sqrt{2}} \tilde{U}(\bar{\mathbf{p}}) \tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1) \right) \\ & + \pi \int_{\bar{P}}^{\epsilon'} \frac{\tilde{U}(\bar{\mathbf{p}}) C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)}{2} + \mathcal{O}(r_s) \\ = & \frac{1}{2n} \int_P \left(\ln \left[1 + \tilde{U}(\mathbf{p}) \tilde{G}_0^{(2)}(\omega, \mathbf{p}; p_F) \right] - \tilde{U}(\mathbf{p}) \tilde{G}_0^{(2)}(\omega, \mathbf{p}; p_F) \right) \\ & + \frac{1}{4n} \int_P^{\epsilon'} \tilde{U}(\mathbf{p}) C_0(\omega, \mathbf{p}; p_F) + \mathcal{O}(r_s). \end{aligned} \quad (6.20)$$

The first term in the right-hand side coincides with the contributions from the rings diagrams. The second term is identical with the contribution from the second-order exchange diagrams. Actually, one has

$$\begin{aligned} \frac{1}{4n} \int_P \tilde{U}(\mathbf{p}) C_0(\omega, \mathbf{p}; p_F) = & \frac{2\pi^2 N_s}{n} \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \frac{\theta(-\xi(\mathbf{p}'')) \theta(-\xi(\mathbf{p}'))}{|\mathbf{p}| |\mathbf{p} + \mathbf{p}' + \mathbf{p}''|} \\ & \times \frac{(1 - \theta(-\xi(\mathbf{p} + \mathbf{p}')))(1 - \theta(-\xi(\mathbf{p} + \mathbf{p}'')))}{\mathbf{p} \cdot (\mathbf{p} + \mathbf{p}' + \mathbf{p}'')}, \end{aligned}$$

which is found to be identical with the expression for the second-order exchange diagrams. Hence, at high-density limit $r_s \rightarrow 0$, our correlation energy gives the same result as that with the Gell-Mann–Brueckner resummation [49, 87], which gives the following exact result at $r_s \rightarrow 0$ [49, 81, 88]:

$$\begin{aligned} \frac{E_{\text{corr}}}{N} &= \ln 2 - 1 + \beta(2) - \frac{8}{\pi^2} \beta(4) - \sqrt{2} \left(\frac{10}{3\pi} - 1 \right) r_s \ln r_s + \mathcal{O}(r_s) \\ &= -0.192496 \dots - 0.0863136 \dots \times r_s \ln r_s + \mathcal{O}(r_s), \end{aligned} \quad (6.21)$$

where $\beta(x)$ is the Dirichlet beta function.

6.4 Numerical results

Our numerical result for the correlation energy are discussed.

6.4.1 Numerical procedure

Before presenting our result, I briefly describe our numerical procedure. One can reduce the computational time to calculate Eq. (6.13) by use of some procedure: As shown in Eq. (6.16), $C_0(P)$ in Eq. (6.13) has the quadruple integral with respect to the momentums. In the case of the Coulomb interaction, this integral can be reduced to a double integral analytically, which largely decrease the computational effort. Moreover, one can easily derive $C_0(P)$ and $\tilde{G}_0^{(2)}(P)$ for various r_s by use of Eqs. (6.17) and (6.18) if $C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)$ and $\tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1)$ are once calculated. Since the system is isotropic, $C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)$ and $\tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1)$ do not depend on the direction of $\bar{\mathbf{p}}$. Therefore, the calculations of $C_0(\bar{\omega}, \bar{\mathbf{p}}; 1)$ and $\tilde{G}_0^{(2)}(\bar{\omega}, \bar{\mathbf{p}}; 1)$ on the $(\bar{\omega}, |\bar{\mathbf{p}}|)$ space are sufficient.

Since the integrand of Eq. (6.13) does not depend on the direction of the momentum, the two-dimensional momentum integral can be reduced to the integral with respect to the norm of the momentum. Moreover, since the integrand of Eq. (6.13) is an even function of the frequency, the domain of the frequency integral can be reduced from $(-\infty, \infty)$ to $[0, \infty)$. To make the domains of the momentum and frequency integrals finite intervals for the numerical calculation, the variables of integrals are changed as $\theta_\omega = (2/\pi) \arctan(\omega^{\alpha_\omega}/s_\omega)$ and $\theta_p = (2/\pi) \arctan(p^{\alpha_p}/s_p)$, where $\alpha_{\omega,p}$ and $s_{\omega,p}$ are arbitral positive numbers. With this change, the domains of the integrals become $\theta_{\omega,p} \in [0, 1]$.

6.4.2 Correlation energy

Figure 6.1 shows the result of the correlation energy per particle as a function of r_s derived by the FRG-DFT with the second-order vertex expansion. Since the FRG-DFT calculation requires relatively small computational efforts, one can obtain the correlation energy for various r_s enough to see the smooth shape of the r_s -dependence

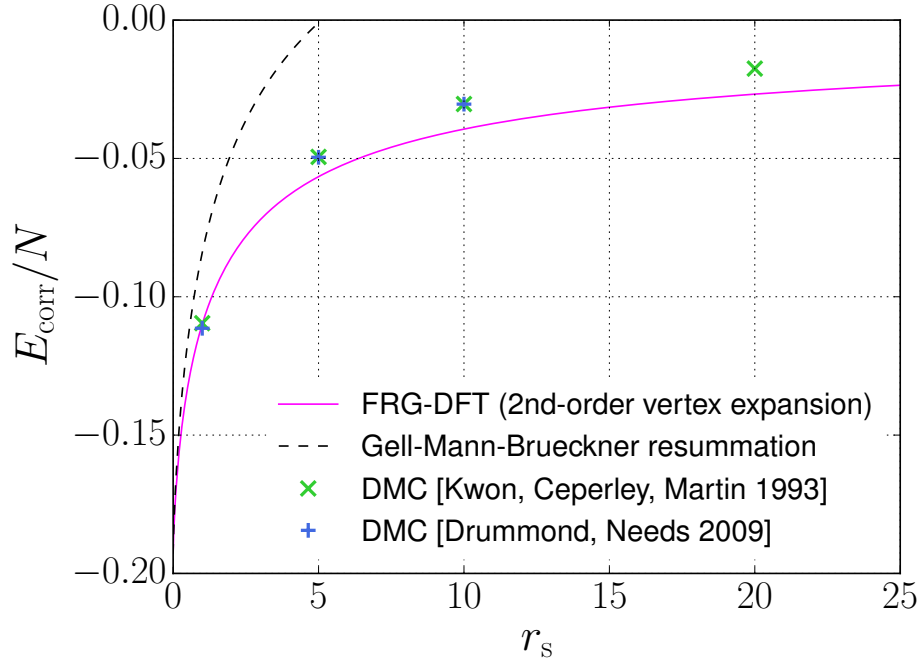


Figure 6.1: Correlation energy per particle derived by the FRG-DFT method (solid magenta line) as the function of the Wigner-Seitz radius r_s . The results derived by Gell-Mann-Brueckner resummation (black dashed line) and the Monte-Carlo calculations are also shown. The green cross marks and blue plus marks are the energies derived by the extrapolations of the results of the DMC calculations to the infinite systems given by Kwon et al. [50] and Drummond et al. [51], respectively.

curve. For comparison, the energies given by the Gell-Mann-Brueckner resummation and the Monte Carlo (MC) calculations are also shown. In the MC calculations, the energies of the infinite matter were calculated by the extrapolations of the energies in the case of finite particle number which were derived by the diffusion Monte Carlo (DMC) method with the backflow correction [50, 51]. As discussed in the previous section, one can see that the FRG-DFT reproduces the exact energy given by the Gell-Mann-Brueckner resummation. For finite r_s , the energy by the FRG-DFT seems to agree with the MC results at $r_s = 1$ a.u., and the deviation between the results of the FRG-DFT and the MC calculations seems to become larger as r_s becomes small.

Table 6.1 shows the numerical values of the correlation energies at some r_s . One finds that the result of the FRG-DFT coincides with both MC results within the errors of the MC calculations at $r_s = 1$ a.u.. The deviation becomes larger as r_s increases: The result given by the FRG-DFT misses by approximately 14% at $r_s = 5$ a.u., 30% at $r_s = 10$ a.u., and 50% at $r_s = 20$ a.u. compared with the MC results. For more accurate description in the case of large r_s , the λ dependences of the higher-order correlation functions $G_\lambda^{(n \geq 3)}$ are needed to be taken into account.

Table 6.1: Numerical value of the correlation energies at the selected Wigner-Seitz radii r_s with the FRG-DFT and the DMC method with the backflow correction [50,51]. The number in the parentheses are errors in the last decimal place.

r_s (a.u.)	1	5	10	20
FRG-DFT	-0.10992	-0.056581	-0.039396	-0.026756
DMC [50]	-0.1096(3)	-0.0495(1)	-0.03034(2)	-0.01753(1)
DMC [51]	-0.1102(6)	-0.04959(3)	-0.030378(6)	-

6.5 Summary

I have shown a demonstration of the FRG-DFT method in a two-dimensional homogeneous infinite system (2DHEG). The FRG-DFT has been applied to the two-dimensional homogeneous electron gas and calculated the correlation energy for various densities with the second-order vertex expansion scheme. The expressions for the correlation energy has been derived by solving the flow equations for the energy and the two-point density correlation function analytically. From the expressions for the correlation energy, Our correlation energy has been analitically found to completely reproduce the exact result given by the Gell-Mann–Brueckner resummation at high-density limit. The reproduction has also been confirmed with the numerical calculation. For finite densities, we have compared our correlation energy with those obtained from the extrapolations of the Monte Carlo (MC) results. Our correlation energy coincides with the MC results at relatively high-density case $r_s = 1$ a.u., whereas the deviation between the results with the FRG-DFT and with the MC calculations becomes larger as the system becomes dilute.

To improve the accuracy when the system is dilute, the inclusion of the flows of the higher-point density correlation functions are needed. In the vertex expansion scheme, one can systematically improve the inclusion of the flows of the density correlation functions. The inclusion of the flow of the three-point density correlation function is the straightforward next step. Another attractive way to include the flows of higher-order correlation functions has been recently proposed [45].

Regarding the electron gas, the extension to the case of spin-polarized case is a significant direction since it is necessary for the investigation of the magnetic phase transition. This can be achieved with introducing different chemical potentials for particles with different spin components.

Our formalism for the infinite matters is flexible and largely extensible: The extension to the three-dimensional system is straightforward, which is important for the analyses of realistic quantum many-body systems. The extension to the case of the finite temperature is also straightforward. In this case, the FRG-DFT becomes a framework to give the Helmholtz free energy.

The 2DHEG is more realistic model than those in any other previous works. Additionally, the demonstration here is the first example showing that the FRG-DFT works even for long-range interaction. In conclusion, our demonstration in this Chapter shows

that the FRG-DFT is a promising way for the analysis of realistic models for quantum many-body systems.

Chapter 7

Conclusion and outlook

This thesis has been devoted to the study of the functional-renormalization-group aided density-functional theory (FRG-DFT). I have summarized the motivation to introduce the FRG-DFT and shown its formalism. I have also elucidated the relation between the FRG-DFT and the adiabatic connection. Some applications of the FRG-DFT to infinite homogeneous matters have been presented.

Although the density functional theory (DFT) is a very powerful method for the analysis of the quantum many-body systems, there are some long-standing problems. In particular, the problem that there is no established methods to derive the energy density functional from microscopic Hamiltonian is very crucial for the establishment of the DFT as a truly ab-initio method. The FRG-DFT is a promising method to give a long-desired solution for the fundamental problems of the DFT based on the functional renormalization group (FRG), which is a tool to connect the information of the microscopic freedoms to the understanding of macroscopic behaviors of a system.

However, whether the FRG-DFT is a practical method for the analysis of realistic quantum many-body systems was not been clarified. To show how powerful method the FRG-DFT is, I have presented two applications. At first with my collaborators, I have formulated the FRG-DFT for infinite homogeneous matters, which is a simple but a practical setup, and demonstrated how it works.

The first application was the analysis of a one-dimensional matter composed of spinless fermions with a non-local interaction exhibiting the qualitative behavior of the nuclear force. We have calculated the equation of state (EOS) at zero temperature, i.e. the density dependence of the ground-state energy, and the spectral function for the density two-point function. We have employed the second-order vertex expansion with a correction to restore the Pauli blocking effect and found that the analytic continuation for the frequencies which is needed to obtain the spectral function can be analytically performed on the level of the flow equation as recently done in the context of the FRG. We have derived the saturation point, i.e. the minimum point of the EOS with respect to the density, and found that the saturation energy derived with the FRG-DFT differs by only 2.7 % in comparison with the Monte Carlo (MC) result. Our result has also shown that the introduction of the correction to restore the Pauli blocking contributes

the improvement of the accuracy. Moreover, we have found that our spectral function reproduces a notable feature of the non-linear Tomonaga–Luttinger liquid that the spectral function diverges at the edge of its support in the lower-energy side.

The other application is the analysis of the two-dimensional homogeneous electron gas. We have calculated the correlation energy by the aid of the second-order vertex expansion. Solving the flow equations analytically, we have found that our correlation energy reproduces the exact result at the high-density limit given by the Gell-Mann–Brueckner resummation. We have also found that our correlation energy coincides with the results of the MC calculation when the density is relatively high, whereas the discrepancy between the results by the FRG-DFT and the MC calculations becomes larger as the system becomes dilute.

Through these demonstration, I have shown that the FRG-DFT formulated for the infinite matters gives a unified way for the analysis of the ground and excited states, and is expected to be a feasible method for the analyses of realistic quantum many-body systems. In addition, the FRG-DFT with the vertex expansion scheme has been found to be powerful at least in the case of high density.

The formulation presented in this thesis is very flexible and largely extensible. For example, the extension to the three-dimensional case is straightforward. Our formulation can also be extended to the system with multi components. With these extensions, the FRG-DFT becomes applicable to various realistic models such as the three-dimensional electron gas, nuclear matter, and cold atomic gas. In particular, the extension to the multi component systems makes the FRG-DFT applicable to the various matters in neutron stars such as asymmetric nuclear matter and nuclear matter with hyperon. The application to the electron gas with arbitrary spin polarization is also a significant direction. Although our demonstrations have been focused on the zero-temperature cases, our formulation can be extended to the case of finite temperature.

One of the advantages of the FRG-DFT is that systematic approximation schemes developed in the FRG are available. In our demonstrations with the second-order vertex expansion, the accuracy seems to become worse as the systems becomes dilute. However, this is not the problem of the FRG-DFT but the approximation scheme, and one can improve the accuracy in the framework of the FRG-DFT. One of the advantage of the vertex expansion scheme is that one can systematically improve the accuracy with taking into account the flows of higher-order density correlation functions. In addition, a more efficient way to include the flows of higher-order density correlation function was recently put forward [45].

As the Hohenberg-Kohn theorem suggests, all the properties of a system are determined in terms of the energy density functional (EDF) even if some symmetry is spontaneously broken and degenerate ground states appear. However, the analysis of a system with symmetry breaking using the energy functional of only total density is practically very difficult. In the DFT, energy functionals of not only the total density but also some other auxiliary fields are often introduced to analyze a system exhibiting some symmetry breaking. For example, the energy functional of the total density

and the fermion pair field is used to analyze the superconducting states. Our FRG-DFT formalism is applicable to the construction of energy functionals of other fields besides the total density. The analyses of a state with symmetry breaking such as the superconductivity with the FRG-DFT are attractive future directions.

The FRG-DFT is also applicable to the finite and isolated systems such as nuclei. In such systems, the effect of the gradient of the density fields is crucial. One of the widely-used approximation including the effect of the gradient is the generalized gradient approximation (GGA). The construction of the GGA functional may be achieved by use of the gradient expansion method developed in the FRG studies.

In conclusion, I have shown some examples which suggest that the FRG-DFT is a promising way. The FRG-DFT will make the DFT a truly ab-initio method for the quantum many-body systems.

Appendix A

The origin of ϵ in Eq. (4.2)

As stated in Chap. 4.1, the normal-ordered Hamiltonian Eq. (4.1) corresponds to the action Eq. (4.2), which has a positive infinitesimal ϵ . In this chapter, we explain the origin of ϵ following the discussion in Ref. [89].

Let us consider a normal-ordered Hamiltonian $\hat{H}(\hat{\psi}_i^*, \hat{\psi}_i)$ with annihilation operator $\hat{\psi}_i$ and creation operator $\hat{\psi}_i^*$ for fermion fields. Here, all the indices of the field including those for the internal degree of freedoms and the coordinates are represented as i . In order to find the action corresponding to this Hamiltonian, we consider the partition function defined as follows:

$$Z = \sum_n \langle n | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle, \quad (\text{A.1})$$

where β is the inverse temperature, μ is the chemical potential, $\hat{N}(\hat{\psi}^*, \hat{\psi}) = \sum_i \hat{\psi}_i^* \hat{\psi}_i$ is the particle-number operator, and $\{|n\rangle\}_{n=0}^\infty$ is the eigenstates of the system.

To find the expression for Eq. (A.1) in the path-integral formalism, I introduce the coherent states $|\psi\rangle$, which is defined as the eigenfunction for $\{\hat{\psi}_i\}_i$ with eigenvalues $\{\psi_i\}_i$:

$$\hat{\psi}_i |\psi\rangle = \psi_i |\psi\rangle.$$

Since $\{\hat{\psi}_i\}_i$ satisfies the anti-commutation relation $\hat{\psi}_i \hat{\psi}_j = -\hat{\psi}_j \hat{\psi}_i$, the eigenvalues $\{\psi_i\}_i$ satisfy $\psi_i \psi_j = -\psi_j \psi_i$. Therefore, $\{\psi_i\}_i$ should be treated as Grassmann numbers. In the same manner, $\langle\psi|$ is defined as follows:

$$\langle\psi| \hat{\psi}_i^* = \langle\psi| \psi_i^*.$$

I briefly summarize the definitions of functions of Grassmann variables and their derivatives and integrals. A function $f(\eta_1, \dots, \eta_N)$ of Grassmann variables $\{\eta_i\}_{i=1}^N$ is defined by the Taylor expansion:

$$f(\eta_1, \dots, \eta_N) = \sum_{k=0}^{\infty} \sum_{i_1, \dots, i_k=1}^N \frac{1}{k!} \left. \frac{\partial^k f}{\partial \eta_{i_1} \dots \partial \eta_{i_k}} \right|_{\eta_1, \dots, \eta_N=0} \eta_{i_1} \dots \eta_{i_k}.$$

Since $\eta_i \eta_i = 0$, $f(\eta_1, \dots, \eta_N)$ can be rewritten as the following form:

$$f(\eta_1, \dots, \eta_N) = f(\eta_1, \dots, \eta_{i-1}, 0, \eta_{i+1}, \dots, \eta_N) + \eta_i g(\eta_1, \dots, \eta_{i-1}, \eta_{i+1}, \dots, \eta_N),$$

where g is a function independent of η_i . Then the derivative of $f(\eta_1, \dots, \eta_N)$ with respect to η_i is defined as follows:

$$\partial_{\eta_i} f(\eta_1, \dots, \eta_N) = g(\eta_1, \dots, \eta_{i-1}, \eta_{i+1}, \dots, \eta_N).$$

For Grassmann variables, the definition of the integral is the same as the derivative:

$$\int d\eta_i f(\eta_1, \dots, \eta_N) = g(\eta_1, \dots, \eta_{i-1}, \eta_{i+1}, \dots, \eta_N).$$

This integral satisfies the partial-integration-like relation:

$$\begin{aligned} & \int d\eta_i (\partial_{\eta_i} f_1(\eta_1, \dots, \eta_N)) f_2(\eta_1, \dots, \eta_N) \\ &= -\zeta(f_1) \int d\eta_i f_1(\eta_1, \dots, \eta_N) \partial_{\eta_i} f_2(\eta_1, \dots, \eta_N), \end{aligned}$$

where

$$\zeta(x) = \begin{cases} -1 & (x \text{ is a Grassmann number.}) \\ 1 & (\text{otherwise}) \end{cases}.$$

Under these definitions, the completeness relation reads as follows:

$$\left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle \psi| = \mathbf{1}, \quad (\text{A.2})$$

where $\mathbf{1}$ is the unit operator. To show that this relation holds, the following expression for the coherent state is useful:

$$|\psi\rangle = e^{-\sum_j \psi_j \hat{\psi}_j^*} |0\rangle, \quad (\text{A.3})$$

where $|0\rangle$ is the vacuum defined by $\psi_i |0\rangle = 0$. Actually, the right-hand side of Eq. (A.3) satisfies

$$\begin{aligned} \hat{\psi}_i e^{-\sum_j \psi_j \hat{\psi}_j^*} |0\rangle &= e^{-\sum_{j \neq i} \psi_j \hat{\psi}_j^*} \hat{\psi}_i (1 - \psi_i \hat{\psi}_i^*) |0\rangle = \psi_i e^{-\sum_{j \neq i} \psi_j \hat{\psi}_j^*} \hat{\psi}_i \hat{\psi}_i^* |0\rangle \\ &= \psi_i e^{-\sum_{j \neq i} \psi_j \hat{\psi}_j^*} |0\rangle = \psi_i e^{-\sum_{j \neq i} \psi_j \hat{\psi}_j^*} (1 - \psi_i \hat{\psi}_i^*) |0\rangle = \psi_i e^{-\sum_j \psi_j \hat{\psi}_j^*} |0\rangle. \end{aligned}$$

Here, the commutation relation $\hat{\psi}_i \hat{\psi}_i^* = -\hat{\psi}_i^* \hat{\psi}_i + 1$ has been used. From Eq. (A.3), one gets the following relation:

$$\hat{\psi}_i^* |\psi\rangle = -\partial_{\psi_i} |\psi\rangle. \quad (\text{A.4})$$

The same relations hold for $\langle\psi|$:

$$\langle\psi| = \langle 0| e^{-\sum_j \hat{\psi}_j \psi_j^*}, \quad (\text{A.5})$$

$$\langle\psi| \hat{\psi}_i = \partial_{\psi_i^*} \langle\psi|. \quad (\text{A.6})$$

The inner product of $\langle\psi|$ and $|\psi'\rangle$ is obtained as follows:

$$\langle\psi|\psi'\rangle = \langle\psi| e^{-\sum_j \psi_j' \hat{\psi}_j^*} |0\rangle = e^{\sum_j \psi_j^* \psi_j'}. \quad (\text{A.7})$$

By use of these relations, let us prove Eq. (A.2). According to the Schur's lemma, the left-hand side of Eq. (A.2) is proportional to the unit operator if and only if it commutes with $\hat{\psi}_i$ and $\hat{\psi}_i^*$. The commutativity with $\hat{\psi}_i$ is shown as follows:

$$\begin{aligned} \hat{\psi}_i \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| &= \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} \hat{\psi}_i |\psi\rangle \langle\psi| \\ &= - \left(\prod_i \int d\psi_i^* d\psi_i \right) \partial_{\psi_i^*} e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| = \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \partial_{\psi_i^*} \langle\psi| \\ &= \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| \hat{\psi}_i. \end{aligned}$$

The commutativity with $\hat{\psi}_i^*$ is also shown as follows:

$$\begin{aligned} \hat{\psi}_i^* \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| &= - \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} \partial_{\psi_i} |\psi\rangle \langle\psi| \\ &= \left(\prod_i \int d\psi_i^* d\psi_i \right) \partial_{\psi_i} e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| = \left(\prod_i \int d\psi_i^* d\psi_i \right) \psi_i^* e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| \\ &= \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| \hat{\psi}_i^*. \end{aligned}$$

Thus, one has

$$\left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\psi\rangle \langle\psi| = C \mathbf{1},$$

where C is a constant. This constant is determined as follows:

$$\begin{aligned} C &= \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} |\langle 0|\psi\rangle|^2 = \left(\prod_i \int d\psi_i^* d\psi_i \right) e^{-\sum_i \psi_i^* \psi_i} \\ &= \prod_i \int d\psi_i^* d\psi_i e^{-\psi_i^* \psi_i} = 1. \end{aligned}$$

Therefore, we have Eq. (A.2).

Let us go back to the partition function. The first step to write the partition function in terms of the path integral is dividing $e^{-\beta(\hat{H}-\mu\hat{N})}$ into $N \gg 1$ pieces:

$$Z = \sum_n \langle n | \prod_{k=1}^N e^{-\delta(\hat{H}-\mu\hat{N})} | n \rangle, \quad (\text{A.8})$$

where $\delta = \beta/N$. I insert the completeness relation Eq. (A.2) between these pieces:

$$\begin{aligned} Z &= \sum_n \langle n | \prod_{k=0}^{N-1} \left(e^{-\delta(\hat{H}-\mu\hat{N})} \left(\prod_i \int d\psi_{ki}^* d\psi_{ki} \right) e^{-\sum_i \psi_{ki}^* \psi_{ki}} | \psi_k \rangle \langle \psi_k | \right) | n \rangle \\ &= \left(\prod_{k=0}^{N-1} \prod_i \int d\psi_{k,i}^* d\psi_{k,i} \right) \sum_n \langle n | e^{-\sum_i \psi_{N-1,i}^* \psi_{N-1,i} - \delta(\hat{H}-\mu\hat{N})} | \psi_{N-1} \rangle \\ &\quad \times \prod_{k=0}^{N-2} \left(\langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle \right) \langle \psi_0 | n \rangle \\ &= \left(\prod_{k=0}^{N-1} \prod_i \int d\psi_{k,i}^* d\psi_{k,i} \right) \sum_n \langle -\psi_0 | n \rangle \langle n | e^{-\sum_i \psi_{N-1,i}^* \psi_{N-1,i} - \delta(\hat{H}-\mu\hat{N})} | \psi_{N-1} \rangle \\ &\quad \times \prod_{k=0}^{N-2} \left(\langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle \right) \\ &= \left(\prod_{k=0}^{N-1} \prod_i \int d\psi_{k,i}^* d\psi_{k,i} \right) \langle -\psi_0 | e^{-\sum_i \psi_{N-1,i}^* \psi_{N-1,i} - \delta(\hat{H}-\mu\hat{N})} | \psi_{N-1} \rangle \\ &\quad \times \prod_{k=0}^{N-2} \left(\langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle \right) \\ &= \int \mathcal{D}\psi_i \mathcal{D}\psi_i^* \prod_{k=0}^{N-1} \langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle. \end{aligned}$$

Here, $\psi_{N,i} = -\psi_{0,i}$, $\psi_{N,i}^* = -\psi_{0,i}^*$, and

$$\int \mathcal{D}\psi_i \mathcal{D}\psi_i^* = \left(\prod_{k=0}^{N-1} \prod_i \int d\psi_{k,i}^* d\psi_{k,i} \right).$$

Since δ is infinitesimally small at $N \rightarrow \infty$, one evaluates $\langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle$ by expanding it with respect to δ :

$$\langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H}-\mu\hat{N})} | \psi_k \rangle = e^{-\sum_i \psi_{ki}^* \psi_{ki}} \langle \psi_{k+1} | (1 - \delta(\hat{H} - \mu\hat{N})) | \psi_k \rangle + \mathcal{O}(\delta^2).$$

Introducing

$$H_k = \frac{\langle \psi_{k+1} | \hat{H} | \psi_k \rangle}{\langle \psi_{k+1} | \psi_k \rangle},$$

and

$$N_k = \frac{\langle \psi_{k+1} | \hat{N} | \psi_k \rangle}{\langle \psi_{k+1} | \psi_k \rangle},$$

one has

$$\begin{aligned} \langle \psi_{k+1} | e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(\hat{H} - \mu \hat{N})} | \psi_k \rangle &= e^{-\sum_i \psi_{ki}^* \psi_{ki} - \delta(H_k - \mu N_k)} \langle \psi_{k+1} | \psi_k \rangle + \mathcal{O}(\delta^2) \\ &= e^{\sum_i (\psi_{k+1,i}^* - \psi_{k,i}^*) \psi_{k,i} - \delta(H_k - \mu N_k)} + \mathcal{O}(\delta^2). \end{aligned}$$

Here, Eq. (A.7) has been used. It is apparent that in the case of a normal-ordered Hamiltonian, H_k is directly obtained from the replacement of $\hat{\psi}^*$ and $\hat{\psi}$ with ψ_{k+1}^* and ψ_k , respectively, in $\hat{H}(\hat{\psi}^*, \hat{\psi})$. N_k is also obtained in the same manner. Therefore, H_k and N_k depend on ψ_{k+1}^* and ψ_k in our case.¹ At the limit $N \rightarrow \infty$, one finally obtains

$$\begin{aligned} Z &= \int \mathcal{D}\psi_i \mathcal{D}\psi_i^* e^{-\delta \sum_{k=0}^{N-1} \left(-\sum_i \frac{\psi_{k+1,i}^* - \psi_{k,i}^*}{\delta} \psi_{k,i} + H(\psi_{k+1}^*, \psi_k) - \mu N(\psi_{k+1}^*, \psi_k) \right)} \\ &= \int \mathcal{D}\psi_i \mathcal{D}\psi_i^* e^{-\delta \sum_{k=0}^{N-1} \left(\sum_i \psi_{k+1,i}^* \frac{\psi_{k+1,i} - \psi_{k,i}}{\delta} + H(\psi_{k+1}^*, \psi_k) - \mu N(\psi_{k+1}^*, \psi_k) \right)} \\ &= \int \mathcal{D}\psi_i \mathcal{D}\psi_i^* e^{-\int_0^\beta d\tau \left(\sum_i \psi_i^*(\tau + \delta) \partial \psi_i(\tau) + H(\psi^*(\tau + \delta), \psi(\tau)) - \mu N(\psi^*(\tau + \delta), \psi(\tau)) \right)}, \end{aligned} \quad (\text{A.9})$$

where the imaginary time $\tau = k\delta$ has been introduced and ψ_k^* and ψ_k are denoted as $\psi^*(\tau)$ and $\psi(\tau)$, respectively. $H(\psi^*, \psi)$ is a function which is obtained by the simple replacement of $\hat{\psi}^*$ and $\hat{\psi}$ with ψ^* and ψ , respectively, in $\hat{H}(\hat{\psi}^*, \hat{\psi})$. From Eq. (A.9), the action corresponding to the normal-ordered Hamiltonian $\hat{H}$ reads

$$S[\psi^*, \psi] = \int_0^\beta d\tau \left(\sum_i \psi_i^*(\tau + \epsilon) \partial \psi_i(\tau) + H(\psi^*(\tau + \epsilon), \psi(\tau)) \right). \quad (\text{A.10})$$

Here, δ has been rewritten as ϵ . As seen in this action, the imaginary time of ψ^* is actually infinitesimally larger than that of ψ .

Since the Hamiltonian Eq. (4.1) satisfies the normal ordering, the positive infinitesimal ϵ appears in the action Eq. (4.2) as Eq. (A.10).

¹ In other choices of the ordering, H_k and N_k may depend on other variables. In the case of a Weyl-ordered Hamiltonian, H_k and N_k depend on ψ_{k+1}^* and $(\psi_{k+1} + \psi_k)/2$, or $(\psi_{k+1}^* + \psi_k^*)/2$ and ψ_k , which is known as the mid-point rule; see Ref. [90] for details of the formalism with the Weyl ordering.

Appendix B

Derivations of the forms of $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$

I present the derivation of the expressions for $\tilde{G}_0^{(2)}(P)$ and $C_0(P)$ given in Eqs. (5.26) and (5.27) in the case of one-dimensional spinless fermions, and in Eqs. (6.15) and (6.16) in the case of two-dimensional spin-1/2 fermions. Since there is no essential difference for the derivation between the of one-dimensional spinless case and two-dimensional spin-1/2 case, I consider a general case: a $(D+1)$ -dimensional spin-unpolarized system composed of spin- N_s fermions with the chemical potential μ_0 . In this case, as Eqs. (5.25) and (6.14), the n -point density correlation functions reads

$$\tilde{G}_0^{(n)}(P_1, \dots, P_{n-1}) = -N_s \sum_{\sigma \in S_{n-1}} \int_P \prod_{k=0}^{n-1} \tilde{G}_{F,0}^{(2)} \left(\sum_{i=1}^k P_{\sigma(i)} + P \right), \quad (\text{B.1})$$

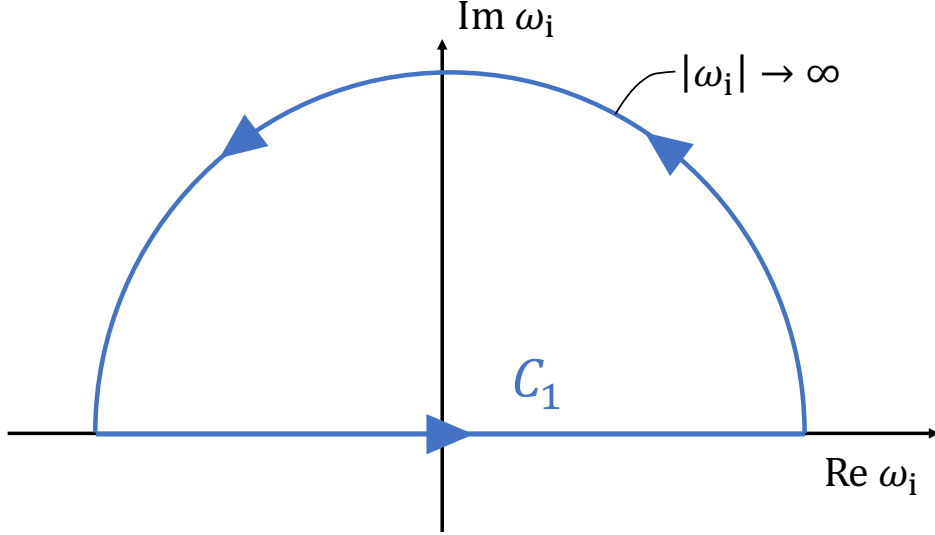
Here, $P = (\omega_i, \mathbf{p})$ with imaginary frequency ω_i and D -dimensional momentum $\mathbf{p}$, $\int_P = \int_{\omega_i} \int_{\mathbf{p}} = \int_{-\infty}^{\infty} d\omega_i / (2\pi) \int d\mathbf{p} / (2\pi)^D$, and $\tilde{G}_{F,0}^{(2)}(P)$ is the two-point propagator of the free fermions:

$$\tilde{G}_{F,0}^{(2)}(P) = \frac{e^{i\omega_i \epsilon}}{i\omega_i - \xi(\mathbf{p})},$$

where $\xi(\mathbf{p}) = \mathbf{p}^2/2 - \mu_0$ and ϵ is a positive infinitesimal.

B.1 Expression for $\tilde{G}_0^{(2)}(P)$

First, the derivation of the expression for $\tilde{G}_0^{(2)}(P)$ is presented. I also confirm whether our expression reproduces the exchange energy of the 2DHEG Eq. (6.9).

Figure B.1: Definition of contour C_1 .

B.1.1 Derivation of $\tilde{G}_0^{(2)}(P)$

From Eq. (B.1), we have

$$\begin{aligned} \tilde{G}_0^{(2)}(P_1) &= -N_s \int_P G_{F,0}^{(2)}(P + P_1) G_{F,0}^{(2)}(P) = -N_s \int_P \frac{e^{i(\omega_i + \omega_{i1})\epsilon}}{i(\omega_i + \omega_{i1}) - \xi(\mathbf{p} + \mathbf{p}_1)} \frac{e^{i\omega_i\epsilon}}{i\omega_i - \xi(\mathbf{p})} \\ &= N_s e^{i\omega_{i1}\epsilon} \int_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{d\omega_i}{2\pi} \frac{e^{2i\omega_i\epsilon}}{[\omega_i + \omega_{i1} + i\xi(\mathbf{p} + \mathbf{p}_1)][\omega_i + i\xi(\mathbf{p})]}. \end{aligned} \quad (\text{B.2})$$

The contour of the ω_i -integral is changed to C_1 which is defined as Fig. B.1. The integrand in the last expression of Eq. (B.2) vanishes at $|\omega| \rightarrow \infty$ in the upper-half plane of ω thanks to the convergence factor $e^{2i\omega_i\epsilon}$. Changing the contour and performing the ω_i -integral, one has

$$\begin{aligned} &N_s e^{i\omega_{i1}\epsilon} \int_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{d\omega_i}{2\pi} \frac{e^{2i\omega_i\epsilon}}{[\omega_i + \omega_{i1} + i\xi(\mathbf{p} + \mathbf{p}_1)][\omega_i + i\xi(\mathbf{p})]} \\ &= N_s e^{i\omega_{i1}\epsilon} \int_{\mathbf{p}} \int_{C_1} \frac{d\omega_i}{2\pi} \frac{e^{2i\omega_i\epsilon}}{[\omega_i + \omega_{i1} + i\xi(\mathbf{p} + \mathbf{p}_1)][\omega_i + i\xi(\mathbf{p})]} \\ &= N_s \int_{\mathbf{p}} \left(\frac{e^{-i\omega_{i1}\epsilon + 2\xi(\mathbf{p} + \mathbf{p}_1)\epsilon} \theta(-\xi(\mathbf{p} + \mathbf{p}_1))}{i\omega_{i1} - \xi(\mathbf{p} + \mathbf{p}_1) + \xi(\mathbf{p})} - \frac{e^{i\omega_{i1}\epsilon + 2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p}))}{i\omega_{i1} - \xi(\mathbf{p} + \mathbf{p}_1) + \xi(\mathbf{p})} \right) \\ &= N_s \int_{\mathbf{p}} \left(\frac{e^{-i\omega_{i1}\epsilon + 2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p}))}{i\omega_{i1} - \xi(\mathbf{p}) + \xi(\mathbf{p} - \mathbf{p}_1)} - \frac{e^{i\omega_{i1}\epsilon + 2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p}))}{i\omega_{i1} - \xi(\mathbf{p} + \mathbf{p}_1) + \xi(\mathbf{p})} \right). \end{aligned} \quad (\text{B.3})$$

Here, the Heaviside functions $\theta(x)$ have appeared since the contour integral along C_1 depends on whether the poles $\omega_i = -\omega_{i1} - i\xi(\mathbf{p} + \mathbf{p}_1)$ and $-i\xi(\mathbf{p})$ reside inside of C_1

or not. In the last equality of Eq. (B.3), the integral variable $\mathbf{p}$ has been shifted to $\mathbf{p} - \mathbf{p}_1$ in the first term of the integrand. With substituting $\mathbf{p}$ to $-\mathbf{p}$ and using that $\xi(\mathbf{p}) = \xi(-\mathbf{p})$, one has

$$\begin{aligned} & N_s \int_{\mathbf{p}} \left(\frac{e^{-i\omega_{i1}\epsilon + 2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p}))}{i\omega_{i1} - \xi(\mathbf{p}) + \xi(\mathbf{p} - \mathbf{p}_1)} - \frac{e^{i\omega_{i1}\epsilon + 2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p}))}{i\omega_{i1} - \xi(\mathbf{p} + \mathbf{p}_1) + \xi(\mathbf{p})} \right) \\ &= N_s \int_{\mathbf{p}} e^{2\xi(\mathbf{p})\epsilon} \theta(-\xi(\mathbf{p})) \left(\frac{e^{-i\omega_{i1}\epsilon}}{i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} + \frac{e^{i\omega_{i1}\epsilon}}{-i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} \right) \\ &= N_s \int_{\mathbf{p}} \theta(-\xi(\mathbf{p})) \left(\frac{e^{-i\omega_{i1}\epsilon}}{i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} + \frac{e^{i\omega_{i1}\epsilon}}{-i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} \right). \end{aligned} \quad (\text{B.4})$$

Here, $e^{2\xi(\mathbf{p})\epsilon}$ has been substituted to 1 in the last equality, since $e^{-2\mu\epsilon} \leq e^{2\xi(\mathbf{p})\epsilon} \leq 1$ owing to the factor $\theta(-\xi(\mathbf{p}))$ and thus $e^{2\xi(\mathbf{p})\epsilon}$ converges to 1 for any ω_{i1} and $\mathbf{p}_1$. For finite ω_{i1} , one has

$$\tilde{G}_0^{(2)}(P_1) = 2N_s \int_{\mathbf{p}} \theta(-\xi(\mathbf{p})) \frac{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})}{\omega_{i1}^2 + (\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p}))^2}. \quad (\text{B.5})$$

since $e^{\pm i\omega_{i1}\epsilon} \rightarrow 1$. This expression coincides with Eq. (5.26) in the case of $D = 1$ and $N_s = 1$, and Eq. (6.15) in the case of $D = 2$ and $N_s = 2$.

The ignorance of the factors $e^{\pm i\omega_{i1}\epsilon}$ alters the behavior of $\tilde{G}_0^{(2)}(P_1)$ at $|\omega_{i1}| \rightarrow \infty$. Thus, one may concern that this ignorance of these factors affects the calculation in the flow equation. These factors, however, can be ignored in the flow equation because ϵ' appearing in the flow equation (4.23) cancels the effect of these factors.

As an example illustrating how the effect of $e^{\pm i\omega_{i1}\epsilon}$ vanishes, let us see the calculation the exchange energy of the 2DHEG, whose expression is given in Eq. (6.6). With keeping the factor $e^{\pm i\omega_{i1}\epsilon}$, Eq. (6.6) reads

$$\begin{aligned} \frac{E_{\text{ex}}}{N} &= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{\omega_i}^{\epsilon'} \tilde{G}_0^{(2)}(P) - n \right) \\ &= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(\int_{\omega_i}^{\epsilon'} 2 \int_{\mathbf{p}} \theta(-\xi(\mathbf{p})) \right. \\ &\quad \times \left(\frac{e^{-i\omega_{i1}\epsilon}}{i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} + \frac{e^{i\omega_{i1}\epsilon}}{-i\omega_{i1} + \xi(\mathbf{p} + \mathbf{p}_1) - \xi(\mathbf{p})} \right) - n \Big) \\ &= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \right. \\ &\quad \times \int_{-\infty}^{\infty} \frac{d\omega_i}{2\pi} e^{i\omega_i \epsilon'} \left(\frac{e^{-i\omega_{i1}\epsilon}}{i\omega_{i1} + \xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')} + \frac{e^{i\omega_{i1}\epsilon}}{-i\omega_{i1} + \xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')} \right) - n \Big). \end{aligned} \quad (\text{B.6})$$

I remind that ϵ' is a positive infinitesimal satisfying $\epsilon' > \epsilon$. The convergence of the integrand of the ω_i -integral at $|\omega_i| \rightarrow \infty$ is dominated by $e^{i\omega_i \epsilon'}$, and does not depend

on the presence of $e^{\pm i\omega_{i1}\epsilon}$ since $\epsilon' > \epsilon$. Therefore, one gets the same result if one uses ϵ -independent expression Eq. (B.5) from the beginning.

B.1.2 Derivation of Eq. (6.9)

To confirm our expression for $\tilde{G}_0^{(2)}(P_1)$ reproduces the exchange energy of 2DHEG Eq. (6.9), let us continue the calculation.

With ignoring $e^{\pm i\omega_{i1}\epsilon}$ in Eq. (B.6), one has

$$\begin{aligned}
\frac{E_{\text{ex}}}{N} &= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \right. \\
&\quad \times \left. \int_{-\infty}^{\infty} \frac{d\omega_i}{2\pi} e^{i\omega_i \epsilon'} \left(\frac{1}{i\omega_{i1} + \xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')} + \frac{1}{-i\omega_{i1} + \xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')} \right) - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \right. \\
&\quad \times \left. \int_{C_1} \frac{d\omega_i}{2\pi i} e^{i\omega_i \epsilon'} \left(\frac{1}{\omega_{i1} - i\xi(\mathbf{p}' + \mathbf{p}) + i\xi(\mathbf{p}')} - \frac{1}{\omega_{i1} + i\xi(\mathbf{p}' + \mathbf{p}) - i\xi(\mathbf{p}')} \right) - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) [\theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}) + \xi(\mathbf{p}'))] - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} [\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) \right. \\
&\quad \left. - \theta(-\xi(\mathbf{p}'))\theta(-\xi(\mathbf{p}' + \mathbf{p}) + \xi(\mathbf{p}'))] - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} [\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) \right. \\
&\quad \left. - \theta(-\xi(\mathbf{p}' - \mathbf{p}))\theta(-\xi(\mathbf{p}') + \xi(\mathbf{p}' - \mathbf{p}))] - n \right).
\end{aligned}$$

In the last equality, $\mathbf{p}'$ has been shifted to $\mathbf{p}' - \mathbf{p}$ in the second term in the integrand of $\mathbf{p}'$ -integral. With changing $\mathbf{p}$ to $-\mathbf{p}$ and using $\xi(\mathbf{p}) = \xi(-\mathbf{p})$, one has

$$\begin{aligned}
&\frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} [\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) \right. \\
&\quad \left. - \theta(-\xi(\mathbf{p}' - \mathbf{p}))\theta(-\xi(\mathbf{p}') + \xi(\mathbf{p}' - \mathbf{p}))] - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} [\theta(-\xi(\mathbf{p}')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}))] \theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \\
&\quad \times \left(2 \int_{\mathbf{p}'} [\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p})) - \theta(\xi(\mathbf{p}'))\theta(-\xi(\mathbf{p}' + \mathbf{p}))] \theta(\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}')) - n \right) \\
&= \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p})) - n \right).
\end{aligned}$$

In the second equality, the following formula has been used:

$$\theta(x) - \theta(y) = \theta(x)\theta(-y) - \theta(-x)\theta(y).$$

By use of $\theta(\xi(\mathbf{p}' + \mathbf{p})) = 1 - \theta(-\xi(\mathbf{p}' + \mathbf{p}))$ and $2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) = n$, one has

$$\begin{aligned} & \frac{1}{2n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \left(2 \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \theta(\xi(\mathbf{p}' + \mathbf{p})) - n \right) \\ &= -\frac{1}{n} \int_{\mathbf{p}} \tilde{U}(\mathbf{p}) \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \theta(-\xi(\mathbf{p}' + \mathbf{p})) = -\frac{1}{n} \int_{\mathbf{p}, \mathbf{p}'} \theta(-\xi(\mathbf{p}')) \theta(-\xi(\mathbf{p})) \tilde{U}(\mathbf{p} - \mathbf{p}') \\ &= -\frac{1}{n} \int_{\mathbf{p}, \mathbf{p}'} \theta(-\xi(\mathbf{p}')) \theta(-\xi(\mathbf{p})) \int_{\mathbf{x}} \frac{e^{-i(\mathbf{p}-\mathbf{p}') \cdot \mathbf{x}}}{|\mathbf{x}|} = -\frac{1}{n} \int_{\mathbf{x}} \frac{1}{|\mathbf{x}|} \left| \int_{\mathbf{p}} \theta(-\xi(\mathbf{p})) e^{-i\mathbf{p} \cdot \mathbf{x}} \right|^2 \\ &= -\frac{1}{(2\pi)^4 n} \int_{\mathbf{x}} \frac{1}{|\mathbf{x}|} \left| \int_0^{2\pi} d\phi \int_0^{p_F} dp p e^{-ip|\mathbf{x}| \cos \phi} \right|^2 \\ &= -\frac{1}{(2\pi)^2 n} \int_{\mathbf{x}} \frac{1}{|\mathbf{x}|} \left| \int_0^{p_F} dp p J_0(p|\mathbf{x}|) \right|^2 = -\frac{1}{(2\pi)^2 n} \int_{\mathbf{x}} \frac{1}{|\mathbf{x}|} \left| \frac{1}{|\mathbf{x}|^2} \int_0^{p_F |\mathbf{x}|} da \frac{d}{da} (a J_1(a)) \right|^2 \\ &= -\frac{p_F^2}{(2\pi)^2 n} \int_{\mathbf{x}} \frac{J_1(p_F |\mathbf{x}|)^2}{|\mathbf{x}|^3} = -\frac{p_F^3}{2\pi n} \int_0^\infty dz \frac{J_1(z)^2}{z^2} = -\frac{\sqrt{2}}{r_s} \int_0^\infty dz \frac{J_1(z)^2}{z^2}, \end{aligned}$$

where $p_F = \sqrt{2\mu_0}$ is the Fermi momentum, $r_s = 1/\sqrt{\pi n} = \sqrt{2}/p_F$ is the Wigner-Seitz radius, and $J_n(x)$ is the Bessel function of the first kind. The integral in the last expression is evaluated as follows [91]:

$$\int_0^\infty dz \frac{J_1(z)^2}{z^2} = \frac{\frac{1}{2} \Gamma(2) \Gamma\left(\frac{1}{2} + \frac{1}{2} + \frac{1}{2} - 1\right)}{2 \Gamma\left(\frac{1}{2} + \frac{1}{2} - \frac{1}{2} + 1\right) \Gamma\left(\frac{1}{2} + \frac{1}{2} + \frac{1}{2} + 1\right) \Gamma\left(\frac{1}{2} + \frac{1}{2} - \frac{1}{2} + 1\right)} = \frac{4}{3\pi},$$

where $\Gamma(x)$ is the gamma function. Finally, one obtains

$$\frac{E_{\text{ex}}}{N} = -\frac{4\sqrt{2}}{3\pi r_s}. \quad (\text{B.7})$$

Therefore, our expression Eq. (B.5) actually reproduces Eq. (6.9).

B.2 Expression for $C_0(P)$

$C_0(P)$ is defined as follows:

$$C_\lambda(P) = -\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \left(\tilde{G}_\lambda^{(4)}(P', -P', P) - \frac{\tilde{G}_\lambda^{(3)}(P', -P') \tilde{G}_\lambda^{(3)}(P, -P)}{\tilde{G}_\lambda^{(2)}(0)} \right), \quad (\text{B.8})$$

where $\tilde{U}(\mathbf{p}')$ is the two-body potential in the momentum representation, and $\int_{P'}^{\epsilon'} = \int_{P'} e^{i\omega' \epsilon'}$ with a positive infinitesimal ϵ' satisfying $\epsilon' > \epsilon$. Here, the density correlation functions with vanishing frequency and momentum should be interpreted as the p limit as I noted below Eq. (5.19). I derive the expression for $C_0(P)$ giving Eqs. (5.27) and (6.15). Our expressions actually satisfy $c_0 = 1$ for c_λ given by Eq. (5.21) is also checked.

B.2.1 Derivation of $C_0(P)$

First, let us calculate $\tilde{G}_0^{(2)}(0)$ appearing in Eq. (B.8). From Eq. (B.5), one has

$$\begin{aligned}
\tilde{G}_0^{(2)}(0) &= \lim_{\mathbf{p}_1 \rightarrow 0} \tilde{G}_0^{(2)}(0, \mathbf{p}_1) = N_s \lim_{\mathbf{p}_1 \rightarrow 0} \int_{\mathbf{p}} \frac{2\theta(-\xi(\mathbf{p}))}{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})} \\
&= N_s \lim_{\mathbf{p}_1 \rightarrow 0} \int_{\mathbf{p}} \left(\frac{\theta(-\xi(\mathbf{p}))}{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})} + \frac{\theta(-\xi(\mathbf{p}))}{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})} \right) \\
&= N_s \lim_{\mathbf{p}_1 \rightarrow 0} \int_{\mathbf{p}} \left(\frac{\theta(-\xi(\mathbf{p}))}{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})} + \frac{\theta(-\xi(\mathbf{p} - \mathbf{p}_1))}{\xi(\mathbf{p}) - \xi(\mathbf{p} - \mathbf{p}_1)} \right) \\
&= -N_s \lim_{\mathbf{p}_1 \rightarrow 0} \int_{\mathbf{p}} \frac{\theta(-\xi(\mathbf{p} + \mathbf{p}_1)) - \theta(-\xi(\mathbf{p}))}{\xi(\mathbf{p}_1 + \mathbf{p}) - \xi(\mathbf{p})} \\
&= N_s \int_{\mathbf{p}} \delta(\xi(\mathbf{p})). \tag{B.9}
\end{aligned}$$

Next, I calculate $\tilde{G}_0^{(3)}(P, -P)$. From Eq. (B.1), $\tilde{G}_0^{(3)}(P_1, P_2)$ reads

$$\begin{aligned}
\tilde{G}_0^{(3)}(P_1, P_2) &= -N_s \int_P \left(\tilde{G}_{F,0}^{(2)}(P) \tilde{G}_{F,0}^{(2)}(P_1 + P) \tilde{G}_{F,0}^{(2)}(P_1 + P_2 + P) \right. \\
&\quad \left. + \tilde{G}_{F,0}^{(2)}(P) \tilde{G}_{F,0}^{(2)}(P_2 + P) \tilde{G}_{F,0}^{(2)}(P_1 + P_2 + P) \right) \\
&= -N_s \int_P \tilde{G}_{F,0}^{(2)}(P) \left(\tilde{G}_{F,0}^{(2)}(P_1 + P) + \tilde{G}_{F,0}^{(2)}(P_2 + P) \right) \tilde{G}_{F,0}^{(2)}(P_1 + P_2 + P).
\end{aligned}$$

Therefore, one has

$$\begin{aligned}
\tilde{G}_0^{(3)}(P, -P) &= \tilde{G}_0^{(3)}(0, P) = \lim_{\mathbf{q} \rightarrow 0} \tilde{G}_0^{(3)}((0, \mathbf{q}), P) \\
&= -N_s \lim_{\mathbf{q} \rightarrow 0} \int_{P'} \tilde{G}_{F,0}^{(2)}(P') \left(\tilde{G}_{F,0}^{(2)}((0, \mathbf{q}) + P') + \tilde{G}_{F,0}^{(2)}(P + P') \right) \\
&\quad \times \tilde{G}_{F,0}^{(2)}((0, \mathbf{q}) + P + P') \\
&= -N_s \lim_{\mathbf{q} \rightarrow 0} \int_{P'} \left(\tilde{G}_{F,0}^{(2)}(P' - (0, \mathbf{q})) \tilde{G}_{F,0}^{(2)}(P') \tilde{G}_{F,0}^{(2)}(P + P') \right. \\
&\quad \left. - \tilde{G}_{F,0}^{(2)}(P' - P) \tilde{G}_{F,0}^{(2)}(P') \tilde{G}_{F,0}^{(2)}((0, \mathbf{q}) + P') \right) \\
&= -N_s \lim_{\mathbf{q} \rightarrow 0} \int_{P'} \int_{-\infty}^{\infty} \frac{d\omega'_i}{2\pi} \left(\frac{e^{i\omega'_i \epsilon}}{i\omega'_i - \xi(\mathbf{p}' - \mathbf{q})} \frac{e^{i(\omega'_i + \omega_i)\epsilon}}{i\omega'_i + i\omega_i - \xi(\mathbf{p}' + \mathbf{p})} \frac{e^{i\omega'_i \epsilon}}{i\omega'_i - \xi(\mathbf{p}')} \right. \\
&\quad \left. - \frac{e^{i\omega'_i \epsilon}}{i\omega'_i - \xi(\mathbf{p}' + \mathbf{q})} \frac{e^{i(\omega'_i - \omega_i)\epsilon}}{i\omega'_i - i\omega_i - \xi(\mathbf{p}' - \mathbf{p})} \frac{e^{i\omega'_i \epsilon}}{i\omega'_i - \xi(\mathbf{p}')} \right) \\
&= N_s \lim_{\mathbf{q} \rightarrow 0} \int_{P'} \int_{C_1} \frac{d\omega'_i}{2\pi i} e^{3i\omega'_i \epsilon} \left(\frac{1}{\omega'_i + i\xi(\mathbf{p}' - \mathbf{q})} \frac{e^{i\omega_i \epsilon}}{\omega'_i + \omega_i + i\xi(\mathbf{p}' + \mathbf{p})} \frac{1}{\omega'_i + i\xi(\mathbf{p}')} \right. \\
&\quad \left. - \frac{1}{\omega'_i + i\xi(\mathbf{p}' + \mathbf{q})} \frac{e^{-i\omega_i \epsilon}}{\omega'_i - \omega_i + i\xi(\mathbf{p}' - \mathbf{p})} \frac{1}{\omega'_i + i\xi(\mathbf{p}')} \right).
\end{aligned}$$

With performing the ω'_i -integral and straightforward but complicated calculation, one has

$$\begin{aligned}
\tilde{G}_0^{(3)}(P, -P) &= iN_s \lim_{q \rightarrow 0} \int_{\mathbf{p}'} \frac{\theta(-\xi(\mathbf{p}' + \mathbf{q})) - \theta(-\xi(\mathbf{p}'))}{\xi(\mathbf{p}' + \mathbf{q}) - \xi(\mathbf{p}')} \\
&\quad \times \left[\frac{1}{\omega_i - i(\xi(\mathbf{p}') - \xi(\mathbf{p}' + \mathbf{p}))} - \frac{1}{\omega_i + i(\xi(\mathbf{p}') - \xi(\mathbf{p}' + \mathbf{p}))} \right] \\
&= -iN_s \int_{\mathbf{p}'} \delta(\xi(\mathbf{p}')) \\
&\quad \times \left[\frac{1}{\omega_i - i(\xi(\mathbf{p}') - \xi(\mathbf{p}' + \mathbf{p}))} - \frac{1}{\omega_i + i(\xi(\mathbf{p}') - \xi(\mathbf{p}' + \mathbf{p}))} \right] \\
&= -iN_s \int_{\mathbf{p}'} \delta(\xi(\mathbf{p}')) \left[\frac{1}{\omega_i + i\xi(\mathbf{p}' + \mathbf{p})} - \frac{1}{\omega_i - i\xi(\mathbf{p}' + \mathbf{p})} \right].
\end{aligned}$$

To evaluate the integral of the term containing $\tilde{G}_0^{(3)}$ in Eq. (B.8), I consider the following integral:

$$\begin{aligned}
\int_{\omega'_i}^{\epsilon'} \tilde{G}_0^{(3)}(P', -P') &= \int_{-\infty}^{\infty} \frac{d\omega'_i}{2\pi} e^{i\omega'_i \epsilon'} \tilde{G}_0^{(3)}(P', -P') \\
&= N_s \int_{-\infty}^{\infty} \frac{d\omega'_i}{2\pi i} e^{i\omega'_i \epsilon'} \int_{\mathbf{p}''} \delta(\xi(\mathbf{p}'')) \left[\frac{1}{\omega'_i + i\xi(\mathbf{p}'' + \mathbf{p}')} - \frac{1}{\omega'_i - i\xi(\mathbf{p}'' + \mathbf{p}')} \right] \\
&= N_s \int_{\mathbf{p}''} \delta(\xi(\mathbf{p}'')) [\theta(-\xi(\mathbf{p}'' + \mathbf{p}')) - \theta(\xi(\mathbf{p}'' + \mathbf{p}'))] \\
&= -N_s \int_{\mathbf{p}''} \delta(\xi(\mathbf{p}'')) \text{sgn}(\xi(\mathbf{p}'' + \mathbf{p}')),
\end{aligned}$$

where

$$\text{sgn}(x) = \begin{cases} 1 & (x > 0) \\ 0 & (x = 0) \\ -1 & (x < 0) \end{cases}.$$

Therefore, the integral of the term containing $\tilde{G}_0^{(3)}$ in Eq. (B.8) reads

$$\begin{aligned}
&\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \frac{\tilde{G}_\lambda^{(3)}(P', -P') \tilde{G}_\lambda^{(3)}(P, -P)}{\tilde{G}_\lambda^{(2)}(0)} \\
&= -\frac{N_s}{\int_{\mathbf{q}} \delta(\xi(\mathbf{q}))} \int_{\mathbf{p}'', \mathbf{p}'''} \left[\int_{\mathbf{p}'} \tilde{U}(\mathbf{p}') \frac{\text{sgn}(\xi(\mathbf{p}''' + \mathbf{p}')) \delta(\xi(\mathbf{p}'')) \delta(\xi(\mathbf{p}''')) (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))}{\omega_i^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))^2} \right].
\end{aligned} \tag{B.10}$$

In this expression, one can substitute $\text{sgn}(\mathbf{p}''' + \mathbf{p}')$ to $\text{sgn}(p_F \mathbf{e} + \mathbf{p}')$, where $\mathbf{e}$ is a constant unit vector, because the norm of $\mathbf{p}'''$ is fixed to p_F by the factor $\delta(\xi(\mathbf{p}'''))$ and

the quantity in the square bracket does not depend on the direction of $\mathbf{p}'''$ since the difference of the direction of $\mathbf{p}'''$ is absorbed by the reselect of the coordinate of $\mathbf{p}'$. Applying this substitution, one has

$$\begin{aligned} & \frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \frac{\tilde{G}_\lambda^{(3)}(P', -P') \tilde{G}_\lambda^{(3)}(P, -P)}{\tilde{G}_\lambda^{(2)}(0)} \\ &= -N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \frac{\text{sgn}(\xi(p_F \mathbf{e} + \mathbf{p}')) \delta(\xi(\mathbf{p}'')) (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))}{\omega_i^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))^2}. \end{aligned} \quad (\text{B.11})$$

Let us evaluate the integral of the term containing $\tilde{G}_0^{(4)}$ in Eq. (B.8). Since the calculation is straightforward but very complicated, the outline of the calculation is briefly presented. From Eq. (B.1), one has

$$\begin{aligned} & -\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \tilde{G}_0^{(4)}(P', -P', P) \\ &= \frac{N_s}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} \\ & \times \left[G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P) \right. \\ & + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' - P) \\ & + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' + P) G_{F,0}^{(2)}(P'' + P) \\ & + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' + P) G_{F,0}^{(2)}(P'' + P') \\ & + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' - P) G_{F,0}^{(2)}(P'' - P) \\ & \left. + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' - P) G_{F,0}^{(2)}(P'' + P') \right] \\ &= \frac{N_s}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} \\ & \times \left[G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' + P) G_{F,0}^{(2)}(P'' + P) \right. \\ & + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' - P) G_{F,0}^{(2)}(P'' - P) \\ & + G_{F,0}^{(2)}(P'')^2 G_{F,0}^{(2)}(P'' + P') \left(G_{F,0}^{(2)}(P'' + P) + G_{F,0}^{(2)}(P'' - P) \right) \\ & \left. + G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P')^2 \left(G_{F,0}^{(2)}(P'' + P' + P) + G_{F,0}^{(2)}(P'' + P' - P) \right) \right] \\ &= N_s \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' + P) G_{F,0}^{(2)}(P'' + P) \\ & + \frac{N_s}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} G_{F,0}^{(2)}(P'')^2 \\ & \times \left(G_{F,0}^{(2)}(P'' + P') + G_{F,0}^{(2)}(P'' - P') \right) \left(G_{F,0}^{(2)}(P'' + P) + G_{F,0}^{(2)}(P'' - P) \right). \end{aligned} \quad (\text{B.12})$$

Performing the frequency integrals, one has following expression for the first term of Eq. (B.12):

$$\begin{aligned}
& N_s \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} G_{F,0}^{(2)}(P'') G_{F,0}^{(2)}(P'' + P') G_{F,0}^{(2)}(P'' + P' + P) G_{F,0}^{(2)}(P'' + P) \\
&= -2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
&\quad \times \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2)(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)}. \quad (\text{B.13})
\end{aligned}$$

In the second term of Eq. (B.12), one meets an contour integral with a pole of second order given by $G_{F,0}^{(2)}(P'')^2$, which should be treated carefully. In order to show how such a contour integral is treated, I consider the following simple integral:

$$\int_{C_1} \frac{d\omega_i}{2\pi i} f(\omega_i) \frac{e^{i\omega_i \epsilon}}{(\omega_i + i\xi)^2},$$

where $\xi \in \mathbb{R}$ and $f(\omega_i)$ is a complex function regular in the upper-half plane of ω_i . In the case of $\xi \neq 0$, this integral gives $f'(-i\xi)\theta(-\xi)$. In the case of $\xi = 0$, however, this integral diverges unless $f(0) = 0$ since the pole $\omega_i = 0$ resides on the contour C_1 . The contribution from such a divergence is evaluated as follows:

$$\begin{aligned}
\int_{C_1} \frac{d\omega_i}{2\pi i} f(\omega_i) \frac{e^{i\omega_i \epsilon}}{(\omega_i + i\xi)^2} &= i \frac{d}{d\xi} \int_{C_1} \frac{d\omega_i}{2\pi i} f(\omega_i) \frac{e^{i\omega_i \epsilon}}{\omega_i + i\xi} = i \frac{d}{d\xi} (f(-i\xi)\theta(-\xi)) \\
&= f'(-i\xi)\theta(-\xi) - i f(-i\xi)\delta(\xi).
\end{aligned}$$

As illustrated in this demonstration, the contour integral involving $G_{F,0}^{(2)}(P'')^2$ yields terms with $\theta'(x) = \delta(x)$. With taking this into account, the second term of Eq. (B.12) is evaluated as follows:

$$\begin{aligned}
& \frac{N_s}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \int_{P''} G_{F,0}^{(2)}(P'')^2 \\
&\quad \times \left(G_{F,0}^{(2)}(P'' + P') + G_{F,0}^{(2)}(P'' - P') \right) \left(G_{F,0}^{(2)}(P'' + P) + G_{F,0}^{(2)}(P'' - P) \right) \\
&= N_s \int_{\mathbf{p}', \mathbf{p}''} U(\mathbf{p}') \text{sgn}(-\xi(\mathbf{p}' + \mathbf{p}'')) \delta(\xi(\mathbf{p}'')) \frac{\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p})}{\omega^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))^2} \\
&\quad + 2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
&\quad \times \frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2}. \quad (\text{B.14})
\end{aligned}$$

In this expression, $\text{sgn}(-\xi(\mathbf{p}' + \mathbf{p}''))$ can be substituted for $\text{sgn}(-\xi(\mathbf{p}' + p_F \mathbf{e}))$ with a constant unit vector $\mathbf{e}$ for the same reason as the derivation of Eq. (B.11). Therefore,

from Eqs. (B.13) and (B.14) one has

$$\begin{aligned}
& -\frac{1}{2} \int_{P'}^{\epsilon'} \tilde{U}(\mathbf{p}') \tilde{G}_0^{(4)}(P', -P', P) \\
& = N_s \int_{\mathbf{p}', \mathbf{p}''} U(\mathbf{p}') \text{sgn}(-\xi(\mathbf{p}' + p_F \mathbf{e})) \delta(\xi(\mathbf{p}'')) \frac{\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p})}{\omega^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' + \mathbf{p}))^2} \\
& + 2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2} \\
& - 2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}')) (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2) (\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)}. \tag{B.15}
\end{aligned}$$

The term including the delta function and Eq. (B.11) cancels each other. Therefore, one finally obtains

$$\begin{aligned}
C_0(P) = & 2N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \left[\frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2} \right. \\
& \left. - \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}')) (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2) (\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)} \right], \tag{B.16}
\end{aligned}$$

which coincides with Eq. (5.27) in the case of $D = 1$ and $N_s = 1$, and Eq. (6.16) in the case of $D = 2$ and $N_s = 2$.

B.2.2 Proof of $c_0 = 1$

I check that c_λ defined by Eq. (5.21) actually satisfies $c_0 = 1$ by use of our expressions Eqs. (B.5) and (B.16).

First, let us evaluate the frequency integral of Eq. (B.16). For convenience, I deform

Eq. (B.16) as follows:

$$\begin{aligned}
C_0(P) = & N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'')) (\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \left[\frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2} \right. \\
& \left. - \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2)(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)} \right] \\
& + N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \theta(-\xi(\mathbf{p}'' - \mathbf{p})) (\theta(-\xi(\mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(-\mathbf{p} + \mathbf{p}' + \mathbf{p}''))) \\
& \times \left[\frac{(\xi(\mathbf{p}'') - \xi(\mathbf{p}'' - \mathbf{p}))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' - \mathbf{p}))^2)^2} \right. \\
& \left. - \frac{(\xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}' - \mathbf{p}))(\xi(\mathbf{p}'') - \xi(\mathbf{p}'' - \mathbf{p})) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}' - \mathbf{p}))^2)(\omega_i^2 + (\xi(\mathbf{p}'') - \xi(\mathbf{p}'' - \mathbf{p}))^2)} \right] \\
= & - N_s \int_{\mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \\
& \times (\theta(-\xi(\mathbf{p}'' + \mathbf{p})) - \theta(-\xi(\mathbf{p}'')))(\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \left[\frac{(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2 - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)^2} \right. \\
& \left. - \frac{(\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \omega_i^2}{(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}'))^2)(\omega_i^2 + (\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}''))^2)} \right].
\end{aligned}$$

By use of this expression, one has

$$\begin{aligned}
& \int_P^{\epsilon'} C_0(P) \\
= & N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \\
& \times (\theta(-\xi(\mathbf{p}'' + \mathbf{p})) - \theta(-\xi(\mathbf{p}'')))(\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) \\
& \times \left[\delta(\xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'')) - \frac{\theta(-\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') + \xi(\mathbf{p}'' + \mathbf{p}')) - \theta(-\xi(\mathbf{p}'' + \mathbf{p}) + \xi(\mathbf{p}''))}{\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}) + \xi(\mathbf{p}'')} \right] \\
= & N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \left[- \frac{(\theta(-\xi(\mathbf{p}'' + \mathbf{p})) - \theta(-\xi(\mathbf{p}'')))(\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')))(\theta(\xi(\mathbf{p}' + \mathbf{p}''))) }{\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}) + \xi(\mathbf{p}'')} \right. \\
& \left. + \frac{\theta(-\xi(\mathbf{p}'' + \mathbf{p}))\theta(\xi(\mathbf{p}''))(\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}''))) }{\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}) + \xi(\mathbf{p}'')} \right] \\
= & - 2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}') \frac{(\theta(-\xi(\mathbf{p}'' + \mathbf{p})) - \theta(-\xi(\mathbf{p}'')))(\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}'')))(\theta(\xi(\mathbf{p}' + \mathbf{p}''))) }{\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}) + \xi(\mathbf{p}'')}.
\end{aligned}$$

where $(\theta(a) - \theta(b))\delta(a - b) = 0$ and $(\theta(a) - \theta(b))\theta(a - b) = \theta(a)\theta(-b)$ have been used.

By exchanging $\mathbf{p}$ and $\mathbf{p}'$, one has

$$\begin{aligned}
& \int_P^{\epsilon'} C_0(P) \\
&= -2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{(\theta(-\xi(\mathbf{p}'' + \mathbf{p}')) - \theta(-\xi(\mathbf{p}'')))\theta(-\xi(\mathbf{p} + \mathbf{p}' + \mathbf{p}''))\theta(\xi(\mathbf{p} + \mathbf{p}''))}{\xi(\mathbf{p}'' + \mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'' + \mathbf{p}) - \xi(\mathbf{p}'' + \mathbf{p}') + \xi(\mathbf{p}'')} \\
&= 2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{(\theta(-\xi(\mathbf{p}' + \mathbf{p})) - \theta(-\xi(\mathbf{p}'')))\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p} + \mathbf{p}''))}{\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}') + \xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')} \\
&= -2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{\theta(\xi(\mathbf{p}' + \mathbf{p}))\theta(-\xi(\mathbf{p}''))\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p} + \mathbf{p}''))}{\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}') + \xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')} \\
&\quad + 2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{\theta(-\xi(\mathbf{p}' + \mathbf{p}))\theta(\xi(\mathbf{p}''))\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p} + \mathbf{p}''))}{\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}') + \xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')}.
\end{aligned}$$

The second term vanishes since the overall sign changes with the changes of variables $\mathbf{p}'$ to $\mathbf{p}' - \mathbf{p}$ and $\mathbf{p}''$ to $\mathbf{p}'' - \mathbf{p}$. Therefore, one has

$$\int_P^{\epsilon'} C_0(P) = -2N_s \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{\theta(\xi(\mathbf{p}' + \mathbf{p}))\theta(-\xi(\mathbf{p}''))\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p} + \mathbf{p}''))}{\xi(\mathbf{p}' + \mathbf{p}) - \xi(\mathbf{p}') + \xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')}. \quad (\text{B.17})$$

Next, I calculate $\int_P^{\epsilon'} \tilde{U}(\mathbf{p}) \tilde{G}_0^{(2)}(P)^2$. From Eq. (B.5), one has

$$\begin{aligned}
& \int_P^{\epsilon'} \tilde{U}(\mathbf{p}) \tilde{G}_0^{(2)}(P)^2 \\
&= \int_P^{\epsilon'} \tilde{U}(\mathbf{p}) \left(2N_s \int_{\mathbf{p}'} \theta(-\xi(\mathbf{p}')) \frac{\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')}{\omega_1^2 + (\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'))^2} \right)^2 \\
&= \int_P^{\epsilon'} \tilde{U}(\mathbf{p}) \left(N_s \int_{\mathbf{p}'} |\theta(-\xi(\mathbf{p}')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}))| \frac{|\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')|}{\omega_1^2 + (\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'))^2} \right)^2 \\
&= N_s^2 \int_P^{\epsilon'} \tilde{U}(\mathbf{p}) \int_{\mathbf{p}', \mathbf{p}''} |\theta(-\xi(\mathbf{p}')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}))| |\theta(-\xi(\mathbf{p}'')) - \theta(-\xi(\mathbf{p}'' + \mathbf{p}))| \\
&\quad \times \frac{|\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')| |\xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')|}{[\omega_1^2 + (\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}'))^2][\omega_1^2 + (\xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}''))^2]} \\
&= -\frac{N_s^2}{2} \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{|\theta(-\xi(\mathbf{p}')) - \theta(-\xi(\mathbf{p}' + \mathbf{p}))| |\theta(-\xi(\mathbf{p}'')) - \theta(-\xi(\mathbf{p}'' + \mathbf{p}))|}{|\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')| + |\xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')|} \\
&= -\frac{N_s^2}{2} \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{1}{|\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}')| + |\xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')|} \\
&\quad \times (\theta(-\xi(\mathbf{p}'))\theta(\xi(\mathbf{p}' + \mathbf{p})) + \theta(\xi(\mathbf{p}'))\theta(-\xi(\mathbf{p}' + \mathbf{p}))) \\
&\quad \times (\theta(-\xi(\mathbf{p}''))\theta(\xi(\mathbf{p}'' + \mathbf{p})) + \theta(\xi(\mathbf{p}''))\theta(-\xi(\mathbf{p}'' + \mathbf{p}))) \\
&= -2N_s^2 \int_{\mathbf{p}, \mathbf{p}', \mathbf{p}''} \tilde{U}(\mathbf{p}) \frac{\theta(\xi(\mathbf{p}' + \mathbf{p}))\theta(-\xi(\mathbf{p}'))\theta(-\xi(\mathbf{p}''))\theta(\xi(\mathbf{p}'' + \mathbf{p}))}{\xi(\mathbf{p} + \mathbf{p}') - \xi(\mathbf{p}') + \xi(\mathbf{p} + \mathbf{p}'') - \xi(\mathbf{p}'')}.
\end{aligned}$$

This is identical with Eq (B.17) in the case of $N_s = 1$.

Therefore, one has $c_0 = 1$ in the case of spinless fermions.

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