Density Renormalization Group for Classical Liquids 1
- Formulation -

Satoshi Iso\textsuperscript{a,b}\textsuperscript{*} and Kiyoharu Kawana\textsuperscript{a}\textsuperscript{†}

\textsuperscript{a}Theory Center, High Energy Accelerator Research Organization (KEK),
\textsuperscript{b}Graduate University for Advanced Studies (SOKENDAI),

Tsukuba, Ibaraki 305-0801, Japan

August 29, 2018

Abstract

Equation of state for gas and liquid gives the relation between pressure and density; and pressure can be calculated from correlation functions. Thus thermodynamical behaviors of liquid can be investigated by scrutinizing how the correlation functions change as the density of the liquid varies. In the present paper, we study response of liquid to a scale transformation, which generates a change of the liquid density, and obtain a set of (density) differential equations for correlation functions. The set of equations, which we call density renormalization group equations (DRGEs), is similar to the BBGKY hierarchy as it relates different multiple-point correlation functions.

\textsuperscript{*}E-mail: satoshi.iso(at)kek.jp
\textsuperscript{†}E-mail: kawana(at)post.kek.jp
1 Introduction

Thermodynamical properties of gas and liquid are described by the equation of state, and the microscopic derivation is one of the most important issues in the liquid theory. Liquid is microscopically described by a collection of interacting particles and the thermodynamical quantities such as pressure, internal energy, and isothermal compressibility can be calculated from density correlation functions [1, 2].

Statistical mechanics of liquid has a long history. The simplest microscopic study of liquid is the virial expansion method, which gives a systematic expansion around the ideal gas. But its convergence is very slow \(^1\) and the method is limited to low density region. In order to describe high density region of liquid, we need to go beyond the virial expansion and take into account effects of strong multi-point density correlations. For this purpose, various integral equations and their approximations have been studied. The Orstein-Zernike equation, which is an integral equation for two-point correlation functions (see Eq. (81)), is often used and various approximations such as the Percus-Yevick approximation [1, 5, 6, 7, 8] or the Hyper-Netted chain approximation [9, 10, 11, 12, 13] are proposed. Another type of integral equations is the BBGKY hierarchy [14, 15, 16, 17, 18], which is a set of integral equations relating different multi-point correlation functions. Thus, in order to solve them, we need to cut the chain of equations at some orders. In the Kirkwood’s superposition approximation [16, 17, 19, 20], 3-point correlation function is assumed to be expressed in terms of a product of 2-point correlation functions so that the hierarchical equations are closed. As explained above, there are various different equations and approximations, but it is not clear when they are justified. No systematic methods to improve these approximations are known. (See [1, 2] and references therein for more details.)

The situation reminds us of the renormalization group (RG) in quantum field theories (QFT): understanding the energy dependence of physical quantities in QFT. Just as an effective coupling varies as a function of the energy scale (i.e. renormalization scale) in QFT, pressure changes as a function of liquid density in liquid theory. In both theories, physical quantities are calculated from correlation functions. Thus we can infer the following analogies between classical liquid theories and quantum field theories:

- Helmholtz free energy \(\leftrightarrow\) Effective potential \(\Gamma\)
- Equation of state \(\leftrightarrow\) RG improved equation of motion for \(\Gamma\)
- Pressure, compressibility, etc. \(\leftrightarrow\) Running couplings

\(^1\) For example, in the case of the hard-sphere potential, the virial expansion becomes [3]

\[
\frac{p}{nT} = 1 + 4\eta + 10\eta^2 + 18.36\eta^3 + 28.22\eta^4 + \cdots ,
\]

where \(\eta\) is the packing fraction defined by \(\eta = \frac{4\pi}{3}\frac{N}{V} = n \times V_p\). For example, setting \(\eta = 0.3\), the contribution of the fifth term is as large as \(\sim 30/80 \sim 0.37\).
• Density $\leftrightarrow$ Renormalization scale $\mu$

Such analogies between statistical mechanics and quantum field theories have been occasionally pointed out, but our present study is strongly stimulated by Nambu’s seminar paper [21] in which an analogy between the renormalization group (RG) equation in gauge theories and thermodynamic equation of state was discussed. (See also [22, 23, 24] and the references therein where the ordinary concept of the RG is applied in the classical liquid/vapor system.)

The purpose of the present paper is to make the analogy more concrete and to propose a set of (density) differential equations for correlation functions by studying response of the liquid to a scale transformation. Since a scale transformation generates a change of liquid density, the resultant equations describe response of correlation functions to a small change of density; thus we call them density renormalization group equations (DRGEs). The physical meaning of DRGEs are the following. In (classical) gas and liquid, when its density is low, the system is well described by the ideal gas, and the density correlation functions are exactly calculated (see Appendix A). As the density increases, correlation functions start to behave nontrivially due to two different reasons. One is, of course, a direct consequence of intermolecular (2-body) potential between particles. This causes a nontrivial behavior for the 2-point density correlation function. But there is another effect. Nontrivial (multi-) correlation (more than 2-point functions) will appear due to finite density effects. Namely, e.g. density fluctuations at 3 different points get correlated mediated by finite density effect at a single point in the middle. This effect becomes stronger in higher density liquid and also when 2-point correlation becomes stronger. Therefore, if we can resum (or accumulate) these effects from low to high density, we will be able to describe the dynamics of high density liquid by solving DRGEs.

The paper is organized as follows. In Section 2, we first briefly review the statistical mechanics of classically interacting particles and then study how a partition function of such a system responds to a scale transformation. In this way, we derive a set of partial differential equations for correlation functions. In Section 3, by using a field theoretical method by Hubbard and Schofield, we calculate perturbative corrections to correlation functions by a small change of density and obtain explicit forms of the density renormalization group equations (DRGEs). We also briefly mention how we can solve the DRGEs to obtain thermodynamical behaviors of liquid. Details are left for future investigations. In Section 4, we perform Legendre transformations to obtain the Helmholtz free energy and derive another type of DRGEs. The Helmholtz free energy generate 1PI diagrams; thus the correlation functions generated by the Helmholtz free energy correspond to the 1PI vertices in QFT. Section 5 is devoted to summary and discussion.
2 Response to Scale Transformations

In this section, we investigate how classical liquid (or gas), i.e. a set of classically interacting particles, responds to scale transformations. A scale transformation generates a change of the liquid density and accordingly we can obtain partial differential equations describing how the system changes according to the change of the density. Thus we call them density renormalization group equations (DRGE).[^1]

In section 2.1 we briefly review various properties of classically interacting particles, and then in section 2.2 obtain the DRGEs for density correlation functions.

2.1 Brief review of classically interacting particles

We consider statistical mechanics of $d$-dimensional classically interacting particles whose Hamiltonian is given by

$$
H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j}^{N} v(x_i, x_j) \tag{2}
$$

where $v(x, y)$ represents two-body interactions. In this paper we assume that $v(x, y)$ is a function of the relative distance $v(x, y) = v(|x-y|)$, which reflects the translational symmetry of the system and the absence of polarizations (i.e. simple liquids). Furthermore we neglect many-body interactions for simplicity.

The grand-canonical partition function is given by

$$
\Xi_v[T, \mu, V; U] = \sum_{N=0}^{\infty} \frac{e^{\beta \mu N}}{N!} \left[ \int_V d^d x_1 \int d^d p_1 \cdots \int_V d^d x_N \int d^d p_N \exp \left( -\beta H_N + \beta \sum_{i=1}^{N} U(x_i) \right) \right] = \sum_{N=0}^{\infty} \frac{z(\mu)^N}{N!} \left[ \int_V d^d x_1 \cdots \int_V d^d x_N \exp \left( -\beta \sum_{i<j} v(x_i - x_j) + \beta \sum_{i=1}^{N} U(x_i) \right) \right], \tag{3}
$$

where $\beta = 1/T$ is the inverse temperature and $z(\mu)$ is defined by

$$
z(\mu) = e^{\beta \mu} (2\pi m T)^{d/2}. \tag{4}
$$

We have introduced the external source $U(x)$ for later convenience. By using the density operator

$$
\rho(x) \equiv \sum_{i=1}^{N} \delta^{(d)}(x - x_i), \tag{5}
$$

[^1]: Please do not be confused with the density matrix renormalization group, in which a density matrix of a quantum state is investigated using renormalization group techniques.
the grand-canonical partition function can be rewritten as

$$\Xi_v[T, \mu, V; U] = \sum_{N=0}^{\infty} \frac{z(\mu + v(0)/2)^N}{N!} \left[ \int_V d^dx_1 \cdots \int_V d^dx_N \exp \left( -\frac{\beta}{2} \langle \rho | v | \rho \rangle + \langle \beta U | \rho \rangle \right) \right],$$

(6)

where

$$\langle \rho | v | \rho \rangle \equiv \int dxdy \rho(x)v(x-y)\rho(y),$$

(7)

$$\langle \beta U | \rho \rangle = \beta \int d^dx U(x)\rho(x).$$

(8)

The functional derivatives of the grand potential,

$$-\beta W_v[T, \mu, V; U] = \log \Xi_v[T, \mu, V; U],$$

(9)

with respect to $$\beta U(x)$$ produce correlation functions of the density fluctuation $$\delta\rho(x) = \rho(x) - \langle \rho(x) \rangle$$:

$$F_1(x) \equiv \left. \frac{\delta(-\beta W_v[T, \mu, V; U])}{\delta(\beta U(x))} \right|_{U=0} = \langle \rho(x) \rangle \equiv n,$$

$$F_l(x_1, \cdots, x_l) \equiv \left. \frac{\delta^l(-\beta W_v[T, \mu, V; U])}{\delta(\beta U(x_1)) \cdots \delta(\beta U(x_l))} \right|_{U=0} = \langle \delta\rho(x_1) \cdots \delta\rho(x_l) \rangle \text{ (for } l \geq 2).$$

(10)

Here we assumed that the translational symmetry is not spontaneously broken at $$U(x) = 0$$ and the particle density $$\langle \rho(x) \rangle$$ does not depend on its position $$x$$, which is written as $$n$$. Note that these correlation functions $$F_l$$ correspond to the connected Green functions in the Hubbard’s field theoretic formulation of classical liquids [25].

The correlation functions are related to the thermodynamical quantities such as the isothermal compressibility. In order to see this, we write the density in presence of the external source $$U = \Delta U(x)$$ as $$n(x)$$ and expand $$\Delta n(x) = n(x) - n$$ with respect $$\Delta U(x)$$:

$$\Delta n(x) = \int d^dy \frac{\delta n(x)}{\delta U(y)} \bigg|_{\Delta U=0} \Delta U(y) + \frac{1}{2} \int d^dy \int d^dz \frac{\delta^2 n(x)}{\delta U(y) \delta U(z)} \bigg|_{\Delta U=0} \Delta U(y) \Delta U(z) + \cdots$$

$$= \int d^dy F_2(x,y)\beta \Delta U(y) + \frac{1}{2} \int d^dy \int d^dz F_3(x,y,z)(\beta \Delta U(y))(\beta \Delta U(z)) + \cdots \quad (11)$$

Setting $$\Delta U(x) = \Delta \mu = \text{const}$$, we have

$$\Delta n = \beta \Delta \mu \int d^dy F_2(x,y) + \frac{\beta^2 \Delta \mu^2}{2} \int d^dy \int d^dz F_3(x,y,z) + \cdots,$$

(12)
from which we obtain the following relations between the thermodynamical quantities and integrals of the correlation functions;

\[ \kappa_T \equiv \frac{1}{n} \frac{\partial n}{\partial (\beta \mu)} \bigg|_{T,V} = \frac{1}{n} \int d^d y F_2(x,y), \]  
(13)

\[ \lambda_l \equiv \frac{1}{n} \frac{\partial^2 n}{\partial (\beta \mu)^{l-1}} \bigg|_{T,V} = \frac{1}{n} \int \cdots \prod_i d^d x_i F_l(x_1, \ldots, x_i), \text{ (for } l \geq 3) \]  
(14)

where \( \kappa_T \) is called the “isothermal compressibility” because it can be rewritten as

\[ \kappa_T = T \frac{\partial n}{\partial p} \bigg|_{T,V} \]  
(15)

by using the thermodynamical relations\[3\]. It is an indicator of the response of the fluid density against a small change of the external pressure. The first equation (13) is well known as the “isothermal compressibility equation”. It is usually written as the following form,

\[ \kappa_T = 1 + n \int \left( \frac{1}{n^2} n^{(2)}(x,0) - 1 \right) = 1 + n \int \cd^d x h_2(x,0), \]  
(18)

where the “two-point distribution function” \( n^{(2)}(x,y) \) and the “total correlation function” \( h_2(x,y) \) are defined by

\[ n^{(2)}(x,y) - n^2 \equiv n^2 h_2(x,y) \equiv F_2(x,y) - n \delta^{(d)}(x - y). \]  
(19)

Note that the total correlation function \( h_2(x,y) \) vanishes for the ideal gas (see Appendix A), and therefore \( \kappa_T = 1 \).

We can similarly define the “\( l \)-point distribution function” \( n^{(l)} \), and the “\( l \)-point total correlation function” \( h_l \) for higher \( l \) by

\[ n^{(l)}(x_1, \ldots, x_l) \equiv n^l \left( h_l(x_1, \ldots, x_l) + 1 \right) \]

\[ = \left( \sum_{i_1} \sum_{i_2 \neq i_1} \cdots \sum_{i_l \neq i_1, \ldots, i_{l-1}} \delta^{(d)}(x_1 - x_{i_1}) \delta^{(d)}(x_2 - x_{i_2}) \cdots \delta^{(d)}(x_l - x_{i_l}) \right). \]  
(20)

---

\[3\]When \( T \) and \( V \) are fixed, the differential form of the grand potential becomes

\[ dW = -pdV + SdT - Nd\mu = -Nd\mu. \]  
(16)

Because of \( W = -pV \), the relation \( Vdp = Nd\mu \) follows for fixed \( T \) and \( V \). Thus we have

\[ \frac{\partial}{\partial p} \bigg|_{T,V} = \frac{1}{n} \frac{\partial}{\partial \mu} \bigg|_{T,V}, \]  
(17)

which relates \(13\) and \(15\).
For an ideal gas, $h_l = 0$ and thus $\lambda_l = 1$.

The relations (13) and (14) tell us that various thermodynamical quantities are expressed as integrals of the correlation functions. In order to evaluate these integrals, various approximations have been exploited such as the Kirkwood’s superposition assumption [16, 17, 19, 20], the Percus-Yevick approximation [4, 5, 6, 7, 8], or the Hyper-Netted chain approximation [9, 10, 11, 12, 13].

These approaches based on integral equations can be applicable to high density regions beyond the ordinary virial expansion method. It is, however, difficult to treat them analytically and most studies have relied on numerical computations with various approximations whose validity are not well understood. In the studies of classical liquids, we often ask the following questions: How does the pressure or the isothermal compressibility vary as a function of the liquid density? How does the phase transition or the critical phenomena occur as we change the density? In order to answer these questions, it will be desirable if we can investigate the system based on a systematic formulation and approximations, and understand the evolution of the thermodynamical quantities as we gradually increase the density. The underlying idea is similar to the renormalization group (RG) in quantum field theories (QFTs) since, in both cases, we are interested in the response of a system against scale transformations. But there is a big difference. In quantum field theory at zero temperature and zero (e.g. baryon) density, scale transformations induce a change of the energy scales; the renormalization scale $\mu$ is changed. On the other hand, in classical liquids at nonzero temperature and nonzero density, the transformations induce a change of the magnitude of the liquid density. Therefore scale transformations in liquid theory lead to differential equations to describe response of thermodynamical quantities against a change of the density $n$ (or the chemical potential $\mu$) instead of the renormalization scale.

### 2.2 Scale transformations

In order to investigate response of the system against a scale transformation, we consider a transformation of the two-body potential: $v(x) \rightarrow v(ax)$. Then the partition function changes as

$$
\Xi_{v(ax)}[T, \mu, V; U(x)]
$$

\[= \sum_{N=0}^{\infty} \frac{z(\mu)^N}{N!} \left[ \int_V d^d x_1 \cdots \int_V d^d x_N \exp \left( -\beta \sum_{i<j} v(a(x_i - x_j)) + \beta \sum_i U(x_i) \right) \right] \]

\[= \sum_{N=0}^{\infty} \frac{z(\mu - dT \log a)^N}{N!} \left[ \int_{aV} d^d x_1 \cdots \int_{aV} d^d x_N \exp \left( -\beta \sum_{i<j} v(x_i - x_j) + \beta \sum_i U(x_i/a) \right) \right] \]

\[= \Xi_v[T, \mu - dT \log a, aV; U(x/a)]. \tag{21}
\]

\(^4\)Amusingly both of the renormalization scale and the chemical potential are denoted by the same sign $\mu$. 


Therefore we see that the change of the potential under the scale transformation, $v(x) \rightarrow v(ax)$, is equivalent to the changes of the chemical potential $\mu$, the volume of the system $V$, and the external source $U(x)$. For an infinitesimal scale transformation $a = 1 + \epsilon$, we have

$$\Xi_{v+\epsilon v}[T,\mu,V;U(x)] = \Xi_v[T,\mu - dT\epsilon,(1 + d\epsilon)V;U(x(1 - \epsilon))]$$

or equivalently

$$-\beta W_{v+\epsilon v}[T,\mu,V;U(x)] = -\beta W_v[T,\mu - dT\epsilon,(1 + d\epsilon)V;U(x(1 - \epsilon))],$$

where $\delta v(x) = x^\mu\partial_\mu v(x)$. Thus, by differentiating it with respect to $\beta U(x)$, we obtain the following relation of the correlation functions,

$$F_l(x_1, \ldots, x_l) + \epsilon \Delta F_l(x_1, \ldots, x_l) = F_l(x_1, \ldots, x_l)\mid_{\mu - dT\epsilon, V + d\epsilon V} + d\epsilon F_l(x_1, \ldots, x_l) + \epsilon \sum_{i=1}^l x_i^\mu \partial_\mu F_l(x_1, \ldots, x_l),$$

where $\Delta F_l(x_1, \ldots, x_l)$ represents perturbative corrections due to $\delta v(x)$, which are explicitly evaluated in the next section. Finally, by taking the $\epsilon \rightarrow 0$ limit, we obtain the following set of partial differential equations for the correlation functions:

$$d \left( -\frac{\partial}{\partial (\beta \mu)} \right)_{T,V} + \frac{\partial}{\partial \ln V} \bigg|_{\mu,T} + l + \frac{1}{d} \sum_{i=1}^l x_i^\mu \partial_\mu \right) F_l(x_1, \ldots, x_l) = \lim_{\epsilon \rightarrow 0} \Delta F_l(x_1, \ldots, x_l).$$

The lhs contains a derivative with respect to the chemical potential $\mu$. Thus they describe how the classical liquids respond to a change of the chemical potential.

By performing the Fourier transform

$$\tilde{F}_l(k_1, \ldots, k_l) = \int d^d x_1 \ldots \int d^d x_l e^{-i\sum_{i=1}^l k_i \cdot x_i} F_l(x_1, \ldots, x_l),$$

we obtain

$$\text{LHS} = F_l(x_1, \ldots, x_l; \mu, V) + \epsilon \Delta F_l(x_1, \ldots, x_l; \mu, V)$$

$$\text{RHS} = \frac{\delta^l \log \Xi_v[T,\mu - dT\epsilon,(1 + d\epsilon)V;v(x),U(x(1 - \epsilon))]}{\delta(\beta U(x_1)) \cdots \delta(\beta U(x_l))}$$

$$= \left( \prod_{i=1}^l \int d^d y_i \frac{\delta(U(y_i) - \epsilon y_i^\mu \partial_\mu U(y_i))}{\delta U(x_i)} \right) F_l(y_1, \ldots, y_l; \mu - dT\epsilon, V + d\epsilon V)$$

$$= F_l(x_1, \ldots, x_l; \mu - dT\epsilon, V + d\epsilon V) + \epsilon \sum_{i=1}^l \partial_\mu (x_i^\mu F_l(x_1, \ldots, x_l; \mu, V))$$

$$= F_l(x_1, \ldots, x_l; \mu - dT\epsilon, V + d\epsilon V) + d\epsilon F_l(x_1, \ldots, x_l; \mu, V) + \epsilon \sum_{i=1}^l x_i^\mu \partial_\mu F_l(x_1, \ldots, x_l; \mu, V).$$
we have
\[ d \left( -\frac{\partial}{\partial (\beta \mu)} \right)_{T,V} + \frac{\partial}{\partial \ln V} \bigg|_{\mu,T} - \frac{1}{d} \sum_{i=1}^{l} k_{i}^{\mu} \frac{\partial}{\partial k_{i}^{\mu}} \bigg) \tilde{F}_{l}(k_{1}, \ldots, k_{l}) = \lim_{\epsilon \to 0} \Delta \tilde{F}_{l}(k_{1}, \ldots, k_{l}). \] (29)

Furthermore, because the chemical potential and the density are related each other through Eq. (13), Eq. (29) can be also written by
\[ d \left( -\kappa_{T} \frac{\partial}{\partial \ln n} \right)_{V,T} + \frac{\partial}{\partial \ln V} \bigg|_{\mu,T} - \frac{1}{d} \sum_{i=1}^{l} k_{i}^{\mu} \frac{\partial}{\partial k_{i}^{\mu}} \bigg) \tilde{F}_{l}(k_{1}, \ldots, k_{l}) = \lim_{\epsilon \to 0} \Delta \tilde{F}_{l}(k_{1}, \ldots, k_{l}), \] (30)

which describes how the system (in particular its correlation functions) changes as we change the density. In the next section, we explicitly evaluate the corrections \( \Delta F_{l} \) to the correlation functions due to change of the potential \( \delta v(x) = x^{\mu} \partial_{\mu} v(x) \). We adopt the field theoretical approach to the classical interacting particles proposed by J. Hubbard and P. Schofield [25], and we will see that the corrections \( \Delta F_{l} \) are written in terms of higher-body correlation functions such as \( F_{l+1} \). Thus the above equations generate a hierarchical structure similar to the BBGKY hierarchy. Note that the volume derivative at fixed \((\mu, T)\) vanishes in the large \( V \) limit.

## 3 Density Renormalization Group Equations

In the previous section, we have derived the density evolution equations (27)(29)(30) from the scale transformation. In this section, we explicitly calculate the perturbative corrections \( \Delta F_{l} \). In particular, we adopt the field theoretical approach proposed by J. Hubbard and P. Schofield [25]. One of the benefits of the approach is that we can use the ordinary field theoretical techniques for calculating the correlation functions such as the Feynman diagram method. The resultant corrections contain contributions from higher-body correlation functions, so the equations generate a hierarchical structure like the ordinary BBGKY equations.

In section 3.1, we briefly review [25] and calculate the perturbative corrections of the correlation functions. In section 3.2, we derive new hierarchical equations by combing all the results of this section and the previous one.

### 3.1 Field theory of classically interacting particles

One of the successful perturbative approaches in the classical liquid/vapor theory is the high temperature expansion from some reference system whose properties are supposed to be already known or exactly solved [26] [27]. In particular, it was shown that this approach can be even applicable to the lower temperature and high density regions. However, this method is usually used to derive global thermodynamical quantities and we need a new framework which enables us to calculate various local quantities such as the correlation functions. One of
useful approaches toward understanding such local quantities is the field theoretical method proposed by J. Hubbard and P. Schofield [25]. In this method, the grand canonical partition function is cleverly transformed into a path integral formulation of a scalar field theory. In the following, we first review the method [25], and then calculate the corrections to the correlation functions.

Suppose that a reference system is described by a two-body potential $v_R(x)$ and then perturbed as

$$v(x) = v_R(x) + \epsilon v_1(x),$$

(31)

where $\epsilon$ is a small parameter and $v_1(x)$ is an arbitrary potential. Note that, in the case of the scale-transformation discussed in the previous section, we take $v_R(x) = v(x)$ itself and $v_1(x) = x^\mu \partial_\mu v(x)$.

Under the shift (31), the partition function Eq.(6) becomes

$$\Xi_{v_R+\epsilon v_1}[T,\mu,V;U(x)]$$

$$= \sum_{N=0}^{\infty} \frac{z(\mu + \epsilon v_1(0)/2)^N}{N!} \int_V \cdots \int_V \prod_{i=1}^N d^d x_i \ e^{-\beta \sum_{i,j} v_R(x_i-x_j)} e^{(-\frac{\beta}{2} \langle \rho | \epsilon v_1 | \rho \rangle + \langle \beta U | \rho \rangle)}$$

$$= \Xi_{v_R}[T,\mu+\frac{\epsilon v_1(0)}{2},V;0] \langle e^{-\frac{\beta}{2} \langle \rho | \epsilon v_1 | \rho \rangle + \langle \beta U | \rho \rangle} \rangle_R,$$

(32)

where $\langle \cdots \rangle_R$ represents the thermodynamical expectation value in the reference system:

$$\langle O \rangle_R = \frac{1}{\Xi_{v_R}[T,\mu+\frac{\epsilon v_1(0)}{2},V;0]} \sum_{N=0}^{\infty} \frac{z(\mu + \epsilon v_1(0)/2)^N}{N!} \int_V \cdots \int_V \prod_{i=1}^N d^d x_i \ e^{-\beta \sum_{i,j} v_R(x_i-x_j)} O.$$

(33)

In order to rewrite the partition function Eq.(32) in a path integral form, we use the following mathematical identity:

$$e^{a x^2} = \left\{ \begin{array}{ll}
\sqrt{2a\pi} \int_{-\infty}^{\infty} dy \ \exp \left( -\frac{y^2}{2a} + xy \right), & \text{for } a > 0 \\
\sqrt{-2a\pi} \int_{-\infty}^{\infty} dy \ \exp \left( \frac{y^2}{2a} + ixy \right), & \text{for } a < 0
\end{array} \right.$$

(34)

where $a > 0$ ($<0$) corresponds to an attractive (repulsive) potential respectively, i.e., $v_1(x) < 0$ ($>0$). In the following, we consider an attractive case for simplicity.\textsuperscript{6}

\textsuperscript{6}In more general liquid/vapor systems such that there is some polarization dependences, we need more careful analysis because the coefficient $a$ can become complex in such a case.

10
By completing the square in the exponent in Eq. (32), we obtain

\[
\exp \left( -\frac{1}{2} \langle \rho | \beta \epsilon v_1 | \rho \rangle + \langle \beta U | \rho \rangle \right)
\]

\[
= \exp \left( -\frac{1}{2} \left( \rho - \frac{1}{\epsilon} U v_1^{-1} \right) | \beta \epsilon v_1 | \rho - \frac{1}{\epsilon} U v_1^{-1} \right) + \frac{1}{2} \left( \beta U | \frac{v_1^{-1}}{\beta \epsilon} | \beta U \right)
\]

\[
= \mathcal{N} e^{\frac{1}{2} \langle \beta U | \frac{v_1^{-1}}{\beta \epsilon} | \beta U \rangle} \int D\phi \exp \left( \frac{1}{2} \left( \frac{v_1^{-1}}{\beta \epsilon} | \phi \right) + \left( \rho - \frac{1}{\epsilon} U v_1^{-1} | \phi \right) \right).
\]

(35)

Here, \(v_1^{-1}\) is an inverse operator acting on functions. Eq. (32) is rewritten in terms of the scalar field path integral:

\[
\Xi_{v_1 + v_1}[T, \mu, V; U(x)] = \mathcal{N} e^{\frac{1}{2} \langle \beta U | \frac{v_1^{-1}}{\beta \epsilon} | \beta U \rangle} \int D\phi \frac{1}{2} \langle \phi | \frac{v_1^{-1}}{\beta \epsilon} | \phi \rangle - \beta U \langle \phi | v_1^{-1} | \phi \rangle \langle e^{\langle \rho | \phi \rangle} \rangle_R ,
\]

(36)

where \(\mathcal{N}\) is a normalization factor. Then, the cumulant expansion of \(\langle e^{\langle \rho | \phi \rangle} \rangle_R\) leads to the following result:

\[
\Xi_{v_1 + v_1}[T, \mu, V; U(x)] = \mathcal{N} \int D\phi \frac{1}{2} \langle \phi | \frac{v_1^{-1}}{\beta \epsilon} | \phi \rangle - \beta U \langle \phi | v_1^{-1} | \phi \rangle
\]

\[
\times \exp \left( \sum_{l=1}^{\infty} \frac{1}{l} \int \prod_{i=1}^{l} \frac{d^d k_i}{(2\pi)^d} \tilde{F}_l(R)(k_1, \cdots, k_i) \tilde{\phi}(k_1) \cdots \tilde{\phi}(k_i) \right),
\]

(37)

where \(\tilde{F}_l(R)(k_1, \cdots, k_i)\) is the Fourier transform of the correlation function of the reference system. This result shows that a classical theory of liquid is equivalent to a quantum field theory with an infinite number of the multiple point operators, each of which corresponds to the correlation function of the reference system.

In this expression, we see that the external source \(U(x)\) originally introduced for the density \(\rho(x)\) now plays a role of the source term for the quantum field \(\phi(x)\). Therefore \(\phi(x)\) can be essentially identified with \(\rho(x)\).\footnote{There is an extra factor \(v_1^{-1}/\epsilon\) in the quadratic and a linear term of \(\phi\) in the Lagrangian \(37\) but these factors are cancelled in \(\epsilon = 0\) limit. Thus \(U\) derivatives give the correlation functions of \(\phi(x)\).} In particular, it is apparent that the correlation function \(F_l(x_1, \cdots, x_i)\) of the density fluctuations corresponds to the connected part of \(\langle \phi(x_1) \cdots \phi(x_i) \rangle\) because it is generated by the generating functional \(-\beta W[U] = \log \Xi[U]\). Therefore, we can calculate the perturbative corrections of these correlation functions in the same manner as the ordinary quantum field theories. Note that this procedure is widely applicable to any perturbed (or transformed) system as long as the resultant potential is given by Eq. (31).

Let us now apply this method to our scale-transformed system, i.e. \(v_{\text{R}}(x) = v(x), v_1(x) = \delta v(x)\). In this case, the correlation functions of the reference system \(\tilde{F}_l^{(R)}(k_1, \cdots, k_i)\) is given
by the exact correlation function $\tilde F_l(k_1, \cdots, k_l)$ at some fixed density. They are, of course, not
yet known. Instead, we investigate how they change under a scale transformation, namely
under a change of the density.

In calculating corrections to the correlators $\Delta \tilde F_l$, it is convenient to use Feynman diagrammatic representations. Associated with the propagator and $l$-point vertices, we introduce the
following graphical representations:

1. For each internal propagator for $\phi(x)$,

$$k = -\int \frac{d^d k}{(2\pi)^d} \beta \epsilon \delta \tilde v(k)$$  \hspace{1cm} (38)

2. For each $l$-th vertex,

$$\tilde F_l(k_1, \cdots, k_l)$$  \hspace{1cm} (39)

where $\tilde F_l(k_1, \cdots, k_l)$ is symmetric under permutations of momenta and vanishes unless mo-
momentum conservation $\sum_{i=1}^l k_i$ is satisfied.

The Fourier transform of $\delta v(x)$ is given by

$$\delta \tilde v(k) = \int d^d x \partial^\mu v(x) e^{-ikx} = -\frac{\partial}{\partial k^\mu} (k^\mu \tilde v(k)) = -d \tilde v(k) + k^\mu \frac{\partial}{\partial k^\mu} \tilde v(k).$$  \hspace{1cm} (40)

Thus we have $\delta \tilde v(0) = -d \tilde v(0)$.

In the graphical representation, there is an important property derived from Eq.(37). When we take the functional derivatives of Eq.(37) with respect to $\beta \tilde U(p)$, an additional
factor $-(\epsilon \delta \tilde v(p))^{-1}$ is added to each of the external legs. However, this additional factor is
completely canceled by the propagator $-\epsilon \delta \tilde v(p)$. This property is depicted as

3. For each external line,

$$p$$

where the blob is any diagram connected with this external line. As a result, the tree-level
correlation functions $\tilde F_l(p_1, \cdots, p_l)$, namely correlation functions without perturbation $\delta v$, can be correctly reproduced.

By using them, we can diagrammatically evaluate the perturbative corrections of the corre-
lation functions, i.e. $\Delta \tilde F_l(x_1, \cdots, x_l)$ in Eqs.(27)(29)(30). Because we are interested in the
\( \epsilon \rightarrow 0 \) limit, it is sufficient to consider the leading order contributions with respect to \( \epsilon \). Such contributions are represented by the diagrams which contain only one internal propagator because it is the only place where an additional \( \epsilon \) factor appears. In other words, if there are more than one internal propagators, the diagram vanishes in the \( \epsilon \rightarrow 0 \) limit. Therefore, we obtain the following results:

(0) **Zero point function** (\( \equiv \) Grand potential):

\[
\Delta F_0 = -\beta \delta W[T, \mu, V] = \begin{array}{c}
\text{vertex} \\
\text{evolution}
\end{array} + \begin{array}{c}
\text{vertex} \\
\text{evolution}
\end{array}
\]

\[
= -\frac{1}{2!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_1(p) \tilde{F}_1(-p) - \frac{1}{2!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_2(p, -p) \tag{42}
\]

(1) **One-point function**:

\[
\Delta \tilde{F}_1(k) = \begin{array}{c}
k \\
\text{evolution}
\end{array} + \begin{array}{c}
k \\
\text{evolution}
\end{array}
\]

\[
= -\frac{2!}{2!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_1(p) \tilde{F}_2(-p, k) - \frac{3}{3!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_3(p, -p, k) \tag{43}
\]

(2) **Two-point correlation function**:

\[
\Delta \tilde{F}_2(k_1, k_2) = \begin{array}{c}
k_1 \\
\text{evolution}
\end{array} + \begin{array}{c}
k_1 \\
\text{evolution}
\end{array} + \begin{array}{c}
k_2 \\
\text{evolution}
\end{array}
\]

\[
= -\frac{3!}{3!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_3(-p, k_1, k_2) - \frac{2!2!}{(2!)^3} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_2(k_1, -p) \tilde{F}_2(p, k_2) - \frac{4 \cdot 3}{4!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{\nu}(p) \tilde{F}_4(k_1, k_2, p, -p) \tag{44}
\]
(3) Three-point correlation function:
\[
\Delta \tilde{F}_3(k_1, k_2, k_3) = \begin{array}{c}
\text{Diagram 1}
\end{array} + \begin{array}{c}
\text{Diagram 2}
\end{array} + \begin{array}{c}
\text{Diagram 3}
\end{array}
\]
\[
= -\frac{4!}{4!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{F}_1(p) \tilde{F}_4(-p, k_1, k_2, k_3)
\]
\[
- \frac{3! \cdot 2!}{3!2!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \left[ \tilde{F}_3(k_1, k_2, -p) \tilde{F}_2(p, k_3) + \tilde{F}_3(k_2, k_3, -p) \tilde{F}_2(p, k_1) + \tilde{F}_3(k_3, k_1, -p) \tilde{F}_2(p, k_2) \right]
\]
\[
- \frac{5 \cdot 4 \cdot 3}{5!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{F}_5(k_1, k_2, k_3, -p, -p)
\tag{45}
\]

(4) Four-point correlation function:
\[
\Delta \tilde{F}_4(k_1, k_2, k_3, k_4) = \begin{array}{c}
\text{Diagram 1}
\end{array} + \begin{array}{c}
\text{Diagram 2}
\end{array} + \begin{array}{c}
\text{Diagram 3}
\end{array} + \begin{array}{c}
\text{Diagram 4}
\end{array}
\]
\[
= -\frac{5!}{5!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{F}_1(p) \tilde{F}_5(p, k_1, k_2, k_3, k_4)
\]
\[
- \frac{3!3!2!}{(3!)^2} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \left[ \tilde{F}_4(k_1, k_2, -p) \tilde{F}_3(p, k_3, k_4) + \tilde{F}_4(k_1, k_3, -p) \tilde{F}_3(p, k_2, k_4) \right.
\]
\[
+ \tilde{F}_4(k_1, k_4, -p) \tilde{F}_3(p, k_2, k_3)
\]
\[
- \frac{4!2!}{4!2!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \left[ \tilde{F}_4(k_1, k_2, k_3, -p) \tilde{F}_2(p, k_4) + \tilde{F}_4(k_1, k_2, k_4, -p) \tilde{F}_2(p, k_3) \right.
\]
\[
+ \tilde{F}_4(k_1, k_3, k_4, -p) \tilde{F}_2(p, k_2) + \tilde{F}_4(k_2, k_3, k_4, -p) \tilde{F}_2(p, k_1) \right]
\]
\[
- \frac{6 \cdot 5 \cdot 4 \cdot 3}{6!} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{F}_6(k_1, k_2, k_3, p, -p)
\tag{46}
\]

(5) \textit{l-point correlation functions} \((l \geq 5)\):
In general, \(\Delta \tilde{F}_{l+1}(k_1, \cdots, k_{l+1})\) can be automatically obtained by taking the functional derivative of the \textit{l-th} diagrams and using the following vertex relation:
\[
\left. \frac{\delta \tilde{F}_l(k_1, \cdots, k_l)}{\delta \beta U(k_{l+1})} \right|_{U=0} = \tilde{F}_{l+1}(k_1, \cdots, k_{l+1}),
\tag{47}
\]
which is diagrammatically represented by

\[ \frac{\delta}{\delta (\beta U(k_{l+1}))} \begin{array}{c} \delta \varepsilon \\ \hspace{1cm} \delta \varepsilon \end{array} \begin{array}{c} k_3 \hspace{0.5cm} k_2 \hspace{0.5cm} k_1 \\ \hspace{1cm} k_i \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm} k_{l+1} \end{array} = \begin{array}{c} k_3 \hspace{0.5cm} k_2 \hspace{0.5cm} k_1 \\ \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm} k_{l+1} \end{array}. \] (48)

In fact, we can straightforwardly check that all the results \((l \leq 4)\) can be rederived by taking the functional derivatives of \(\Delta F_0 = -\beta \Delta W\).

### 3.2 DRGEs as hierarchical equations

By substituting the results of the previous section into Eqs. (27), (29), (30), we obtain a sequence of the differential equations that govern the changes of the correlation functions against a variation of the density (or chemical potential). In order to separate the momentum conservation from the correlation functions, we introduce the following notations:

\[ -\beta \frac{W}{nV} = \frac{p}{nT} \equiv \lambda, \]
\[ \tilde{F}_1(k) = (2\pi)^d \delta^{(d)}(k)n, \] (49)
\[ \tilde{F}_2(k_1, k_2) = (2\pi)^d \delta^{(d)}(k_1 + k_2)\kappa(k_1, k_2) = (2\pi)^d \delta^{(d)}(k_1 + k_2)n\kappa(k_1, k_2). \] (50)

Especially, the 2-point function at zero momentum \(\kappa(k) = 0\) is identified with \(\kappa_T\). For higher \(l \geq 3\), we define

\[ \tilde{F}_l(k_1, \ldots, k_l) = (2\pi)^d \delta^{(d)} \left( \sum_{i=1}^{l} k_i \right) \tilde{\lambda}_l(k_1, \ldots, k_l) = (2\pi)^d \delta^{(d)} \left( \sum_{i=1}^{l} k_i \right) n\lambda_l(k_1, \ldots, k_l). \] (51)

Note that \(\lambda, \kappa\) and \(\lambda_l\) \((l \geq 3)\) are dimensionless. Especially, their initial values at \(n = 0\) \((\mu = -\infty)\), namely the values for the ideal gas, are given by

\[ \lambda|_{n=0} = 1, \quad \kappa(k_1, k_2)|_{n=0} = 1, \quad \lambda_l(k_1, \ldots, k_l)|_{n=0} = 1 \quad (l \geq 3), \] (52)

as can be easily checked from the correlation functions for the ideal gas (see Appendix A).

By substituting Eqs. (49)-(52) into Eq. (29) or (30), we obtain the following set of hierar-
For $l = 0$, we get an equation of state of the classical liquid:

$$\frac{p}{T} - n = \frac{1}{2} \beta \tilde{v}(0)n^2 - \frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{\kappa}(p, -p), \quad (55)$$

which relates the pressure with an integral of two-point correlation function. Here we have used $\delta \tilde{v}(0) = -d \tilde{v}(0)$.

For $l \geq 1$ we have the following set of partial differential equations. First we define the differential operator $\mathcal{D}$ as

$$\mathcal{D} \equiv d \left( -\frac{\partial}{\partial (\beta \mu)} \right)_{V,T} + \frac{\partial}{\partial \log \frac{V}{V_{\mu,T}}} + 1 - \frac{1}{d} \sum_{i=1}^{l} k_{i}^{\mu} \frac{\partial}{\partial k_{i}^{\mu}} \right). \quad (56)$$

Here we note that the volume derivative in the differential operator $\mathcal{D}$ can be neglected in the large $V$ limit since local quantities such as the density $n$ or the correlation functions do not depend on the total volume when $(\mu, T)$ are fixed.

For $l = 1$, we get

$$\mathcal{D} n = d \beta \tilde{v}(0)n \tilde{\kappa}(k, 0) - \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{\lambda}_{3}(p, -p, k). \quad (58)$$

Because of the assumption of the translational invariance, it vanishes unless $k = 0$. Since $\mu$ derivative in the left hand side for $k = 0$ is written in terms of $\kappa_{T} = \kappa(0)$, the equation relates $\kappa_{T}$ with an integral of the 3-point function $\lambda_{3}$.

For $l = 2$, we have

$$\mathcal{D} \tilde{\kappa}(k_1, k_2) = d \beta \tilde{v}(0)n \tilde{\lambda}_{3}(k_1, k_2, 0) - \frac{1}{2} \tilde{\kappa}(k_1, k_2) \sum_{i=1}^{2} \beta \delta \tilde{v}(k_{i}) \tilde{\kappa}(k_{i}, -k_{i})$$

$$- \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \beta \delta \tilde{v}(p) \tilde{\lambda}_{4}(k_1, k_2, p, -p), \quad (59)$$

---

8 The momentum derivative in the LHS of Eq. (29) or (30) is given by

$$- \sum_{i=1}^{l} k_{i}^{\mu} \partial_{\mu} \left( \delta^{(d)} \left( \sum_{i=1}^{l} k_{i} \right) \tilde{\lambda}_{l} \right) = - \tilde{\lambda}_{l} \sum_{i=1}^{l} k_{i}^{\mu} \partial_{\mu} \delta^{(d)} \left( \sum_{i=1}^{l} k_{i} \right) - \sum_{i=1}^{l} k_{i}^{\mu} \delta^{(d)} \left( \sum_{i=1}^{l} k_{i} \right) \partial_{\mu} \tilde{\lambda}_{l}$$

$$= \delta^{(d)} \left( \sum_{i=1}^{l} k_{i} \right) \left( d \tilde{\lambda}_{l} - \sum_{i=1}^{l} k_{i}^{\mu} \partial_{\mu} \tilde{\lambda}_{l} \right). \quad (54)$$
which relates a density response of $\kappa(k)$ with an integral of 3- and 4-point functions. For $l = 3$ and $l = 4$, we have

$$D\tilde{\lambda}_3(k_1, k_2, k_3) = d\beta\tilde{v}(0)n\tilde{\lambda}_4(k_1, k_2, k_3, 0) - \tilde{\lambda}_3(k_1, k_2, k_3) \sum_{i=1}^{3} \beta\delta\tilde{v}(k_i)\kappa(k_i, -k_i) - \frac{1}{2} \int \frac{d^dp}{(2\pi)^d} \beta\delta\tilde{v}(p)\tilde{\lambda}_5(k_1, k_2, k_3, p, -p),$$

and

$$D\tilde{\lambda}_4(k_1, k_2, k_3, k_4) = -\beta\delta\tilde{v}(0)n\tilde{\lambda}_5(k_1, k_2, k_3, k_4, 0) - \left[\tilde{\lambda}_3(k_1, k_2, k_3 + k_4)\tilde{\lambda}_3(k_1 + k_2, k_3, k_4) \Re[\beta\delta\tilde{v}(k_1 + k_2)] + (k_1 \leftrightarrow k_3) + (k_1 \leftrightarrow k_4) + (k_1 \leftrightarrow k_3)\right]$$

$$- \tilde{\lambda}_4(k_1, k_2, k_3, k_4) \sum_{i=1}^{4} \delta\tilde{v}(k_i)\kappa(k_i, -k_i) - \frac{1}{2} \int \frac{d^dp}{(2\pi)^d} \beta\delta\tilde{v}(p)\tilde{\lambda}_6(k_1, k_2, k_3, k_4, p, -p),$$

where $\Re$ is the real part and $(k_a \leftrightarrow k_b)$ denotes interchanging the momenta, $k_a$ and $k_b$.

These hierarchical equations describe the response of the system to a small change of the density. Though we have used perturbative technique, they are the exact (non-perturbative) equations and offer us an alternative formulation of the classical liquid/vapor system. Our next step is to solve them by using physically reasonable approximations or assumptions.

### 3.3 Towards solving DRGEs

In this section, we briefly discuss how we can attack to solve the set of differential equations (DRGE) derived in the previous section; more details are left for future investigations.

There are two difficulties in solving the DRGEs. The first one is a mixture with higher-point correlation functions, and some approximations are necessary to close the hierarchical equations. Another is the momentum integration, which originates in the loop diagrams. The second difficulty can be avoided by noticing that various integrals have similar forms; integrants always contain $\delta\tilde{v}(p)$. Thus, we can regard a special set of integrals as couplings that govern the system. One of the most important examples is given by the following integral

$$\kappa_I \equiv \frac{1}{2^d} \int \frac{d^dp}{(2\pi)^d} \beta\delta\tilde{v}(p)\kappa(p, -p).$$

It is interpreted as a "coupling" of the liquid system as well as $\kappa(0) = \kappa_T$. Other quantities appearing in the integrals of Eqs.[58]-[61] at zero external momenta $k_i = 0$ are related to $\kappa_I$.
as follows;

\[
\frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \beta \delta \bar{v}(p) \tilde{\lambda}_3(p, -p, 0) = \frac{\partial (n\kappa_I)}{\partial (\beta \mu)}, \tag{63}
\]

\[
\frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \beta \delta \bar{v}(p) \tilde{\lambda}_4(p, -p, 0, 0) = \frac{\partial^2 (n\kappa_I)}{\partial (\beta \mu)^2}, \tag{64}
\]

\[
\frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \beta \delta \bar{v}(p) \tilde{\lambda}_5(p, -p, 0, 0, 0) = \frac{\partial^3 (n\kappa_I)}{\partial (\beta \mu)^3}. \tag{65}
\]

In deriving these equations, we used the relation

\[
\frac{\partial}{\partial (\beta \mu)} \tilde{\lambda}_l(k_1, \cdots, k_l) \bigg|_{V,T} = \tilde{\lambda}_{l+1}(k_1, \cdots, k_l, 0), \tag{66}
\]

which can be proved by using the fact that the chemical potential \(\mu\) and the zero mode of \(U(x)\) can be identified. In other words, the relation

\[
\frac{\partial}{\partial (\beta \mu)} = \int dy \frac{\partial}{\partial (\beta U(y))} \tag{67}
\]

is satisfied, and then Eq.(66) is derived.

By using these relations in Eq.(55) and Eq.(58), we get the following equations:

\[
-n + \frac{p}{T} = \frac{1}{2} \beta \bar{v}(0)n^2 - n\kappa_I, \tag{68}
\]

\[
- \kappa_T n + n = \beta \bar{v}(0)n^2\kappa_T - \frac{\partial (n\kappa_I)}{\partial (\beta \mu)} \bigg|_{V,T}, \tag{69}
\]

Setting the external momenta \(k_i = 0\) and using these relations for \(l \geq 2\), e.g., in Eq.(59), we get a similar equation

\[
- \tilde{\lambda}_3 + \tilde{\kappa} = \beta \bar{v}(0)n\tilde{\lambda}_3 + \tilde{\kappa}^2 \beta \bar{v}(0) - \frac{\partial^2 (n\kappa_I)}{\partial (\beta \mu)^2} \bigg|_{V,T}. \tag{70}
\]

But it is not independent from Eq.(69) since Eq.(70) can be derived by taking a \((\beta \mu)\) derivative of Eq.(69). Eq.(68) and Eq.(69) are not independent either, and there is a single independent equation for vanishing external momenta. Thus another relation between \(\kappa_T\) and \(\kappa_I\) is necessary to solve the equation.

An independent equation can be obtained, e.g., by multiplying \(\beta \delta \bar{v}(k)\) on Eq. (59) with \(k_1 = -k_2 = k\) and integrating over \(k\). Then, defining two new couplings by the following integrals

\[
\kappa_{I2} = \frac{n}{2d^2} \int \frac{d^d p}{(2\pi)^d} (\beta \delta \bar{v}(p)\kappa(p, -p))^2, \tag{71}
\]
and
\[ \lambda_4 \equiv \frac{1}{(2\pi)^d} \int \frac{d^dp}{(2\pi)^d} \int \frac{d^dk}{(2\pi)^d} \beta \delta \tilde{v}(p) \beta \delta \tilde{v}(k) \lambda_4(p, -p, k, -k), \quad (72) \]
we get the following equation
\[ \left( -\frac{\partial}{\partial(\beta\mu)} + 1 \right) (n\kappa_I) = \beta \tilde{v}(0)n \frac{\partial(n\kappa_I)}{\partial(\beta\mu)} - n\kappa_{I2} - n\lambda_4. \quad (73) \]
In this way we can generate independent differential equations, but at the same time more new couplings are introduced and we need some approximations to close the equations; it is the destiny of the hierarchical equations and further investigations are left for future publications. In the next section we will make Legendre transformations to one-particle irreducible (1PI) diagrams in which multipoint 1PI vertices are expected to become local and closure of the hierarchical equations becomes more tractable and reliable.

4 Legendre Transformation and 1PI Potential

In quantum field theory, it is usually much more convenient to discuss the dynamics of a system based on the effective action \( \Gamma[\phi] \) which is obtained by the Legendre transformation of \( iW[J] = \log Z[J] \); \( \Gamma[\phi] \) represents the generating functional of the 1PI diagrams. The 1PI effective action \( \Gamma[\phi] \) is especially useful and inevitable when a spontaneous symmetry breaking occurs. Similarly 2PI effective action is important when we discuss a nontrivial behavior of the propagator \(^{28}\). In this paper, we concentrate on \( \Gamma[\phi] \) and leave analysis of 2PI actions for future.

In the case of the classically interacting particles, such a transformation corresponds to the thermodynamical Legendre transformation of the grand potential \(-\beta W[U]\) to the Helmholtz free energy \(-\beta \Gamma[\rho]\) where the thermodynamical parameters are transformed from \((T, V, \mu)\) to \((T, V, N)\). Either thermodynamical potential has its advantage and we can use them as the situation demands. Here we generalize the thermodynamical Legendre transformation including the local external source term \( U(x) \). Thus, \(-\beta W_v[U]\) is transformed to a generating functional of 1PI correlations functions of density, i.e. \(-\beta \Gamma[\rho]\). Up to trivial contributions from the ideal gas, such 1PI correlation functions are called the direct correlation functions in the liquid theory.

In the following, in order to make the discussions simpler, we absorb the chemical potential \( \mu \) into the zero mode of the external source \( U(x) \) and denote \(-\beta W_v[T, \mu, V; U]\) as \(-\beta W_v[T, V; U]\). Also we introduce the correlation functions of density fluctuations in the presence of external source terms and denote them as
\[ F_l^U(x_1, \ldots, x_l) \equiv \frac{\delta^l(-\beta W_v[U])}{\delta(\beta U(x_1)) \cdots \delta(\beta U(x_l))}. \quad (74) \]
Setting \( U(x) = \mu \), they coincide with the previous ones \( F_l(x_1, \ldots, x_l) \).
4.1 Direct correlation functions

We define the (generalized) Helmholtz free energy $-\beta \Gamma_v[T,V;\rho]$ by the Legendre transformation of $-\beta W_v[T,V;U]$:

$$-\beta \Gamma_v[T,V;\rho] = \min_U \left( -\beta W_v[T,V;U] - \beta \int d^d x U(x) \rho(x) \right)$$

$$= -\beta W_v[T,V;U^\rho] - \beta \int d^d x U^\rho(x) \rho(x), \quad (75)$$

where $\rho(x)$ represents a density field, and $U^\rho(x)$ is a solution of

$$\frac{\delta (-\beta W_v[T,V;U])}{\delta \rho(x)} = \rho(x). \quad (76)$$

Then, we can define new correlation functions by taking the functional derivatives of $-\beta \Gamma_v[T,V;\rho]$ with respect to $\rho(x)$:

$$\delta^l (x_1,x_2,\cdots,x_l) \equiv \left. \frac{\delta^l (-\beta \Gamma_v[T,V;\rho])}{\delta \rho(x_1) \delta \rho(x_2) \cdots \delta \rho(x_l)} \right|_{\rho(x)=n}. \quad (77)$$

In the following, we call them the $l$–point 1PI vertices for $l \geq 3$. In particular, $c_2(x,y)$ and $c_3(x,y,z)$ satisfy the following relations

$$\int d^d z F_2(x,z) c_2(z,y) = -\delta^{(d)}(x-y), \quad (78)$$

$$F_3(x,y,z) = \int d^d w \int d^d w' \int d^d w'' F_2(x,w) F_2(y,w') F_2(z,w'') c_3(w,w',w'') \quad (79)$$

where $F_2$ and $F_3$ are the (connected) correlation functions defined in the previous section. These relations are the direct consequences of the Legendre transformation. The first relation is called the “Ornstein-Zernike equation” in the liquid/vapor theory. In order to rewrite it in a standard form, we note that the two-point “direct correlation function” $c^D_2(x,y)$ is defined by

$$c^D_2(x,y) = c_2(x,y) + n^{-1} \delta^{(d)}(x-y). \quad (80)$$

The direct correlation function $c^D_2$ vanishes for the ideal gas (see Appendix A). Then using the definition of the total correlation function $h_2$ in Eq.(19) which also vanishes for the ideal gas, Eq.(78) becomes

$$h_2(x,y) = c_2^D(x,y) + n \int d^d y c_2^D(z,y) h_2(x,z), \quad (81)$$

which is the standard form of the Ornstein-Zernike equation.

Similarly we define $l$–point direct 1PI vertices (for $l \geq 3$), $c^D_l$, by

$$c^D_l(x_1,\cdots,x_l) = c_l(x_1,\cdots,x_l) - \frac{(-1)^{l+1}(l-2)!}{n^{l-1}} \prod_{i=2}^l \delta^{(d)}(x_1-x_i). \quad (82)$$

The direct 1PI vertices are defined so as to vanish for the ideal gas (see Appendix A).
4.2 Scale transformations of 1PI potential

Now let us consider a scale transformation of the potential $v(x) \rightarrow v(x) + \epsilon \delta v(x)$ and its consequence to the Helmholtz free energy $-\beta \Gamma_v[T;V;\rho]$. Here, we should recall the relation Eq.(23) between $-\beta W_v[T;V;U]$ and $-\beta W_v[T;V;U]$: 

$$-\beta W_{v+\epsilon\delta v}[T;V;U(x)] = -\beta W_v[T, (1+\epsilon) V; U(x(1-\epsilon)) - dT \epsilon].$$  

(83)

The Legendre transformation of the LHS gives $-\beta \Gamma_{v+\epsilon\delta v}[T;V;\rho(x)]$ by definition. On the other hand, the Legendre transformation of the RHS is

$$\text{Min}_U \left[ -\beta W_v[T, (1+\epsilon) V; U(x(1-\epsilon)) - dT \epsilon] - \beta \int_V d^d x U(x) \rho(x) \right]$$

$$= \text{Min}_U \left[ -\beta W_v[T, (1+\epsilon) V; U(x(1-\epsilon)) - dT \epsilon] - (1-\epsilon) \beta \int_{1+\epsilon}^V d^d x (U(x(1-\epsilon)) - dT \epsilon) \rho(x(1-\epsilon)) \right] - d \epsilon \int_V d^d x \rho(x)$$

$$= -\beta \Gamma_v[T, (1+\epsilon) V; (1-\epsilon) \rho(x(1-\epsilon)))] - d \epsilon \int_V d^d x \rho(x),$$  

(84)

where we have regarded $\tilde{U}(x) = U(x(1-\epsilon)) - dT \epsilon$ as a new external source and performed the Legendre transformation with respect to it. Thus, we obtain

$$-\beta \Gamma_{v+\epsilon\delta v}[T;V;\rho(x)] = -\beta \Gamma_v[T, (1+\epsilon) V; (1-\epsilon) \rho(x(1-\epsilon))] - d \epsilon \int_V d^d x \rho(x) + O(\epsilon^2),$$  

(85)

and, by differentiating it with respect to $\rho(x)$, we obtain the following differential equation of the 1PI vertices:

$$\left( \frac{d}{\partial \ln V} \left|_{T,N} \right. + \sum_{i=1}^t x_i \partial_{\mu_i} \right) c_l(x_1, \cdots, x_t) - d \delta_{l0} N - \delta_{l1} d = \Delta c_l(x_1, \cdots, x_t),$$  

(86)

where $\Delta c_l(x_1, \cdots, x_t)$ represents the perturbative corrections caused by $\delta v(x)$. They are explicitly calculated in the next section. Note that the $V$ derivative in the LHS is equivalent to the $n(= \langle N \rangle / V)$ derivative

$$\frac{\partial}{\partial \ln V} = - \frac{\partial}{\partial \ln n}$$  

(87)

because $\langle N \rangle$ is fixed here. Thus the equation describes a response of various 1PI quantities against a small change of density. For the ideal gas, the LHS is shown to vanish (see Appendix A).
4.3 Derivations of $\Delta c_l(x_1, \cdots, x_l)$

In this section, we will explicitly calculate the corrections $\Delta c_l(x_1, \cdots, x_l)$. In order for this, we use the previous result of the correction to the grand potential;

$$-\beta W_{v+\delta v}[T, V; U] = -\beta W_v[T, V; U] - \beta \Delta W_v[T, V; U],$$

where $-\beta \Delta W_v[T, V; U]$ is given by Eq. (88). Then, from the definition of the Legendre transformation, we have

$$-\beta \Gamma_{v+\delta v}[T, V; \rho] = \text{Min}_{U(x)} \left[ -\beta W_v[T, V; U] - \beta \Delta W_v[T, V; U] + O(\epsilon^2) - \beta \int d^d x U(x) \rho(x) \right]$$

$$= -\beta W_v[T, V; U^{v+\delta v}_{\rho}] - \beta \Delta W_v[T, V; U^{v+\delta v}_{\rho}] - \beta \int d^d x U^{v+\delta v}_{\rho}(x) \rho(x) + O(\epsilon^2)$$

where $U^{v+\delta v}_{\rho}(x)$ is a solution of

$$\frac{\delta(-\beta W_v[T, V; U] - \beta \Delta W_v[T, V; U])}{\delta(U(x))} = \rho(x).$$

Thus, by denoting the difference between $U^{v+\delta v}_{\rho}(x)$ and $U^{v}_{\rho}(x)$ as $\Delta U^{v}_{\rho}(x)$, we have

$$-\beta \Gamma_{v+\delta v}[T, V; \rho] = -\beta W_v[T, V; U^{v}_{\rho}] + \int d^d x \frac{\delta(-\beta W_v[T, V; U])}{\delta(U(x))} \bigg|_{U=U^{v}_{\rho}} \beta \Delta U^{v}_{\rho}(x)$$

$$- \beta \Delta W_v[T, V; U^{v}_{\rho}] - \beta \int d^d x (U^{v}_{\rho}(x) + \Delta U^{v}_{\rho}(x)) \rho(x) + O(\epsilon^2)$$

$$= -\beta \Gamma_v[T, V; \rho] - \beta \Delta W_v[T, V; U^{v}_{\rho}] + O(\epsilon^2),$$

where we used Eq. (76). From Eq. (42), the second term $-\beta \Delta W_v[T, V; U^{v}_{\rho}]$ is given by $9$

$$-\beta \Delta W_v[T, V; U^{v}_{\rho}] = -\frac{1}{2!} \int d^d x \int d^d y \rho(x) \beta \delta v(x - y) \rho(y) - \frac{1}{2!} \int d^d x \int d^d y \beta \delta v(x - y) F^2_{1, v}(x, y).$$

Therefore, by functionally differentiating Eq. (91) with respect to $\rho(x)$ and putting $\rho(x) = n$, we can obtain $\Delta c_l(x_1, \cdots, x_l)$. In order for systematic calculations, we introduce the following graphical representations:

$9$Here, $F^{\nu}_{1, v}(x)$ in Eq. (42) becomes $\rho(x)$ by the definition;

$$F^{\nu}_{1, v}(x) = \frac{\delta(-\beta W_v[T, V; U])}{\delta(U(x))} \bigg|_{U=U^{v}_{\rho}} = \rho(x).$$
• For the perturbative potential, we use the wavy line:

\[ \beta \delta v(x - y) = \]

\[ (94) \]

• For the two-point (exact) correlation function, a straight line with a blob is used:

\[ F_2^{\nu, \rho}(x, y) = \]

\[ (95) \]

• For the 1PI vertices, shaded polygons are used:

\[ c_l(x_1, x_2, \ldots, x_l) = \]

\[ (96) \]

These graphical representations are used to express \( \Delta c_l \) in the following.

Here we note that the functional derivative of \( c_l(x_1, \ldots, x_l) \) with respect to the density field \( \rho \) is given by

\[ \frac{\delta c_l(x_1, \ldots, x_l)}{\delta \rho(x_{l+1})}\bigg|_{\rho(x)=n} = c_{l+1}(x_1, \ldots, x_{l+1}), \]

which is graphically represented by

\[ (97) \]

Finally, because the functional derivative with respect to \( \rho(x) \) can be also written as

\[ \frac{\delta}{\delta \rho(x)} = \int d^d y \frac{\delta (\beta U_\rho^\nu(y))}{\delta \rho(x)} \frac{\delta}{\delta (\beta U_\rho^\nu(y))} = -\int d^d y c_2(x, y) \frac{\delta}{\delta (\beta U_\rho^\nu(y))}, \]

\[ (99) \]
the functional derivative of $F_2^{U^\rho}(x,y)$ with respect to $\rho(z)$ becomes

$$\left. \frac{\delta F_2^{U^\rho}(x,y)}{\delta \rho(z)} \right|_{\rho(x)=n} = \int d^d w \int d^d w' F_2^{U^\rho}(x,w)c_3(w,z,w')F_2(w',y),$$

where we have used Eqs. (78),(79). It is graphically represented by

Now we calculate $\Delta c_l(x_1, \cdots, x_1)$ and represent them graphically.

(0) **Zero-point** $l = 0$ 1PI function (Helmholtz free energy):

$$\Delta(-\beta \Gamma) = -\frac{n^2}{2} \int d^d x \int d^d y \beta \delta v(x-y) - \frac{1}{2}$$

(1) **One-point** $l = 1$ 1PI function (density):

$$\Delta c_1(x) = -n \int d^d y \beta \delta v(x-y) - \frac{1}{2}$$

$$= -n \int d^d y \beta \delta v(x-y) - \frac{1}{2} \int d^d y \int d^d z \int d^d w \int d^d w' c_3(x,w,w')F_2(y,w)F_2(z,w')\beta \delta v(y-z)$$
(2) Two-point $l = 2$ direct correlation function:

$$
\Delta c_2(x, y) = - \beta \delta v(x - y) - \frac{1}{2}
$$

The graphical representation is read as:

$$
\begin{align*}
\Delta c_2(x, y) &= - \beta \delta v(x - y) \\
&\quad - \frac{1}{2} \int d^d z \int d^d z' \int d^d w \int d^d w' c_4(x, y, w, w') F_2(z, w) F_2(z', w') \beta \delta v(z - z') \\
&\quad - \int d^d z \int d^d z' \int d^d w \int d^d w' \int d^d X \int d^d X' c_3(x, w, X) F_2(X, z) F_2(z', X') \beta \delta v(z - z') \\
&\quad \times F_2(z', X') F_2(w, w') c_3(w', X', y).
\end{align*}
$$

(3) $l$-point 1PI vertex ($l \geq 4$):

In general, $\Delta c_l(x_1, \cdots, x_l)$ can be systematically obtained by taking the functional derivatives of the $(l-1)$-th diagrams and using Eqs. (98)-(101). The $l = 3$ and $l = 4$ cases are given in Appendix B.

4.4 DRGEs for 1PI correlation functions

We now summarize the differential equations that the Legendre transformed correlation functions satisfy. By substituting the corrections $\Delta c_l$ into Eq. (86) and performing the Fourier transform, we obtain the hierarchical equations for the 1PI correlation functions. In the last two diagrams consisting of $c_4$ and $(c_3 F_2 c_3)$ can be combined with a single term $(c_2)^4 F_4$. But the coefficients are different and they cannot. It is because, in Eq. (103), the structure of the legs associated with the 3-point functions $c_3$ are asymmetric, i.e., two legs contain $F_2$ terms (the blobs) but the last one is amputated and there is no $F_2$ term and, when taking derivatives with respect to $\rho$, an asymmetry between legs appears. It is also true in the following higher order correlation functions.
following, we use \( g_l(k_1, \ldots, k_l) \) defined by
\[
\tilde{c}_l(k_1, \ldots, k_l) = \int d^d x_1 \cdots \int d^d x_l e^{-i \sum_{i=1}^l k_i \cdot x_i} c_l(x_1, \ldots, x_l)
\equiv (2\pi)^d \delta^{(d)} \left( \sum_{i=1}^l k_i \right) g_l(k_1, \ldots, k_2),
\tag{106}
\]
in which the momentum conservation is factorized. For the ideal gas (see Appendix A), \( g_l \)'s are constants Eq. (120) and do not have dependence on the external momenta.

For \( l = 0 \), we have
\[
\frac{pV}{T} - N = V \left( \frac{n^2}{2} \beta \bar{\nu}(0) + \frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \frac{\beta \delta \bar{\nu}(p)}{g_2(p,-p)} \right),
\tag{107}
\]
where we have used \((\partial (-\beta \Gamma v[T, V, N]) / \partial \ln V)\big|_{T, N} = pV/T\). Noticing that \( g_2(p, -p) = -1/\kappa(p, -p) \), it is equivalent to Eq. (55).

For \( l = 1 \), we have
\[
\left. \frac{\partial g_1(k)}{\partial \ln V} \right|_{T, N} - 1 = n \beta \bar{\nu}(0) - \frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \frac{g_3(k, p, -p)}{g_2(p, -p)} \beta \delta \bar{\nu}(p),
\tag{108}
\]
which is equivalent to Eq. (58) since
\[
g_1(0) = \frac{1}{V} \int d^d x \frac{\delta (-\beta \Gamma[p])}{\delta \rho(x)} \bigg|_{T, V} = \left. \frac{\partial (-\beta \Gamma[n])}{\partial N} \right|_{T, V} = -\beta \mu,
\tag{109}
\]
and we have
\[
\left. \frac{\partial g_1(k)}{\partial \ln V} \right|_{T, N} - 1 = n \left. \frac{\partial (\beta \mu)}{\partial n} \right|_{T, N} - 1 = \kappa^{-1} - 1
\tag{110}
\]
from which we can easily check that Eq. (108) coincides with Eq. (58).

For \( l = 2 \), namely the response of the 1PI 2-point correlation to a small change of the liquid density is given by
\[
\left( \frac{\partial}{\partial \ln V} \right)_{T, N} - 1 - \frac{1}{2d} \sum_{i=1}^2 \frac{k_i^\mu}{\partial k_i^\mu} \frac{\partial}{\partial \ln V} \left. g_2(k_1, k_2) = -\beta \frac{\partial}{\partial \ln V} (\delta \bar{\nu}(k_1) + \delta \bar{\nu}(k_2)) - \frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} \frac{g_4(k_1, k_2, p, -p)}{g_2(p, -p)^2} \beta \delta \bar{\nu}(p)
\right.
\]
\[
+ \frac{1}{d} \int \frac{d^d p}{(2\pi)^d} \frac{g_3(k_1, k_2 - p, p) g_3(k_2, k_1 + p, -p)}{g_2(p, -p)^2 g_2(k_1 + p, k_2 - p)} \beta \delta \bar{\nu}(p).
\tag{111}
\]
This can be rewritten as
\[
\left( \frac{\partial}{\partial \ln n} \right)_{T, N} + 1 + \frac{1}{2d} \sum_{i=1}^2 \frac{k_i^\mu}{\partial k_i^\mu} \frac{\partial}{\partial \ln n} \left. g_2(k_1, k_2) = \beta \frac{\partial}{\partial \ln n} (\delta \bar{\nu}(k_1) + \delta \bar{\nu}(k_2))
\right.
\]
\[
+ \frac{1}{2d} \int \frac{d^d p}{(2\pi)^d} g_4(k_1, k_2, p, -p) \kappa(p, -p)^2 \beta \delta \bar{\nu}(p)
\]
\[
+ \frac{1}{d} \int \frac{d^d p}{(2\pi)^d} |g_3(k_1, p, -k_1 - p)|^2 \kappa(p, -p)^2 \kappa(k_1 + p, -k_1 - p) \beta \delta \bar{\nu}(p).
\tag{112}
\]
The DRGEs for \( l = 3 \) and \( l = 4 \) point 1PI vertices are given in Appendix C.

In Eq.\((112)\), we can see an advantage of using 1PI quantities to Eq.\((59)\). Even when higher-point vertex functions such, \( g_3 \) and \( g_4 \), are replaced by the ideal gas vertices, long-range correlations in the multi-point correlation functions \( F_3 \) or \( F_4 \) can be at least partially taken into account through a product of two-point function \( F_2(x, y) \). Indeed, if we replace \( g_3 \) and \( g_4 \) by the ideal gas vertices and set \( k_2 = -k_1 \), Eq.\((112)\) becomes (we write \( \kappa(k) = \kappa(k, -k) \) and \( g_2(k) = g_2(k, -k) \))

\[
\left( \frac{\partial}{\partial \ln n} \bigg|_{T, N} + 1 + \frac{1}{d} k_1^\mu \frac{\partial}{\partial k_1^\mu} \right) g_2(k_1) = \left( \frac{\partial}{\partial n} n + \frac{1}{d} k_1^\mu \frac{\partial}{\partial k_1^\mu} \right) g_2(k_1)
= \frac{\beta}{d} \delta \tilde{v}(k_1) - \frac{1}{d n} \int \frac{d^dp}{(2\pi)^d} \kappa(p)^2 \beta \delta \tilde{v}(p) + \frac{1}{d n} \int \frac{d^dp}{(2\pi)^d} \kappa(p)^2 \kappa(k_1 + p) \beta \delta \tilde{v}(p). \tag{113}
\]

It is a closed equation for the two-point correlation function. Validity of the approximation to replace multi-point vertices by the ideal gas needs to be checked by studying the DRGEs for these vertices. Further details are studied in a separate paper.

5 Summary and Discussion

In this paper, we proposed a new formulation of statistical mechanic of classical liquid based on a scale transformation method. Scale transformations generate an analogue equation to the Ward-Takahashi identity of scale transformations in QFTs; and consequently we have obtained the density renormalization group equations (DRGEs). The set of equations describes response of various physical quantities and correlation functions to a change of the liquid density. The response itself depends on the density. Thus if we can integrate the equations from low to high density, we can accumulate the effects of finite density, which corresponds to a resummation of quantum effects in the renormalization group method in QFT.

The DRGEs are a set of differential equations which contain multi-point correlation functions. It is similar to the BBGKY hierarchy. Namely the equations must be appropriately closed at some orders. Hence, our next necessary step is to introduce reasonable approximations for higher order correlation functions. A simple but physically reasonable approximation is to replace higher order (more than 2-point functions) 1PI vertices by those of the ideal gas (times a density-dependent function). It will be reasonable because in this approximation multiple-correlation effects of the liquid can be partially taken into account. This approximation will be systematically improved by slightly taking nonlocal effects of multiple-point 1PI vertices. Also it is interesting to see how we can perform resummation of the virial expansion by solving DRGEs. We will investigate these issues in separate papers.
Acknowledgements

We would like to thank Yoshio Kuramoto for useful discussions. This work of SI is supported in part by Grants-in-Aid for Scientific Research (No. 16K05329) and (No. 18H03708) from the Japan Society for the Promotion of Science. The work of KK is supported by the Grant-in-Aid for JSPS Research Fellow, Grant Number 17J03848.

Appendix A  Correlation Functions of the Ideal Gas

In order to confirm the consistency of the DRGEs [27], we calculate the correlation functions for the ideal gas. In this case, the correlation functions must satisfy

\[ d \left( -\frac{\partial}{\partial (\beta \mu)} \right)_{T,V} + \frac{\partial}{\partial \ln V} + l + \frac{1}{d} \sum_{i=1}^{l} x_i^\mu \partial_{\mu} \right) F_l(x_1, \cdots, x_l) = 0, \tag{114} \]

which we will explicitly check in the following.

The grand canonical partition function with the external source \( U(x) \) can be evaluated as

\[ \Xi_{\text{ideal}}[U] = \sum_{N=0}^\infty \frac{z(\mu)^N}{N!} \int_V d^d x_1 \cdots d^d x_N \exp(\beta \sum_{i=1}^{N} U(x_i)) = \exp \left( z(\mu) \int d^d x e^{\beta U(x)} \right) \]

\[ \therefore -\beta W_{\text{ideal}}[U] = \log \Xi_{\text{ideal}}[U] = z(\mu) \int d^d x e^{\beta U(x)}. \tag{115} \]

Thus, the correlation functions are given by

\[ F_l(x_1, \cdots, x_l) = n \delta^{(d)}(x_2 - x_1) \delta^{(d)}(x_3 - x_1) \cdots \delta^{(d)}(x_l - x_1), \tag{116} \]

where \( n = z(\mu) = (2\pi m T)^{d/2} \). Thus, we have

\[ F_l((1 + \epsilon)x_1, (1 + \epsilon)\cdots, (1 + \epsilon)x_l) = n \delta^{(d)}((1 + \epsilon)(x_2 - x_1)) \delta^{(d)}((1 + \epsilon)(x_3 - x_1)) \cdots \delta^{(d)}((1 + \epsilon)(x_l - x_1)) \]

\[ = (1 - (l-1)\epsilon) F_l(x_1, \cdots, x_l), \]

\[ \therefore \sum_{i=1}^{l} x_i^\mu \partial_{\mu} F_l(x_1, \cdots, x_l) = -(l-1)dF_l(x_1, \cdots, x_l), \tag{117} \]

from which we can easily check that the LHS of Eq. (114) vanishes.

Next, let us consider the Legendre transformation. In the ideal gas case, we can easily find the minimum of \( -\beta W[U] \), and the resultant free energy is

\[ -\beta F[\rho] = \min_U (-\beta W[U] - \beta \int d^d x U(x) \rho(x)) \]

\[ = \int d^d x \left[ \rho(x) - \rho(x) \log \left( \frac{\rho(x)}{(2\pi m T)^{d/2}} \right) \right], \tag{118} \]
from which we obtain the following direct correlation functions:

\[ c_1(x) = -\log \left( \frac{n}{(2\pi m T)^{d/2}} \right), \quad c_2(x, y) = -\frac{\delta(d)(x - y)}{n}, \quad \cdots, \]

\[ c_l(x_1, \cdots, x_l) = \frac{(-1)^{l+1}(l-2)!}{n^{l-1}} \delta(d)(x_1 - x_l) \delta(d)(x_2 - x_l) \cdots \delta(d)(x_{l-1} - x_l). \] (119)

Thus, the log \( V \) derivative in Eq. (86) gives \( d(l - 1)c_l(x_1, \cdots, x_l) \) which is canceled by the third term in the LHS.

For the ideal gas, \( g_l(k_1, \cdots, k_l) \)'s defined by Eq. (106) are given by constants

\[ g_l(k_1, \cdots, k_l) = \frac{(-1)^{l+1}(l-2)!}{n^{l-1}} \] (120)

and do not have dependence on the external momenta.

Appendix B  Corrections to \( l = 3, 4 \) 1PI vertices

The correction to the \( l = 3 \) 1PI vertex \( \Delta c_3(x, y, z) \) is graphically given by

\[ \Delta c_3(x, y, z) = -\frac{1}{2} y \]

\[ + (x \leftrightarrow z) + (y \leftrightarrow z) \] (121)
The correction to the $l = 4$ 1PI vertex $\Delta c_4(x, y, z, w)$ is graphically given by

\[
\Delta c_4(x, y, z, w) = -\frac{1}{2} \left[ (x \leftrightarrow w) + (y \leftrightarrow w) + (z \leftrightarrow w) \right]
\]

\[
+ (x \leftrightarrow z) + (x \leftrightarrow w) + (y \leftrightarrow z) + (y \leftrightarrow w) + (x \leftrightarrow z \& y \leftrightarrow w) \right]
\]

\[
- 2 \left[ (x \leftrightarrow y) + (x \leftrightarrow z) + (y \leftrightarrow w) + (z \leftrightarrow w) + (x \equiv y \& z \equiv w) \right].
\]
Appendix C  DRGEs for $l = 3, 4$ 1PI vertices

The DRGE for $l = 3$ 1PI vertex can be read from Eq.(121) and given by

$$
\left. \left( \frac{\partial}{\partial \ln n} \right) \right|_{T,N} + 2 + \frac{1}{n} \sum_{i=1}^{3} k_i^\mu \frac{\partial}{\partial k_i^\mu} \right) g_3(k_1, k_2, k_3) = \left( \frac{1}{n} \frac{\partial}{\partial n} n^2 + \frac{1}{d} \sum_{i=1}^{3} k_i^\mu \frac{\partial}{\partial k_i^\mu} \right) g_3(k_1, k_2, k_3)
$$

$$
= \frac{1}{2d} \int \frac{dp}{(2\pi)^d} \frac{g_5(k_1, k_2, k_3, p, -p)}{g_2(p, -p)^2} \beta \delta \bar{v}(p) - \frac{1}{d} \left[ \int \frac{dp}{(2\pi)^d} \frac{g_4(k_1, k_2, p, -k_3 - p, k_3 - p)}{g_2(-k_3 + p, k_3 - p) g_2(p, -p)^2} \beta \delta \bar{v}(p) + (k_1 \leftrightarrow k_3) + (k_2 \leftrightarrow k_3) \right]
$$

$$
+ \frac{1}{d} \left[ \int \frac{dp}{(2\pi)^d} \frac{g_3(k_1, p, -k_1 - p, -k_2 - p) g_2(k_2, k_1 + p, k_2 - p) g_2(-k_3 + p, -p, k_3 - p) g_2(p, -p)^2}{g_2(k_1 + p, -k_1 - p) g_2(-k_3 + p, k_3 - p) g_2(p, -p)^2} \beta \delta \bar{v}(p) + (k_1 \leftrightarrow k_2) + (k_2 \leftrightarrow k_3) \right].
$$

(123)

For $l = 4$ 1PI vertex, the DRGE is given by

$$
\left. \left( \frac{\partial}{\partial \ln n} \right) \right|_{T,N} + 3 + \frac{1}{d} \sum_{i=1}^{4} k_i^\mu \frac{\partial}{\partial k_i^\mu} \right) g_4(k_1, k_2, k_3, k_4) = \left( \frac{1}{n^2} \frac{\partial}{\partial n} n^2 + \frac{1}{d} \sum_{i=1}^{4} k_i^\mu \frac{\partial}{\partial k_i^\mu} \right) g_4(k_1, k_2, k_3, k_4)
$$

$$
= \frac{1}{2d} \int \frac{dp}{(2\pi)^d} \frac{g_6(k_1, k_2, k_3, k_4, p, -p)}{g_2(p, -p)^2} \beta \delta \bar{v}(p) - \frac{1}{d} \left[ \int \frac{dp}{(2\pi)^d} \frac{g_5(k_1, k_2, k_3, k_4, p, -p)}{g_2(-k_4 + p, k_4 - p) g_2(p, -p)^2} \beta \delta \bar{v}(p) + (k_1 \leftrightarrow k_4) + (k_2 \leftrightarrow k_4) + (k_3 \leftrightarrow k_4) \right]
$$

$$
+ \frac{1}{d} \left[ \int \frac{dp}{(2\pi)^d} \frac{g_4(k_1, k_2, k_3, p, -k_1 - k_2 - p) g_4(k_1 + k_2, k_3, k_4, p)}{g_2(k_1 + k_2 + p, -k_1 - k_2 - p) g_2(-k_4 + p, k_4 - p) g_2(p, -p)^2} \beta \delta \bar{v}(p) + (k_1 \leftrightarrow k_3) + (k_1 \leftrightarrow k_4) + (k_2 \leftrightarrow k_3) + (k_2 \leftrightarrow k_4) + (k_1 \leftrightarrow k_3 & k_2 \leftrightarrow k_4) \right]
$$

$$
+ \int \frac{dp}{(2\pi)^d} \frac{g_4(k_1, k_2, k_3, -k_1 - k_2 - p) g_3(k_1 + k_2 + p, k_4, k_3 - p) g_3(-k_3 + p, k_4, k_3, p)}{g_2(k_1 + k_2 + p, -k_1 - k_2 - p) g_2(-k_3 + p, p, k_4 - p) g_2(p, -p)^2} \beta \delta \bar{v}(p) + (k_1 \leftrightarrow k_3) + (k_1 \leftrightarrow k_4) + (k_2 \leftrightarrow k_3) + (k_2 \leftrightarrow k_4) + (k_1 \leftrightarrow k_3 & k_2 \leftrightarrow k_4) \right]
$$

$$
+ \int \frac{dp}{(2\pi)^d} \frac{g_4(k_1, k_2, p, -k_1 - k_2 - p) g_3(k_1 + k_2, k_3, k_4, p) g_3(-k_3 + p, k_4, k_3, p)}{g_2(k_1 + k_2 + p, -k_1 - k_2 - p) g_2(-k_3 + p, k_4 - p) g_2(p, -p)^2} \beta \delta \bar{v}(-k_4 + p, k_4, -p)
$$

$$
+ (k_1 \leftrightarrow k_3) + (k_1 \leftrightarrow k_4) + (k_2 \leftrightarrow k_3) + (k_2 \leftrightarrow k_4) + (k_1 \leftrightarrow k_3 & k_2 \leftrightarrow k_4) \right].
$$

(124)

Here, $(k_1 \leftrightarrow k_2)$ represents interchanging $k_1$ and $k_2$. The sign $(k_1 \leftrightarrow k_2 & k_3 \leftrightarrow k_4)$ means interchanging both of $(k_1, k_1)$ and $(k_3, k_3)$. 

31
References

[1] J.A. Barker and D. Henderson, What is liquid? Understanding the states of matter, Rev. Mod. Phys. 48, 587-671 (1967)

[2] J.-P. Hansen and I. R. McDonald, Theory of Simple Liquids (Elsevier Science, 2006).

[3] Clisby, N., and B. M. McCoy, 2006, “Ninth and Tenth Order Virial Coefficients for Hard Spheres in D Dimensions, J. Stat. Phys. 122, 15 - 57.

[4] J.K. Percus and G.J. Yevick, “Analysis of classical statistic mechanics by means of collective coordinates”, Phys. Rev. 110, 1-13 (1958).

[5] M. S. Wertheim, Exact solution of the Percus-Yevick integral equation for hard spheres, Phys. Rev. Lett. 10, 321 - 323 (1963).

[6] E. Thiele, Equation of state for hard spheres, J. Chem. Phys. 39, 474 - 479 (1963).

[7] L. Verlet and D. Levesque, “On the theory of classical fluids VI”, Physica 36, 254 (1967).

[8] L. Verlet, “Computer ”Experiments” on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules”, Phys. Rev. 159, 98 (1967).

[9] T. Morita, “Theory of Classical Fluids: Hyper-Netted Chain Approximation, I: Formulation for a One-Component System”, Prog. Theor. Phys. 20 (1958), 920.

[10] T. Morita, “Theory of Classical Fluids: Hyper-Netted Chain Approximation. III: A New Integral Equation for the Pair Distribution Function”, Prog. Theor. Phys. 23, 829 (1960).

[11] T. Morita and K. Hiroike, “A New Approach to the Theory of Classical Fluids. I”, Prog. Theor. Phys. 23, 1003 (1960).

[12] J.M.J. van Leeuwen, J. Groeneveld, and J. De Boer, “New method for the calculation of the pair correlation function. I”, 1959, Physica 25, 792.

[13] D. Henderson, W. G. Madden, and D. D. Fitts, “Monte Carlo and hypernetted chain equation of state for the squarewell fluid”, J. Chem. Phys. 64, 5026 (1976).

[14] N.N. Bogolyubov, ”Kinetic Equations”, J. Phys. (URSS) 10, 256 (1946).

[15] N. N. Bogoliubov, “The Dynamical Theory in Statistical Physics”, Hindustan Pub. Corp., Delhi, 1965.

[16] H. Born, H. S. Green, “A General Kinetic Theory of Liquids”, Proc. Roy. Soc. A188 (1946) 10.

[17] J. G. Kirkwood, “Statistical Mechanics of Fluid Mixtures”, J. Chem. Phys. 3, 300 (1935).

[18] J. Yvon, “Actualities Scientijiques et Indillstrielles”, Hermann and Cie, Paris, 1935.

[19] J. G. Kirkwood, “The Statistical Mechanical Theory of Transport Processes I. General Theory”, J. Chem. Phys. 14 (1946) 180.
[20] B. Schrodt and K. D. Luks, “Square-Well Potential. I. An Yvon-Born-Green Square-Well Equation of State”, J. Chern. Phys. 57, 200 (1972).

[21] Y. Nambu, “THERMODYNAMICAL ANALOGY IN QUANTUM FIELD THEORY”, Phys. Reports 104 (1984) 237.

[22] A. Parola and L. Reatto, “Hierarchical reference theory of fluids and the critical point”, Phys. Rev. A 31 (1985) 3309.

[23] A. Parola and L. Reatto, “Liquid state theories and critical phenomena”, Adv. in Phys. 44 (1995) 211.

[24] J. M. Caillol, “Non-Perturbative Renormalization Group for Simple Fluids”, Mol. Phys. 104, 1931 (2006).

[25] J. Hubbard and P. Schofield, “Wilson theory of a liquid-vapour critical point”, Phys. Lett. 40A (1972) 245.

[26] R. Zwanzig, “High-Temperature Equation of State by a Perturbation Method. I. Nonpolar Gases”, J. Chem. Phys. 22, 1420 (1954).

[27] J. A. Barker and D. Henderson, “Perturbation Theory and Equation of State for Fluids: The Square-Well Potential”, J. Chem. Phys. 47, 2856 (1967).

[28] J. Berges, “Introduction to nonequilibrium quantum field theory,” AIP Conf. Proc. 739, 3 (2005) doi:10.1063/1.1843591 [hep-ph/0409233].