RENORMALIZATION OF THE GAS-LIQUID TRANSITION

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I. The flow equations

The understanding of the mechanism of phase transitions and critical phenomena has deepened substantially by the renormalization approach. The spectacular success of the field theoretic methods in calculating the universal properties \(^1\)\(^-\)\(^4\) and the power of real space renormalization in computing phase diagrams \(^5\),\(^6\) has brought the feeling that most of the problems of phase transitions have now been understood.

The theory of the gas-liquid phase transition has the oldest history starting with the van der Waals equation. Several approximation schemes have subsequently been developed which are able in varying degree of success to locate critical points and phase boundaries but which all predict the classical universal properties. There is little doubt however about the universality class to which the gas-liquid transition belongs as its order parameter (the density) has one component and therefore its universality class should be the same as that of Ising models. This gives an independent means of determining the universal properties as the Ising model is optimally suited for series-analysis of its critical properties. The experiments confirm the universal predictions of the renormalization theory and the analysis of the Ising model.

We have now a situation where both universal and non-universal properties of the gas-liquid transition are well understood. But a theory encompassing a complete picture does not exist. The Landau-Ginzburg-Wilson description of the fluid is not in a transparant way connected to its microscopic properties as e.g. the interparticle potential. The Ising description of the fluid through the lattice gas is too simple a model for a fluid to produce also the location of the phase transition accurately.

A theory which gives a complete picture of the fluid will be hard to conceive but it would be desirable to have a description which is comparably accurate to the classical approximation further away and comparably accurate to real space renormalization theories in the vicinity of the phase transition. Such a description would yield valuable information of the size of the critical region where the properties are universal and of the crossover to nonuniversal behavior further away from criticality.
In our opinion it would be most desirable that a renormalization procedure could be formulated on a microscopic level involving particle positions as variables and particle interactions as hamiltonian. Such a scheme should in no way use a lattice in order to acknowledge fully the character of the particle positions as continuous variables.

There has been a limited effort in applying the renormalization techniques directly to fluids. Schofield and Hubbard have constructed a map by which the fluid properties are associated with an Ising model. M.S. Green studied the problem in the context of MacMillans solution theory and this thesis is in spirit most similar to Green's attempt (cf. also Parola and Reatto).

A naive approach would be a transcription of the real space renormalization for Ising systems to fluids through the lattice gas. One could imagine the continuous space subdivided in a cell-like partitioning and mimic in such a way an Ising model: an occupied cell is a spin +1 and an empty cell a spin -1. In the transition to the continuum limit this would lead however to a totally unmanageable Ising model. Real particles have a strong repulsion for short distances (hard core) and the lattice gas would become extremely dilute in cell occupation as well as the interaction of the particles extremely long ranged when measured in cell distances. It is well known that extension of the core in the lattice gas (e.g. hard hexagons) leads to complications where the lattice structure more tends to represent the solid than the liquid arrangement.

Nevertheless the renormalization scheme we propose for the fluid is inspired on the existing procedures in the Ising model. First of all it has the basic ingredients one would expect from any renormalization technique: reduction of the number of degrees of freedom under simultaneous reduction of the size of the system. Already in this respect there is however a fundamental difference between the Ising model and the fluid. In the Ising model a combination of spins to a block spin immediately dictates the reduction of the size of the system as the ratio of block distance to site distance. In the fluid there exists, as we will show, an exact scale equivalence which allows to reduce the size (volume) of the system arbitrarily and unrelated to the reduction of the number of degrees of freedom.
Secondly we will try to reduce the degrees of freedom in such a way that the cluster structure near criticality is self-similar on original and renormalized scale. This is the hard part and concerns finding an equivalent of e.g. the majority rule in Ising systems. We will achieve this in essence by the principle of weighted decimation.

The renormalization approach of course is not satisfied with a formal approach. The method of implementation of the renormalization scheme is essential. One of the most powerful and versatile methods is the Monte Carlo Renormalization [11], combining renormalization ideas and Monte Carlo simulations. The attractive feature of this method is that it does not require the difficult task of finding the fixed points but it is sufficient that the procedure allows to make a connection between renormalized and original degrees of freedom. To apply Monte Carlo Renormalization to the fluid was one of our motivations to set up a Renormalization Scheme which can be used for fluid simulations.

From the Ising model it is well known that simple decimation does not lead to satisfactory renormalization and the difficulties as well as the means to overcome these are studied in this chapter. By introducing weights in the decimation process we can cure the difficulties of decimation as well as deal with another intrinsical problem of the fluid: how to conserve the hard core of the interaction under renormalization. It is obvious that the reduction of spatial distances will tend to decrease the core size and this is another drawback of simple decimation as we will show.

In this chapter we derive renormalization flow equations which on the one hand are explicit and on the other hand are sufficiently general to cope with the above-mentioned problems for the fluid. In section 1.1 we will give the necessary definitions for the fluid properties. In section 1.2 we outline the most general transformations and the reduction to flow equations by studying the infinitesimal generators. This is a feature where the fluid distinguishes itself favorably from the Ising model where due to the lattice structure infinitesimal transformation can seldom be realised. The advantage is that the structure of the infinitesimal transformation can be made explicit in contrast to finite transformations.
In section 1.3 and section 1.4 we define the two basic ingredients: spatial rearrangement and weighted decimation. The general transformations can always be decomposed in a weighted decimation and a rearrangement of the remaining particles. Section 1.5 is devoted to the consequences for the correlation functions. From this and additional requirements the global properties of the decimation weights can be deduced. The chapter closes with a discussion and an outline of the consequences of the flow equations to be studied in later chapters.
1.1. Description of the classical fluid in d-dimensions

For the description of the state of the fluid, we start with the definition of the N-particle Hamiltonian $H$:

$$ H(p_1,\ldots,p_N, r_1,\ldots, r_N) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \Phi(r_1,\ldots, r_N) \quad (1.1.1) $$

The potential $\Phi$ is a function of the N-dimensional coordinates $r_i$ only. $\Phi$ can be separated into one-, two- and more-particle contributions:

$$ \Phi(r_1,\ldots, r_N) = -\sum_i \mu(r_i) + \sum_{i<j} \psi(r_i, r_j) + \cdots \psi(r_1,\ldots, r_N). \quad (1.1.2) $$

The one-particle potential is called $-\mu(r)$ in view of its role as the chemical potential. For spatially homogeneous systems $\mu$ is a constant and the $\psi(r_i, r_j)$ ($j \geq 2$) are translational invariant. We assume the $\psi(r_i, r_j)$ ($j \geq 2$) to have cluster properties, i.e. to vanish sufficiently fast for all $r_i$ well separated. Moreover we will assume that $\Phi$ has a "hard core", i.e. that $\Phi$ goes to infinity very fast when particles approach each other too closely. This property guarantees that the fluid is not compressible to arbitrary small volumes.

The thermodynamics of the fluid will be described in the grand-canonical formalism. Doing the momentum integrations and absorbing factors like $m$, $\hbar$ etc. in $\mu$ gives us the following grand-canonical partition function:

$$ Z_{gc}(\Phi, V, T) = e^{\frac{pV}{k_BT}} = \sum_{N=0}^{\infty} \frac{1}{N!} \int_V dr_1 \ldots dr_N \psi(r_1,\ldots, r_N) \quad (1.1.3) $$

The Boltzmann weight $W$ is defined by:

$$ W(r_1,\ldots, r_N) = \exp \left\{ -\frac{1}{k_BT} \Phi(r_1,\ldots, r_N) \right\} \quad (1.1.4) $$
Hereafter the factor $k_BT$ is incorporated in the potential $\Phi$, the pressure $p$ and the chemical potential $\mu$. The minus sign in (1.1.4) is as well incorporated in the $\Phi(r_1 \ldots r_{j-1})$ ($j \geq 2$).

The quantity $\rho(r_1 \ldots r_N)$ defined by

$$
\rho(r_1 \ldots r_N) = \frac{1}{N!} e^{-pV} W(r_1 \ldots r_N)
$$

(1.1.5)

is the properly normalized probability density for finding the $N$-particle configuration $\{r_1 \ldots r_N\}$. This function will be the object of the renormalization procedure, introduced in the next sections.

Next we define the usual reduced probability functions $n(r_1 \ldots r_k)$:

$$
n(r_1 \ldots r_k) = \sum_{N=k}^{\infty} \frac{N!}{(N-k)!} \int \frac{d\mathbf{r}_{k+1} \ldots d\mathbf{r}_N}{N!} \rho(r_1 \ldots r_N)
$$

(1.1.6)

The $k$-particle correlation function $g(r_1 \ldots r_k)$ then follows as:

$$
g(r_1 \ldots r_k) = n(r_1 \ldots r_k) / [n(r_1) \ldots n(r_k)]
$$

(1.1.7)

The correlation functions have the property of approaching 1 when all the positions $\mathbf{r}_i$ are well separated in a spatially homogeneous system with short ranged potentials. At the critical point the approach to 1 is slow and governed by a singular power of the distance, e.g. the two point correlation function is known to decay as:

$$
g(r_1, r_2) = 1 + A_2 \frac{1}{|r_1 - r_2|^{d-2+\eta}}, \quad |r_1 - r_2| \to \infty
$$

(1.1.8)

In the next section we introduce a stochastic process which will enable us to define a renormalization procedure.
1.2. **General form of the renormalization scheme**

The renormalization scheme will essentially be defined as an operation which reduces the degrees of freedom and the size of the system. Hamiltonians using spin variables are usually renormalized by defining block spin variables, being combinations of site variables. Most of these schemes used so far are projective, which means that a given configuration of site spins defines a unique configuration of block spins. In general, the schemes need not be projective, and our choice will use the possibility of defining the more general stochastic process as a renormalization procedure.

For this purpose we consider an operator $\mathcal{G}$ working on the configuration probability densities $\rho(\vec{r}_1, \ldots, \vec{r}_N)$ (1.1.5) with the following form:

$$\mathcal{G}: \rho'(\vec{r}_1, \ldots, \vec{r}_M) = \sum_{N=M}^{\infty} \int d\vec{r}_1 \ldots d\vec{r}_N \, \mathcal{P}(\vec{r}_1, \ldots, \vec{r}_M | \vec{r}_1, \ldots, \vec{r}_N) \rho(\vec{r}_1, \ldots, \vec{r}_N)$$  \hspace{1cm} (1.2.1)

We see from this that $\mathcal{G}$ links a configuration to a new one with equal or lesser particles. The process should have the following properties:

- To assure that under $\mathcal{G}$ the $\rho$ stay normalized we require:

$$\sum_{M=0}^{N} \int d\vec{r}_1 \ldots d\vec{r}_M \, \mathcal{P}(\vec{r}_1, \ldots, \vec{r}_M | \vec{r}_1, \ldots, \vec{r}_N) = 1$$  \hspace{1cm} (1.2.2)

- To assure that $\rho$ remains positive we use positive functions $\mathcal{P}$:

$$\mathcal{P}(\vec{r}_1, \ldots, \vec{r}_M | \vec{r}_1, \ldots, \vec{r}_N) \geq 0 \quad \forall \vec{r}_1, \ldots, \vec{r}_M, \vec{r}_1, \ldots, \vec{r}_N$$  \hspace{1cm} (1.2.3)

Eqs. (1.2.1), (1.2.2), (1.2.3) together define a stochastic process. $\mathcal{G}$ is defined by the transition probability density $\mathcal{P}(\vec{r}_1, \ldots, \vec{r}_M | \vec{r}_1, \ldots, \vec{r}_N)$ of going from the $N$-particle configuration $\{\vec{r}_1\}$ to the $M$-particle configuration $\{\vec{r}_1\}$. The fact that we have only non-zero $\mathcal{P}$ for $M \leq N$ enables us to denote the process $\mathcal{G}$ as a renormalization process. Note that projective renormalization procedures are a special case of this general form.

Equation (1.2.1) defines what is called the renormalization transformation.
Equation (1.2.1) contains a hierarchy (as $M \leq N$) of equations of which we write down the first few:

$M = 0$:

$$
\rho'(\cdot) = e^{-p'V'} = e^{-pV} \sum_{N=0}^{\infty} \frac{1}{N!} \int dr_1^r, .. dr_N^r \mathbb{P}(\cdot | r_1^r, .. r_N^r) W(r_1^r, .. r_N^r) \tag{1.2.4a}
$$

$M = 1$:

$$
\rho'(r_1^r) = e^{-p'V'+\mu'(r_1^r)} = e^{-pV} \sum_{N=1}^{\infty} \frac{1}{N!} \int dr_1^r, .. dr_N^r \mathbb{P}(r_1^r | r_1^r, .. r_N^r) W(r_1^r, .. r_N^r) \tag{1.2.4b}
$$

$M = 2$:

$$
\rho'(r_1^r, r_2^r) = \frac{1}{2} e^{-p'V'+\mu'(r_1^r)+\mu'(r_2^r)} e^{\varphi'(r_1^r, r_2^r)} = e^{-pV} \sum_{N=2}^{\infty} \frac{1}{N!} \int dr_1^r, .. dr_N^r \mathbb{P}(r_1^r, r_2^r | r_1^r, .. r_N^r) W(r_1^r, .. r_N^r) \tag{1.2.4c}
$$

etc.

Eq. (1.2.4a) is similar to changes in the free energy in spin models, with $p$ replacing the free energy. The $\ell$-th equation can be viewed as the defining equation for $\varphi'(r_1^r, r_2^r)$, since it appears for the first time in the $\ell$-th equation. A $N$-body potential couples to all other potentials. Generally, if at the beginning $\Phi$ consists of two-body contributions $\varphi(r_1^r, r_j^r)$ only, one renormalization step will produce arbitrary high $N$-body potentials $\varphi(r_1^r, .. r_N^r)$.

To remain in the class of functions $\Phi$, discussed in section 1.1 we have to give certain properties to the functions $\mathbb{P}$, like:
- $\mathbb{P}$ itself must have cluster properties to assure that the $\varphi'(r_1^r, r_2^r)$ have cluster properties.
- $\mathbb{P}$ must conserve the hard core properties of the potentials.

At this point we want to mention a special property of the fluid functions. The $\rho'(r_1^r, r_N^r)$ are functions of the continuous variables $r_1^r$, in contrast to
spin variables at the lattice points. In spin systems it is therefore hard to define a renormalization scheme which is continuous in "time". In the fluid this is different.

The stochastic process characterized by the transition probability density \( P \) can be made continuous by defining the transition rate \( T \) in the usual way:

\[
P_{\Delta t}(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o, \vec{r}_N^o) = \sum_{MN} \delta(\vec{r}_1^f - \vec{r}_1^o) \cdots \delta(\vec{r}_N^f - \vec{r}_N^o) + T(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o, \vec{r}_N^o) \Delta t \quad (1.2.5)
\]

The renormalization transformation then becomes a differential equation, which will be called the renormalization flow equation:

\[
\frac{d}{dt} \rho(\vec{r}_1^f, \vec{r}_N^f) = \sum_{MN} \int d\vec{r}_1^o \cdots d\vec{r}_N^o T(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o \cdots \vec{r}_N^o) \rho(\vec{r}_1^o, \vec{r}_N^o) \quad (1.2.6)
\]

Eqs. (1.2.2) and (1.2.3) have their equivalence for \( T \) in:

\[
\sum_{M=0}^{N} \int d\vec{r}_1^o \cdots d\vec{r}_M^o T(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o \cdots \vec{r}_N^o) = 0 \quad (1.2.7)
\]

\[
T(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o \cdots \vec{r}_N^o) \geq 0 \quad \text{if} \quad M \neq N \quad (1.2.8)
\]

For \( T \) the same remarks apply as for \( P \), concerning the cluster properties, the hard core etc.

Eq. (1.2.6) has some advantage above eq. (1.2.1) because:

- It can be written as a flow of the potentials. As \( \dot{\Phi} = \dot{W}/W \) we find:

\[
\frac{W(\vec{r}_1^f, \vec{r}_N^f)}{M!} \frac{d}{dt} [\Phi(\vec{r}_1^f, \vec{r}_M^f) - pV] = \sum_{MN} \int d\vec{r}_1^o \cdots d\vec{r}_N^o T(\vec{r}_1^f, \vec{r}_N^f | \vec{r}_1^o \cdots \vec{r}_N^o) \frac{W(\vec{r}_1^f, \vec{r}_N^f)}{N!} \quad (1.2.9)
\]

In the next section we will show that (1.2.9) can be worked out further.
The sum of two transition rates is again a transition rate. This means that we can study different processes and later on combine them to form a final scheme. Of course (1.2.1) defines a wider class of processes than (1.2.6). Nevertheless it does not seem a large restriction to consider the infinitesimal generators only; so from now on we will mainly concentrate on the renormalization flow (1.2.6) and define a few basic processes in the next sections.
1.3. Spatial rescaling and spatial rearrangements

In section 1.1 we have defined the fluid state. The spatial scale of the fluid can be varied with trivial concomitant changes in the pressure $p$, the volume $V$ and the chemical potential $\mu$. The transformation of scaling by a factor $b$ and its consequences are:

\[(r'_i)_b = r_i / b \Rightarrow V_b = V / b^d, \quad p_b = p b^d, \quad \mu_b = \mu + \log b^d\]

\[
\begin{align*}
\varphi_b((r'_1)_b, \ldots, (r'_j)_b) &= \varphi(r_1 \cdots r_j), \\
\Xi_b((r'_1)_b, \ldots, (r'_j)_b) &= \Xi(r_1 \cdots r_j)
\end{align*} \tag{1.3.1}
\]

Spatial rescaling will be used, as in spin models, after each renormalization step. The new system can then be compared with the old system. Rescaling therefore builds in the possibility of fixed points under the renormalization transformation.

Uniform spatial rescaling as (1.3.1) is an example of a transformation of $N$ to $N$ particle configurations. The remaining part of this section deals with a generalization of rescaling called spatial rearrangement. The starting point is equation (1.2.1) for $M = N$:

\[
\mathcal{P} : \rho'(r'_{1\cdots N}) = \int dr'_{1\cdots N} \mathcal{P}(r'_{1\cdots N}|r_{1\cdots N}) \rho(r_{1\cdots N}) \tag{1.3.2}
\]

The transformation $\mathcal{P}$ is chosen such that particles are moved over an infinitesimal distance from old to new positions according to some velocity field $\vec{v}_i(r'_{1\cdots N})$:

\[
\mathcal{P}_{\Delta t}(r'_{1\cdots N}|r_{1\cdots N}) = \prod_{i=1}^N \delta(r_{i'} - r_i - \vec{v}_i(r_{1\cdots N}) \Delta t) \quad (\Delta t \to 0) \tag{1.3.3}
\]
The resulting flow can be viewed as a conservation of probability with the quantity $\bar{\mathbf{v}}_i p$ as the probability current:

$$\dot{\rho}_i (\mathbf{r}_T, \mathbf{r}_N) = - \sum_{i=1}^{N} \bar{\mathbf{v}}_i \cdot (\bar{\mathbf{v}}_i \rho (\mathbf{r}_T, \mathbf{r}_N)) \quad N = 1, 2, \ldots \quad (1.3.4)$$

The flow equation (1.3.4) can be written in terms of the potentials as:

$$\frac{d}{dt} [\Phi(\mathbf{r}_T, \mathbf{r}_N) - p \mathbf{v}] = - \sum_{i=1}^{N} \bar{\mathbf{v}}_i \Phi (\mathbf{r}_T, \mathbf{r}_N) \cdot \bar{\mathbf{v}}_i (\mathbf{r}_T, \mathbf{r}_N) - \sum_{i=1}^{N} \bar{\mathbf{v}}_i \cdot \bar{\mathbf{v}}_i (\mathbf{r}_T, \mathbf{r}_N) \quad (1.3.5)$$

Uniform spatial rescaling is a special case. The choice $\bar{\mathbf{v}}_i = -\mathbf{r}_i$ gives the infinitesimal equivalent of (1.3.1) (the subscript $s$ denotes that we deal with scaling):

$$\dot{p}_s = dp, \quad (1.3.6^a)$$

$$\dot{\mu}_s = d, \quad (1.3.6^b)$$

$$\dot{\Phi}_s (\mathbf{r}_T, \mathbf{r}_N) = \sum_{i=1}^{N} \mathbf{r}_i \cdot \bar{\mathbf{v}}_i \Phi (\mathbf{r}_T, \mathbf{r}_N) \quad (1.3.6^c)$$

In the more general case we have a velocity field $\bar{\mathbf{v}}_i$ which depends on more than one particle, and which is translationally invariant for spatially homogeneous systems. The functions $\bar{\mathbf{v}}_i (\mathbf{r}_1, \ldots, \mathbf{r}_N)$ should be chosen such that (1.3.5) changes the potentials $\Phi$, but does not destroy its general properties. For mathematical simplicity we consider velocity fields that are derivable from a potential $\Psi$:

$$\bar{\mathbf{v}}_i (\mathbf{r}_1, \ldots, \mathbf{r}_N) = - \bar{\mathbf{v}}_i \Psi (\mathbf{r}_1, \ldots, \mathbf{r}_N) \quad (1.3.7^a)$$

for which the expansion exists:
\[ \Psi(r_1, \ldots, r_N) = \sum_{i=1}^{N} \phi_1(r_i) + \sum_{1<j} \phi_2(r_i, r_j) + \ldots \] (1.3.7b)

Note that uniform spatial rescaling uses \( \phi_1(r) = \frac{1}{r^n} \). We will restrict the term spatial rearrangements to the case when \( \phi(r_1, \ldots, r_N) \) goes to zero (fast enough to be integrable) when the particles are well separated (i.e. the first term in (1.3.7b) yields the spatial rescaling and the other terms the spatial rearrangements). This means that spatial rearrangement does not change the pressure or the chemical potential (which is easily seen by putting \( N = 0 \) and \( 1 \) in (1.3.5)). The flow equation for spatial rearrangement (denoted by a subscript \( R \)) then becomes:

\[ \dot{\rho}_R = \dot{\mu}_R = 0 \] (1.3.8a)

\[ \dot{\psi}_R(r_1, \ldots, r_N) = \left( \sum_{i=1}^{N} \nabla_i \phi_1 \cdot \nabla_i + \sum_{i=1}^{N} \nabla_i^2 \right) \Psi(r_1, \ldots, r_N) (N = 1, 2, \ldots) \] (1.3.8b)

As a special case we write down the hierarchy when \( \phi_2 \) is the only contribution in (1.3.7b):

\[ \dot{\psi}(r_1, r_2) = \dot{\psi}(r_1, r_2) = 2 \frac{\partial \phi_2}{\partial r_{12}} (r_{12}) + 2\nu_1 \psi_2 (r_{12}) \] (1.3.9a)

\[ \dot{\psi}(r_1, r_2, r_3) = \nabla_1 \psi_2 (r_{12}) \cdot \nabla_1 \psi_2 (r_{13}) + \nabla_1 \psi_2 (r_{13}) \cdot \nabla_1 \psi_2 (r_{12}) \]

\[ + \nabla_3 \psi_2 (r_{13}) \cdot \nabla_3 \psi_2 (r_{23}) + \text{terms involving 3-body potentials} \] (1.3.9b)

\[ \dot{\psi}(r_1, \ldots, r_j) = \text{sum of terms involving (j-1)- and j-body potentials} \] (1.3.9c)

We see that hierarchy stops when there are no higher body potentials \( \Psi(r_1, \ldots, r_j) \) (\( j \geq 3 \)).
Uniform rescaling and spatial rearrangement will be used together with the decimation process of the next section to define a complete renormalization scheme. We want to reiterate here that there is a great advantage in using transition rates, since addition of several transition rates $T$ results in a new transition rate, which defines a full renormalization scheme. Moreover the infinitesimal generators $T$ of such processes can be written down explicitly.
1.4. **Weighted decimation**

This section will be used to define renormalization transformations to which we will refer as weighted decimation. The idea is that particles will be left out of the system with a probability depending on the state of that system. A special case is the decimation of only one particle. Many particle decimation can in most cases be seen as repetitions of this basic step. The transition rate $T$ defined in section 1.2 for this process consists of gain terms ($N \rightarrow N-1$) and loss terms ($N \rightarrow N$), which are determined by the gain terms. They respectively are:

$$
T\left(\vec{r}_1 \ldots \vec{r}_N | \vec{r}_1 \ldots \vec{r}_N \right) = \sum_{j=1}^{N} S(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N) \delta(\vec{r}_j - \vec{r}_1) \ldots \delta(\vec{r}_{j-1} - \vec{r}_{j+1}) \ldots \delta(\vec{r}_{N-1} - \vec{r}_N) 
$$

(1.4.1a)

$$
T\left(\vec{r}_1 \ldots \vec{r}_N | \vec{r}_1 \ldots \vec{r}_N \right) = -\left( \sum_{j=1}^{N} S(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N) \right) \delta(\vec{r}_1 - \vec{r}_1) \ldots \delta(\vec{r}_{N} - \vec{r}_{N}) 
$$

(1.4.1b)

$S(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N)$ is the rate with which $j$ is eliminated in the configuration $(\vec{r}_1 \ldots \vec{r}_N)$.

We see that (1.4.1a) and (1.4.1b) are such that (1.2.7) holds. Furthermore we must assume that the function $S$ is positive in view of (1.2.8) The $\delta$-functions simplify the flow equations for the potentials (1.2.9) considerably:

$$
\frac{d}{dt} [\Phi(\vec{r}_1 \ldots \vec{r}_N) - pv] = -\sum_{j=1}^{N} S(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N) + 
$$

$$
\int d\vec{r} \frac{W(\vec{r} \ldots \vec{r}_N)}{W(\vec{r}_1 \ldots \vec{r}_N)}
$$

(1.4.2)

If we want the cluster properties (1.1.2) to hold for $\Phi$, $S$ must be expandable as:
\[ S(\vec{r}; \vec{r}_1, \ldots, \vec{r}_N) = s + \sum_{i} s(\vec{r}; \vec{r}_i) + \sum_{i < j} s(\vec{r}; \vec{r}_i \vec{r}_j) + \ldots s(\vec{r}; \vec{r}_1, \ldots, \vec{r}_N) \]  

(1.4.3)

In a homogeneous system \( s(\vec{r}; \vec{r}_1, \ldots, \vec{r}_j) \) should be translational invariant. Equation (1.4.2) defines a hierarchy (like (1.2.4)) for the flow of \( p \), \( \mu \), and the \( \phi \), which can be written down using the following notation:

\[ f(\vec{r}_1, \ldots, \vec{r}_j) = e^{\phi(\vec{r}_1, \ldots, \vec{r}_j)} - 1, \quad z = e^\mu, \]  

(1.4.4)

the functions \( f(\vec{r}_1, \ldots, \vec{r}_j) \) are called the Mayer functions and \( z \) the fugacity.

The flow equations are:

\[ \dot{p} = -sz \]  

(1.4.5a)

\[ \dot{z} = -s + z \int d\vec{r}_2 \left[ sf(\vec{r}_{12}) + s(\vec{r}_2; \vec{r}_1)e^{\phi(\vec{r}_{12})} \right] \]  

(1.4.5b)

\[ \dot{\phi}(\vec{r}_{12}) = -[s(\vec{r}_2; \vec{r}_1) + s(\vec{r}_1; \vec{r}_2)] + z \int d\vec{r}_3 \left[ sf(\vec{r}_{13})f(\vec{r}_{23}) + s(\vec{r}_3; \vec{r}_1)e^{\phi(\vec{r}_{13})}f(\vec{r}_{23}) + s(\vec{r}_3; \vec{r}_2)e^{\phi(\vec{r}_{23})}f(\vec{r}_{13}) + s(\vec{r}_3; \vec{r}_1) e^{\phi(\vec{r}_{13})\phi(\vec{r}_{23})} + \right. \]  

\[ \left. + \chi(\vec{r}_{13}) + \chi(\vec{r}_{23}) \right] (1.4.5c) \]

\[ \dot{\phi}(\vec{r}_{12}\vec{r}_3) = -[s(\vec{r}_3; \vec{r}_1) + s(\vec{r}_2; \vec{r}_3) + s(\vec{r}_1; \vec{r}_2) + s(\vec{r}_1; \vec{r}_3)] + z \int d\vec{r}_4 \left[ sf(\vec{r}_{14})f(\vec{r}_{24})f(\vec{r}_{34}) + s(\vec{r}_4; \vec{r}_1) e^{\phi(\vec{r}_{14})}f(\vec{r}_{24})f(\vec{r}_{34}) + \ldots s(\vec{r}_4; \vec{r}_1) e^{\phi(\vec{r}_{14})\phi(\vec{r}_{24})\phi(\vec{r}_{34})} + \chi(\vec{r}_{14}) + \chi(\vec{r}_{24}) + \chi(\vec{r}_{34}) \right] + \text{terms involving} \]  

\[ f(\vec{r}_1\vec{r}_2\vec{r}_3), f(\vec{r}_1\vec{r}_3\vec{r}_4), f(\vec{r}_2\vec{r}_3\vec{r}_4) \text{ and } f(\vec{r}_1\vec{r}_2\vec{r}_3\vec{r}_4) \]  

(1.4.5d)

etc.
We see that the equation for $\dot{\phi}(r_1, ..., r_j)$ couples to the $\phi(r_1, ..., r_j)$ for $j \leq \mathbb{Z}$. In general it is such that if at $t = 0$, $\phi$ consists of two body potentials $\phi(r_{1j})$ only, the $\phi(r_1, ..., r_j)$ with $j \geq 3$ will be produced for $t > 0$ unless by a suitable choice of the weights $S$ this is prevented.

The flow equations (1.4.5) are explicit, which is a consequence of the differential formalism we used. This is in contrast with spin models where finite transformations are mostly used. They therefore lead to implicit transformations of the coupling constants, which only after approximations can be made explicit.
1.5. **The behavior of the correlation functions under renormalization**

The correlation functions, or the reduced probability densities, change under renormalization. In this section we will derive a hierarchy for the correlation function flow. The starting point is the differentiation of equation (1.2.7) for \( \phi(r_1 \ldots r_N) \) with respect to \( t \). The result is:

\[
\dot{\phi}(r_1 \ldots r_N) = e^{-pV} \sum_{N=1}^\infty \frac{1}{(N-1)!} \int dr_{N+1} \ldots dr_N W(r_1 \ldots r_N) \frac{d}{dt} \left[ \phi(r_1 \ldots r_N) - pV \right] \tag{1.5.1}
\]

This is to be used in conjunction with the flow equations for the potentials (1.2.9) in which one should substitute (1.3.5) or (1.3.8) successively for spatial rearrangement and (1.4.2) for weighted decimation. We do this in the following subsections starting with spatial rescaling.

1.5.1. **Spatial rescaling**

When we substitute in (1.5.1) the flow equation for spatial rescaling (\( s \) means scaling):

\[
\dot{\phi}_s(r_1 \ldots r_N) = [N d + \sum_{i=1}^N r_i \dot{V}] \phi_s(r_1 \ldots r_N) \tag{1.5.2}
\]

it gives for \( \dot{n}(r_1 \ldots r_N) \):

\[
\dot{n}_s(r_1 \ldots r_N) = [d + \sum_{i=1}^l r_i \dot{V}] n_s(r_1 \ldots r_N) \tag{1.5.3}
\]

and for the correlation functions \( g(r_1 \ldots r_N) \):

\[
\dot{g}_s(r_1 \ldots r_N) = \sum_{I=1}^l \frac{r_I \dot{V}}{r_I} g_s(r_1 \ldots r_N) \tag{1.5.4}
\]

We see that the correlation functions are just rescaled as the \( \phi(r_1 \ldots r_N) \).
1.5.2. Spatial rearrangement

The general case of spatial rearrangement is given by equation (1.3.4)
or (1.3.5). When this is inserted into (5.1) we get (R means rearrangement):

\[ \frac{d N}{d t} (\mathbf{r}_1, \ldots, \mathbf{r}_L) = - \sum_{i=1}^{L} \left( \frac{\partial}{\partial \mathbf{r}_i} \psi \right) e^{-pV} \sum_{N=L}^{\infty} \frac{1}{(N-L)!} \int d\mathbf{r}_{L+1} \ldots d\mathbf{r}_N \psi_{1}(\mathbf{r}_1, \ldots, \mathbf{r}_N) W(\mathbf{r}_1, \ldots, \mathbf{r}_N) \]

(1.5.5)

If we use the potential \( \psi \) of equations (1.3.7a) and (1.3.7b) up to \( \psi_2 \) we obtain:

\[ \frac{d N}{d t} (\mathbf{r}_1, \ldots, \mathbf{r}_L) = \sum_{i=1}^{L} \left( \frac{\partial}{\partial \mathbf{r}_i} \psi \right) \left\{ \psi_{i}^{*}(\mathbf{r}_i) + \sum_{j \neq i}^{L} \psi_{j}(\mathbf{r}_i, \mathbf{r}_j) \right\} n(\mathbf{r}_1, \ldots, \mathbf{r}_L) + \int d\mathbf{r}_1 \psi_{2}(\mathbf{r}_1, \mathbf{r}_L) n(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_L) \]

(1.5.6)

The reduced probability density functions couple to those of one order higher. The same of course holds for the correlation functions. If we had used a potential \( \psi \) containing \( L \)-particle terms \( \psi_{L}(\mathbf{r}_1, \ldots, \mathbf{r}_L) \) there would have been a coupling between \( n(\mathbf{r}_1, \ldots, \mathbf{r}_L) \) and \( n(\mathbf{r}_1, \ldots, \mathbf{r}_k) \) for \( k \leq L+1 \).

1.5.3. Weighted decimation

When the flow equation for weighted decimation (1.4.2) is inserted into (1.5.1) we get (D stands for decimation):

\[ \frac{d N}{d t} (\mathbf{r}_1, \ldots, \mathbf{r}_L) = e^{-pV} \sum_{N=L}^{\infty} \frac{1}{(N-L)!} \int d\mathbf{r}_{L+1} \ldots d\mathbf{r}_N \left[ - \sum_{j=1}^{L} \frac{1}{S(\mathbf{r}_j; \mathbf{r}_1, \ldots, \mathbf{r}_j-1, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_N)} W(\mathbf{r}_1, \ldots, \mathbf{r}_N) \right. \]

\[ + \left. \int d\mathbf{r} S(\mathbf{r}; \mathbf{r}_1, \ldots, \mathbf{r}_N) W(\mathbf{r}_1, \ldots, \mathbf{r}_N) \right] \]

(1.5.7)
In the first summation between the brackets for \( N = M + 1 \) there are \((N-\ell)\) terms which are also present in the second summation for \( N = M \) (after relabeling). This means that those terms, where a \( \vec{r}_i \) with \( i = 1 \) to \( \ell \) is at the first entry in \( S \) (i.e. the position of the decimated particle), are the only terms that are not canceled. This results in:

\[
\hat{n}(\vec{r}_1 \ldots \vec{r}_\ell) = -e^{-pV} \sum_{N=\ell}^{N=M} \frac{1}{(N-\ell)!} \int d\vec{r}_{\ell+1} \ldots d\vec{r}_N [\sum_{j=1}^{\ell} S(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N)] W(\vec{r}_1 \ldots \vec{r}_N)
\] (1.5.8)

This can be simplified further using the expansions (1.4.3) for \( S \). We use the definition of the reduced probability functions (1.1.1) to express the flow in terms of the \( n(\vec{r}_1 \ldots \vec{r}_m) \). We give the cases \( \ell = 1 \) and \( \ell = 2 \) explicitly; the general formulae will be clear from these examples.

\[
\hat{n}(\vec{r}_1) = -\sum_{k=1}^{\infty} \frac{1}{(k-1)!} \int d\vec{r}_2 \ldots d\vec{r}_k s(\vec{r}_1; \vec{r}_2 \ldots \vec{r}_k) n(\vec{r}_1 \ldots \vec{r}_k)
\] (1.5.9a)

\[
\hat{n}(\vec{r}_1, \vec{r}_2) = -\sum_{k=2}^{\infty} \frac{1}{(k-2)!} \int d\vec{r}_3 \ldots d\vec{r}_k [s(\vec{r}_1, \vec{r}_2; \vec{r}_3 \ldots \vec{r}_k) + s(\vec{r}_2, \vec{r}_3; \vec{r}_1 \vec{r}_4 \ldots \vec{r}_k)] + s(\vec{r}_1; \vec{r}_2 \vec{r}_3 \ldots \vec{r}_k) + s(\vec{r}_2; \vec{r}_1 \vec{r}_3 \ldots \vec{r}_k) n(\vec{r}_1 \ldots \vec{r}_k)
\] (1.5.9b)

At this point we want to mention a special case of decimation weights in which only \( s(\vec{r}_1) \) and \( s(\vec{r}_1; \vec{r}_2) \) are present. The hierarchies (1.5.9) are then such that \( n(\vec{r}_1 \ldots \vec{r}_j) \) couples to \( n(\vec{r}_1 \ldots \vec{r}_k) \) for \( k = j \) and \( k = j+1 \) only.

We write them for later convenience in terms of \( n(\vec{r}) \) and \( g(\vec{r}_1 \ldots \vec{r}_j) \):

\[
\hat{n}(\vec{r}_1) = -s(\vec{r}_1)n(\vec{r}_1) - n(\vec{r}_1) \int d\vec{r}_2 s(\vec{r}_1, \vec{r}_2; \vec{r}_2) n(\vec{r}_2) g(\vec{r}_1, \vec{r}_2)
\] (1.5.10a)
\[ g_D(\vec{r}_1;\vec{r}_2) = -[s(\vec{r}_1;\vec{r}_2) + s(\vec{r}_2;\vec{r}_1)]g(\vec{r}_1;\vec{r}_2) - \int d\vec{r}_3 n(\vec{r}_3) \]

\[ \{s(\vec{r}_1;\vec{r}_3)[g(\vec{r}_1;\vec{r}_2;\vec{r}_3) - g(\vec{r}_1;\vec{r}_3)g(\vec{r}_1;\vec{r}_2)] + \]

\[ + s(\vec{r}_2;\vec{r}_3)[g(\vec{r}_1;\vec{r}_2;\vec{r}_3) - g(\vec{r}_2;\vec{r}_3)g(\vec{r}_1;\vec{r}_2)] \} \]

(1.5.10b)

The equations show that the correlation functions \( g(\vec{r}_1;\vec{r}_3) \) only change due to the higher order \( s(\vec{r}_1;\vec{r}_2) \) etc. in \( S \), a conclusion already known for decimation in spin models. Thus it is the weighted decimation that opens the possibility for a useful renormalization scheme. So we have to use more complicated weights than \( S = s \), (pure decimation). In appendix A is shown how pure decimation develops a potential \( \Phi \) which for \( t \to \infty \) approaches to the potential of average force, i.e.:

\[ W(\vec{r}_1;\vec{r}_N) \to \infty \rightarrow g(\vec{r}_1;\vec{r}_N) \to 0 \]

(1.5.11)

It indicates that for pure decimation many-particle potentials \( \Phi(\vec{r}_1;\vec{r}_j) \) (for \( j \geq 3 \)) are produced in as much as deviations from Kirkwood's superposition arise.

In the next section further restrictions on the weights \( S \) for weighted decimation are discussed. In particular weights \( S \) consisting of \( s(\vec{r}_1) \) and \( s(\vec{r}_1;\vec{r}_2) \) only leading to the equations (1.5.10) for the correlation functions are discussed in some detail in view of their usefulness in practical calculations.
1.6. Discussion

In this chapter renormalization transformations are presented as a stochastic process, reducing the number of variables in the fluid. The process can be viewed as a superposition of weighted decimation, spatial rescaling and rearrangement. The weighted decimation and the rescaling are the essential features. Without the decimation weights (pure decimation) no fixed point will result. Combining the ingredients we have the following flow equation for the pressure:

\[ \dot{p} = dp - s_1 z \]  \hspace{1cm} (1.6.1)

For the potentials we get a renormalization flow (for the homogeneous isotropic case):

\[ \dot{\varphi}(r) = d - s_1 + z \int dr [ s_1 f(r) + s_2 (r) e^{\varphi(r)} ] \]  \hspace{1cm} (1.6.2a)

\[ \dot{\varphi}(r_{12}) = [r_{12} + z \varphi(r_{12})] \varphi(r_{12}) + \frac{1}{2} \frac{\partial^2}{\partial r_{12}^2} - 2s_2 (r_{12}) + z \int dr_3 [ s_1 f(r_{13}) f(r_{23}) + s_2 (r_{13}) f(r_{23}) + s_2 (r_{23}) f(r_{13}) ] + ... \]  \hspace{1cm} (1.6.2b)

\[ \dot{\varphi}(r_{123}) = \frac{1}{2} \varphi(r_{12}) \varphi(r_{13}) + \frac{1}{3} \varphi(r_{13}) \varphi(r_{23}) - s_1 (r_{31}) + s_2 (r_{21}) - s_2 (r_{13}) + z \int dr_4 [ s_1 f(r_{14}) f(r_{24}) f(r_{34}) + s_2 (r_{14}) f(r_{24}) f(r_{34}) + ... + s_2 (r_{41}) e^{\varphi(r_{24})} f(r_{34}) + ... + s_2 (r_{41}) e^{\varphi(r_{24})} f(r_{34}) + ... \]  \hspace{1cm} (1.6.2c)
The functions $s_1$, $s_2(r)$, $s(r_1^{-1} r_2^{-1})$ etc. are the decimation weights, determining the decimation probability for one particle. The function $\phi(r)$ is the potential for rearrangement flow, which we restricted to a two-particle potential here. In appendix B we give the full flow equation with the three- and more-body potential terms present. Equation (1.6.2) is complete for the case that $\Phi(r_1^{-1} \ldots r_j^{-1}) = 0$ for $j \geq 3$.

The flow of the reduced probability densities can also be written down explicitly:

\[
\dot{n} = (d-s_1)n - \int d\vec{r}_2 s_2(r_{12})n(\vec{r}_1^{-1} \vec{r}_2^{-1}) - \frac{1}{2} \int dr_2 dr_3 s(r_1^{-1} r_2^{-1} r_3^{-1})n(\vec{r}_1^{-1} \vec{r}_2^{-1} \vec{r}_3^{-1}) \ldots 
\]  

(1.6.3a)

\[
\dot{n}(\vec{r}_1 \vec{r}_2) = (2d+\vec{v}_1 \cdot \dot{\vec{v}}_1 + \vec{v}_2 \cdot \dot{\vec{v}}_2)n(\vec{r}_1^{-1} \vec{r}_2^{-1}) + \vec{v}_1 \cdot \int dr_2 \vec{v}_1 \Phi(r_{12})n(\vec{r}_1^{-1} \vec{r}_2^{-1}) + \vec{v}_2 \cdot \int dr_3 \vec{v}_2 \Phi(r_{23})n(\vec{r}_1^{-1} \vec{r}_2^{-1} \vec{r}_3^{-1})
\]

\[
+ \vec{v}_3 \cdot \int dr_3 \vec{v}_3 \Phi(r_{23})n(\vec{r}_1^{-1} \vec{r}_2^{-1} \vec{r}_3^{-1})
\]

(1.6.3b)

In comparison to real space renormalization of spin systems it is remarkable that the flow equations are explicit and that the dimension only appears in the integrations to be carried out (apart from factors $d$ in rescaling). The only approximations which have to be made are a treatment of the influence of the three and higher body potentials. In practice equations as (1.6.2a) and (1.6.2b) can be handled quite well, but including $\Phi(\vec{r}_1 \vec{r}_2 \vec{r}_3^{-1})$ would make the equations immediately much more involved. Therefore one would like to restrict the flow to one and two particle potentials only. The scheme we have developed is sufficiently flexible to achieve this in principle by an adaption of $s(\vec{r}_j^{-1} \vec{r}_1^{-1} \ldots \vec{r}_{j-1}^{-1})$ to make $\Phi(\vec{r}_1^{-1} \ldots \vec{r}_j^{-1}) = 0$ when $\Phi(\vec{r}_1^{-1} \ldots \vec{r}_j^{-1}) = 0$. The problems related to such procedure are discussed
later on. Chapter II will deal with the choice of the weights and with the problem of finding fixed points of the flow equations and their properties.

The value of \( s_1 \) and the functions \( s_2(r) \) and \( \Phi_2(r) \) are free to choose but restrictions exist. We should take them such that there is an attractive trivial fixed point. The easiest way to achieve this is to locate such a point at zero density (\( z = n = 0 \)). To assure that such a fixed point is attractive for small enough density (or fugacity) we should take \( s_1 > d \), as is easily seen from (1.6.2a) and (1.6.3a) The choice of \( s_2(r) \) and \( \Phi_2(r) \) (being complementary in many respects) is based on the requirements:

- that the dilute phase fixed point (\( z = n = 0 \)) has a potential \( \Phi^*(r) \) which has a hard core
- that the critical fixed point has positive density (\( n \)) and fugacity (\( z \)) and a potential with a hard core and a short ranged attracting tail.

(Here we assume that only two particle potentials develop.)

To see that \( s_2(r) \) is restricted we consider the case that \( s(r; \vec{r}_1, ..., \vec{r}_j) = 0 \) for \( j \geq 3 \). The density then changes according to the exact relation (1.5.10a)

For a positive fixed point density and \( s_1 > d \) the expression \( \int s_2(r)g_2(r)dr \) has to be negative, which means (since \( g_2(r) \) is positive everywhere) that \( s_2(r) \) must have a regime in which \( s_2(r) < 0 \). Let \( r_m \) be the point where \( s_2(r) \) reaches its minimum. Since the total weight is \( S(\vec{r}; \vec{r}_1, ..., \vec{r}_j) = s_1 + \sum_{i=1}^{j} s_2(\vec{r} - \vec{r}_i) \) for this case, \( S \) can become negative for some configuration \( (\vec{r}; \vec{r}_1, ..., \vec{r}_j) \). This could violate our requirement that \( S \) should be positive when a large number of particles are at a distance \( r_m \) from \( \vec{r} \). However, in chapter II we arrive at a formulation for weighted decimation, in which positivity is no stringent requirement anymore.

For more general cases where \( s(\vec{r}, \vec{r}_1, ..., \vec{r}_j) \) for \( j \geq 2 \) are present, the restrictions as deduced from the fact that \( s_1 > d \), \( n > 0 \) and \( S > 0 \) are less stringent. In a later chapter we construct such weights, and we will see that although there seems to be a large freedom in choosing the weights, in practice there are but a few possibilities left.
As a last point we want to mention generalizations of the processes we have given in this chapter. First of all, many particle weighted decimation in which $j$ particles are decimated out of $N$ particles at once with a weight $S(\mathbf{r}_1, \ldots, \mathbf{r}_j, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_N)$. Secondly, finite rearrangement (called reconstruction) which can be seen as a finite motion of particles governed by a probability distribution (this is also a $N$- to $N$ particle transformation). Both can be made explicit but do not seem to add new mathematical ingredients nor are advantageous from a physical point of view. In particular in the case of the reconstruction process the hard core is less easy to preserve and it is less elegant than the way it is (automatically) achieved in the cases of rearrangement and decimation.
II. Results for some renormalization schemes

In chapter I we have constructed a renormalization scheme for the fluid with the aid of two independent processes: weighted decimation and spatial rearrangement. Two so far unspecified functions enter in the theory: the decimation weight \( S(\mathbf{r}; \mathbf{r}_1 \ldots \mathbf{r}_N) \) and the vector field \( \mathbf{V}(\mathbf{r}; \mathbf{r}_1 \ldots \mathbf{r}_N) \) for spatial rearrangement. \( S \) must be positive and both \( \mathbf{S} \) and \( \mathbf{V} \) must be cluster expandable, but are otherwise free.

We start to show in section 2.1 that the spatial rearrangements can be incorporated in a larger class of not necessarily positive decimation weights \( S \). The freedom in choosing \( S \) can then be used in two ways. Firstly, one can choose \( S(\mathbf{r}; \mathbf{r}_1 \ldots \mathbf{r}_N) \) on basis of physical plausibility and then study the consequences for the flow. This will be the strategy of the remaining part of this chapter. Secondly, one can use the freedom in choosing \( S(\mathbf{r}; \mathbf{r}_1 \ldots \mathbf{r}_N) \) to simplify the flow equations, which will be the subject of chapter III and partly of chapter IV.

Sections 2.2 and 2.3 will discuss the results of an approximation to the general equations which is based on neglect of the influence of many body potentials on the renormalization process. Such an approximation seems justified in view of similar calculations in spin models on a lattice where indeed the influence of multi-spin interactions is minor for many renormalization schemes \(^5, 12-14\).

To improve on the results of above approximations, one has to take into account the many body potentials. In section 2.4 we will treat in a heuristic way how the production of many particle potentials in the renormalization process can be tamed. It will as well be a first step to a more systematic treatment of the many body potentials, as given in chapters III and IV.
2.1. Relations between spatial rearrangement and weighted decimation

In the previous chapter we have introduced the renormalization scheme. The resulting flow equations were given in terms of the decimation weight \( S(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) \) and the rearrangement weight \( \overline{V}(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) \) and read (eqs. (1.3.6) and (1.4.2)):

\[
\frac{d}{dt} [\phi(\vec{r}_1 \ldots \vec{r}_N) - pV] = - \sum_{j=1}^{N} \{ \overline{V}_{\vec{r}_j} \phi(\vec{r}_1 \ldots \vec{r}_N) + \overline{V}(\vec{r}_j; \vec{r}_1 \ldots \vec{r}_{j-1} \vec{r}_{j+1} \ldots \vec{r}_N) + \}
\]

\[
+ \int d\vec{r} \frac{\phi(\vec{r}; \vec{r}_1 \ldots \vec{r}_N)}{e^{\phi(\vec{r}; \vec{r}_1 \ldots \vec{r}_N)}}
\]

Eq. (2.1.1) defines the flow for the pressure \( p \quad (N=0) \) and for the \( N \)-particle potential \( \phi(\vec{r}_1 \ldots \vec{r}_N) \) \( (N=1,2,\ldots) \). The functions \( \phi, S \) and \( V \) are assumed to have cluster properties, i.e.:

\[
\phi(\vec{r}_1 \ldots \vec{r}_N) = N \mu + \sum_{i<j} \phi_{ij} + \sum_{i<j<k} \phi_{ijk} + \ldots \quad (2.1.2^a)
\]

\[
S(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) = s + \sum_{i} s(r; \vec{r}_i) + \sum_{i<j} s(r; \vec{r}_i \vec{r}_j) + \ldots \quad (2.1.2^b)
\]

\[
\overline{V}(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) = \overline{v}(r) + \sum_{i} \overline{v}(r; \vec{r}_i) + \sum_{i<j} \overline{v}(r; \vec{r}_i \vec{r}_j) + \ldots \quad (2.1.2^c)
\]

where the lower cast functions (\( \phi, s, \overline{v} \)) vanish when one argument is separated far from the others.

The two stages in the scheme have, although different in origin, much in common. To show this, we write down the following transformation from \( S \) to \( \overline{S} \):

\[
S(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) = \overline{S}(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) + \overline{V}_{\vec{r}} \phi(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) + \overline{V}_{\vec{r}} \overline{V}(\vec{r}; \vec{r}_1 \ldots \vec{r}_N) \quad (2.1.3)
\]

Substituted in eq. (2.1.1) we see that the first two sums amount to a sum over \( \overline{S} \) only, while the integral becomes:
\[ \int d\mathbf{r} \mathcal{S}(\mathbf{r}; \mathbf{r}_1 \cdots \mathbf{r}_N) \frac{e^{\Phi(\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_N)}}{\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N)} = \int d\mathbf{r} \mathcal{S}(\mathbf{r}; \mathbf{r}_1 \cdots \mathbf{r}_N) \frac{e^{\Phi(\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_N)}}{\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N)} \\
+ \int d\mathbf{r} [\mathcal{V}(\mathbf{r}; \mathbf{r}_1 \cdots \mathbf{r}_N) \frac{e^{\Phi(\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_N)}}{\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N)}] \] (2.1.4)

The second integrand on the right-hand side is a divergence. When \( \Phi \) and \( \mathcal{V} \) are, for \( \mathbf{r} \) far apart from the positions \( \{\mathbf{r}_1 \cdots \mathbf{r}_N\} \), fast enough decaying (and we assume such), the integral of it vanishes according to Gauss' theorem. The flow equation then becomes:

\[ \frac{d}{dt} [\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N) - p \mathcal{V}] = - \sum_{j=1}^{N} \mathcal{S}(\mathbf{r}_j; \mathbf{r}_1 \cdots \mathbf{r}_{j-1} \mathbf{r}_{j+1} \cdots \mathbf{r}_N) + \]

\[ + \int d\mathbf{r} \mathcal{S}(\mathbf{r}; \mathbf{r}_1 \cdots \mathbf{r}_N) \frac{e^{\Phi(\mathbf{r}, \mathbf{r}_1 \cdots \mathbf{r}_N)}}{\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N)} \] (2.1.5)

Equation (2.1.5) is a flow equation for the potentials with a decimation weight \( \mathcal{S} \) and no spatial rearrangement. However, the decimation weight \( S \) was assumed to be positive since it defines a transition rate, but \( \mathcal{S} \) is not necessarily positive everywhere as one sees from eq. (2.1.3).

This shows that spatial rearrangements may be seen as a subset of the generalized weighted decimations. The strategy for proceeding may now be to choose \( \mathcal{S} \) either on physical plausibility arguments or such that the flow equations become convenient. One then can check afterwards whether the choice can be built up from a positive weight and spatial rearrangement. The positivity of the decimation weight was to guarantee the potentials to remain real valued under renormalization flow. We therefore will not check positivity as long as the potentials do not become complex. In the remainder of this thesis we thus concentrate on weighted decimation and the so following flow equations.
2.2. Simple weight for preservation of the hard core

The general flow equations for weighted decimation (eq. (2.1.5) combined with spatial rescaling) are hard to solve. In fact, this problem is even harder than the original problem of finding the relation between the pressure $p$ and the state $\Phi$ of the fluid. Therefore, we are forced to make approximations. The neglect of many particle potentials, i.e. to set $\Phi(r_k) = 0$ for $k \geq 3$, seems a promising approximation in view of its success in spin models. The flow equations are then (using the cluster properties (2.1.2)) found to be (eq. 1.6.2.):

$$\dot{\mu} = d - s_1 + z \int d\vec{r} \left[ s_1 f(r) + s_2(r) e^{\Phi(r)} \right]$$ \hspace{1cm} (2.2.1a)

$$\dot{\psi}(r_{12}) = r \frac{\partial \psi}{\partial r}(r_{12}) - 2s_2(r_{12}) + z \int d\vec{r}_3 \left[ s_1 f(r_{13}) f(r_{23}) + 2f(r_{13}) s_2(r_{23}) e^{\Phi(r_{23})} + s_3(r_3; r_{12}) e^{\Phi(r_{13}) + \Phi(r_{23})} \right]$$ \hspace{1cm} (2.2.1b)

As one notices, there are still three decimation weights to be chosen being $s_1$, $s_2(r)$ and $s_3(r_3; r_{12})$.

Likely, the three particle decimation weight $s(r_3; r_{12})$ is of comparable importance as the three particle potential. Therefore we will set $s(r_3; r_{12}) = 0$, as a first approximation, since we also have assumed $\Phi(r_{12}; r_3) = 0$. As argued in chapter I, $s_2(r)$ is essential for the existence of a critical fixed point. Furthermore we found that $s_2(r)$ must assume also negative values, and has to be chosen such that under renormalization the hard core of the potential is preserved.

To assure the existence of a trivial fixed point at zero density we examine equations (2.2.1) for $z = 0$ (or zero density):

$$\dot{\mu} = d - s_1$$ \hspace{1cm} (2.2.2a)

$$\dot{\psi}(r) = r \frac{\partial \psi}{\partial r}(r) - 2s_2(r)$$ \hspace{1cm} (2.2.2b)

This trivial fixed point is required to be attractive for all neighbouring states, and its potential must have a core. For $s_1 > d$, $\dot{\mu}$ is negative
such that for $z \to 0$, the value of $z$ is driven to smaller and smaller values, as it should for an attractive fixed point. The fixed point potential is found from eq. (2.2.2b), or, turning the argument around, $s_2(r)$ follows from a reference potential $\varphi_R(r)$. The weights thus satisfy:

$$s_1 > d$$  \hspace{1cm} (2.2.3a)

$$s_2(r) = \frac{1}{2} r \frac{\partial \varphi_R}{\partial r}(r)$$  \hspace{1cm} (2.2.3b)

Before we answer the question whether this choice leads to a zero density attractive fixed point, we must consider the possibility to move the weights along with the state $\Phi$.

When one allows the weights $s_1$ and $s_2(r)$ to depend on $u$ and $\varphi(r)$ one may be tempted to choose for the two-particle decimation weight $s_2(r) = \frac{1}{2} r \frac{\partial \varphi}{\partial r}$ for all $\varphi(r)$. Then any $\varphi(r)$ is a fixed point for $z = 0$. However, such a choice would lead, when substituted in eq. (2.2.1b), to the following flow equation for $\varphi(r)$:

$$\dot{\varphi}(r_{12}) = z \int dr_3 f(r_{13}) [s_1 f(r_{23}) + r \frac{\partial f}{\partial r}(r_{23})]$$  \hspace{1cm} (2.2.4)

This equation has a fixed point for $z \neq 0$ only when $f(r) = 0$, i.e. $\varphi(r) = 0$. Such a choice thus does not lead to the existence of a critical fixed point.

It teaches us to be careful with a choice in which the weights move with the state. In this section, which must be looked upon as a search for rough guidelines, we will use from now on fixed weights. Then one easily proves that the trivial fixed point is attractive, i.e. any $\varphi(r)$ will be attracted to $\varphi_R(r)$ for $z \to 0$. To see this, we write down the flow equation for $\varphi(r)$, eq.(2.2.2b), using eq. (2.2.3b):

$$\frac{d}{dt} \varphi(r) = \frac{d}{dt} [\varphi(r) - \varphi_R(r)] = r \frac{\partial}{\partial r} [\varphi(r) - \varphi_R(r)]$$  \hspace{1cm} (2.2.5)
Considering the combination $\psi(r) - \psi_R(r)$ as one function, it follows that the operation of eq. (2.2.5) means nothing but rescaling that function until it disappears for $t \to \infty$, which means that $\psi(r) \to \psi_R(r)$ for $t \to \infty$.

As we committed ourselves in this section to fixed weights the flow equations (2.2.1) become, with the choice for $s_1$ and $s_2(r)$ satisfying eqs. (2.2.3) and setting $s(r_1; r_2, r_3) = 0$:

\[ \dot{\psi} = d - s_1 + z \int dr \left[ s_1 f(r) + \frac{1}{2} r \frac{\partial \psi}{\partial r} e^{\psi(r)} \right] \]  

(2.2.6a)

\[ \dot{\psi}(r) = r \frac{\partial}{\partial r} \left[ \psi(r) - \psi_R(r) \right] + z f \ast [s_1 f + r \frac{\partial \psi}{\partial r} e^{\psi}] (r) \]  

(2.2.6b)

Here we used the convolution notation:

\[ (f \ast f)(r_{12}) = \int dr_3 f(r_{13}) f(r_{23}) \]  

(2.2.7)

The convolution term in eq. (2.2.6b) is finite everywhere. When $\psi(r)$ has a core, i.e. $\psi(r) \to -\infty$ for $r \to 0$, $\psi_R(r)$ must have a similar core to let $\psi(r)$ keep its core under renormalization.

An attractive choice for $\psi_R(r)$ seems a function that possesses a core only. For instance one could take (with an eye on 12-6 Lennard-Jones potentials)

\[ \psi_R(r) = -\left( \frac{\sigma}{r} \right)^{12} \]  

(2.2.8)

However, this choice would lead to a two particle weight $s_2(r)$ which is positive everywhere, namely $s_2(r) = 6 \left( \frac{\sigma}{r} \right)^{12}$. This we know to be unacceptable when there are no further weights $s(r; r_1, \ldots, r_k)$ for $k \geq 3$. Nevertheless we will come back later on this choice.

A well known potential, and therefore an attractive choice, is a 12-6 Lennard-Jones potential for $\psi_R(r)$. In the notation of chapter I, with $\frac{1}{T}$ included in the potentials, it reads 21):

\[ \psi_R(r) = \frac{4}{T_R} \left[ \left( \frac{\sigma}{r} \right)^6 - \left( \frac{\sigma}{r} \right)^{12} \right] \]  

(2.2.9)
The function \( s_2(r) \), given by eq. (2.2.3), has the desired shape. The reduced reference temperature \( T_R \) is now a free parameter in the flow equations, which together with \( s_1 \) and the dimension \( d \) define three parameters of which one must examine their influence on the flow equations. The parameter \( \sigma \), appearing in eqs. (2.2.8) and (2.2.9), is irrelevant to the problem since it sets the scale of the functions appearing in the fluid. When \( \sigma \) is changed, one gets equivalent results by rescaling of \( \Phi \) as done in chapter I. When \( \sigma \rightarrow \infty \) and \( T_R \rightarrow \infty \) such that \( \sigma^{12}/T_R = \text{const.} \) one regains the choice (2.2.8).

The flow equations (2.2.6) cannot be treated analytically. To treat them numerically, we have discretized the potential \( \Phi(r) \) by sampling it at \( P \) positions \( (r_1\ldots r_P) \):

\[
\Phi_i = \Phi(r_i), \quad i = 1\ldots P
\]  

(2.2.10)

Together with \( \mu \), which we shall call \( \Phi_0 \) for the moment, the flow equations (2.2.6) become \( P+1 \) equations for \( P+1 \) unknowns:

\[
\begin{align*}
\dot{\mu} &= \Phi_0 (\mu_1 \Phi_1 \ldots \Phi_p) = \Phi_0 (\Phi_\Phi \ldots \Phi_p) \\
\dot{\Phi}_i &= \Phi_i (\mu_1 \Phi_1 \ldots \Phi_p) = \Phi_i (\Phi_\Phi \ldots \Phi_p) \quad i = 0,1\ldots P
\end{align*}
\]

(2.2.11)

In appendices C and D we discuss how \( (r_1\ldots r_p) \) can be chosen as to make the calculation of the necessary integrals fast and simple with the use of Laguerre integration.

The existence of a fixed point can be examined by solving

\[
\dot{\Phi}_0 = \dot{\Phi}_1 = \ldots \dot{\Phi}_p = 0
\]

for a certain set \( \Phi_0, \Phi_1, \ldots, \Phi_p \), which in practice means solving a set of nonlinear equations. The linearization matrix \( L \), at the fixed point, is defined by:

\[
L: L_{ij} = \frac{\partial \Phi_i}{\partial \Phi_j} (\Phi_k^*) \quad i,j = 0,1\ldots P
\]

(2.2.12)

This \((P+1)\times(P+1)\) matrix yields the eigenvalues \( y_i (i = 0,1\ldots P) \) related to the critical exponents. For a critical fixed point one must have two positive (relevant) eigenvalues \( y_H \) and \( y_T \) for \( d < 4 \) \((y_H > y_T > 0)\). The remaining eigenvalues \((P-1)\) should all be zero (marginal) or negative (irrelevant).
The two positive eigenvalues $y_H$ and $y_T$ are known to be related to the familiar critical exponents $(\alpha, \beta, \gamma, \delta)$ and $(\eta, \nu)$ as $^{1-5,15}$:

\[
\begin{align*}
\alpha &= 2 - \frac{d}{y_T} \\
\beta &= \frac{d - y_H}{y_T} \\
\gamma &= \frac{2y_H - d}{y_T} \\
\delta &= \frac{y_H}{d - y_H} \\
\eta &= d + 2 - 2y_H \\
\nu &= \frac{1}{y_T}
\end{align*}
\]

They may not depend on the precise form of the renormalization scheme as long as its fixed point potential is short-ranged. They thus must be independent of the choice of the decimation weights, i.e. be independent of $s_1$ and $T_R$ defined above. The eigenvalues should however depend on the dimension $d$ in a very precise way. The fluid exponents are believed to be equal to the ones of the Ising model (table 1). Since our calculational scheme, as defined in appendices C and D, is designed such that it can treat the flow equations in any, also fractional dimensions, we can check this dependence for any $d$.

<table>
<thead>
<tr>
<th>$d$</th>
<th>$y_H$</th>
<th>$y_T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.875</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>2.484</td>
<td>1.587</td>
</tr>
</tbody>
</table>
| 4   | 3.0   | 2.0   | Onsager's solution$^{16)}$  
| $3d/4$ | $d/2$ |  

|  
| mean field$^{15)}$  
|  
|  

Table 1. Best known relevant eigenvalues of the Ising model.

As we neglected many-particle effects, our scheme is approximate and this may result in eigenvalues $y_H$ and $y_T$ that depend on the weights, i.e. $s_1$ and $T_R$. To check this, we start with the $d = 2$ case for which $y_H$ and $y_T$ are known exactly (Onsager's solution, table 1). Within a certain range of values for $s_1$ and $T_R$ we indeed have found fixed points, of which the linearization matrix has two relevant eigenvalues.
Fig. 1. The Mayer function $f(r)$ for a Lennard-Jones potential at its two dimensional critical point. For $d = 2$:
$T_c = 0.56$ and $z_c \int dr^2 f_c(r) = 0.48$.

To compare with what we get for the fixed points, we have plotted in fig. 1 the Mayer potential $f(r)$ of two dimensional Lennard-Jones at its critical temperature ($T_c = 0.56$, as known from computer simulations$^1$). In figs. 2 we show $f^*(r)$ for a few fixed points $({\mu^*}, {\varphi^*}(r))$, as found numerically with the method of appendices C and D, for $d = 2$ and some values of $s_1$ and $T_R$. For instance fig. 2a shows $f^*(r)$ for the more or less characteristic choice $s_1 = 3.5$ and $T_R = 1.56$ (the two-dimensional Lennard-Jones-Boyle temperature).

For all cases the function $f^*(r)$ is obviously longer in range than the one for critical Lennard-Jones in fig. 1. The reason for that is the appearance of the convolution term in eq. (2.2.6$^b$). Nevertheless, its shape is sufficiently similar to assume that it corresponds to a critical fixed point. Also the values of the chemical potential $\mu^*$, or rather the values of scale invariant quantity $z \int dr^2 f(r)$, point in that direction. (The value for critical Lennard-Jones, $z \int dr^2 f(r) = 0.48$ for $d = 2$ (fig. 1), estimated from a Padé approximation for the critical isotherm $p = p(n, T_c)$, as given in ref. 18).
Fig. 2a. Fixed point Mayer function $f(r)$ for $d = 2$, $a_1 = 3.50$, $T_R = 1.56$:
$z \int dr f(r) = 0.3942$, $y_H = 4.9329$, $y_T = 0.3530$.

Fig. 2b. Fixed point Mayer function $f(r)$ for $d = 2$, $a_1 = 3.50$, $r^{12}$-core:
$z \int dr f(r) = 0.3592$, $y_H = 6.2487$, $y_T = 0.4846$. 
Fig. 2\textsuperscript{c}. Fixed point Mayer function $f(r)$ for $d = 2$, $s_1 = 3.25$, $T_R = 1.56$: $\int dr \ f(r) = 0.3377$, $y_H = 5.4612$, $y_T = 0.3614$.

Fig. 2\textsuperscript{d}. Fixed point Mayer function $f(r)$ for $d = 2$, $s_1 = 3.75$, $T_R = 1.56$: $\int dr \ f(r) = 0.4435$, $y_H = 4.604$, $y_T = 0.3144$. 
For the case of fig. 2, $s_1 = 3.5$ and $T_R = 1.56$, we see that there are two relevant eigenvalues for the linearization matrix at the fixed point, which confirm that one is dealing with a critical fixed point. However, the values of $y_H$ and $y_T$ are far from what is expected. The value of $y_H$ is too large while $y_T$ is too small as can be seen from table 2 (fig. 2) compared with table 1. Also, many of the irrelevant eigenvalues are complex, but to this we shall come back later in this section. A crucial check now will be the dependence of the eigenvalues of the parameters $s_1$, $T_R$ and $d$.

<table>
<thead>
<tr>
<th>$d$</th>
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<th>$y_T$</th>
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</tr>
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<tr>
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<td>3.9129</td>
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<td>0.3614</td>
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<td>4.9329</td>
<td>0.3530</td>
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<td>1.56</td>
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<td>0.3144</td>
</tr>
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<td>HC</td>
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<td>0.7258</td>
</tr>
<tr>
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<td>5.25</td>
<td>3.39</td>
<td>6.2256</td>
<td>0.5703</td>
</tr>
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<td>5.50</td>
<td>3.39</td>
<td>6.0452</td>
<td>0.4629</td>
</tr>
</tbody>
</table>

Table 2. Relevant eigenvalues for several choices of the weights.

(HC-result for the $r^{14}$-core potential for $q_R$, eq. (2.2.8)).
Dependence on \( T_R \)

It appears that for a large region, \( T_R \geq 1.56 \) the fixed point and the eigenvalues \( y_H \) and \( y_T \) change only moderately with \( T_R \). In fig. 2\(^b\) we plotted the case when \( \varphi_R(r) \) is a \( r^2 \) –core potential (eq. (2.2.8) or \( T_R = \infty \)). The fixed point \( f(r) \) resembles the case of fig. 2\(^a\) very much, while for instance the eigenvalue \( y_H \) has worsened (see also table 2). Compared to the enormous change in \( T_R \) however, this change is not spectacular.

For values of \( T_R \) smaller than the Boyle temperature, i.e. \( T_R \leq 1.56 \), the values of \( y_H \) and \( y_T \) begin to change much more rapidly with \( T_R \). In table 2 we have given the case \( s_1 = 3.50 \) and \( T_R = 1.0 \). For that case the eigenvalue has changed in the range from \( T_R = 1.56 \) to 1.0 as much as from \( T_R = \infty \) to 1.56, and this will continue. The fixed point \( f(r) \) however changes very mildly with \( T_R \). The behaviour of this dependence for low \( T_R \) will be found to be very much similar to the dependence on a parameter \( d_1 \) which will be introduced in section 2.3. Further discussions will therefore be postponed to that section.

Dependence on \( s_1 \)

The results for the fixed points as well as for the eigenvalues \( y_H \) and \( y_T \) depend strongly on \( s_1 \). In fig. 2\(^c\) we show \( f^*(r) \) for the case \( T_R = 1.56 \) again, but with \( s_1 = 3.25 \), while fig. 2\(^d\) pictures the case \( s_1 = 3.75 \). It is clear that with increasing \( s_1 \), \( f^*(r) \) becomes smaller in the well and longer in range. The eigenvalues, especially \( y_H \), change quite rapidly with \( s_1 \) (compared with the variation for \( T_R \geq 1.56 \)). The value of \( z \int dr^2 f(r) \) remains more or less of the order that can be expected for a critical fluid.

We have found a critical fixed point in the region \( 3 \leq s_1 \leq 4 \) for all \( T_R \geq 1.56 \). For \( s_1 \leq 3 \) \( f^*(r) \) becomes very high in the well which is with our method numerically unmanageable. For \( s_1 \geq 4 \) \( f^*(r) \) becomes long in range for which as well the numerical method cannot be trusted. Within this range the eigenvalues change with \( s_1 \) rather fast. No values of \( s_1 \) and \( T_R \) can be found for which the eigenvalues are near the anticipated values which is clear when one compares table 2 and table 1.
Fig. 3. Fixed point Mayer function $f(r)$ for $d = 3$, $s_1 = 5.25$, $T_R = 3.39$.
\[ z \int dr r^2 f(r) = 0.4131, \quad y_H = 6.2256, \quad y_T = 0.5703. \]

Dependence on dimension $d$

To get results in $d$ dimensions which are comparable with the case $d = 2$, we made the following choices for $s_1$ and $T_R$. We denote the d-dimensional Boyle temperature by $T_B$. Then $T_R \simeq T_B$ is a representative value since $T_B > T_C$ in any $d$. One can expect the dependence of the renormalization scheme for $T_R \geq T_B$ to be moderate. For $s_1$ one cannot take a fixed value for all dimensions since one should obey $s_1 > d$. For this reason, and reasons that will appear later on, we have compared results in different dimensions for a fixed value of $s_1/d$. In fig. 3 we have plotted the fixed point Mayer function $f^*$ for the case $d = 3$, $s_1 = 5.25$ and $T_R = T_B = 3.39$ ($d = 3$ Boyle temperature). This result should be compared to the case of fig. 2a ($s_1/d = 1.75$).

The result for $d = 3$ is strikingly similar to the $d = 2$ case, i.e. a potential with a large well and eigenvalues of which $y_H$ is too large and $y_T$ is too small (table 2). Critical Lennard-Jones in $d = 3$ has a temperature $T_C = 1.25$, which is much higher than the $d = 2$ value for $T_C (T_C = 0.56)$. Therefore one expects the Mayer function for $d = 3$
to be smaller in the well than for \( d = 2 \), which clearly is not the case. When the value of \( s_1 \) is increased, the behavior is similar to the \( d = 2 \) case, \( f^*(r) \) becomes smaller in the well and longer in range. Also, the eigenvalues change rapidly with \( s_1 \) as for \( d = 2 \). The results indeed do not change much with \( T_R \) when \( T_R \gtrsim T_B \), and we found fixed points again in the range \( 4.5 \lesssim s_1 \lesssim 6 \) for all \( T_R \gtrsim T_B \).

Generally we have found for \( 2 \leq d < 4 \) fixed points in the range \( 1.5 \lesssim s_1/d \lesssim 2 \) when \( T_R \gtrsim T_B \) \( (T_B \) for \( d \)-dimensions). The fixed point Mayer functions resemble the results of the figures 2 and 3. The eigenvalue \( \nu_H \) is too large while \( \nu_T \) is too small; for \( T_R \gtrsim T_B \) they depend much more on \( s_1 \) than on \( T_R \).

To investigate the influence of the numerical scheme used, we varied the number of points \( P \), i.e. \( \{ r_i \} \) \( i = 1, \ldots, P \). This had only a minor influence on the outcome. Another calculational scheme, more primitive than the one described in appendices C and D, gave results similar to the ones above. However, the numerical representation of the operator \( r \frac{\partial}{\partial r} \) appearing in eq. (2.2.6) has influence on some of the irrelevant eigenvalues, but not on the relevant ones. This has made us believe that at least some of the complex irrelevant eigenvalues are due to the poor representation of the \( r \frac{\partial}{\partial r} \). Since the relevant results did not depend much on this numerical representation of \( r \frac{\partial}{\partial r} \), we have not payed more attention to this problem.
2.3. More sophisticated weights

In section 2.2 the choice for \( s_2(r) \) was based on the desire to preserve the hard core of the potential under renormalization. No further adjustment of \( s_2(r) \) was made, in particular \( s_2(r) \) was taken fixed for all states \((\mu, \varphi(r))\). In this section we explore the freedom in choosing \( s_2(r) \) under the constraint that the core remains fixed. We thus write perturbatively:

\[
\varphi(r) = \varphi_R(r) + \varphi_I(r)
\]

\[
s_2(r) = \frac{1}{r} \frac{\partial \varphi_R}{\partial r}(r) + s_2^{(I)}(r)
\]

The potential \( \varphi_R(r) \) is now considered as to be the reference potential similar to the choices in section 2.2 (eqs. (2.2.8) and (2.2.9)).

As in section 2.2 we assume the many particle decimation weights as well as many particle potentials to be absent. Substitution of eqs. (2.3.1) in eq. (2.2.1) results in the following flow equations for \( \mu \) and \( \varphi_I(r) \):

\[
\dot{\mu} = d - s_1 + z \int dr [s_1 f(r) + \frac{1}{r} \frac{\partial \varphi_R}{\partial r}(r)e^{\varphi(r)} + s_2^{(I)}(r)e^{\varphi(r)}]
\]

\[
\dot{\varphi}_I(r) = r \frac{\partial \varphi_I}{\partial r}(r) - 2s_2^{(I)}(r) + z[f(s_1 f + r \frac{\partial \varphi_R}{\partial r} e^{\varphi} + 2s_2^{(I)} e^{\varphi}](r)
\]

The advantage of eqs. (2.3.2) is that the functions \( \varphi_I(r) \) and \( s_2^{(I)}(r) \) can be taken to be well behaved for \( r \rightarrow 0 \). Since the convolution terms are well behaved for \( r \rightarrow 0 \) the flow of \( \varphi_I(r) \) remains finite for \( r \rightarrow 0 \). The terms in the convolution are regular since \( \varphi_R(r) \), which is singular in the core, appears only in combination with \( \exp \varphi(r) \). The choice \( s_2^{(I)}(r) = 0 \) reduces the flow equation to the case treated in section 2.2. In section 2.2 we have found that the fixed points and eigenvalues do not depend much on the choice of \( \varphi_R(r) \) (for \( T_R > T_B \)). Therefore, one does not expect these properties of the flow equations to depend much on any \( s_2^{(I)}(r) \) as long as it is kept fixed during the renormalization flow. That may be different when \( s_2^{(I)}(r) \) is a function of the potentials, e.g. on \( \varphi_I(r) \).
There are few guide lines for such a choice for $s_2(I)(r)$. In this section we limit ourselves to the form:

$$s_2(I)(r) = q_1 r \frac{\partial}{\partial r} \varphi_I(r) - q_2 \varphi_I(r)$$  \hspace{1cm} (2.3.3)

The second term on the right hand side is added on the general idea that $s_2(I)(r)$ should help to keep the form of $\varphi_I(r)$ invariant under flow. When substituted in eq. (2.3.2b), one sees that the term $-q_2 \varphi_I(r)$ in first instance drives $\dot{\varphi}_I(r)$ in the direction of $\varphi_I(r)$ (which explains the minus sign in front of $q_2$). The origin of the first term in eq. (2.3.3) is more mathematical in nature. It compensates the action of the scaling term $r \frac{\partial \varphi_I}{\partial r}$ in eq. (2.3.2b) which we have found to be very dominant in the eigenvalue structure. Physically, eq. (2.3.3) means that particles are decimated from the system on basis of the virial (local pressure) and the (local) energy respectively. During the flow we will take $q_1$ and $q_2$ fixed (as well as $s_1$ and $T_R$). The numerical treatment of the flow equations (2.3.2) is similar to the one discussed in section 2.2.

Dependence on $q_1$

As a first case we examine the influence of $q_1$ on the fixed points and their properties, while $q_2 = 0$ in eq. (2.3.3). The range in which $q_1$ has been varied is $0 \leq q_1 \leq \frac{1}{2}$. For $q_1 = \frac{1}{2}$ (and $q_2 = 0$) the total two particle weight would read $s_2(r) = \frac{1}{2} r \frac{\partial \varphi}{\partial r}(r)$. In section 2.2 we already found that this weight does not lead to the existence of a critical fixed point. For $\varphi_R(r)$ we have chosen as before a Lennard-Jones potential at its d-dimensional Boyle temperature ($T_R = T_B$ in eq. (2.2.9)), or the $r^\infty$-core potential (eq. (2.2.8)). For $s_1$ we have chosen again the values in the range $1.5 \leq s_1/d \leq 2$.

For $d = 2$ we have plotted in fig. 4 the results for $s_1 = 3.5$ and $T_R = T_B = 1.56$, while $q_1 = 0.3$ and $q_1 = 0.41$. These results should be compared with that of $q_1 = 0$, discussed in section 2.2, of which the fixed point $f(r)$ is plotted in fig. 2a. The change in $f^*(r)$, as well as in the eigenvalues of the linearization matrix are dramatic. The fixed point develops for larger $q_1$ a double well and this resembles hardly a critical Lennard-Jones $f(r)$ (fig. 1) anymore. This is not so much a problem in itself, since a fixed point may be situated in principle anywhere on the critical surface.
<table>
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Table 3. Eigenvalues for several values of $a_1$, $q_1$, $q_2$ and $T_R$. 
More alarming is that with increasing \( q_1 \), \( f^*(r) \) becomes even longer in range than for \( q_1 = 0 \). This can cause fundamental as well as numerical problems.

For the eigenvalues the trend is that they improve for increasing \( q_1 \). In table 3 we have given the change in the eigenvalues \( y_H \) and \( y_T \) when \( q_1 \) increases while \( s_1 \), \( T_R \), \( q_2 \) and \( d \) are fixed (among other results). Let us concentrate on \( d = 2 \) of which some examples were given in fig. 4. One sees that \( y_H \) becomes smaller while \( y_T \) becomes larger, which means that both eigenvalues improve. For \( s_1 = 3.5 \) and \( T_R = T_B = 1.56 \), \( q_1 = 0.41 \) is the value that approaches well the known exact results (table 1).

For \( q_1 \) larger than this "optimal" value, \( y_H \) and \( y_T \) deviate again from the exact values, i.e. \( y_H \) becomes too low and \( y_T \) too large. For \( q_1 \to \frac{1}{2} \) the fixed point disappears for reasons mentioned above.

Another numerical result is that the irrelevant eigenvalues, of which many had a complex part for \( q_1 = 0 \), become less complex for \( q_1 \) increasing. This fact is due to the reduced influence of the operator \( r \frac{\partial}{\partial r} \) in eq. (2.3.2) which we blame for the complexity of these irrelevant eigenvalues as pointed out in section 2.2.

Dependence on \( q_2 \)

We discuss briefly the cases where \( q_2 \neq 0 \) in eq. (2.3.3). When \( q_1 = 0 \), \( s_1/d = 1.75 \) and \( T_R = T_B \) (d-dimensional Boyle temperature) we find for \( 0 \leq q_2 \leq 1 \) fixed points which resembled \( q_1 = q_2 = 0 \) very much, although for \( q_2 \) larger the \( f^*(r) \) becomes a little longer in range. The eigenvalues only improve marginally with increasing \( q_2 \) as given in table 3. When \( q_1 \neq 0 \), the results resemble \( q_2 = 0 \) also. The reason why \( q_2 \) seems less important than \( q_1 \) probably is that the operator \( r \frac{\partial}{\partial r} \) is so dominant for minor changes in \( \psi_T(r) \) at longer distances. (It is therefore more resistant against the long range character of the convolutions appearing in eq. (2.3.2b)). Because of its minor role, we will set \( q_2 = 0 \) again in the rest of this section.
Fig. 4a. Fixed point Mayer function $f(r)$ for $d = 2$, $s = 3.50$, $T_R = 1.56$, $q_1 = 0.30$, $q_2 = 0$: $z \int dr^2 f(r) = 0.5223$, $y_H = 2.4223$, $y_T = 0.5015$.

Fig. 4b. Fixed point Mayer function $f(r)$ for $d = 2$, $s = 3.50$, $T_R = 1.56$, $q_1 = 0.41$, $q_2 = 0$: $z \int dr^2 f(r) = 0.5594$, $y_H = 1.8740$, $y_T = 0.9893$. 
Dependence on $T_R$

The dependence of above results on $T_R$, when $T_R \geq T_B$ and $q_1 \neq 0$, is larger than for $q_1 = 0$, although still moderate. Since $s_2(r)$ is no longer positive definite for $q_1 \neq 0$ it is legitimate to examine also the $r^{12}$-core case. In search for the optimal value of $q_1$ for this case ($T_R \rightarrow \infty$) we have found, however, that we must approach $q_1 = \frac{1}{2}$, i.e. the limit where fixed points disappear. When $T_R$ decreases, the value of $q_1$, where the eigenvalues are in best agreement with the exact values, also decreases somewhat. When $T_R < T_B$, this dependence on $T_R$ sets in more rapidly although the change in $f^*(r)$ still is negligible. In this region changes in $T_R$ are more or less equivalent to changes in $q_1$, which may be explained by the fact that changes in $\varphi_R(r)$ are transferred to $\varphi_I(r)$ in eqs. (2.3.1), such that the renormalization flow does not change much. (This explains also the $T_R \leq T_B$ dependence discussed in section 2.2.)

Dependence in $s_1$

Changes in $s_1$ cause effects for $q_1 \neq 0$ which are similar to those for $q_1 = 0$ (section 2.2). The fixed point Mayer function $f^*(r)$ becomes lower in the well for increasing $s_1$. However, for $q_1 = 0.41$ the eigenvalues increase now approximately linear with $s_1$ (a little different from $q_1 = 0$). Therefore we are unable to find eigenvalues $y_H$ and $y_T$ which are of the right magnitude for all $s_1$ in the range $1.5 \leq s_1/d \leq 2$. The one-particle decimation weight $s_1$ thus must have a rather definite value, being $s_1 \approx 3.5$ in two dimensions, irrespective the choice for $T_R$ and accompanying optimal $q_1$. 
Fig. 5. Fixed point Mayer function \( f(r) \) for \( d = 3, s_1 = 5.25, T_R = 3.39, q_1 = 0.41, q_2 = 0 \): \( z \int dr f(r) = 0.5584, y_H = 2.8300, y_T = 1.0278 \).

Fig. 6. Eigenvalues \( y_H \) and \( y_T \); the \( x \) are the ones calculated from the renormalization scheme with \( x = s_1/d = 1.75, q_1 = 0.41 \) and \( T_R = T_B \). The \( o \) are the best known Ising values and the dashed lines are the classical values: \( d/2 \) and \( 3d/4 \).
Dependence on d

As before, we will compare results in different dimensions, for fixed value of \( s_1/d \) while \( T_R = T_B \) (in d-dimensions). The value of \( q_1 \) we will take fixed in different dimensions. In fig. 5 we have the result for the \( d = 3 \), \( s_1 = 5.25 \) (\( s_1/d = 1.75 \)), \( q_1 = 0.41 \) and \( T_R = 3.39 \) (\( d = 3 \) Boyle temperature). The function \( f^*(r) \) is more or less similar to the \( d = 2 \) case again, although it is a little smaller in the well and a little longer in range (as for \( q_1 = 0 \)). Similar results were found in other dimensions. The dimensions in which calculations were done are \( d = 2, 2\frac{1}{2}, 3, 3\frac{1}{2} \) and 4. For \( d = 4 \) the fixed point \( f^*(r) \) becomes so small and long ranged that the numerical calculations cannot be trusted anymore. In table 3 we give the results for the relevant eigenvalues \( y_H \) and \( y_T \) for above cases. In fig. 6 we plot these values together with the best known Ising values and the mean field (classical) values (table 1).

What appears clearly, is that the dimensional dependence of \( y_H \) is predicted quite well but that the values of \( y_T \) are too much independent of the dimension \( d \). This, however, is for cases where \( s_1/d = 1.75 \) and \( T_R = T_B \), which in principle is a rather arbitrary choice. Therefore, it is interesting to see that it is possible to move \( y_H \) and \( y_T \) towards the Ising values for \( d > 2 \) by raising \( s_1/d \) a bit above the \( d = 2 \) value, i.e. when one takes \( s_1/d > 1.75 \). For \( d = 3 \), for instance, we find an optimal case for \( s_1 = 5.4 \), \( q_1 = 0.41 \) and \( T_R = 2.13 \), while \( f^*(r) \) still resembles the \( d = 2 \) case for several values of \( T_R \) in the range \( T_C < T_R < T_B \). For \( T_R \) too large one gets as for \( d = 2 \) that the optimal value of \( q_1 \) approaches \( q_1 = \frac{1}{2} \). For \( T_R \) too small (\( T_R < T_C \)) both eigenvalues \( y_H \) and \( y_T \) approach to each other and become complex.

In section 2.2 we mentioned that in a proper renormalization scheme the relevant eigenvalues (\( y_H \) and \( y_T \)) have to be independent of the choice of the decimation weights. In that sense our scheme fails. For that we must blame the many particle terms which we neglected so far. In the next section we will treat, in a heuristic way, how the production of many particle potentials may be reduced.
2.4. The influence of many particle potentials

In the previous sections we have observed a sensitivity of the results on the choice of the decimation weights. As the only approximation made is the neglect of the many particle potentials, we inspect in this section the many particle potential flow. It is sufficient to see how the many particle potentials develop in a situation where they themselves are absent. If one could manage to arrive at vanishing higher potential flow, a self consistent approximation would be realized.

In chapter I we have given the three particle potential flow for the case that no many particle potentials are present (eq. (1.6.2c)). Since we assumed so far as well \(\varphi(r_1, r_2, r_3) = 0\) as \(s(r_1; r_2, r_3) = 0\) for \(k \geq 3\), we get for three particle potential the following flow:

\[
\frac{\dot{\varphi}(r_1, r_2, r_3)}{s_3} = z \int dr_4 \left[ \frac{\varphi(r_4)}{s_3} f(r_4) f(r_{34}) + \frac{\varphi(r_{24})}{s_2} f(r_{24}) f(r_{34}) + \frac{\varphi(r_{34})}{s_1} f(r_{34}) \right]
\]

(2.4.1)

We thus see that \(\dot{\varphi}(r_1, r_2, r_3) \neq 0\) in general, as we assumed in the previous sections, unless \(s_2(r)\) is chosen in a very particular way, i.e. chosen as:

\[
s_2(r) e^{-\varphi(r)} = -q_0 s_1 f(r)
\]

(2.4.2)

with \(q_0 = 1/3\).

It is remarkable that with this choice of \(s_2(r)\) the \(\dot{\varphi}(r_1, r_2, r_3)\) can be made identically zero. We have made elaborate calculations with the expression (2.4.2). There are some problems with this choice. Firstly, it is inconsistent with the wish to have a critical fixed point with a "hard" core. For this case the \(r \frac{\partial \varphi}{\partial r}\) term is not able to compensate the exponential rise of \(s_2(r)\) in the core \((s_2(r) \sim q_0 s_1 e^{-\varphi(r)}\) when \(r \to 0\)). Secondly, we were unable to find a fixed point for this case, even when we skipped the demand to have a "hard" core preserved.
Finally, this choice generates a flow of four and more particle potentials. This means that after some "time" there are four particle potentials created which gives rise to a modification of eq. (2.4.1), leading to a production of $\varphi(r_1, r_2, r_3)$, etc. (see appendix B).

To see that $\varphi(r_1, r_2, r_3) \neq 0$, we write down the general equation for $\hat{\varphi}(r_1, r_2, r_3)$ when $\varphi(r_1, r_2, r_3) = s(r_1, r_2, r_3) = 0$ for $k \geq 3$:

$$
\hat{\varphi}(r_1, r_2, r_3) = \mathcal{Z} \int dr_{k+1} [s_1 f(r_{1,k+1})...f(r_{k,k+1}) + \varphi(r_{1,k+1}) s_2(r_{1,k+1})...f(r_{k,k+1}) + \ldots + f(r_{1,k+1})...f(r_{k-1,k+1}) s_2(r_{k,k+1})...s_2(r_{k+1})...]
$$

(2.4.3)

Thus to get $\hat{\varphi}(r_1, r_2, r_3) = 0$, one could take $s_2(r)$ as defined in eq. (2.4.2) with $q_0 = 1/k$, which would mean in return that $\varphi(r_1, r_2, r_3) \neq 0$ when $l \neq k$ ($l \geq 3$). Therefore one is in principle unable to fulfill our assumption concerning many particle terms by a choice of $s_1$ and $s_2(r)$ alone. As we shall see in the next chapters, one always needs many particle weights $s(r_1, r_2, r_3)$ to make $\hat{\varphi}(r_1, r_2, r_3) = 0$ exactly for $k \geq 3$. Then eq. (2.4.3) is modified as we shall see and a systematic approach to the problem is possible.

Before doing so, let us come back to the idea of compensation of many particle terms. Although it is impossible to get all $\varphi(r_1, r_2, r_3) = 0$ for $k \geq 3$ by adjusting $s_1$ and $s_2(r)$, it may be that the production of $\varphi(r_1, r_2, r_3)$ and $\varphi(r_1, r_2, r_3)$ can be minimized. Then one expects that the influence of the higher potentials on the eigenvalues is reduced, which hopefully gives rise to better values of $y_H$ and $y_T$.

A heuristic attempt is to let the flow of $\varphi(r_1, r_2, r_3)$ and $\varphi(r_1, r_2, r_3)$ be zero on the average. As equation (2.4.2) cannot be fulfilled for all $r$ let us impose only the integrated form of eq. (2.4.2):

$$
\int d\mathbf{r} s_2(r) e^{\varphi(r)} = -q_0 s_1 \int d\mathbf{r} f(r); \quad \frac{1}{4} \leq q_0 \leq \frac{1}{3}
$$

(2.4.4)
where the range in $q_0$ is taken such as to compromise between compensation of three- and four particle terms.

To examine this in the light of the results of sections 2.2 and 2.3, we take $s_2(r) = q_1 r \frac{\partial \varphi}{\partial r}(r) \geq 0$. This means more or less the case $q_2 = 0$ in eq. (2.3.3) of section 2.3. With this choice we get:

$$s_2(r) \varphi(r) = q_1 \frac{\partial \varphi}{\partial r}(r) (r \geq \sigma)$$

(2.4.5)

Substitution in eq. (2.4.4), and the use of the fact that $\int d^3r \frac{\partial f}{\partial r} (r) = -d \int df f(r)$ gives us the following approximate relation:

$$q_1 \approx q_0 s_1/d; \quad \frac{1}{3} \leq q_0 \leq \frac{1}{3}$$

(2.4.6)

We see that this very rough attempt to minimize the influence of the three- and four particle potential leads to a condition on the parameter $q_1$ when the value of $s_1/d$ is given.

Relation (2.4.6) works two ways: it is a condition on $q_1$ since we know that $s_1/d > 1$, and it is a condition on $s_1/d$ since we know that $0 \leq q_1 < \frac{1}{3}$ from section 2.3. We thus get the bounds:

$$1 < s_1/d \leq 2$$

(2.4.7a)

$$\frac{1}{3} \leq q_1 < \frac{1}{2}$$

(2.4.7b)

The optimal values of $s_1$ and $q_1$ found in the previous section fall indeed near the region given by the bounds (2.4.7). For the optimal value of $s_1/d$ on $d = 2$, i.e. $s_1/d = 1.75$, the bound (2.4.7b) leads to $0.4375 \leq q_1 < 0.5$. For $T_R \geq 1.80$ (where $\varphi_R(r)$ becomes less important outside the core and therefore leads to a good approximation of $s_2(r) = q_1 r \frac{\partial \varphi}{\partial r}(r)$ to the form (2.3.3)) we have found our optimal value of $q_1$ to lie in this region (for $d = 2$).
We close this chapter with a summary and then draw some conclusions. The renormalization scheme has been restricted to the flow of the chemical potential \( \mu \) and the pair potential \( \varphi(r) \). All decimation weights, except \( s_1 \) and \( s_2(r) \), have been set equal to zero. The possible \( s_2(r) \) have been represented by a number of variable parameters \( (T_R, q_1, q_2) \) and a fixed shape \( (12-6 \) Lennard-Jones). In this context, critical fixed points have been found for wide ranges of the free parameters. The fixed point potential is in many cases of the form one expects for a critical system, although the range of the fixed point potential is generally substantially longer than the range of the input weight function.

A problem we meet is the occurrence of a critical fixed point for the case that \( s_2(r) \) is a positive function everywhere. Then one can rigorously prove that only a zero density fixed point can exist and not a critical one. The fact that we find a critical fixed point even in a case where one should not, must be the result of our approximations: i.e. the neglect of the many particle terms. One may wonder whether the fixed points we get for the other cases will not be spoiled by the many particle terms. However, the shape of the fixed point potential and the fact that we always find two relevant eigenvalues, has convinced us that we deal with really existing critical fixed points, whose properties may be influenced by the many particle terms.

The associated critical exponents are in general far from the expected values, unless the free parameters of the renormalization scheme are carefully chosen. A substantial reduction in the freedom of the parameters follows by heuristical inspection of the growth of the many particle potentials. The successful parameter values fall near the window suggested by the higher order flow equations. The window is, however, still too wide to exclude large variations in the exponents, in particular the variation in \( s_1 \). For fixed \( s_1/d \) the dimensional dependence of the largest "magnetic" eigenvalue \( y_H \) is acceptable, whereas the thermal eigenvalue \( y_T \) shows an incorrect dependence of \( d \).

We have not been able to answer the question whether the decimation weights must depend on the state of the system. In our present approach the eigenvalues are affected by the dependence of the decimation weights of the state \( \Phi \). One can take for instance a choice \( s_1^\Phi \) and \( s_2^\Phi(r) \) which are fixed and result in a fixed point \( (\mu^\Phi, \varphi^\Phi(r)) \). One arrives at the same fixed point when one deviates \( s_1 \) and \( s_2(r) \) from \( s_1^\Phi \) and \( s_2^\Phi(r) \) outside this.
fixed point. However, this affects the eigenvalues $y_H$ and $y_T$. A reflection of this may be that the eigenvalues $y_H$ and $y_T$ behave differently as a function of the free parameters in section 2.2, where the weights are fixed, than in section 2.3, where the weight $s_2(r)$ depends on $\Phi(r)$.

All these shortcomings must be blamed on the unjustified neglect of the many particle potentials, in particular $\Phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$, which directly couples to the flow of $\Phi(r)$. In the next chapters we will concentrate on the inclusion of the many particle terms in a systematic way.
III. Compensation of many particle potentials

In the previous chapters we found that weighted decimation combined with spatial rescaling is a plausible renormalization scheme. In the assumption that many particle terms could be neglected, we found a dependence of what should be universal quantities, on the precise scheme. In the search for an optimal scheme we found that it is inconsistent to neglect many particle decimation weights when many particle potentials are assumed to be absent and vice versa.

For practical calculations, inclusion of many particle potentials is very hard. If one examines the flow of the three body potential \( \phi(r_1, r_2, r_3) \), as given in appendix B, one sees that this equation is much more difficult than the flow of the pair potential \( \phi(r) \). Numerically, the search for a fixed point of the flow equations as defined in sections 2.2 and 2.3 is already time-consuming. One therefore may state that, as far as the numerical method is developed, inclusion of many particle potentials is not a first option.

The alternative is to prevent that many particle potentials develop. To do this, we now know that many particle decimation weights must necessarily be defined. In this chapter we will investigate in a general way the consequences of constraints on the flow equations in the critical region. As we shall see, these constraints will impose conditions on the a priori free weights. In chapter IV we will investigate the convergence of the procedure of adjusting weights. Especially this will serve as a powerful reduction of the too large freedom in choosing the decimation weights.

3.1. General approach to constrained flow equations

In this section we formulate the construction of a renormalization scheme with the exact absence of many particle potentials. The starting point is the flow equation for a combination of weighted decimation (eqs. (1.4.2) or (2.1.5)) and spatial rescaling (eq. (1.3.6)):

\[ \dot{p} = dp - s_z \]  

(3.1.1)
\[
\begin{align*}
\Phi(r_1, \ldots, r_N) &= \text{N} (r_1 \wedge \mathbf{v}_1 + \ldots + r_N \wedge \mathbf{v}_N) + \sum_{j=1}^{N} S(r_j; r_{j+1} \ldots r_{j-1} r_j r_{j+1} \ldots r_N) \\
&\quad + \int dr \left[ \frac{e S(r_1, \ldots, r_N)}{\Phi(r_1, \ldots, r_N)} - s_i e^\mu \right] 
\end{align*}
\]

(3.1.2)

With the use of the cluster properties, eqs. (2.1.2), we have derived in chapter I the flow equations for \(\mu, \Phi(r_{12}), \Phi(r_1 r_2 r_3), \) etc., as a hierarchy. We write down the case that no three- and more particle potentials are present (for a homogeneous and isotropic system):

\[
\begin{align*}
\dot{\mu} &= d - s_1 + z \int dr_2 \left[ s_1 f(r_{12}) + s_2 f(r_{12}) \right] \\
\dot{\Phi}(r_{12}) &= r \frac{\partial f}{\partial r}(r_{12}) - 2s_2 f(r_{12}) + z \int dr_3 \left[ s_1 f(r_{13}) f(r_{23}) + s_3 f(r_{13}) + \Phi(r_{23}) \right] \\
\dot{\Phi}(r_{12} r_3) &= s_3 f(r_{12}; r_3) - s_3 f(r_1; r_2 r_3) - s_3 f(r_2; r_1 r_3) + z \int dr_4 \left[ s_1 f(r_{14}) f(r_{24}) f(r_{34}) + s_2 f(r_{14}) f(r_{24}) f(r_{34}) \right. \\
&\quad + s_3 f(r_{14}) f(r_{24}) f(r_{34}) + \Phi(r_{14}) + \Phi(r_{24}) + \Phi(r_{34}) \\
&\quad + \ldots + s_3 f(r_{14}; r_{24} r_3) \Phi(r_{14}) + \Phi(r_{24}) + \Phi(r_{34}) \right] 
\end{align*}
\]

(3.1.3)

Here, \(f(r) = e^{\Phi(r)} - 1\) is the Mayer function and \(z(= e^\mu)\) is the fugacity again.

From eq. (3.1.2) we see that the flow equations are linearly depending on the decimation weights \(S\). Consequently the flow equations (3.1.3) are linear in the weights \(s_1, s_2(r), s_3(r_1; r_2 r_3), \) etc. We want to examine whether it is possible to make \(\Phi(r_1, \ldots, r_k) = 0\) for \(k \geq 3\) by adjustment of the decimation weights. When the hierarchy defined by the equations (3.1.3) for that case could be terminated at some finite \(k = K\), this problem would reduce to a coupled set of inhomogeneous many dimensional linear integral equations for \(s(r_1; r_2, \ldots, r_k) (k \leq K)\). Under normal conditions such a system has one solution. However, for \(K = \infty\) the situation is more delicate as we shall see.
In section 2.4 we have seen that it is possible to adjust $s_2(r)$ such that $\dot{\Phi}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = 0$, but this gives rise to undesired properties of the flow equations. Another strategy is adjustment of $s(\vec{r}_1, \vec{r}_2, \vec{r}_3)$. Generally, we will thus adjust $s(\vec{r}_1, \vec{r}_2, \vec{r}_k)$ to get $\dot{\Phi}(\vec{r}_1, \vec{r}_2, \vec{r}_k) = 0$ for $k \geq 3$. In the next chapter we will explicitly do so, and discuss the consequences of various approximations. In this chapter we will only assume that there exist flow equations, in $\mu$ and $\Phi(r)$ only, given by (2.1.3a) and (2.1.3b), where $s(\vec{r}_1, \vec{r}_2)$ is a function depending on $\mu$, $\Phi(r)$, $s_1$ and $s_2(r)$. Both $s_1$ and $s_2(r)$ are then assumed to be free to choose.

A curious point of the flow equations is that the freedom in choosing the decimation weights seems so large that one is able to let the flow of all potentials $\Phi$ vanish. To be precise, one might set $\mu = 0$ by adjusting $s_1$ and $\Phi(r) = 0$ by adjusting $s_2(r)$, etc., i.e. generalize the above scheme to all $\dot{\Phi}(\vec{r}_1, \vec{r}_k)$, $k \geq 1$. In that case every state $\Phi$ would be a fixed point of the flow equations. Of course such a procedure is against the spirit of renormalization. The price one has to pay is indeed that the decimation weights become singular functions of the state $\Phi$. This will be shown in section 3.2.

We will proceed to relax gradually the constraints. Section 3.3 will deal with flow constraints in the $\mu$-direction, i.e. $\mu \neq 0$ while $\dot{\Phi}(\vec{r}_1, \vec{r}_k) = 0$ for $k \geq 2$. In section 3.4 we introduce $(\mu, T)$ flow where $\mu \neq 0$ and $\Phi(r)$ is restricted to flow in the temperature ($T$) direction only. The last section deals with the more realistic case of $(\mu, \Phi_2)$ flow, i.e. when $\dot{\Phi}(\vec{r}_1, \vec{r}_k) = 0$ for $k \geq 3$.

The general tendency will be that the more constraints are imposed on the flow, the more weights become singular functions of the potentials.

All cases will be investigated from an alternative flow relation for the pressure $p$. Viewing the grand canonical partition function $Z_{gr}(e^{pV})$ as a functional of the potentials, and using that the reduced probability densities (defined by eq. (1.1.6)) are the functional derivatives of $\ln Z_{gr}(e^{pV})$ with respect to the potentials, one has:

$$\dot{p} = \mu + \frac{1}{2T} \int d\vec{r}_2 n(\vec{r}_1, 2^2, \vec{r}_2) \dot{\Phi}(\vec{r}_{12}) + \frac{1}{3!} \int d\vec{r}_2 d\vec{r}_3 n(\vec{r}_1, 2^3, \vec{r}_3) \dot{\Phi}(\vec{r}_1, \vec{r}_2, \vec{r}_3) + \ldots$$

(3.1.4)
This equation must match expression (3.1.1). The more the flow is constrained, i.e. the fewer terms in eq. (3.1.4) contribute, the stronger connections between the weights, appearing in the flow, and the correlation functions can be drawn.

3.2. Zero flow situation

In this section we will construct a renormalization scheme in which adjustment of \( s(\vec{r}_1; \vec{r}_2; \ldots; \vec{r}_k) \) in eqs. (3.1.3) sets \( \dot{\phi}(\vec{r}_1; \ldots; \vec{r}_k) = 0 \) for all \( k \geq 1 \). Since any point is a fixed point then, there is no information in the linearization around the fixed point (all eigenvalues are zero). Such a renormalization theory does not explain the singular behaviour of thermodynamic quantities at criticality in terms of the flow. The price one pays is that the singularities now enter in the decimation weights, as we will show.

Since there is no flow of the potentials, there is no flow of the pressure (as one sees from eq. (3.1.4)). When \( \dot{\phi} = 0 \) during renormalization, this means that for all states \( \phi \) we should have, according to eq. (3.1.1):

\[
s_1 = \frac{\dot{p}}{z}
\]  

As \( p \) is at criticality a singular function of \( \phi \), e.g. as function of the chemical potential \( \mu \) and the temperature \( T \), \( s_1 \) becomes a singular function of \( \phi \). The same is easily seen for \( s_2(r) \) using that \( \dot{\mu} = 0 \). Substitution of eq. (3.2.1) in eq. (3.1.3\( ^a \)) yields:

\[
z \int d\vec{r} \, s_2(r) e^{\phi(r)} = \frac{\dot{p}}{z} [1 - z \int d\vec{r} \, f(r)] - d
\]  

As for \( s_1 \) we see that this integral is a singular function of the state \( \phi \) near criticality through \( p \). This means that the function \( s_2(r) \) depends singularly on \( \phi \), either as a function of \( r \) at fixed \( \phi \) (e.g. through the development of a long tail), or at fixed \( r \) as function of \( \phi \) (similar to \( s_1 \), or both.

We have not found a closed expression for \( s_2(r) \) which fulfils \( \dot{\phi}(r) = 0 \), but one can find a diagrammatic expression in powers of the fugacity \( z \), similar to the method which will be treated in section 4.1.
The diagram series are similar to the cluster expansion series for the correlation functions which lead us to believe that the weights \( s_2(r), s_3(r_1; r_2, r_3), \) etc., which set \( \mu = 0 \), have behaviour similar to that of the correlation functions, i.e. singular as function of \( \phi \) and long-ranged near criticality \(^{19}\).

This picture is strengthened by the observation that, when eq. (2.2.5) is differentiated twice with respect to \( \mu \) or \( T \), the right-hand side will contain \( \frac{\partial^2 \rho}{\partial \mu^2} \) and \( \frac{\partial^2 \rho}{\partial T^2} \) respectively. At criticality both quantities, being the isothermal compressibility and (apart from trivial factors) the specific heat, are known to be divergent \(^{15, 19}\). The consequence is:

\[
\frac{\partial^2 \rho}{\partial \mu^2} z \int dr \ s_2(r) e^\mu(r) \to \infty
\]

at criticality \( (3.2.3) \)

\[
\frac{\partial^2 \rho}{\partial T^2} z \int dr \ s_2(r) e^\phi(r) \to \infty
\]

This strongly suggests that \( \frac{\partial^2 \rho}{\partial \mu^2} s_2(r) \) and \( \frac{\partial^2 \rho}{\partial T^2} s_2(r) \) become longer in range than \( r^{-d} \), which indicates long-rangedness of \( s_2(r) \) itself.

We have not entered into the question whether the weights \( S \), constructed as above, are physically admissible (\( s_1 \) given by eq. (2.2.4) certainly is). Positivity of decimation weight \( S \) (as meant in section 2.1) should in principle be fulfilled but on the other hand is of not much interest here where the potentials are fixed and thus remain real valued under renormalization.

A more serious problem is whether the procedure converges, i.e. as a function of \( j \) do the functions \( s(r_1; r_2, \ldots, r_j) \) behave reasonably for large \( j \)? To this problem we shall come back in a somewhat wider context, in chapter IV. Within the approximation made there, we find that for a scheme as above, the weights \( s(r_1; r_2, \ldots, r_j) \), or rather \( \int dr_1 \cdots dr_j s(r_1; r_2, \ldots, r_j) e^{\phi(r_1 - r) + \cdots + \phi(r_j - r)} \), diverge as a function of \( j \).
3.3. Flow of the chemical potential

The procedure of this section is similar to the one in section 3.2. We will set \( \dot{\mu}(\mathbf{r}_1, \ldots, \mathbf{r}_k) = 0 \) by adjusting \( s(\mathbf{r}_1; \mathbf{r}_2, \ldots, \mathbf{r}_k) \) for \( k \geq 2 \), which means that only \( \mu \neq 0 \). Therefore \( \mu \neq 0 \) for arbitrary \( \Phi \) and thus in principle there is no condition on \( s_1 \) as before (eq. 3.2.1). Now, still a few conclusions can be drawn about the flow using the general property that the flow of the pressure can be expressed in eq. (3.1.1) as well as in eq. (3.1.4). In this case only \( \mu \neq 0 \) and thus one has:

\[
\dot{\mu} = n \dot{\mu} = dp - s_1 z
\]  

(3.3.1)

So we know the flow of \( \mu \) in terms of \( p, n \) and \( z \)

\[
\dot{\mu} = \frac{dp - s_1 z}{n}
\]  

(3.3.2)

Unless \( s_1 \) prevents so, the flow of \( \mu \) is a singular function of \( \mu \) at criticality since \( p \) as well as \( n \) are singular functions of \( \Phi \) and thus also of \( \mu \).

We thus have the choice between a simple scheme with \( s_1 \) fixed but a flow singularly depending on the state when it is near criticality, or a scheme with no (leading) singularity in the flow of \( \mu \) but an \( s_1 \) which depends in a complicated way on the state \( \Phi \). The last solution is as difficult as the original problem of finding the thermodynamic functions of the fluid, as we show now.

Let us start with a state \( \Phi \) which is critical, specifically a state at its critical value of the chemical potential \( \mu_c \) and with a potential at its critical temperature. As only the chemical potential can flow, we inspect the dependence of \( \mu \) on \( \mu \), in particular we will inspect the singular behaviour of the pressure \( p \) and the density \( n \) on \( \mu \).

The pressure \( p \) is known to behave near criticality, in lowest order in \( \mu - \mu_c \) as \[15]:

\[
p(\mu) = p_c + n_c(\mu - \mu_c) + \ldots A \mu |\mu - \mu_c|^{1+1/\delta} + \ldots
\]  

(3.3.3)
IV. Connection of constrained flow with virial series

In this chapter we will proceed with a renormalization scheme that is constrained to flow in \(\mu\) and \(\varphi(r)\), as introduced in section 3.5. For the decimation weights it means that \(s(\vec{r}_1;\vec{r}_2;...;\vec{r}_k)\) is adjusted to make \(\varphi(\vec{r}_1;...;\vec{r}_k) = 0\) for \(k \geq 3\). In section 4.1 we show that there is a systematic approach possible, which leads to a diagram expansion for the weights \(s(\vec{r}_1;\vec{r}_2;...;\vec{r}_k)\) \((k \geq 3)\) in powers of the fugacity \(z\). In particular, we are interested in the diagram expansion for \(s(\vec{r}_1;\vec{r}_2;\vec{r}_3)\) which enters in the flow of \(\varphi(r)\), given by eq. (3.1.3b).

In many respects the expansion resembles the cluster expansion for the pressure \(p\), or the reduced probability densities \(n(\vec{r}_1;...;\vec{r}_k)^{21-25}\). Inspired on that theory, we can make two types of approximation. The first one is to take into account only a few orders in \(z\) of the fugacity expansion for \(s(\vec{r}_1;\vec{r}_2;\vec{r}_3)\). We will comment on such a scheme in section 4.1. The second strategy is to take into account only relatively simple diagrams, but to all orders in \(z\). Since especially such an approach has proven to be useful, the remainder of this chapter will deal with it.

In sections 4.2 and 4.3 we try the simplest of such an approximation, namely the Cayley tree approximation. It accounts for diagrams with no loops only, and will result in a soluble flow equation. This flow will teach us that there are conditions on the a priori free weight \(s_2(r)\) and that one has to take loops into account for the description of a critical theory.

Section 4.4 will include in the flow the simplest loop to all orders. The resulting flow equations have a critical fixed point with (classical) mean field exponents. The conditions on \(s_2(r)\) survive and will be understood in the context of chapter III. We will meet a difficulty in both approximations, namely the divergence of the quantity \(\xi_j = \int dr_2...dr_j\{s(r_1;r_2;...;r_j) \exp \sum_{1<j} \varphi(r_{ij})\}\) as a function of \(j\) for \(j \to \infty\), via a deep minimum. This fact that the \(s_j\) seem to form an asymptotic series indicates that \((\mu,\varphi)\) flow may not be imposed too strictly.

We close in section 4.5 with a discussion of the relation between the results of this chapter to those of chapter II, and a general discussion on constrained flow equations.
4.1. Diagrammatic approach to \((\mu, \varphi)\) flow

In chapter III we have introduced constrained flow. The assumption is that it is possible to make \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = 0\) by adjustment of \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\). We have found that the adjustment leads to undesired flow properties if one imposes constraints on \(\dot{\mu}\) (\(k = 1\)) and \(\dot{\varphi}(\vec{r})\) (\(k = 2\)). In this chapter we proceed with \((\mu, \varphi)\) flow as introduced in section 3.5, with \(\varphi(\vec{r}_1, \ldots, \vec{r}_k) = 0\) for \(k \geq 3\). The flow equations are then defined by eqs. (3.1.3).

The most important unknown in the flow of \(\varphi(\vec{r})\) is \(s(\vec{r}_1; \vec{r}_2, \vec{r}_3)\), which will be fixed by the condition \(\dot{\varphi}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = 0\) in our set-up.

We thus obtain a hierarchy of equations for the weights \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\) while we are interested especially in \(s(\vec{r}_1; \vec{r}_2, \vec{r}_3)\). As a first step to a systematic approach to the problem we write down the general flow equation for \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k)\) for \(k \geq 3\):

\[
0 = \dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = - \sum_{j=1}^{k} s(\vec{r}_j; \vec{r}_1, \ldots, \vec{r}_{j-1}, \vec{r}_{j+1}, \ldots, \vec{r}_k) + z \int d\vec{r}_{k+1} \sum_{n=0}^{\infty} \frac{\varphi(\vec{r}_{i_1, \ldots, i_k}; \vec{r}_{1, \ldots, n})}{\{i_1, \ldots, i_k\} \in \{1, \ldots, k\}}
\]

\[
\int d\vec{r}_{k+1} s(\vec{r}_{k+1}; \vec{r}_{1}, \ldots, \vec{r}_n) f(\vec{r}_{i_{n+1}, \ldots, n+1}) f(\vec{r}_{1, \ldots, n})
\]

We consider \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = 0\) as the defining equation for \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\).

The function \(s(\vec{r}_j; \vec{r}_1, \ldots, \vec{r}_{j-1}, \vec{r}_{j+1}, \ldots, \vec{r}_k)\) must be symmetric in the arguments \(\{\vec{r}_1, \ldots, \vec{r}_{j-1}, \vec{r}_{j+1}, \ldots, \vec{r}_k\}\) since the particles are identical. It need not be symmetric in all the arguments, \(\vec{r}_j\) included, since the \(j\)-th particle is the one that is decimated and therefore plays a special role. Equation (4.1.1) only tells that the symmetric sum of asymmetric functions vanishes.

Therefore we may write:

\[
s(\vec{r}_k; \vec{r}_1, \ldots, \vec{r}_{k-1}) = \frac{1}{k} z \int d\vec{r}_{k+1} \sum_{j=0}^{k} \frac{1}{\{i_1, \ldots, i_k\} \in \{1, \ldots, k\}} s(\vec{r}_{k+1}; \vec{r}_{i_1}, \ldots, \vec{r}_{i_j})
\]

\[
\varphi(\vec{r}_{i_1, \ldots, i_j}) \varphi(\vec{r}_{j, \ldots, k}) f(\vec{r}_{i_{j+1}, \ldots, k}) f(\vec{r}_{i_1, \ldots, i_j}) +
\]

\[
\chi(\vec{r}_k; \vec{r}_1, \ldots, \vec{r}_{k-1})
\]

(4.1)
The only parameters that can be chosen in principle are \( s_1 \) and \( B \); they may be chosen to depend on the state \((\mu,T)\). In section 3.3 we learned that to prevent singularities in the flow, one had to adjust the a priori free parameters, in that case \( s_1 \). Our aim is to examine this for this more general case. It is an important question since flow in \((\mu,T)\) is the least one should have to define a proper renormalization theory for the critical fluid. Moreover, it would give a justification of eventual phenomenological renormalization attempts on the fluid.

Now we follow a path similar to that of section 3.3 and use the expression for \( \dot{p} \) in terms of \( \dot{\mu} \) and \( \dot{\varphi}(r) \) in eq. (3.1.4) (up to \( \varphi(r) \)) for this case, combined with eq. (3.1.1):

\[
\dot{p} = n \dot{\mu} + \frac{1}{2} B \int dr_2 \, n(r_1, r_2) \varphi(r_{12}) = dp - s_1 z
\]  

(3.4.3)

A first consequence is that again one can express \( \dot{\mu} \) in terms of thermodynamic quantities (for \( B = 0 \) we get the results of section 3.3):

\[
\dot{\mu} = \frac{dp - s_1 z}{n} + Bu
\]  

(3.4.4)

Here, \( u \) is the potential energy per particle:

\[
u = -\frac{1}{2n} \int dr_2 \, n(r_1, r_2) \varphi(r_{12})
\]  

(3.4.5)

The quantities \( p, n \) and \( u \) are known to be singular functions of \((\mu,T)\) near critical point \((\mu_c, T_c)\). Therefore, the flow of \( \mu \), eq. (3.4.4), is singular unless \( s_1 \) and \( B \), which are the only a priori free parameters, are chosen carefully, as was shown for \( s_1 \) in section 3.3.

Before we go into that more deeply, we look at another consequence of eq. (3.4.4) in combination with the flow equation (3.1.3) for \( \mu \) for weighted decimation:

\[
\dot{\mu} = d - s_1 + z \int dr \, [s_1 f(r) + s_2 r e^{\varphi(r)}] = \frac{dp}{n} - s_1 \frac{z}{n} + Bu
\]  

(3.4.6)
In the idea that $s_1$ and $B$ are free and independent variables, this suggests that the weight $s_2(r)$ which realizes $\hat{s}(r) = B\varphi(r)$, can be written as:

$$s_2(r) = s_2^{(0)}(r) + s_2^{(s)}(r) + B s_2^{(B)}(r)$$  \hspace{1cm} (3.4)

Substituted in the flow $\hat{s}(r)$ for weighted decimation, eq. (3.1.3b) combined with eq. (3.4.2), it means that $s_2^{(0)}(r)$ compensates the $r \frac{\partial \varphi}{\partial r} (r)$ term in $\hat{s}(r)$, $s_2^{(s)}(r)$ the pure decimation terms and $s_2^{(B)}(r)$ the flow term $B\varphi(r)$, in the same way as compensation occurs in the sections 3.2 ($B = 0$, $s_1 = \frac{dp}{d}$) and 3.3 ($B = 0$, $s_1$ free):

$$z \int dr\ s_2^{(0)}(r)e^{\varphi(r)} = d \frac{2-n}{n}$$  \hspace{1cm} (3.4.1)

$$z \int dr\ s_2^{(s)}(r)e^{\varphi(r)} = 1 - z \int dr\ f(r) - z/n$$  \hspace{1cm} (3.4.2)

$$z \int dr\ s_2^{(B)}(r)e^{\varphi(r)} = u$$  \hspace{1cm} (3.4.3)

It is generally known that $\frac{\partial n}{\partial \mu}$ (compressibility) and $\frac{\partial u}{\partial T}$ (specific heat) diverge at criticality, but also $\frac{\partial n}{\partial T}$ and $\frac{\partial u}{\partial \mu}$ diverge, unless the singularities in $p$ are exact in the $\mu$- and the T-direction (i.e. they are the scaling field as e.g. in the Ising model. The situation is therefore worse than for the case of section 3.2 (zero flow), where only the second derivatives with respect to $\mu$ and $T$ diverge at criticality. Thus the first derivatives of $z \int dr\ s_2(r)e^{\varphi(r)}$ with respect to $\mu$ and $T$ diverge at criticality unless or prevents so by adjustment of $s_1$ and $B$ (using eq. (3.4.7)).

The procedure of adjusting $s_1$ and $B$ such that there are no singularities in the flow nor the weight $s_2(r)$ is similar to that of section 3.3, except that instead of inspecting the $\mu$- and $T$-direction one has to inspect Wagne's scaling fields 19). The conclusion is that it is possible to have a regular $\{\mu,T\}$ flow when the seemingly free parameters $s_1$ and $B$ are chosen deliberately for such a choice one needs to know $\{\mu_c,T_c\}$, i.e. the critical chemical potential and -temperature, and $p$, $n$, $u$, etc. at criticality, while it should be the aim of the theory to calculate these quantities.
Finally we remark that a two parameter flow, like \((\mu, T)\) flow is, necessarily misses the corrections to scaling (the irrelevant eigenvalues). In the next section we will treat flow constrained to \(\mu\) and \(\phi(r)\) in which the corrections to scaling are present.

3.5. Flow in \(\mu\) and \(\phi(r)\) only

This section deals with flow that is restricted to \(\mu\) and \(\phi(r)\) only, and thus assumes adjustment of \(s(r_1; r_2, \ldots, r_k)\) to get \(\phi(r_1, \ldots, r_k) = 0\) for \(k \geq 3\). It is more or less a cornerstone for the remainder of this thesis. We have to investigate whether the restriction to \((\mu, \phi)\) flow gives rise to singular behaviour of the flow, as before, which limits the a priori freedom in choosing \(s_1\) and \(s_2(r)\). The set-up of this section is therefore quite similar to that of section 3.4.

We, firstly, split up eqs. (3.1.3\textsuperscript{a},b) in the rescaling part and the weighted decimation part. The rescaling part is:

\[
\begin{align*}
\dot{p}_s &= dp \\
\dot{\mu}_s &= d \\
\dot{\phi}_s(r) &= r \frac{\partial \phi}{\partial r}(r)
\end{align*}
\]  

The weighted decimation flow is:

\[
\begin{align*}
\dot{p}_d &= -s_1 z \\
\dot{\mu}_d &= -s_1 + s_1 z \int dr f(r) + z \int dr s_2(r) e^{\phi(r)} \\
\dot{\phi}_d(r_{12}) &= -2s_2(r_{12}) + s_1 z (f s f)(r_{12}) + 2z (f s_2 e^\phi)(r_{12}) + \\
&+ z \int dr_3 s_3(r_3; r_1, r_2) e^{\phi(r_{13}) + \phi(r_{23})}
\end{align*}
\]

Now we use eq. (3.1.4) for the flow of the pressure up to the second term, which is exact for \((\mu, \phi)\) flow:
\[ \dot{\Phi} = n \dot{u} + \frac{1}{2} \int d^2 r \, n(r_1 r_2) \Phi(r_{12}) \]  

(3.5.3)

Substitution of eqs. (3.5.1) gives rise to the well-known trivial expression in d dimensions:

\[ p = n + \frac{1}{2d} \int d^2 r \, n(r_1 r_2) r \frac{\partial \Phi}{\partial r}(r_{12}) \]  

(3.5.4)

Therefore it does not give a new result. Eqs. (3.5.2) however give rise to a non trivial expression, being:

\[ -s_1 z = n[-s_1 + s_1 z \int d^2(r) + z \int d^2 s(r) \Phi(r)] - \frac{1}{2} \int d^2 n(r_1 r_2) [-2s_2 (r_{12}) + s_1 z(r^2 f(r)) (r_{12}) + 2z(r^2 s_2 e^2) (r_{12}) + z \int d^2 s_3 (r_3 r_1 r_2) \Phi(r_{13}) \Phi(r_{23}) ] \]  

(3.5.5)

The functions \( s_1 \) and \( s_2 (r) \) are so far free functions, while \( s(r_3 r_1 r_2) \) is used to make \( \Phi(r_1 r_2 r_3) = 0 \). The weight \( s(r_3 r_1 r_2) \) depends on \( n, \Phi(r), s_1 \) and \( s_2 (r) \) in a rather difficult way which will be treated in more detail in chapter IV.

The weight \( s_1 \) is in contrast with former cases, a multiplicative constant in eq. (3.5.5). This has its origin in the fact that the constraint \( \Phi(r_1 ... r_k) \) with \( \Phi(r_1 ... r_k) = 0 \) does not involve rescaling terms. One sees for instance from eq. (3.1.3) that the rescaling term is absent and that \( \Phi(r_1 r_2 r_3) = 0 \) is linear homogeneous in the weights. If one defines:

\[ \tilde{s}(r_1 r_2 ... r_k) = s(r_1 r_2 ... r_k) / s_1 \]  

(3.5.6)

then the \( \tilde{s}(r_1 r_2 ... r_k) \) are independent of \( s_1 \) (when \( s(r_1 r_2 ... r_k) \) makes indeed \( \Phi(r_1 ... r_k) = 0 \) for \( k \geq 3 \)).

So now we have one in principle free function \( s_2 (r) \) which must fulfill:
\[ z = n[1 - z \int \mathbf{dr} f(r) - z \int \mathbf{dr} s_2(r)e^\phi(r)] + \frac{1}{n^2} \int \mathbf{dr} g(r_{12}) [2s_2(r_{12})] \]

\[ -z(f^*f)(r_{12}) - 2z(f^*s_2e^\phi)(r_{12}) - z \int \mathbf{dr} s_3(r_{3}^*; r_1^*r_2^*)e^{\phi(r_{13})+\phi(r_{23})} \]

(3.5.7)

Here we used \( n(r_1^*r_2^*) = n^2g(r_{12}) \) with \( g(r) \) the pair correlation function. At criticality, we know that both \( n \) and \( g(r) \) are singular functions of \( \mu \) and \( \phi(r) \). The left-hand side of eq. (3.5.7) is regular, and to keep the flow of \( \phi(r) \) regular we must also demand \( \frac{\mathbf{r}_2}{s_2(r_{12})} \) and \( \frac{\mathbf{r}_3^*; r_1^*r_2^*}{s_3(r_{3}^*; r_1^*r_2^*)} \) to be regular. The question is whether \( s_2(r) \) can be chosen freely, and regular, or are there conditions on \( s_2(r) \) to keep \( s_3(r_{3}^*; r_1^*r_2^*) \) regular, similar to the conditions found in sections 3.3 and 3.4.

No definite statements, as in sections 3.3 and 3.4, can be made about the question whether \( s_2(r) \) is totally free to choose, but eq. (3.5.7) points in the direction that there are conditions on \( s_2(r) \). It is namely unlikely that for a totally free \( s_2(r) \) the right-hand side of eq. (3.5.7) loses its singularities without building them up in \( s_3(r_{3}^*; r_1^*r_2^*) \). As argued in section 3.2 for \( s_2(r) \) we now see that \( s_3(r_{3}^*; r_1^*r_2^*) \) may build up correlation function (i.e. \( n(r_1^*r_2^*) \)) like singularities, to compensate the ones of \( n \) and \( g(r) \) in eq. (3.5.7). If so, this means that there are at least two (the number or relevant eigenvalues) conditions on \( s_2(r) \) as in section 3.4.

The above is not a proof but a warning against too rigorous constraints on the flow. We may conclude that \((\mu, \phi)\) flow is a good candidate for further investigations. In contrast to \((\mu, T)\) flow, we do not have to know the location of a critical point since for \((\mu, \phi)\) flow there is a critical sheet with infinitely many dimensions (co-dimension 2). Therefore there is no unique value of the critical pressure, such that one must have a very precise prescription of \( s_1 \) (see eq. 3.3.7), etc. Moreover, \((\mu, \phi)\) flow allows for the possibility of studying the corrections to scaling (irrelevant eigenvalues).

In the next chapter we will look at the realization of \((\mu, \phi)\) flow for weighted decimation. Approximations made there show that there are indeed conditions, on a priori free weights, for this sort of constrained flow, but they are of a different origin. They are a consequence of demands on the quantity \( \int \mathbf{dr} s_2(r_{12}) + \ldots + \phi(r_{1j}) \) as a function of \( j \).
for $j \to \infty$ (as already mentioned in section 3.2). These conditions, due to exact absence of higher order flow, must also be imposed outside the critical region, in contrast with the eventual consequences of eq. (3.5.7). It will serve us with the reduction of freedom in choosing the weights searched for heuristically in section 2.4.
IV. Connection of constrained flow with virial series

In this chapter we will proceed with a renormalization scheme that is constrained to flow in \( \mu \) and \( \varphi(r) \), as introduced in section 3.5. For the decimation weights it means that \( s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k) \) is adjusted to make \( \varphi(\vec{r}_1, \ldots, \vec{r}_k) = 0 \) for \( k \geq 3 \). In section 4.1 we show that there is a systematic approach possible, which leads to a diagram expansion for the weights \( s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k) \) \( (k \geq 3) \) in powers of the fugacity \( z \). In particular, we are interested in the diagram expansion for \( s(\vec{r}_1; \vec{r}_2, \vec{r}_3) \) which enters in the flow of \( \varphi(r) \), given by eq. (3.1.3b).

In many respects the expansion resembles the cluster expansion for the pressure \( p \), or the reduced probability densities \( n(\vec{r}_1, \ldots, \vec{r}_k) \) \( (21-25) \).

Inspired on that theory, we can make two types of approximation. The first one is to take into account only a few orders in \( z \) of the fugacity expansion for \( s(\vec{r}_1; \vec{r}_2, \vec{r}_3) \). We will comment on such a scheme in section 4.1. The second strategy is to take into account only relatively simple diagrams, but to all orders in \( z \). Since especially such an approach has proven to be useful, the remainder of this chapter will deal with it.

In sections 4.2 and 4.3 we try the simplest of such an approximation, namely the Cayley tree approximation. It accounts for diagrams with no loops only, and will result in a soluble flow equation. This flow will teach us that there are conditions on the a priori free weight \( s_2(r) \) and that one has to take loops into account for the description of a critical theory.

Section 4.4 will include in the flow the simplest loop to all orders. The resulting flow equations have a critical fixed point with (classical) mean field exponents. The conditions on \( s_2(r) \) survive and will be understood in the context of chapter III. We will meet a difficulty in both approximations, namely the divergence of the quantity \( \tilde{s}_j = \int d\vec{r}_2 \ldots d\vec{r}_j \{(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_j) \exp \sum_{i<j} \varphi(\vec{r}_{ij}) \} \) as a function of \( j \) for \( j \to \infty \), via a deep minimum. This fact that the \( s_j \) seem to form an asymptotic series indicates that \( (\mu, \varphi) \) flow may not be imposed too strictly.

We close in section 4.5 with a discussion of the relation between the results of this chapter to those of chapter II, and a general discussion on constrained flow equations.
4.1. Diagrammatic approach to \((u, \varphi)\) flow

In chapter III we have introduced constrained flow. The assumption is that it is possible to make \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = 0\) by adjustment of \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\). We have found that the adjustment leads to undesired flow properties if one imposes constraints on \(\dot{u}\) (\(k = 1\)) and \(\dot{\varphi}(r)\) (\(k = 2\)). In this chapter we proceed with \((u, \varphi)\) flow as introduced in section 3.5, with \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = 0\) for \(k \geq 3\). The flow equations are then defined by eqs. (3.1.3).

The most important unknown in the flow of \(\varphi(r)\) is \(s(\vec{r}_1; \vec{r}_2, \vec{r}_3)\), which will be fixed by the condition \(\dot{\varphi}(\vec{r}_1; \vec{r}_2, \vec{r}_3) = 0\) in our set-up.

We thus obtain a hierarchy of equations for the weights \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\), while we are interested especially in \(s(\vec{r}_1; \vec{r}_2, \vec{r}_3)\). As a first step to a systematic approach to the problem we write down the general flow equation for \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k)\) for \(k \geq 3\):

\[
0 = \dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = - \sum_{j=1}^{\ell} s(\vec{r}_j; \vec{r}_1, \ldots, \vec{r}_{j-1}, \vec{r}_{j+1}, \ldots, \vec{r}_k) + \int \! dr_{\ell+1} \sum_{n=0}^{\ell} \phi(\vec{r}_{1, \ell+1}) s(\vec{r}_{\ell+1}; \vec{r}_1, \ldots, \vec{r}_n) e^{f(\vec{r}_{n+1, \ell+1}) \ldots f(\vec{r}_{\ell, \ell+1})} \tag{4.1}
\]

We consider \(\dot{\varphi}(\vec{r}_1, \ldots, \vec{r}_k) = 0\) as the defining equation for \(s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)\).

The function \(s(\vec{r}_j; \vec{r}_1, \ldots, \vec{r}_{j-1}, \vec{r}_{j+1}, \ldots, \vec{r}_k)\) must be symmetric in the argument \(\{\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_k\}\) since the particles are identical. It need not be symmetric in all the arguments, \(\vec{r}_j\) included, since the \(j\)-th particle is the one that is decimated and therefore plays a special role. Equation (4.1.1) only tells that the symmetric sum of asymmetric functions vanishes. Therefore we may write:

\[
s(\vec{r}_\ell; \vec{r}_1, \ldots, \vec{r}_{\ell-1}) = \frac{1}{\ell} z \int \! dr_{\ell+1} \sum_{j=0}^{\ell} s(\vec{r}_{\ell+1}; \vec{r}_1, \ldots, \vec{r}_j) e^{\varphi(\vec{r}_1, \ell+1) \ldots \varphi(\vec{r}_j, \ell+1)} f(\vec{r}_{j+1, \ell+1}) \ldots f(\vec{r}_{\ell, \ell+1}) + \chi(\vec{r}_\ell; \vec{r}_1, \ldots, \vec{r}_{\ell-1}) \tag{4.1}
\]
where the function $\chi(r_{1}, r_{2}, \ldots, r_{k})$ satisfies

$$\chi(r_{1}, r_{2}, \ldots, r_{k}) + \chi(r_{2}, r_{1}, r_{3}, \ldots, r_{k}) + \cdots + \chi(r_{k}, r_{1}, \ldots, r_{k-1}) = 0 \quad (4.1.3)$$

For $\chi = 0$ one obtains a solution $s(r_{1}, r_{2}, \ldots, r_{k})$ which is symmetric in all its arguments $r_{j}$, $j = 1, \ldots, k$.

With the condition (4.1.3) for $\chi$, eq. (4.1.2) indeed leads to eq. (4.1.1). A function $\chi$, having the property (4.1.3), can be constructed from a general function $\tilde{\chi}(r_{1}, r_{2}, \ldots, r_{k})$ which is symmetric in $\{r_{1}, \ldots, r_{k}\}$, but not in the full $\{r_{1}, r_{2}, \ldots, r_{k}\}$ (i.e., $r_{1}$ is a special coordinate) as follows:

$$\chi(r_{1}, r_{2}, \ldots, r_{k}) = \tilde{\chi}(r_{1}, r_{2}, \ldots, r_{k}) - \frac{1}{k-1} \sum_{j=2}^{k} \chi(r_{j}, r_{1}, r_{2}, \ldots, r_{j-1}, r_{j+1}, \ldots, r_{k}) \quad (4.1.4)$$

The function $\tilde{\chi}$ is thus still quite general, which means that there is a substantial freedom in making $\tilde{\phi}(r_{1}, r_{k}) = 0$ for $k > 3$.

The set equations (4.1.2) is an open (infinite) hierarchy which has no unique solution as we shall see (even if we consider the $\chi(r_{1}, r_{2}, \ldots, r_{k})$ as given). If we truncate the set at finite $k$ we have $k+1$ unknown functions in $k$ equations. We then can set $s(r_{1}, \ldots, r_{k}) = 0$ in the $k$-th equation and consider it as a $k$-dimensional inhomogeneous integral equation for $s(r_{1}, \ldots, r_{k-1})$. Substituting the so found $s(r_{1}, \ldots, r_{k-1})$ in the $(k-1)$th equation, etc., we may roll down the solution till we obtain the desired $s(r_{3}, r_{2})$ in terms of the state $(\mu, \phi)$ and the two weights $s_{1}$ and $s_{2}(r)$. The meaning of such a solution depends on the convergence for $s(r_{3}, r_{2})$ when we let the truncation level $k \rightarrow \infty$.

For $z \rightarrow 0$ indeed a unique solution exists. Then we can make an expansion in powers of $z$, writing:

$$s(r_{1}, \ldots, r_{k-1}) = \sum_{m=1}^{\infty} z^{m} s^{(m)}(r_{1}, \ldots, r_{k-1}) \quad (4.1.5a)$$

$$\chi(r_{1}, \ldots, r_{k-1}) = \sum_{m=1}^{\infty} z^{m} \chi^{(m)}(r_{1}, \ldots, r_{k-1}) \quad (4.1.5b)$$

(One may start eqs. (4.1.5) with an $m = 0$ term. However, there is no need
at \( z = 0 \) for a decimation weight when there are no particles. Inclusion of \( \ell = 0 \) would modify the remainder of this section. Inserting the expansion (4.1.5) into eq. (4.1.2) leads to a closed hierarchy for the \( s(n)(\vec{r}_e;r_1,\ldots,r_{\ell-1}) \). The first order approximation \( s^{(1)}(\vec{r}_e;r_1,\ldots,r_{\ell-1}) \) is determined by the terms involving \( s_1 \) and \( s_2(r) \) (\( \ell \geq 3 \)):

\[
s^{(1)}(\vec{r}_e;r_1,\ldots,r_{\ell-1}) = \frac{1}{\ell} z \int d\vec{r}_{\ell+1} \left[ s_1 f(r_1,\ell+1) + \ldots + f(r_{\ell+1}) + s_2(r_1,\ell+1) e^{\psi(r_1,\ell+1)} f(r_2,\ell+1) \ldots f(r_{\ell},\ell+1) + \ldots + f(r_1,\ell+1) \ldots f(r_{\ell-1},\ell+1) s_2(r_{\ell},\ell+1) e^{\psi(r_{\ell},\ell+1)} \right] + x^{(1)}(\vec{r}_e;r_1,\ldots,r_{\ell-1})
\]

(4.1.6)

The second approximation \( s^{(2)}(\vec{r}_e;r_1,\ldots,r_{\ell-1}) \) involves \( s^{(1)}(\vec{r}_m;r_1,\ldots,r_{m-1}) \) for \( 3 \leq m \leq \ell+1 \) etc. We get, for instance, for \( s^{(2)}(\vec{r}_3;r_1,\vec{r}_2) \):

\[
s^{(2)}(\vec{r}_3;r_1,\vec{r}_2) = \frac{1}{3} z \int d\vec{r}_3 \left[ s^{(1)}(\vec{r}_3;r_1,\vec{r}_2) e^{\psi(r_1) + \psi(r_2)} f(r_3) + s^{(1)}(\vec{r}_3;r_1,\vec{r}_2) e^{\psi(r_1) + \psi(r_2)} f(r_3) + s^{(1)}(\vec{r}_3;r_1,\vec{r}_2) e^{\psi(r_1) + \psi(r_2)} f(r_3) + s^{(1)}(\vec{r}_3;r_1,\vec{r}_2) e^{\psi(r_1) + \psi(r_2)} f(r_3) + s^{(1)}(\vec{r}_3;r_1,\vec{r}_2) e^{\psi(r_1) + \psi(r_2)} f(r_3) \right] + x^{(2)}(\vec{r}_3;r_1,\vec{r}_2)
\]

(4.1.7)

The expressions for \( s^{(m)}(\vec{r}_e;r_1,\ldots,r_{\ell-1}) \) are most easily represented with the help of Mayer cluster diagrams \( \vec{\alpha}_1,\ldots,\vec{\alpha}_m \), having the rules:

\[
0 \longrightarrow 0 = f(r_{12}) = e^{\psi(r_{12}) - 1} \quad 0 \longrightarrow 0 = e^{\psi(r_{12}) - 1 + f(r_{12})}
\]

(4.1.8)

\[
\sigma \sigma = \frac{1}{s_1} s_2(r_{12}) e^{\psi(r_{12})}
\]

(4.1.9)

An open dot in the diagram represents a coordinate, while a closed dot
means integration over such a coordinate. For instance, one gets for 
\( l = 3 \) and \( l = 4 \) in eq. (4.1.6):

\[
s^{(1)}(\vec{r}_3; \vec{r}_1, \vec{r}_2)/s_1 = \frac{1}{3} \left[ \begin{array}{c}
+ x^{(1)}(\vec{r}_3; \vec{r}_1, \vec{r}_2)/s_1 \\
\end{array} \right] (4.1.9a)
\]

\[
s^{(1)}(\vec{r}_4; \vec{r}_1, \vec{r}_2, \vec{r}_3)/s_1 = \frac{1}{4} \left[ \begin{array}{c}
+ x^{(1)}(\vec{r}_4; \vec{r}_1, \vec{r}_2, \vec{r}_3)/s_1 \\
\end{array} \right] + x^{(1)}(\vec{r}_4; \vec{r}_1, \vec{r}_2, \vec{r}_3)/s_1 (4.1.9b)
\]

Substitution of the expressions (4.1.9) in eq. (4.1.7) yields:

\[
s^{(2)}(\vec{r}_3; \vec{r}_1, \vec{r}_2)/s_1 = \frac{1}{9} \left[ \begin{array}{c}
+ \text{all permutations in (123)} \\
\end{array} \right] + \frac{1}{12} \left[ \begin{array}{c}
+ \frac{1}{3s_1} \int dr_4 \left[ x^{(1)}(\vec{r}_4; \vec{r}_1, \vec{r}_2)e^{\varphi(r_{14})+\varphi(r_{24})}f(r_{34})+\ldots \right] \\
\end{array} \right] \\
\]

\[
+ x^{(2)}(\vec{r}_3; \vec{r}_1, \vec{r}_2)/s_1 (4.1.10)
\]
These expressions for $s^{(m)}(\vec{r}_3; \vec{r}_1, \vec{r}_2)$ can be substituted in the flow for $\dot{\varphi}(r_{12})$, eq. (3.1.3), leading to a diagram expansion for the flow ($\dot{\mu}$ is still given by eq. (3.1.3a)):

$$
\dot{\mu} = d - s_1 + z \int dr \left[ s_1 f(r) + s_2(r) e^\varphi(r) \right] 
$$

(4.1.1)

$$
\dot{\varphi}(r_{12}) = r \frac{\partial}{\partial r} (r_{12}) - 2s_2(r_{12}) + s_1 z(f^*f)(r) + 2z(f^*s_2\varphi)(r)
$$

$$+ z^2 \int dr_3 s(1)(r; \vec{r}_3; \vec{r}_1, \vec{r}_2) e^{\varphi(r_{13})+\varphi(r_{23})} +
$$

$$+ z^3 \int dr_3 s(2)(r; \vec{r}_3; \vec{r}_1, \vec{r}_2) e^{\varphi(r_{13})+\varphi(r_{23})} + \ldots 
$$

(4.1.1)

In terms of this expansion, we have treated in chapter II this flow equations up to the first order in $z$ only. The choice $\chi^{(m)}(r_2; r_1, \ldots, r_{L-1}) = 0$ can be seen from eq. (4.1.10) to give rise to so called chain diagrams. As mentioned in chapter III this can be dangerous since they could make the flow operate long in range (as they are primarily responsible for long-rangedness of the correlation functions). The freedom in choosing the function $\chi(r; \vec{r}_1, \ldots, \vec{r}_{L-1})$ at every level $L$, makes that there are many realizations of ($\mu, \varphi$) flow. With the help of $\chi(r_1, r_2, \ldots, r_L)$, leading with eq. (4.1.4) to a $\chi(r_1; r_2, \ldots, r_L)$, one can, for instance, try to reduce the influence of some chain diagrams (their combinatorial factors). However, due to relation (4.1.3), one is not able to remove all chain diagrams.

Again we have to make approximations to calculate the flow for ($\mu, \varphi$) numerically. There are two ways to proceed. The first is to stop at a certain power of $z$ in eq. (4.1.1b). However, with our procedure of calculation, as explained in section 2.2, some of the resulting diagrams are hard to handle. (Note that for the search after a fixed point such diagrams must be calculated many times). Moreover, these difficult diagrams (i.e. the ones that are completely filled with $f(r)$ functions) are usually small compared to the convolution like diagrams in the region we are interested in.

Taking only these into account in lowest order in $z$, has given results comparable with the ones of chapter II. In fact, one finds that the more of these diagrams are included, the more the results depend on $s_1$ and $s_2(r)$. This can be understood in the light of what will follow.
The second method for making approximations is to take only certain types of diagrams into account, but to all orders in \( z \). The first and simplest of such an approximation is the Cayley tree, or no-loop approximation. This will be treated in sections 4.2 and 4.3. We will learn that for a study of critical phenomena one at least needs to take into account the simplest loop to all orders (section 4.4).

4.2. The Cayley tree approximation

The simplest approximation which takes into account infinitely many orders of the fugacity \( z \) in eq. (4.1.11) is the Cayley tree approximation. It means that no loops are allowed in the diagrams, since usually these diagrams give the largest contribution. In the Cayley tree approximation all terms with \( 1+f(r) \) are set equal to 1 (i.e. all dotted lines in eq. (4.1.10) are removed). The problem has then been reduced to finding the combinatorial factors of the diagrams. This follows most easily by studying eq. (4.1.2).

The Cayley tree approximation can be obtained from eq. (4.1.2) by removing all \( e^{\Phi(r)} \) terms, except the one accompanied by \( s_2(r) \). However, in the remainder of this section we will write \( s_2(r)e^{\Phi(r)} \) simply as \( s_2(r) \). Eq. (4.1.2) now becomes:

\[
\begin{align*}
\bar{s}_2(r_1, r_2, \ldots, r_{L-1}) &= \frac{1}{L^z} \int d\vec{r}_{L+1} \sum_{j=0}^{L} \left( \frac{L}{\{j_1, \ldots, j_L\}} \right)_{\{1, \ldots, L\}} \left( \{s_{j+1}(r_{L+1}; r_1, \ldots, r_j) \right. \\
& \quad + f(r_{j+1, L+1}) \cdot f(r_1, L+1) \cdot f(r_{L+1, L+1}) + x(r_{L+1}; r_1, \ldots, r_{L-1}) \\
\end{align*}
\]

(4.2.1)

So what remains is an expression which, due to its convolution character, is most easily solved in Fourier space. Therefore we define:

\[
\begin{align*}
\bar{s}_2(k_1, k_2, \ldots, k_{L-1}) &= \int d\vec{r}_1 \ldots d\vec{r}_{L-1} s(\vec{r}_2; r_1, \ldots, r_{L-1}) e^{ik_1 \cdot (r_1 - r_2)} + \ldots + e^{ik_{L-1} \cdot (r_{L-1} - r_L)} \\
\end{align*}
\]

(4.2.2)

Equation (4.2.1) simplifies considerably since the integral of \( \vec{r}_{L+1} \) can be
performed, leading to a δ-function as a consequence of translational invariance (therefore \( \vec{k}_2 = -\vec{k}_1 = \cdots = \vec{k}_{L-1} \)):

\[
\hat{s}_k(\vec{k}_1, \ldots, \vec{k}_{L-1}) = \frac{1}{L} \sum_{j=0}^{L-1} \frac{1}{(l_1, \ldots, l_j) \in \{1, \ldots, L\}} \left[ \hat{s}_{j+1}((\vec{k}_1, \ldots, \vec{k}_j) \hat{f}(\vec{k}_{j+1} \ldots \hat{f}(\vec{k}_1)) \right] \hat{\chi}_k = -\vec{k}_1 = \cdots = \vec{k}_{L-1} \]

\[(4.2.3)\]

Here \( \hat{f}(k) \) is the Fourier transform of \( f(r) \).

As before we are interested in the effect of the approximations on the flow of \( \varphi(r) \), which now reads (eq. (3.1.3b)):

\[
\dot{\varphi}(r_{12}) = \frac{\partial \varphi}{\partial r}(r_{12}) - 2s_2(r_{12}) + zf^s[s_1f + 2s_2](r_{12}) + z\int d^3r_3 s_3(r_3; r_1 r_2)
\]

\[(4.2.4)\]

In Fourier language this means that we have to know the function \( \hat{s}_3(\vec{k}, \vec{k}) \), i.e. \( \vec{k}_1 = -\vec{k}_2 = \vec{k} \). To find this function, one should study eq. (4.2.3) for all \( \hat{s}_k(\vec{k}_1, \vec{k}_2, \vec{k}_3 = 0, \vec{k}_{L-1} = 0) \) to which it couples, namely the three cases: \( \vec{k}_1 = -\vec{k}_2 = \vec{k}; \vec{k}_1 = \vec{k}_2, \vec{k}_2 = 0; \vec{k}_1 = \vec{k}_2 = 0 \). However, one easily checks that one also needs \( \hat{\chi}_k(\vec{k}_1, \ldots, \vec{k}_{L-1}) \) for these cases. Due to the fact that \( \chi \) can be written in terms of a free function \( \chi \), as done in eq. (4.1.4), one can prove the following relations:

\[
\hat{\chi}_k(\vec{k}, 0, \ldots, 0) = \frac{1}{L-1} \left[ \hat{\chi}_k(\vec{k}, \vec{k}, 0, \ldots, 0) - \hat{\chi}_k(\vec{k}, 0, \ldots, 0) \right]
\]

\[(4.2.5a)\]

\[
\hat{\chi}_k(\vec{k}, -\vec{k}, 0, \ldots, 0) = \frac{2}{L-1} \left[ \hat{\chi}_k(\vec{k}, -\vec{k}, 0, \ldots, 0) - \hat{\chi}_k(\vec{k}, 0, \ldots, 0) \right] = 2\hat{\chi}_k(\vec{k}, 0, \ldots, 0)
\]

\[(4.2.5b)\]

This means that \( k = 0 \) is special since \( \hat{\chi}_k(0, \ldots, 0) = 0 \). Thus for \( k = 0 \) the results do not depend on the choice of \( \chi \), where as \( k \neq 0 \) they do.

For finite \( k \) one has moreover coupling to the \( k = 0 \) result (see appendix E). Therefore we will concentrate on the \( k = 0 \) case.
When all \( \bar{K}_1 = 0 \) (\( i = 1, \ldots, l-1 \)), eq. (4.2.3) simply becomes:

\[
\sum_{j=0}^{l-1} \frac{\Gamma_j}{(j)!} s_{j+1}^{l-j} = z \sum_{j=0}^{l} \frac{u}{(j)!} s_{j+1}^{l-j} \quad (4.2.6)
\]

where we abbreviated \( \sum_{j=0}^{l} \frac{\Gamma_j}{(j)!} s_{j+1}^{l-j} = \tilde{s}_l \) (\( \bar{K}_1 = 0, \ldots, \bar{K}_{l-1} = 0 \)) and \( \tilde{\chi} = \tilde{\chi}(0) \). This recurrence relation can be treated by the use of a generation function:

\[
S(u) = \sum_{l=0}^{\infty} \frac{u^l}{l!} \tilde{s}_{l+1} \quad (4.2.7)
\]

Multiplication of eq. (4.2.6) with \( \frac{u}{(j)!} s_{j+1}^{l-j} \) and summation over \( l \geq 1 \) (and correction for \( l=1 \) and \( l=2 \)) yields:

\[
u \cdot S(u) = \sum_{l=1}^{\infty} \frac{u^l}{l!} \left[ \sum_{j=0}^{l} \frac{u}{(j)!} s_{j+1}^{l-j} \right] - u \cdot S(u) \tilde{s}_1^\chi - S_2^\chi
\]

\[
= \frac{-u^2 z [s_1^\chi + s_2^\chi + s_3^\chi]}{1 - u \cdot S(u)} \quad (4.2.8)
\]

The sum term on the right-hand side can be worked out as follows:

\[
\sum_{l=1}^{\infty} \frac{u^l}{l!} \left[ \sum_{j=0}^{l} \frac{u}{(j)!} s_{j+1}^{l-j} \right] = \sum_{l=1}^{\infty} \frac{u^l}{l!} \left[ \sum_{j=0}^{l} \frac{u}{(j)!} s_{j+1}^{l-j} - s_1 z \right]
\]

\[
= \sum_{j=0}^{\infty} \frac{u^j}{j!} s_{j+1}^{\chi} \sum_{l=j}^{\infty} \frac{(u \cdot S(u))^{l-j}}{(l-j)!} - s_1 z
\]

\[
= S(u) e^{u \cdot S(u)} - s_1 z \quad (4.2.9)
\]

Substitution of this into eq. (4.2.8) leads to the following expression for \( S(u) \):

\[
S(u) = \frac{s_1 [u - z - u \cdot S(u)] + u s_2 [u - z - u \cdot S(u)] - i u^2 z s_3}{(u - z \exp u \cdot S(u))} \quad (4.2.10)
\]

Equation (4.2.10) teaches us something very important, namely the existence of poles in \( S(u) \). A (simple) pole due to a zero at \( u = u_0 \) in the denominator of \( S(u) \) yields a finite radius of convergence. If \( u_0 \) is the closest pole to the origin, the coefficients \( s_l / l! \), defined through eq. (4.2.7), behave as:
\[
\frac{s_k}{k!} \approx A u^{-k} / 0 \quad (k \to \infty)
\]

This implies that the \( s_k \) increase as a factorial for \( k \to \infty \). Such weights are physically unacceptable. Thus the zeroes of the denominator of \( S(u) \) must be compensated through the following demand:

\[
[v_1 - 1 - (v_1 x)^{1/2} (v_1 x)^2] + v_1 \frac{s_3}{s_2} [v_1 - 1 - (v_1 x)] - \frac{1}{2} v_1^{s_3} = 0
\]

whenever \( v_1 (= u/z) \) fulfills:

\[
v_1 = e^{x_1} (= u/z = e^{u_1})
\]

Furthermore we used the abbreviations:

\[
x = z = z f(r) = z f(r)
\]

\[
\frac{s_3}{s_2} = \frac{1}{s_1} z \frac{\nu}{s_2} = \frac{1}{s_1} \int dr s_2(r) e^{\nu(r)}
\]

\[
\frac{s_3}{s_2} = \frac{1}{s_1} z \frac{\nu}{s_3} = \frac{1}{s_1} \int dr ds_3(r_3) e^{\nu_1(r_3, r_1 r_2)}
\]

So when the denominator of eq. (4.2.11) is zero, leading to eq. (4.2.12b), one must have the numerator zero, leading to eq. (4.2.12a).

Eq. (4.2.12a) must hold for all roots \( v_1 \) of eq. (4.2.12b), also complex ones. The number of conditions is the number of roots \( v_1 \), which we will investigate for a value of \( x \) in the region \( 0.3 \leq x \leq 0.5 \), i.e. roughly when one can expect the critical value (see e.g. section 2.2). One easily checks that there are for \( x < 1/e \) two real roots \( v_1 \) of eq. (4.2.12b). For \( x = 1/e \) they merge into \( v_{1,2} = e \), and for \( x > 1/e \) they become two complex conjugate ones \( (v_1^* = v_2) \). For \( x > 1/e \) there are no real valued roots \( v_1 \) anymore. However, one can prove that there are more (conjugate) complex roots than the ones found above. The ones that are in absolute value closest to \( v_{1,2} = e \) (= 2.7182), for \( x = 1/e \), are:

\[
v_{3,4} = 8.3963 \pm 20.2824 \quad ; \quad |v_{3,4}| x = 8.0756
\]

\[
v_{5,6} = 9.9600 \pm 37.7272 \quad ; \quad |v_{5,6}| x = 14.3546
\]
Roughly the absolute value of $|v_{2n-1,2n}|x$ $(n = 2, 3, \ldots)$ increases every next root with a value $2x$. More generally one finds the same behavior for $|vx|$ for all $x$.

The set of roots of the denominator (4.2.10) requires a discussion. If we could restrict ourselves to the smallest root, one would have one condition (4.2.12$^a$) by which $\hat{s}_3$ could be expressed in terms of $\hat{s}_2$. This is the situation which was anticipated: the 2-particle weight $s_2$ is free and the higher weights, e.g. $s_3$ are expressed in $s_2$.

If we could limit ourselves to the two smallest roots, we should adjust $\hat{s}_2$ and $\hat{s}_3$ to fulfill eq. (4.2.12$^a$). It is surprising that convergence imposes a requirement on the seemingly free weight $\hat{s}_2$. As we shall see in the next section, this makes the flow scheme however fully determined (in the Cayleytree approximation) and a satisfactory picture results.

The multitude of conditions due to the other roots cannot be met and we see this as an indication that strict $(u, p)$ flow is not possible without unphysically increasing weights $s_l$ for $l \to \infty$. A positive point is that the other roots are relatively far away from the one we will use. This means that the divergence of the $s_l$ goes via a reasonably deep minimum as will be shown in section 4.3., and, for a more general case, in section 4.4. It indicates that one deals with an asymptotic series. In the next section we will proceed with the two conditions fixing $\hat{s}_2$ and $\hat{s}_3$ as a function of $x$, and study the consequences of it on the flow equations.

Finally we mention that it is possible to derive a recurrence relation, similar to eq. (4.2.6), for $\hat{s}_2(k, \hat{k}, 0, \ldots, 0)$ and $\hat{s}_3(k, 0, \ldots, 0)$. In appendix E we have given the results for finite $k$. The fact that $x$ stays in these equations as a freedom, has convinced us that there will not follow stringent conditions for $\hat{s}_2(k)$ and $\hat{s}_3(\hat{k}, \hat{k})$ as for $\hat{k} = 0$. Since our experiences from chapter II are that especially these conditions are important, we will not concentrate on finite $k$ further.
4.3. Flow in the Cayley tree approximation

In this section we study the consequences for the flow of the conditions on the weights \( s_2 \) and \( s_3 \) as found in section 4.2. The flow will be treated, as there, in the Cayley tree approximation. In that case, we neglect the \( f(r) \) in all \( e^\phi(r) = 1 + f(r) \), which means that there is no difference in \( \dot{\phi}(r) \), given by eq. (4.2.4), and \( \dot{f}(r) \), as well as between \( r \frac{\partial \phi}{\partial r}(r) \) and \( r \frac{\partial f}{\partial r}(r) \). As a consequence we may change the \( \phi(r) \) in eq. (4.2.4) in \( f(r) \) everywhere.

There are only conditions for the Fourier transforms \( \hat{s}_2(k) \) and \( \hat{s}_3(k, -k) \) at \( k = 0 \). Since the flow of \( \hat{f}(k=0) \) does not couple to \( \hat{\phi}(k\neq0) \) (in this approximation), we only inspect \( \hat{f}(k=0) \). This flow is found from eq. (4.2.4) and reads in the notation of section 4.2 (\( \mu \) given by eq. (3.1.3b)):

\[
\begin{align*}
\dot{\mu} &= d - s_1 + z[s_1 \hat{\phi} + \hat{s}_2] \quad (4.3.1a) \\
\dot{\hat{\phi}} &= -d \hat{\phi} - 2s_2 + z[s_1 \hat{\phi} + 2f \hat{s}_2 + \hat{s}_3] \quad (4.3.1b)
\end{align*}
\]

We know that the fluid is invariant under changes in scale \((r \rightarrow r/b)\). As the variable \( z \hat{\phi} \) is scaling invariant, the flow \( \dot{\mu} \) is, but \( \dot{\hat{\phi}} \) is not scaling invariant. For that reason, we go over to the flow of the variable \( z \hat{\phi} \). Introduction of the combinations defined in eq. (4.2.13), which are all scaling invariant, results in:

\[
\begin{align*}
\dot{\mu} &= d + s_1 [-1 + x + \hat{s}_2] \quad (4.3.2a) \\
\dot{x} &= s_1 [-x - 2s_2 + 2x^2 + 3x \hat{s}_2 + \hat{s}_3] \quad (4.3.2b)
\end{align*}
\]

We observe that the flow of \( x \) decouples from the flow of \( \mu \). Thus eq. (4.3.2b) can be considered separately. As \( \mu \) does not occur in eq. (4.3.2a) either, one is able to make \( \dot{\mu} = 0 \) by adjustment of \( s_1 \), when \( \dot{x} = 0 \) for \( x = x^* \). A fixed line then results for all \( \mu, \hat{\phi} \) such that \( z \hat{\phi} = x^* \).

Thus \( s_1 \) has to have a definite value, as we will see.
We will discuss first the scheme where both \( \hat{s}_2 \) and \( \hat{s}_3 \) are found from the conditions \((4.2.12)\), being:

\[
\left[ v_1 - v_1 x - \frac{1}{2}(v_1 x)^2 \right] + v_1 \hat{s}_2 \left[ v_1 - v_1 x \right] - \frac{1}{2} v_1^2 \hat{s}_3 = 0 \tag{4.3.3a}
\]

\[
v_1 = e^{v_1 x}, \quad i = 1, 2 \tag{4.3.3b}
\]

where \( v_{1,2} \) are the roots that are smallest in absolute value.

Later on we shall discuss the scheme where only one root is used.

The flow of \( x \) is a non trivial problem, however, one finds a fixed point for \( x = 1/e \). This is the point where the two roots of \((4.3.3b)\) coincide, i.e. \( v_1 = v_2 = e \), as mentioned before. To get then two conditions (to set the values of \( \hat{s}_2 \) and \( \hat{s}_3 \)), one has to recall the original problem, the pole in the generating function \( S(u) \) in eq. \((4.2.10)\). Rewritten in the variables \( v, \hat{s}_2, \hat{s}_3 \) and \( x \) it reads

\[
(v-e^{vx})S(v) = [v_1 - v_1 x - \frac{1}{2}(vx)^2] + v\hat{s}_2 [v_1 - v_1 x] - \frac{1}{2} v^2 \hat{s}_3 \tag{4.3.4}
\]

For \( x = 1/e \) we thus have that \( c(v) = v-e^{v/e} \) is quadratic at \( v = e \) (i.e. \( c(e) = c'(e) = 0 \)). Differentiation of eq. \((4.3.4)\) with respect to \( v \) and setting \( v = e \) gives, together with the equation at \( v = e \), two conditions, being \( (x = 1/e, \ vx = 1) \):

\[
(e-2) + e\hat{s}_2 [e-2] - \frac{1}{2} e^2 \hat{s}_3 = 0 \tag{4.3.5a}
\]

\[
(e-2) + e\hat{s}_2 [2e-3] - e^2 \hat{s}_3 = 0 \tag{4.3.5b}
\]

One gets for \( \hat{s}_2 \) and \( \hat{s}_3 \):

\[
\hat{s}_2 = \frac{e-3}{e} = -0.103638 \tag{4.3.6a}
\]

\[
\hat{s}_3 = \frac{2e^2-8e+7}{e^2} = 0.004311 \tag{4.3.6b}
\]
Substitution of this in equation (4.3.2^b) indeed gives that \( \dot{x} = 0 \) for this case. To get \( \dot{\tilde{y}} = 0 \) for these values we use eq. (4.3.2^a):

\[
s_1/d = x^* = \frac{1}{1-x-\hat{s}_2} \bigg|_{x=0} = e/2 = 1.359141
\]

(4.3.7)

Thus \( s_1 \) (or rather \( s_1/d \)) must have definite value at this fixed point. Then one has a fixed line for all values of \( z \) and \( \tilde{\gamma} \) with \( x = \tilde{\gamma}^2 = 1/e \), which is a consequence of scaling invariance.

To proceed we want to know \( \frac{\delta s}{\delta x} \) for the fixed point \( x = 1/e \). To calculate \( \frac{\delta s_2}{\delta x} \) and \( \frac{\delta s_3}{\delta x} \) we have to differentiate eq. (4.2.21) with respect to \( x \), and then carry out the above procedure again. However, in the next section we will describe the same procedure for a more general case. Therefore we give the calculated \( \frac{\delta s_2}{\delta x} \) and \( \frac{\delta s_3}{\delta x} \), and skip the derivation (see also appendix F). The answers are:

\[
\frac{\delta s_2}{\delta x} = -\frac{1}{3}
\]

(4.3.8^a)

\[
\frac{\delta s_3}{\delta x} = \frac{2}{3} \frac{1-4e}{e}
\]

(4.3.8^b)

Substitution in the expression for \( \frac{\delta s}{\delta x} \bigg|_{x=1/e} \) derived from eq. (4.3.2^b), one gets for the eigenvalue \( y_{CT} \) for the Cayley tree case:

\[
y_{CT} = \frac{\delta x}{\delta x} \bigg|_{x=1/e} = dx^* \left[ -1+4x+3\hat{s}_2 + (3x-2) \frac{\delta s_2}{\delta x} + \frac{\delta s_3}{\delta x} \right]_{x=1/e} = \frac{2d}{3}
\]

(4.3.9)

Note that variation of \( s_1 \), away from the fixed point has no influence, since \( s_1 \) appears multiplicative in eq. (4.3.2^b).

To interpret this result we go back to the starting point: the Cayley tree approximation. Inspection of the types of diagrams which are generated in the integration of the pressure from the flow, eq.(3.1.3^a), tells us that the pressure is approximated as well by a Cayley tree diagram expansion in the fugacity. A well-known result is the following
The pressure is approximated by the first two terms of the virial expansion (i.e. p(n) relation):

\[ p(n) = n - \frac{1}{2}fn^2 \]  \hspace{1cm} (4.3.10a)

while the fugacity is expressed by:

\[ z = n \exp[-\gamma n] \]  \hspace{1cm} (4.3.10b)

Then one has indeed a self consistent approximation, i.e. \[ \frac{\partial p}{\partial \mu} = z \frac{\partial p}{\partial z} = n, \]
which involves the most simple cluster diagram \[ e \rightarrow f = \int dr f(r). \]

It is easy to check that eqs. (4.3.10) are compatible with the flow of the pressure \( \dot{z} = dp - s_z z \) using eqs. (4.3.2).

The set equations (4.3.10) describes a system which does not have a critical point, for which \[ \frac{\partial p}{\partial n} (n^*) = \frac{\partial^2 p}{\partial n^2} (n^*) = 0 \] must be fulfilled.

Now one can only have \[ \frac{\partial p}{\partial n} (n^*) = 0, \] which leads to:

\[ n^* n^* = 1 \]  \hspace{1cm} (4.3.11)

Using eq. (4.3.10b) we then obtain

\[ n^*/z^* = e \]  \hspace{1cm} (4.3.12a)

\[ z^* n^* = 1/e \]  \hspace{1cm} (4.3.12b)

Eq. (4.3.12b) is exactly our value \( x^* = 1/e \) where we have found a fixed point, i.e. \( x = 0 \) in eq. (4.3.2b). The variable \( v \) must be interpreted as \( n/z, \) as can be seen by comparing eq. (4.3.10b) and eq. (4.2.12b). In the Cayley tree approximation one thus finds that the generating function \( S(u) \), defined in eq. (4.2.7) has poles at \( u = n \), where in principle also complex solutions of that \( z(n) \) relation, eq. (4.3.10b), should be counted.

The eigenvalue \( y_{CT} \) is now easily interpreted. The \( p(n) \) relation is quadratic in \( n. \) So when \[ \frac{\partial p}{\partial n} (n^*) = 0, \] one has \[ p(n) = p(n^*) + \frac{1}{2} \frac{\partial^2 p}{\partial n^2} (n^*) (n-n^*)^2. \]

Inspecting the definition of the critical exponent \( \delta, \) we find \( \delta = 2. \)

In section 2.2 we have given the relation between \( y_H \) and \( \delta, \) being for \( \delta = 2: \)

\[ y_H = \frac{\delta}{\delta+1} d = \frac{2}{3} d \]  \hspace{1cm} (4.3.13)
Thus \( y_H = y_{CT} \), given by eq. (4.3.9).

Now, also the special value of \( s_1 \) can be understood since we know from the flow of \( p (p = dp - s_1 z) \) that one must have at the fixed point, using eqs. (4.3.12):

\[
x^* = s_1^*/d = p^*/z^* = (p^*/n^*)(n^*/z^*) = e/2
\]

(4.3.14)

So by studying the flow at \( k = 0 \), using the two roots \( v_{1,2} \) given by (4.3.3b), we obtain all already known results, i.e. results from the truncated virial- and cluster expansions for the pressure at Cayley tree level.

The results of this section may be clarified by making the connection with chapter III, where we derived the general consequence from restricting the flow to the \((\mu, \psi)\) space. In order that the pressure flow equation is consistent with the flow \((\mu, \psi)\), eq. (3.5.7) has to be obeyed. Now one observes that inserting for the pair correlation function the expression:

\[
g(r) = \exp \psi(r)
\]

(4.3.15)

condition (4.3.3a) follows exactly, with \( n/z \) replaced by \( v \). This result is altogether not surprising since the pressure, as calculated from the virial theorem (3.5.4) and using eq. (4.3.15), precisely yields the Cayley tree approximation for the pressure. This means that the set eqs. (4.3.10) is a solution of the flow equations \( \dot{s} = dp - s_1 z \) and (4.3.1) for \( s_1 \) and \( s_2 \) provided that \( s_2 \) and \( s_3 \) obey (4.3.3a).

However, (4.3.3a) should hold for all roots, whereas for the pressure expression (4.3.10) it is sufficient that (4.3.3a) is obeyed for the root corresponding to the physical density. The role of the other roots deserve a further discussion. There are two aspects to the issue.

Firstly, one cannot satisfy (4.3.3a) for all roots as mentioned earlier. As a result, the \( s_2 \) diverge for large \( l \). We have computed the \( s_2 \) for the fixed point and in table 4 we show the quantities \( s_2 = z^{-1} \gamma / s_1 \) for several \( l \). One observes the divergence, but after having passed through a very low minimum, indicating that the difficulties only arise at reasonably high potentials. Nevertheless it is an essential argument against imposing constraints on the flow.
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</tr>
<tr>
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</tr>
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</table>

Table 4. Behavior of $\hat{s}_l = \frac{1}{s} s_{l-1} / s$
for $l \leq 20$.

Secondly, with the maximum of two roots satisfying (4.3.3²), a basic new element is added to the flow properties (not to the pressure). This can be seen by investigating the flow in the neighbourhood of the fixed point $x = 1/e$. Writing

$$x = 1/e - \delta x$$  \hspace{1cm} (4.3.16)

the roots are

$$v_\pm = e \left[ 1 \pm 2e\delta x \right]^{1/2} + \frac{5}{6} \left( 2e\delta x \right) + \frac{47}{72} \left| 2e\delta x \right|^{3/2} + \ldots $$  \hspace{1cm} (4.3.17)

The smallest (physical) root has the minus sign. For $\hat{s}_2$ and $\hat{s}_3$ we can expand similarly ($l = 2, 3,$):

$$\hat{s}_l = a_l + b_l \left| 2e\delta x \right|^{1/2} + \ldots$$  \hspace{1cm} (4.3.18)
The requirement that both roots (4.3.17) satisfy (4.3.3) implies that the half integer powers in $\delta^2$ are absent ($b_3 = 0$). Thus the flow (involving $\delta^1$ and $\delta^3$) is then regular, whereas the roots singularly depend on $x$. See that the requirements of convergence of the $\delta^2$ and regularity of the flow go hand in hand.

The pressure, as given by eq. (4.3.10), shows that the Cayley tree approximation is too poor to describe a critical theory. In section 4.4 we include the most simple loop, i.e. the third virial coefficient in the flow. It will turn out that it is then possible to obtain the mean field exponents, by studying the flow of these diagrams only. Of course this is (as the flow of $x$) not the full problem. The hope is to find so a starting point for a more correct formulation of $(\mu, \varphi)$ flow.

4.4. Inclusion of the simplest loop to all orders in $z$

In this section we will define a renormalization scheme on the level of diagrams, which is able to incorporate the results of mean field theory. The approach is equivalent to the one of sections 4.2 and 4.3, but we will start with the classical virial expansion, the final point of section 4.3. Our aim is to define a flow in variables which are representative for the state. Its properties will help us in defining an optimal renormalization scheme.

Section 4.2 has taught us that loops in Mayer cluster diagrams are necessary for the description of a critical point. The simplest of such theories that exhibits a critical point is the approximation of the virial expansion by its first three terms, being $^{21-28)}$:

$$p(n) = n - \frac{1}{2} \beta_2 n^2 - \frac{1}{3} \beta_3 n^2$$  \hspace{1cm} (4.4.1)

where $\beta_2$ and $\beta_3$ are the following diagrams:

$$\beta_2 = \quad \quad = \int dr^2 f(r)$$  \hspace{1cm} (4.4.2a)

$$\beta_3 = \quad \quad = \int dr^2 \int dr_3 f(r_{12})f(r_{13})f(r_{23})$$  \hspace{1cm} (4.4.2b)

The fugacity is found selfconsistently as a function of the density $n$
to be \[ (\text{i.e. } n = z \frac{\partial P}{\partial z}) \]

\[ z = n \exp[-\beta_2 n - \frac{1}{2} \beta_3 n^2] \]  

\[ (4.4.3) \]

The critical point follows from the condition \[ \frac{\partial P}{\partial n} = \frac{\partial P}{\partial n^2} (n^*) = 0. \]

The critical conditions, as found from eq. \[(4.4.1)\] are:

\[ n^* = -\frac{1}{3} \beta_2, \quad (\beta_2^*)^2 = -4 \beta_3, \quad p^*/n^* = 1/3, \quad n^* \beta_2^* = 2 \]  

\[ (4.4.4) \]

With the help of eq. \[(4.3.3)\] one arrives at:

\[ n^*/z^* = e^{3/2}, \quad p^*/z^* = \frac{1}{3} e^{3/2}, \quad z^* \beta_2^* = 2e^{-3/2} \]  

\[ (4.4.5) \]

To characterize the state of the fluid we thus approximate it with \( u \) (or \( z \)), \( \beta_2 \) and \( \beta_3 \). As for the Cayley tree, we lose one parameter because of scaling invariance.

We have chosen for the following parameters to define the state of the fluid in a scaling invariant way:

\[ x = z \beta_2, \quad \Gamma = \beta_2^*/\beta_3 \]  

\[ (4.4.6) \]

The critical values are found from eqs. \[(4.4.4)\] and \[(4.4.5)\]:

\[ x^* = 2e^{-3/2} = 0.44626, \quad \Gamma^* = -\frac{1}{4} \]  

\[ (4.4.7) \]

The renormalization scheme in \( x \) and \( \Gamma \) which we will define, must take into account all diagrams formed from \( \beta_2 \) and \( \beta_3 \) exactly to obtain eqs. \[(4.4.1)\] and \[(4.4.3)\].

The starting point for the approximation is eq. \[(4.1.2)\] for the functions \( s(r^*_2; r^*_1, \ldots r^*_l) \), and the flow for \( f(r) \) defined by eq. \[(4.2.4)\].

One finds for instance the flow for \( \beta_3 \) as follows:

\[ \beta_3 = 3 \int dr^*_2 dr^*_3 f(r^*_2) f(r^*_1) f(r^*_3) = 3 \int dr f(r) (f^* f)(r) \]  

\[ (4.4.8) \]

which means that the flow of \( \beta_3 \) (and thus of \( \Gamma \)) is found by integration of
eq. (4.2.4) after multiplication with \((f*f)(r)\). The strategy will be to neglect diagrams which are more complex combinations of \(\beta_2\) and \(\beta_3\). This means that diagrams like:

\[
\frac{1}{s_1} \int dr (f*f)(r)e^{\phi(r)}(f*f)(r)
\]

are neglected. However, the following diagram will be taken into account:

\[
\frac{1}{s_1} \int dr f(r)(f*s_2 e^\phi)(r)
\]

since it is of comparable importance as \(\beta_3\).

The basic observation will be that expressions like

\[
\int dr_1 dr_2 dr_3 s(r_3; r_1, r_2) e^{\phi(r_1) + \phi(r_2)} (f*f)(r_{12})
\]

consist of neglectable diagrams only, as can for instance be seen from eq. (4.1.6) for \(s^{(1)}(r_3; r_1, r_2)\).

This is true for all \(s(r_{\ell}; r_{1}, \ldots r_{\ell-1})\) with \(\ell \geq 3\). Using this principle, we get the following equations:

\[
\dot{\mu} = d + s_1[-1 + x + \delta_2]
\]

\[
\dot{x} = s_1[-x - 2\delta_2 + 2x^2 + 3x\delta_2 + 3x\delta_2 + \Gamma x^2 + 2\beta_3 + \delta_3]
\]

\[
\dot{\Gamma} = - \frac{s_1}{x} \left[ 6 \frac{\beta_3}{x} + 2\Gamma (-2\delta_2 + \Gamma^2) + 2x\delta_2 + 2\beta_3 + \delta_3 \right]
\]

with the following quantities (compare with eqs. (4.2.13)):
\[ s_2 = \frac{1}{s_3} z z \int \bar{r}^2 s_2(r) e^{\Phi(r)} \]  
\[ s_3 = \frac{1}{s_3} z^2 \int \bar{r}^2 \bar{r}^3 s_3(r, \bar{r}_1, \bar{r}_2) e^{\Phi(r_{12}) + \Phi(r_{13}) + \Phi(r_{23})} \]  
\[ \beta_3 = \frac{1}{s_3} z^2 \int \bar{r}^2 \bar{r}^3 s_2(r_{12}) e^{\Phi(r_{12})} f(r_{13}) f(r_{23}) \]  

From eq. (4.1.7), or more general eq. (4.1.2), one sees that \( s_3 \) is coupled to the integral of \( \int d\bar{r}_1 \ldots d\bar{r}_{\ell-1} \Phi(r, \bar{r}_1, \ldots, \bar{r}_{\ell-1}) \) only, since the \( s_i \) terms are neglected when combined with \( f^i \Phi(r_{ij}) \).

Therefore we define the scaling invariant quantity:

\[ s_\ell = \frac{1}{s_3} z^{\ell-1} \int \bar{r}_1 \ldots d\bar{r}_{\ell-1} s(\bar{r}_1, \ldots, \bar{r}_{\ell-1}) e^{\Phi(\bar{r}_1, \ldots, \bar{r}_\ell)} \]  
\[ \Phi(\bar{r}_1, \ldots, \bar{r}_\ell) = \sum_{i < j} \Psi(r_{ij}) \]  

As for the Cayley tree approximation, one has that

\[ \int d\bar{r}_1 \ldots d\bar{r}_{\ell-1} \chi(\bar{r}_1, \ldots, \bar{r}_{\ell-1}) e^{\Phi(\bar{r}_1, \ldots, \bar{r}_\ell)} = 0 \]  
(\( \chi e^{\Phi(\bar{r}_1, \ldots, \bar{r}_\ell)} \) also obeys eq. (4.1.3)).

The integral over \( \bar{r}_1, \ldots, \bar{r}_{\ell-1} \) of eq. (4.1.2) multiplied with \( e^{\Phi(\bar{r}_1, \ldots, \bar{r}_\ell)} \) gives rise to the following recurrence relation for the quantities \( s_\ell \):

\[ s_\ell = \frac{1}{s_3} \sum_{j=0}^{\ell-1} \frac{1}{s_{j+1}} z^{\ell-1} \int d\bar{r}_1 \ldots d\bar{r}_{\ell-1} \Phi(r, \bar{r}_{1j}, \ldots, \bar{r}_{\ell-1}) e^{\Phi(\bar{r}_1, \ldots, \bar{r}_{\ell-1})} \]  
\[ + \frac{1}{s_3} [z^{\ell-1} \int d\bar{r}_1 \ldots d\bar{r}_{\ell-1} s_2(r_{1j}, \ldots, \bar{r}_{\ell-1}) e^{\Phi(r_{1j}, \ldots, \bar{r}_{\ell-1})} f(r_{2, \ell+1}) f(r_{3, \ell+1}) e^{\Phi(\bar{r}_1, \ldots, \bar{r}_{\ell})} ] \]  

(4.13)

The second term (\( j=1 \)) is special, as it takes into account the diagram \( \Phi(r_{ij}) \) (4.4.9). Through the \( \Phi(\bar{r}_1, \ldots, \bar{r}_{\ell-1}) \) there is a connection \( e^{\Phi(r_{ij})} \) for all \( \Phi(r_{ij}) = 1 + f(r_{ij}) \), we see that the Cayley tree approximation only accounts for the 1 (section 4.2). To get diagrams up to \( s_3 \) we may take \( f(r_{ij}) \) into account for all distinct pairs \( (r_{ij}) \in \{\bar{r}_1, \ldots, \bar{r}_{\ell-1}\} \). The combinatorics for that is:

\[ \# \text{ ways to choose } n \text{ distinct pairs } = \frac{(2n)!}{2^n n!} \]  

(4.14)
\((2n! \binom{\ell-j}{2n} = 2n \text{ points from } \ell-j \text{ positions}, \ 2^n = \text{ permutations of } n \text{ pairs } r_{ij}, \ n! = \text{ permutation of the } f(r_{ij})\).

With this combinatorial factor one finds for \(\hat{S}_\ell\) the following recurrence relation (sum over all possible pairs; and \(j=1\) is special):

\[
\ell \hat{S}_\ell = \sum_{j=0}^{\ell} \binom{\ell}{j} \hat{S}_{j+1} (z\beta_2)^{\ell-j} \left[ \frac{\ell-1}{2n!} \frac{1}{(2n)!} \binom{\ell-j}{\ell-j} \frac{n^{n}}{2^n} (x \beta_3^n) \right] \\
+ (z\beta_2)^{\ell-2} \sum_{n=0}^{\ell-2} \frac{\ell!}{(\ell-2-2n)!} \frac{1}{2^n} \frac{\beta_3^n}{n!} \frac{1}{\ell-z^2} \frac{1}{s_1} \int dr_2 dr_3 (s_2 e^r) (r_{12}) (r_{3\ell}) (r)
\]

In terms of the variables defined in (4.4.11) and \(x\) and \(\Gamma\) (eq. (4.4.6)) this recurrence relation becomes

\[
\ell \hat{S}_\ell = \sum_{j=0}^{\ell} \binom{\ell}{j} \hat{S}_{j+1} x^{\ell-j} \left[ \frac{(2n)!}{n!} \frac{(x \beta_3^n)}{(2n)(\ell)} \right] \\
+ \ell! x^{\ell-2} \beta_3 \sum_{n=0}^{\ell-2} \frac{1}{(\ell-2-2n)!} \frac{\Gamma^n}{(x\beta_3^n)} (\ell \geq 3)
\tag{4.4.15}
\]

This relation can be compared with the one of the Cayley tree case. For \(\Gamma = 0\) one indeed retrieves eq. (4.2.6) (then also \(\beta_3 = 0\)).

The recurrence relation (4.4.15) can be treated exactly with the same method as in section 4.2. We define a generating function \(S(v)\) as:

\[
S(v) = \sum_{\ell=0}^{\infty} \frac{v^\ell}{\ell!} \hat{S}_{\ell+1}
\tag{4.4.16}
\]

The calculation made in section 4.2 by eqs. (4.2.8) and (4.2.9) can be repeated to a large extent. The answer is:

\[
(v-e^{vx+\frac{1}{2}\Gamma(vx)^2}) S(v) = [v-1-vx-\frac{1}{2}(vx)^2 (1+\Gamma)] + v\hat{S}_2 [v-1-vx] \\
+ v^2 \beta_3 [e^{vx+\frac{1}{2}\Gamma(vx)^2} - 1] - \frac{1}{2} v^3 \hat{S}_3
\tag{4.4.17}
\]

For \(\Gamma = \beta_3 = 0\) this leads to eq. (4.2.10) as it should.
As for the Cayley tree case we find the $S(v)$ has a simple pole when:

$$c(v)^{x, \Gamma} = v - e^{vx + \frac{i}{2} \Gamma (vx)^2} = 0, \quad \text{for } v = v_i \quad (i = 1, 2, 3) \quad (4.4.17^b)$$

Inspection of eq. (4.4.3) teaches us that again one has a pole when $v_i = n/z$. However, the $v_i$ may be complex, while the density $n$ is a real quantity. The function $c(v)$, defined through eq. (4.4.17^b), has at most three real valued roots, as is easily checked by plotting $c(v)$ as a function of $v \in \mathbb{R}$. However, as for the Cayley tree case one can prove that there are infinitely many complex roots, which in the region for $x$ and $\Gamma$ we are interested in, have larger absolute value then the three roots we shall use hereafter. These three roots shall be removed by adjustment of $\hat{s}_2$, $\hat{s}_3$ and $\hat{s}_3$ such that the flow equations (4.4.10) are completely determined. Later on we shall comment on this decision.

Guided by our experience of section 4.2, we inspect eqs. (4.4.17) at the critical point $(x^*, \Gamma^*)$ as found in eq. (4.4.7). Indeed for $x = 2e^{-3/2}$ and $\Gamma = -\frac{1}{4}$, eq. (4.3.17^b) has three coinciding roots:

$$v^* = e^{3/2} = \exp[v^* 2e^{-3/2} - \frac{1}{2} (v^*)^2 e^{-3}] \quad v_{1, 2, 3} = v^* \quad (4.4.18)$$

The function $c^*(v) = c(v)^{x^*, \Gamma^*}$ is such that $c^*(v^*) = \frac{dc^*}{dv}(v^*) = \frac{d^2c^*}{d(v^*)^2}(v^*) = 0$. We can find $\hat{s}_2$, $\hat{s}_3$ and $\hat{s}_3$ by making the 0th, 1st and 2nd derivative with respect to $v$ at the right-hand side of eq. (4.4.17^a) zero (assuming that these coinciding roots are the three we need).

In appendix F we perform the calculations to find $\hat{s}_2$, $\hat{s}_3$ and $\hat{s}_3$ and their derivatives with respect to $x$ and $\Gamma$. The results are:

$$\hat{s}_2 = 1 - 5e^{-3/2} = -0.115651 \quad (4.4.19^a)$$

$$\hat{s}_3 = e^{-9/2} = 0.011109 \quad (4.4.19^b)$$

$$\hat{s}_3 = 2 - 14e^{-3/2} + 23e^3 - 2e^{-9/2} = -0.000938 \quad (4.4.19^c)$$

for $x$ and $\Gamma$ fulfilling eq. (4.4.7). The flow for $x$ and $\Gamma$ (4.4.10^b, c) indeed is zero, i.e. $\dot{x} = \dot{\Gamma} = 0$. The flow for $\mu$ is made zero by adjusting $a_1$ (which does not have effect on $x^*, \Gamma^*$):
\[ s^*_1/d = x^* = \frac{1}{1-x^*} = \frac{1}{3} e^{3/2} = 1.493896 \]  \hspace{1cm} (4.4.1)

This indeed equals \( p^*/z^* \) at the critical point as given in eq. (4.4.5).

With the help of \( \delta \delta_2^*/\delta x, \delta \delta_2^*/\delta \Gamma, \) etc., one can calculate the linearization matrix at the fixed point. The result, as found in appendix F, is:

\[
T = \begin{pmatrix}
\frac{\delta x^*}{\delta x} & \frac{\delta x^*}{\delta \Gamma} \\
\frac{\delta \Gamma^*}{\delta x} & \frac{\delta \Gamma^*}{\delta \Gamma}
\end{pmatrix} = d
\begin{pmatrix}
\frac{189}{240} & \frac{23}{20} e^{-3/2} \\
-\frac{3}{320} e^{3/2} & \frac{111}{240}
\end{pmatrix}
\hspace{1cm} (4.4.2)

The eigenvalues of this matrix are easily found to be:

\[ y_H = \frac{3d}{4}, \quad y_T = \frac{d}{2} \]  \hspace{1cm} (4.4.3)

Indeed these are the mean field (classical) eigenvalues, leading to the critical exponents \( \delta = 3 \) (since \( p(n) \) is cubic) and \( \alpha = 0 \) (not a logarithmic divergence of \( c_v \) as \( T \to T_c \), as for the Ising model).

One is able to draw the flow lines with the help of the flow equations (4.4.10) and the conditions defined through (4.4.17).

---

**Fig. 7.** Flow pattern for \((x, \Gamma)\)-flow near its critical point \((x^* = 2e^{-3/2}, \Gamma^* = -\frac{1}{4})\). In the shaded region eq. (4.4.17b) has three real-valued roots. The heavy drawn line is the flow line which runs from \((x^*, \Gamma^*)\) to the Cayley tree fixed point \((x = 1/e, \Gamma = 0)\) and separates the gas- and liquid phase (separatrix). Also the right eigenvectors of \( y_H \) and \( y_T \) are drawn.
In fig. 7 this is done for the flow \( \left( \frac{x}{s_1}, \frac{t}{s_1} \right) \) (note that \( s_1 \) and \( d \) are both unimportant for the topology of the picture through the redefinition of \( t' = s_1 t \)). The point \( (x = 1/e, \Gamma = 0) \), which is the fixed point of the Cayley tree case, is a sort of phase separating fixed point. It has one relevant eigenvalue \( y_{CT} = \frac{2d}{3} \) and an irrelevant one \( y = -\frac{d}{2} \).

The flow line from the critical point \( (x^*, \Gamma^*) \) to this (Cayley tree) point, the separatrix, separates the fluid and the gas phase. It runs through the region where there are three real valued roots of eq. (4.4.17), which we have studied in the picture. Outside this region they are one real root and two complex conjugated ones.

Let us now comment on the scheme as defined above. One can understand, as in section 4.3, the conditions on \( \hat{s}_2, \hat{p}_3 \), and \( \hat{s}_3 \) in a different way. Therefore we return to eq. (3.5.7) and use the following approximation for the two point correlation functions (compare eq. (4.3.15)). 21-25):

\[
g(\vec{r}_1, \vec{r}_2) = e^{i\phi(r_{12})} [1 + n(r)(r_{12})]
\]

(4.4.23)

which leads to the density series for the pressure up to the third virial coefficient, eq. (4.4.1). Substitution of eq. (4.4.23) in eq. (3.5.7) yields an equation that is equivalent to the conditions found from eqs. (4.4.17) with \( v \) replaced by \( n/z \), and \( n/z \) given by eq. (4.4.3). However, eq. (4.4.3) has only meaning at the physical realized density. As in section 4.3, regularity of the flow near \( (x^*, \Gamma^*) \) will turn out to be equivalent with demanding the such found relation for three roots of eq. (4.4.3), resulting in the earlier used scheme.

<table>
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</table>

Table 5. Behavior of \( \hat{B}_{\ell} = z^{\ell-1} B_{\ell}/s_1 \) for \( \ell \leq 12 \), at \( (x^*, \Gamma^*) \).
Above method, however, would not give us the meaning of the other complex roots of eq. (4.4.17). As in sections 4.2 and 4.3, we are unable to compensate all these poles in the generating function $S(v)$. Also here one can show that the roots we have not accounted for, are well separated from the ones we do take into account (for $(x, \Gamma)$ in the critical region). Therefore the weights $\hat{S}_k$ behave as explained in section 4.3. Table 5, in which we give the $\hat{S}_k$ for $k \leq 0$, confirms such behavior.

In the next section we comment on the results of this chapter in relation to those of chapter II. In chapter V (conclusions) we discuss further consequences for the results on flow constrained to $\mu$ and $\varphi(r)$.

4.5. Connection with the results of chapter II

In chapter II we have treated the numerical results of a scheme that neglects all many particle terms as well as potentials $\varphi(r_1, \ldots, r_k)$ and decimation weights $s(r_1, r_2, \ldots, r_k)$ for $k \geq 3$. For the choice $s_2(r)$ given by the combination of eqs. (2.3.1) and (2.3.3) we have found that the properties of the fixed points depend on $s_1$, $q_1$ and $T_R(q_2 = 0)$, but that there are values which lead to the anticipated Ising critical exponents. In section 2.4 we have treated in a heuristic way how the role of the $\varphi(r_1, \ldots, r_k)$ can be minimized leading to a window for the a priori free parameters $(s_1, q_1, \text{and } T_R)$. For the choice (closely related to the expression for $s_2(r)$ in chapter II):

$$s_2(r) \propto q_1 r \frac{\partial \varphi}{\partial r}(r) \quad (r \geq \sigma)$$  \hspace{1cm} (4.5.1)

we have found a window given by (2.4.6):

$$\frac{1}{4} \leq \frac{q_1 d}{s_1} \leq \frac{1}{3}$$  \hspace{1cm} (4.5.2)

We can compare these results with the ones of this chapter by substituting eq. (4.5.1) in the conditions, as found in sections 4.3 and 4.4., in the expression for $\hat{S}_2$, being:
\[ S_2 = \frac{1}{s_1} z \int d^2 r \sigma(r) \varphi(r) = \frac{q_1}{s_1} z \int d^2 r \frac{\delta\varphi}{\delta r}(r) \varphi(r) = -\frac{q_1 d}{s_1} z \int d^2 f(r) \quad (4.5.3) \]

In the notation of sections 4.3 and 4.4 this means for the respective 
(x-, and (x,τ)-flow) fixed points:

\[ q_1 d/s_1 = \left( -S_2/x \right)^* = \frac{3-e}{2} / 0.2817 \quad (\text{Cayley-tree}) \]

\[ \qquad \frac{5-e^{3/2}}{2} = 0.2592 \quad ((x,\tau)-flow) \quad (4.5.4) \]

as can be seen from eqs. (4.3.6) and (4.4.19). These values both fall in 
the window given by (4.5.2). Moreover, we have found that the value of 
\[ S_3 = \frac{1}{s_1} z^2 \int d^2 r d^2 r' s(r_3; r_1^r_2) \exp[\varphi(r_{12})+\varphi(r_{13})+\varphi(r_{23})] \]
is small (compared to \( S_2 \)) for both the Cayley tree and the (x,τ)-flow fixed points. This means 
that there is some justification for the neglect of \( s(r_3; r_1^r_2) \) in the 
flow of \( \varphi(r) \).

In chapter II we have found for \( s_1 \), or rather \( s_1/d \), the (unsatisfactory) 
window given by eq. (2.4.7). This chapter results in only one value of 
\( s_1/d \), at which there exists a fixed point (or, better, due to scaling 
invariance, a fixed line). For all dimensions, this value of \( s_1/d \) is the 
same, since \( d \) appears trivially in the flow equations. For the Cayley tree 
case it reads \( s_1/d = e/2 = 1.3592 \ldots \), while for (x,τ)-flow we found \( s_1/d = 
\frac{1}{3} e^{3/2} = 1.494 \ldots \). (eqs. (4.3.14) and (4.4.20), resp.). Both values are much lower 
than the "optimal" value of \( s_1/d \), that, as we have seen in section 2.3, 
depends on the dimension and equals \( s_1/d = 1.75 \) for \( d = 2 \) and \( s_1/d = 1.80 \) 
for \( d = 3 \).

So far we have only compared the conditions at the fixed point. 
That means that we have checked only whether the fixed point has no pro-
duction of many particle potentials. Essential for the calculation of the 
critical exponents is that also in the neighbouring states this production 
is minimal. Therefore one has to vary the weights with the state. Indeed 
this appears to be essential for obtaining the mean field exponents in the 
case of (x,τ)-flow. However, one can prove that if we would move the 
weights of chapter II (introducing also a \( s(r_1^r_2; r_3^r_4) \)) consistently with 
the requirements of section 4.4., we would get either a fixed point with 
mean field exponents or no fixed point at all.
From the ample evidence that the fluid does not behave classically at its critical points, one must conclude that strict enforcement of the conditions of section 4.4. excludes a critical fixed point. This also follows from a consideration on the nature of the conditions for strict \((\mu, \psi)\) flow. For well behaved weights, one has to meet a condition for all solutions of the fugacity-density relation \(z = z(n)\) in the complex \(n\)-plane. In a classical fluid the critical point is a situation where three (or, more generally, a finite number of) roots coincide. In a non-classical fluid one has a singularity in the \(z(n)\) relation, which is not described by the coalescence of a finite number of roots. So one has to meet infinitely many conditions.

A compromise is possible by moving the weights with the state \((\mu, \psi)\) by imposing the conditions only for a finite number of roots of the \(z(n)\) relation. This defines weights and a flow pattern which is dominantly \((\mu, \psi)\)-flow. It can be used as a starting point for a full discussion involving many particle potentials, in which they are treated perturbatively. Some of the choices for the free parameters \(s_1\), \(q_1\) and \(T_R\) in chapter II may serve as such an optimal starting point. To see this, we return to eq. (4.5.3), which in the notation of section 4.4. leads to:

\[
\frac{\delta s_2}{\delta x} = -\frac{q_1 d}{s_1} = -0.2592.. \tag{4.5.5}
\]

when we use eq. (4.5.4) for the \((x, \Gamma)\)-flow case. In appendix F we calculate for \((x, \Gamma)\)-flow what \(\delta s_2/\delta x\) must really be at \((x^*, \Gamma^*)\). The result is

\[
\frac{\delta s_2}{\delta x} = -\frac{9}{160} = -0.06025 \ (eq. (F.11)),
\]

which is fairly consistent with eq. (4.5.5). In other words, the way \(s_2(r)\) is varied with the state for an "optimal" set \(s_1\), \(q_1\) and \(T_R\) is reasonable. Exploratory calculations have been made along these lines, but a full implementation falls outside the scope of this thesis.
V. Conclusions

In this thesis we have investigated the possibilities of a renormalization method based on weighted decimation. The flow equations of this scheme are explicit expressions for the flow of the pressure $p$, the thermodynamic potential $\mu$ and the $k$-particle potential $\varphi({\vec r}_1,..{\vec r}_k)$ in terms of $\mu$ and $\varphi({\vec r}_1,..{\vec r}_j)$. The equations involve decimation weights $s(r_1;r_2,..r_k)$ ($k = 1,2,..$) which must be chosen such that the renormalization procedure becomes useful for the description of a critical fluid. We have addressed ourselves mainly to the following questions:

a) Is it possible to choose the weights such that the flow equations exhibit a critical fixed point?

b) Can we develop an approximation scheme for the critical exponents in arbitrary dimension?

The answers are subject to the restriction that the weights and flow are regular functions of the potentials. An essential characteristic of this and other many-particle-problems is that the hierarchy of the flow equations is open. Therefore some closure must be introduced to turn them to useful equations, and as a consequence both questions depend crucially on the role of the higher potentials $\varphi({\vec r}_1,..{\vec r}_k)$ for $k \geq 3$.

The answer to a) is positive within the limits of physically always necessary approximations. In chapter II we neglect all many particle terms ($k \geq 3$) and show that plausible choices for the weights $s_1$ and $s_2(r)$ (numerically) lead to a fixed point for the potentials $\mu$ and $\varphi(r)$, which have typically the properties to be expected for a critical system. The fixed point two particle potential has a hard core and an attractive, reasonably short-ranged, tail, not unlike the shape of the potentials encountered in noble gases.

However, for the critical exponents in question b) we have results that are far from the anticipated (Ising) exponents. Moreover, they depend strongly on arbitrary parameters in the weights, which only have moderate influence on the fixed point. This is the opposite of what one expects for a renormalization procedure: the fixed point may change with the weights, but the critical exponents should be independent of the way the renormalization is realized.
The explicit character of the flow equations leaves the role of many particle potentials as the only source of error. Indeed we find (heuristically) that in a relatively small window of the free parameter values the three particle potential is not produced in an average sense. In this window the exponents come closer to the Ising values, although, for the present-day accuracy, it is still quite far. Especially the value of the one particle weight $s_1$ (rather $s_1/d$), which, depending on the dimension, must be chosen carefully to result in the Ising exponents, is unexplained on these global grounds.

Two ways are open to resolve the difficulties:

1) To take into account the effect of higher order potentials, $\varphi(\mathbf{r}_1,..,\mathbf{r}_k)$ for $k \geq 3$.

2) To prevent the higher order potentials from developing, by adjustment of the weights $s(\mathbf{r}_1;\mathbf{r}_2,..,\mathbf{r}_k)$.

In this thesis the second option, namely flow constrained to $\mu$ and $\varphi(r)$ is investigated systematically; firstly since it stays closer to the fluid description based on a pair potential, and secondly since numerically many particle potentials are hard to handle.

In chapter III we come to the conclusion that constraints on the flow, which limit the flow to an even smaller Hamiltonian space than $(\mu,\varphi(r))$, like e.g. $(\mu,T)$-flow, force the weights to be chosen very precisely and such that knowledge of singular thermodynamic quantities is essential, otherwise the flow becomes singular. Thus the singularities, which should be explained by the renormalization approach, enter in the renormalization transformation itself.

For flow equations which are strictly constrained to $\mu$ and $\varphi(r)$ we derive in chapter IV a systematic diagrammatic expansion in powers of the fugacity $z$ (near the ideal gas limit) for the weights $s(\mathbf{r}_1;\mathbf{r}_2,\mathbf{r}_3)$, leaving $s_1$ and $s_2(r)$ free. Inspecting this series by taking subsets of diagrams (e.g. the Cayley tree) shows that (diagrammatic combinations of) the weights $s(\mathbf{r}_1;\mathbf{r}_2,..,\mathbf{r}_k)$, which make $\Phi(\mathbf{r}_1,..,\mathbf{r}_k) = 0$ for $k \geq 3$, diverge as a function of $k$ ($k \to \infty$) unless the two particle weight $s_2(r)$ obeys a set of necessary (not sufficient) conditions.

These conditions can be associated with the location of the roots of the fugacity-density relation $z(n)$, in the complex $n$-plane. Again we encounter the difficulty that one has to know a singular thermodynamic relation.
(z(n)) in order to constrain the flow. Thus the conclusion is that no systematic calculation of the critical exponents is possible without flow of the many particle potentials.

A by-product of this analysis is, that a consistent flow scheme is possible involving a finite set of virial coefficients. In chapter IV we have treated flow based on the second and third virial coefficients which leads to (classical) mean field exponents with $\alpha = 0$ and $\delta = 3$. One can make plausible that including more virial coefficients would lead to a cascade of fixed points with $\delta = 4, 5, \ldots$.

A real potential has, however, never a finite set of virial coefficients. Thus these classical fixed points are not realized. It remains an interesting question how well a potential (or set of potentials) can be approximated by a finite set of virial coefficients and how one could see crossover behavior from the true fixed point to the neighbouring classical fixed point.\(^\text{29}\)

Since we cannot constrain the flow to $(\mu, \psi(r))$ flow too strictly, we enter into the question which scheme of chapter II can be denoted at as an optimal starting point for a perturbative treatment of the many particle potentials. It will be the $(\mu, \psi(r))$ flow in which the least many particle potentials are produced. For a given two particle weight function, involving a number of free parameters, one has to find the values which give the least divergence in the many particle weight functions under strict absence of many particle potentials.
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Appendix A: Pure decimation

For pure decimation it is advantageous to use the formalism in which the stochastic process is defined with a conditional probability density \( P_\text{D} \). Pure decimation takes out of the system particles without prejudice. This means that we can define the \( P_\text{D} \) to be:

\[
P_\text{D}(\vec{r}_{j}^1, \ldots, \vec{r}_{M}^1; \vec{r}_{j}^N, \ldots, \vec{r}_{N}^N) = \frac{1}{M!} \sum_{\{j_1, \ldots, j_M\} \in \mathbb{N}} \delta(\vec{r}_{j_1}^1 - \vec{r}_{j_1}^M) \cdots \delta(\vec{r}_{j_M}^M - \vec{r}_{j_M}^1) \frac{\omega^M}{(1 + \omega)^N} (M \leq N) \quad (A.1)
\]

(A.1) says that \( M \) particles are taken out of \( N \), and then are renumbered. The \( M! \) is the number of ways the renumbering can be done. The factor \( \frac{\omega^M}{(1 + \omega)^N} \) is chosen such that \( P_\text{D} \) is normalized according to (1.2.2).

We get back the infinitesimal generator by taking \( \Delta t = \frac{1}{1 + \omega} \) and \( \omega \to \infty \). Then \( P_\text{D} \to 1 + T_\text{D} \Delta t \) where \( T_\text{D} \) is the probability rate of decimation defined in section 1.4 with the weight \( S = s_1 = 1 \). In that limit only one step \( \Delta N \) per unit of time is done. A finite number of repetitions of this process gives again a process of pure decimation but with different \( \omega \), called \( \omega' \) with \( \omega' < \omega \). This means that the limit of infinitely many repetitions is equivalent to \( \omega \to 0 \) in (A.1).

If (A.1) is substituted into (1.2.1) we see that using the definition of the correlation functions we get:

\[
z' = \omega n(z), \quad p' = p - p(\bar{z}, [\omega])
\]

\[
W'(\vec{r}_{j_1}^1, \ldots, \vec{r}_{M}^1; \bar{z}, [\omega])
\]

\[
\text{where } \bar{z} = \frac{z}{1 + \omega}
\]

(A.2a)

(A.2b)

(A.2c)

Here \( z \) is the old and \( z' \) the new fugacity. The new Boltzmann weight is related to the correlation function \( g \) of the old system of Boltzmann weights but for a fugacity smaller than \( z \) being \( \bar{z} \) given by (A.2c).

For \( t \to \infty \) we see that \( \bar{z} \to z \) and thus for \( t \to \infty \) the new Boltzmann weights are exactly the old correlation functions. In section 1.5 we already
saw that the correlation function does not change, and that the density changes exponentially under pure decimation. For \( t \to \infty \) the density and the pressure go to zero, since there are no particles left. The potentials keep their hard core when there is no rescaling of the positions of the particles. They develop however for critical potentials a long range tail like the original correlation functions have.
Appendix B: The exact flow equations for the potentials

In section 1.6 we gave the flow equations for the case that spatial rescaling, spatial rearrangement and weighted decimation are combined, and restricted to two-particle flow. Here we give the total flow equations for $\dot{p}$, $\dot{u}$, $\dot{\phi(r_{12})}$ and $\dot{\phi(r_{12}r_{23})}$ in the case that also higher order potentials are present:

$$\dot{p} = dp - s_1 z \quad \text{(B.1)}$$

$$\dot{u} = d - s_1 + z \int d\bar{r}_{12} \left[ s_1 r_{12} + s_2 (\bar{r}_{12}) e^{\phi(\bar{r}_{12})} \right]$$

$$\dot{\phi(r_{12})} = (\bar{r}_{12} + 2\bar{\phi}) \cdot \bar{\phi(r_{12})} + 2\bar{\phi} (\bar{r}_{12}) - 2s_2 (\bar{r}_{12}) + z \int d\bar{r}_{23} \left[ s_1 r_{23} + s_2 (\bar{r}_{23}) e^{\phi(\bar{r}_{23})} \right]$$

$$\quad + s_2 (\bar{r}_{13}) e^{\phi(\bar{r}_{13})} f(r_{23}) + s_2 (\bar{r}_{23}) e^{\phi(\bar{r}_{23})} f(r_{13}) + s_2 (r_{23}; r_{12}) e^{\phi(\bar{r}_{13}) + \phi(\bar{r}_{23})}$$

$$\quad + z \int d\bar{r}_{3} S(r_{3}; r_{12}) e^{\phi(\bar{r}_{3}) + \phi(\bar{r}_{23})} f(r_{12} r_{23}) \quad \text{(B.2)}$$

$$\dot{\phi(r_{12}r_{23})} = (\bar{r}_{12} + \bar{r}_{23}) \cdot \bar{\phi(r_{12}r_{23})} + [\bar{\phi}_{12} \phi_{12} + \bar{\phi}_{23} \phi_{23}] \cdot \bar{\phi(r_{12}r_{23})}$$

$$\quad + \bar{\phi}_{12} \phi_{12} + \bar{\phi}_{23} \phi_{23} \cdot \bar{\phi(r_{12}r_{23})}$$

$$\quad - s(r_{3}; r_{12}) - s(r_{23}; r_{12}) - s(r_{12}; r_{23}) \quad \text{(B.3)}$$
Here again we used Mayer functions $f(\vec{r}_1 \ldots \vec{r}_j) = e^{\phi(\vec{r}_1 \ldots \vec{r}_j)} - 1$ and the fugacity $z$. The spatial rearrangement is used with a $\phi_2(\vec{r})$ only. We assumed the system to be homogeneous.
Appendix C: Laguerre integration

This appendix concerns a way to handle integro differential equations, like e.g. eqs. (2.2.1). The scheme must be able to calculate of a function, specified in a number of points as indicated in section 2.2, the integral and integral transforms in any dimension. As an example one may think of Fourier-, Legendre- and Laguerre transforms, which all can be used for calculating Mayer cluster diagrams (as introduced in section 4.1).

The class of functions on which we want to perform these operations are the Mayer functions \( f(r) \), defined by eq. (1.4.4). These functions are finite everywhere and decaying fast (exponentially) such that they can be approximated by:

\[
f(x) = P(x) e^{-x}
\]

where \( P \) is a polynomial of \( n^{th} \)-degree. We calculate integrals by a Gauss-Laguerre summation \(^{30, 31}\):

\[
\int_{0}^{\infty} dx \ x^{\alpha} e^{-x} P(x) = \sum_{i=1}^{N} w_i^{(N)} P(x_i) + R_N
\]

The constant \( R_N \) is a rest term. The \( x_i \) and \( w_i^{(N)} \) form a set of \( 2N \) constants which will be chosen such that the representation of \( P(x) \) at \( x_i \) will give \( R_N = 0 \) for \( P(x) \) a polynomial of degree \( n \), with \( n \leq 2N-1 \).

For integrals as defined in (C.2) the Laguerre polynomials, defined by \(^{30}\):

\[
L_n^{(\alpha)}(x) = \sum_{m=0}^{n} (-1)^m \frac{(n+\alpha)_m}{(n-m)_m} \frac{x^m}{m!} = \frac{1}{e^{-x} x^\alpha} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha})
\]

form an orthogonal basis

\[
\int_{0}^{\infty} dx \ x^{\alpha} e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) = \delta_{nm} \frac{\Gamma(n+\alpha+1)}{n!}
\]
To find the optimal choice for \( x_i \) and \( w_i^{(N)} \) we will look at the polynomial \( P(x) = L_N^{(a)}(x) \ L_m^{(a)}(x) \) with \( m < N \). This is a polynomial of order \( N+m \leq 2N-1 \), for which one can have \( R_N = 0 \) when \( P(x) \) is substituted in (C.2). However, then also the left-hand side of (C.2) is zero for all \( m < N \) as a consequence of (C.4). Evidently one must choose for \( x_i \) the \( N \) zeros of the polynomial \( L_N^{(a)}(x) \):

\[
x_i : \quad L_N^{(a)}(x_i) = 0 \quad (i = 1, \ldots, N) \tag{C.5}
\]

Now that the \( x_i \) are fixed we concentrate on the \( w_i^{(N)} \) introduced in eq. (C.2).

For that purpose we write the polynomial \( L_N^{(a)}(x) \) in terms of its zeros:

\[
\omega_N(x) = \prod_{i=1}^{N} (x-x_i) = (-1)^N N! \ L_N^{(a)}(x) \tag{C.6}
\]

Next we define a function \( \phi_{K,N}(x) \) which is zero at all \( x_i \) except \( x_k \):

\[
\phi_{K,N}(x) = \frac{\omega_N(x)}{x-x_k} \tag{C.7}
\]

From the fact \( \phi_{K,N} \) is a polynomial of order \( N-1 \) we can calculate its integral by the use of (C.2) with \( R_N = 0 \). As only \( i = k \) contributes we get:

\[
\omega_k^{(N)} = \frac{\int_{-\infty}^{\infty} x^\alpha \ e^{-x} \ \phi_{K,N}(x)^2 \ dx}{\phi_{K,N}(x_k)} \tag{C.8}
\]

From (C.7) we know that \( \omega_N'(x_k) = \phi_{K,N}(x_k) \). With the use of (C.6) we obtain for (C.8):

\[
\omega_k^{(N)} = \frac{\int_{-\infty}^{\infty} x^\alpha \ e^{-x} \ [L_N^{(a)}(x)^2/(x-x_k)^2] \ dx}{[(x-k) \ L_N^{(a)}(x_k)]^2} \tag{C.9}
\]
This expression for the $w_k^{(N)}$ can be simplified with integration by parts

$$\begin{align*}
w_k^{(N)} \left[ \frac{d}{dx} L_N^{(a)}(x_k) \right]^2 &= - \left[ \frac{x e^{-x} L_N^{(a)}(x)}{x-x_k} \right]_0^\infty + \int_0^\infty dx \alpha e^{-x} \left[ \frac{1}{x(x-x_k)} \right] L_N^{(a)}(x) \\
&= - \frac{1}{x-x_k} L_N^{(a)}(x)^2 + 2 \frac{1}{x-x_k} \left[ \frac{d}{dx} L_N^{(a)}(x) \right] L_N^{(a)}(x) \)
\end{align*}$$

(C.10)

The last two terms between the $\{\}$ in the right-hand side of eq. (C.10) are polynomials of degree $(2N-1)$ and $(2N-2)$ respectively, with zeroes at all the $x_i$ of (C.5). So these integrals vanish as one can apply (6.2) with $R_N = 0$. With the use of (C.6) and (C.7) one obtains for the other terms:

$$\begin{align*}
w_k^{(N)} \left[ \frac{d}{dx} L_N^{(a)}(x_k) \right]^2 &= \delta_{a,0} \frac{\alpha}{x_k} - \alpha \int_0^\infty dx \alpha e^{-x} \frac{L_N^{(a)}(x)^2}{x(x-x_k)} \)
\end{align*}$$

(C.11)

This integral appearing in (C.11) can be treated as follows:

$$I_k^{(N)} = -\alpha \int_0^\infty dx \frac{x}{x-x_k} e^{-x} L_N^{(a)}(x)^2 = \alpha \frac{x}{x_k} \int_0^\infty dx \frac{x}{x-x_k} e^{-x} \left[ \frac{L_N^{(a)}(x)^2}{x} - \frac{L_N^{(a)}(x)^2}{x-x_k} \right]$$

With (C.2) the second term on the right-hand side becomes zero and what remains is (for $\alpha > 0$) expressed as:

$$I_k^{(N)} = + \frac{\alpha}{x_k} \int_0^\infty dx \frac{x}{x-x_k} e^{-x} L_N^{(a)}(x)^2$$

(integrating by parts)

$$= + \frac{1}{x_k} \int_0^\infty dx \frac{x}{x-x_k} e^{-x} L_N^{(a)}(x)^2 + \text{a term which is zero due to (C.2)}$$

$$= + \frac{1}{x_k} \int_0^\infty dx \frac{x}{x-x_k} e^{-x} L_N^{(a)}(x)^2 = \text{(use (C.3))}$$

$$= + \frac{1}{x_k} \frac{\Gamma(N+\alpha+1)}{N!}$$

(C.12)
Finally, we express \( \frac{d}{dx} L^{(\alpha)}_N(x_k) \), appearing in eq. (C.10), in \( L_N(x_k) \) using the following general properties of Laguerre polynomials:

\[
\begin{align*}
  x \frac{d}{dx} L^{(\alpha)}_n(x) &= nL^{(\alpha)}_n(x) - (n+\alpha) L^{(\alpha)}_{n-1}(x) \\
  (n+1)L^{(\alpha)}_{n+1}(x) &= (2n+1+\alpha-x)L^{(\alpha)}_n(x) - (n+\alpha)L^{(\alpha)}_{n-1}(x)
\end{align*}
\]  
(C.13)

This expression for \( w^{(N)}_k \), given by (C.11), becomes with the use of eqs. (C.12) and (C.13) the following (Note that \( \alpha = 0 \) is the limit of \( \alpha > 0 \)):

\[
w^{(N)}_k = \frac{\Gamma(N+\alpha+1)}{N!} \frac{x_k}{(N+1)L^{(\alpha)}_{N+1}(x_k)} = \frac{\Gamma(N+\alpha+1)}{N!} \frac{x_k}{(N+\alpha)L^{(\alpha)}_{N-1}(x_k)}
\]
(C.14)

With \( x_i \) defined by (C.5) and \( w^{(N)}_k \) defined by (C.14) we are thus able to calculate integrals of the form (C.2) for polynomials of degree \( n \leq 2N-1 \) exactly.

For functions \( f(x) \) which are not exactly given by (C.1) we may approximate integrals of \( f(x) \) as follows:

\[
\int_0^\infty dx \ x^\alpha f(x) = \sum_{i=1}^N (w^{(N)}_i x_i) f(x_i) + R_N
\]
(C.15)

The rest term \( R_N \) will be proportional with the \( (2N)^{th} \) derivative of \( f(x)e^x \) at some representative point. Of course \( f(x) \) must be well defined for all \( x \in [0,\infty[ \) and decay sufficiently fast for \( x \to \infty \).
Appendix D: Calculation of integral transforms

For calculation of the flow of the potential $\varphi(r)$, as given in chapter II, we have to handle numerically the convolution of two Mayer functions $f(r)$, defined by eq. (2.2.7). The convolution can be treated using Fourier transforms

$$(F \tilde{f})(k) = \tilde{f}(k) = \int \, dr \, e^{ik \cdot r} f(r)$$ \hspace{1cm} (D.1)

Then one has:

$$F(f \ast f)(k) = (\tilde{f}(k))^2 \iff (f \ast f)(r) = \frac{dk}{(2\pi)^d} e^{ik \cdot r} \tilde{f}(k)^2$$ \hspace{1cm} (D.2)

The Mayer functions $f(r)$ are well behaved for all $r \in [0, \infty]$. Therefore we apply the numerical development of integrals as given in appendix C. For that purpose we approximate $f(r)$ in terms of a finite (i.e. $N < \infty$) Laguerre transform as:

$$f(r) = \sum_{n=0}^{N} A_n^{(\alpha)} L_n^{(\alpha)}(r^2) e^{-r^2/2}$$ \hspace{1cm} (D.3)

The constants $A_n^{(\alpha)}$ can be found as any orthogonality of $L_n^{(\alpha)} ((C.4))$:

$$A_n^{(\alpha)} = \frac{2n!}{\Gamma(n+\alpha+1)} \int_0^{\infty} dr \, r^{2\alpha+1} f(r) \, L_n^{(\alpha)}(r^2) e^{-r^2/2}$$ \hspace{1cm} (D.4)

This expression resembles an integral in d-dimensions, which for spherical symmetric functions reads:

$$\int dr^d f(r) = \Omega_d \int_0^{\infty} r^{d-1} f(r); \quad \Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$ \hspace{1cm} (D.5)

($\Omega_d$ is the surface of a d-dimensional sphere).

This means that the integrals in (D.4) are d-dimensional when:

$$\alpha = \frac{d}{2} - 1$$ \hspace{1cm} (D.6)
For this choice of $\alpha$ we shall need for the calculation of the flow only $d$-dimensional integrals, as we shall see.

Having obtained the coefficients $A_n^{(\alpha)}$, one has at the same time Fourier transforms of $f(r)$, since generally:

$$\mathcal{F}[L_n^{(\alpha)} r^2 e^{-r^2/2}](k) = (-1)^n (2\pi)^{d/2} L_n^{(\alpha)}(k^2) e^{-k^2/2}$$  \hspace{1cm} (D.7)

which is proven most easily from the generating function of the Laguerre polynomials:

$$\sum_{n=0}^{\infty} L_n^{(\alpha)}(x) z^n = \frac{xz}{(1-z)^{1+\alpha} e^{-z}}$$  \hspace{1cm} (D.8)

With the help of the evaluation of integrals numerically, as treated in appendix C, eq. (C.15), we obtain:

$$A_n^{(\alpha)} = \frac{n!}{\Gamma(n+\alpha+1)} \int_0^\infty dx x^\alpha f(\sqrt{x}) L_n^{(\alpha)}(x) e^{-x/2} = \sum_{i=1}^{N} (w_i^{(N)} x_1^i) f(\sqrt{x_1^i}) L_n^{(\alpha)}(x_1^i) e^{-x_1^i}$$

Renaming $x_1 = r_1^2$ and $w_i = w_i^{(N)} x_1^i$, we get:

$$A_n^{(\alpha)} = \frac{n!}{\Gamma(n+\alpha+1)} \sum_{i=1}^{N} w_i f(r_i^2) L_n^{(\alpha)}(r_i^2) e^{-r_i^2/2}$$  \hspace{1cm} (D.9)

Using (D.6) for $d$-dimensions, this means that we are thus able to calculate with the use of the same $r_i$ and $w_i$ ($i = 1, \ldots, N$), integrals of $f(r)$ (necessary for the flow of $u$) as well as Fourier transforms (necessary for the flow of $\varphi(r)$). The $r_i$, $w_i$ and $L_n^{(\alpha)}(r_i^2) e^{-r_i^2/2}$ have to be calculated only once for every dimension of interest.
Appendix E: Cayley tree recurrence relation for \( \tilde{s}_k \) at finite \( \vec{k} \)

In this appendix we will derive some properties of the weights \( s(\vec{r}_1; \vec{r}_1, \ldots, \vec{r}_{l-1}) \) which make \( \Phi(\vec{r}_1, \ldots, \vec{r}_l) = 0 \) in the Cayley tree approximation, as treated in section 4.2. The starting point is eq. (4.2.3) for the Fourier transform \( \tilde{s}_k(\vec{k}_1, \ldots, \vec{k}_{l-1}) \). Then we found that one needs \( \tilde{s}_k(\vec{k}_1, \vec{k}_2, 0, \ldots, 0) \) for the cases \( \vec{k}_1 = -\vec{k}_2 = \vec{k}; \vec{k}_1 = \vec{k}, \vec{k}_2 = 0 \) and \( \vec{k}_1 = \vec{k}_2 = 0 \). The last case can be treated exactly. The first two cases need a study of equation (4.2.3) for the number of possibilities to choose \( k_1 \) and \( k_2 \) inside or outside \( \{k_1, \ldots, k_j \} \), while \( \{i_1, i_2\} \subseteq \{1, \ldots, l\} \). This gives rise to the following two recurrence relations:

\[
\tilde{s}_k(\vec{k}, -\vec{k}, 0, \ldots, 0) = \frac{1}{k} \sum_{j=0}^{l} \frac{z}{2} (s_{j+1}(\vec{k}, -k, 0, \ldots, 0) \hat{f}(k=0)^{l-j} + \hat{f}(k^2=0)^{l-j-1} + \hat{f}(k=0)^{l-j-2}) + \chi_k(\vec{k}, -\vec{k}, 0, \ldots, 0)
\]

(E.1)

\[
\tilde{s}_k(\vec{k}, 0, \ldots, 0) = \frac{1}{k} \sum_{j=0}^{l} \frac{z}{2} (s_{j+1}(\vec{k}, -k, 0, \ldots, 0) \hat{f}(k=0)^{l-j} + \hat{f}(k^2=0)^{l-j-1} + \hat{f}(k=0)^{l-j-2}) + \chi_k(\vec{k}, 0, \ldots, 0)
\]

(E.2)

Use of eq. (4.2.5), \( \chi_k(\vec{k}, -\vec{k}, 0, \ldots, 0) = 2\chi_k(\vec{k}, 0, \ldots, 0) \equiv 2\chi_k(\vec{k}) \), yields the following relation from eqs. (E.1) and (E.2) (\( \tilde{s}_k(\vec{k}) \equiv \tilde{s}_k(\vec{k}, 0, \ldots, 0) \)):

\[
\tilde{s}_k(\vec{k}, -\vec{k}, 0, \ldots, 0) = \tilde{s}_k(\vec{k}, 0, \ldots, 0) + \chi_k(\vec{k}, 0, \ldots, 0) \equiv \tilde{s}_k(\vec{k}) + \chi_k(\vec{k})
\]

(E.3)

For \( \tilde{s}_k(\vec{k}) \) we then get an uncoupled recurrence relation:
\[ \varpi^*_{\ell}(\mathbf{k}) = z \sum_{j=0}^{\ell} \left\{ (\ell-2) s_{j+1}(\mathbf{k}) f(0) \ell^{-j-1} + 2(\ell-2) s_{j+1}^{*}(\mathbf{k}) f(0) \ell^{-j} \right\} \\
+ \left( \ell^{-2} \right) s_{j+1}(\mathbf{k}) f(k) f(0) \ell^{-j-2} + \ell s_{\ell}^{*}(\mathbf{k}) + z \sum_{j=0}^{\ell} \left( \ell^{-2} \right) s_{j+1}^{*}(\mathbf{k}) f(0) \ell^{-j} \]

(E.4)

For \( k = 0 \) this recurrence relation equals indeed eq. (4.2.6) (remember that \( s_{\ell}^{*}(\mathbf{k}=0) = 0 \)).

For the case \( \mathbf{k} = 0 \) one is able to treat the problem exactly using a generating function technique. Following the same route we derive a differential equation with the use of the generating functions:

\[ S(\mathbf{u},\mathbf{k}) = \sum_{\ell=0}^{\infty} \frac{\mathbf{u}^{\ell}}{\ell!} s_{\ell+1}(\mathbf{k}) \]  
\[ X(\mathbf{u},\mathbf{k}) = \sum_{\ell=2}^{\infty} \frac{\mathbf{u}^{\ell}}{\ell!} x_{\ell+1}(\mathbf{k}) \]  

(E.5a)  
(E.5b)

Multiplying (E.4) with \( \mathbf{u}^{\ell}/\ell! \) and summing over \( \ell \), leads to the differential equation:

\[ (u - z e^{\mathbf{u} f(0)} \frac{\partial}{\partial u} s_{2}(\mathbf{u},\mathbf{k}) + 2(1 - z e^{\mathbf{u} f(0)} f(k)) \frac{\partial}{\partial u} s_{3}(\mathbf{u},\mathbf{k}) + s_{4} \mathbf{u} f(k) + 2(-1 - z f(k)) s_{5}(\mathbf{u},\mathbf{k}) + z s_{3}(\mathbf{u},\mathbf{k}) + \mathbf{u}^{*} x_{3}(\mathbf{u},\mathbf{k}) + (u - z e^{\mathbf{u} f(0)} \frac{\partial}{\partial u} x_{2}(\mathbf{u},\mathbf{k}) + z \frac{\partial}{\partial u} x_{3}(\mathbf{u},\mathbf{k}) - z e^{\mathbf{u} f(0)} \mathbf{u} f(k) S(u,0) = 0 \]

(E.6)

The function \( S(u,0) \) is given by eq. (4.2.10). Equation (E.6) is a linear first order in homogeneous differential equation for \( \frac{\partial}{\partial u} s_{2}(\mathbf{u},\mathbf{k}) \). The function \( X(u,k) \) is, except for the fact that \( X(u,0) = 0 \), assumed to be a free function.

We have not been able to solve eq. (E.6) for arbitrary \( X(u,k) \) (or \( \varpi_{\ell}^{*}(\mathbf{k}) \)). Since \( X(u,k) \) is basically arbitrary, it shows that there are no conditions on \( \varpi_{2}^{*}(\mathbf{k}) \) and \( \varpi_{3}^{*}(\mathbf{k}) \) as there are for \( \mathbf{k} = 0 \), as found in section 4.2, which lead to far reaching consequences for the flow, as treated in sections 4.3 and 4.4.
Appendix F: Eigenvalues $\lambda_H$ and $\lambda_T$ for $(x, \Gamma)$ flow

The basic relations of this appendix are the flow for $x$ and $\Gamma$, as defined by eqs. (4.4.10$^b$, $^c$) and (4.4.11):

\[
\frac{1}{a} \frac{\partial u}{\partial t} = 1 + x[-1 + x + \delta_2] \quad (F.1^a)
\]

\[
\frac{1}{a} \frac{\partial x}{\partial t} = x[-x - 2\delta_2 + 2x^2 + 3x\delta_2 + \Gamma x^2 + 2x^2 p_3 + \delta_3] \quad (F.1^b)
\]

\[
\frac{1}{a} \frac{\partial \Gamma}{\partial t} = \frac{x}{x} [6p_3 x + 2\Gamma(-2\delta_2 + x^2 (1 + \Gamma) + 2\delta_2 + 2x^2 p_3 + \delta_3)] \quad (F.1^c)
\]

We have defined $p_3 = \delta_2/x^2$ ($\delta_2$ defined by eq. (4.4.11$^c$)), while $x = s_1/d$. The quantities $\delta_2$, $p_3$ and $\delta_3$ are fixed by the removal of three poles of the generating function $S(v)$, defined by eq. (4.4.17$^a$), which reads:

\[
(v - e^{vx + \frac{1}{2}\Gamma(vx)^2})S(v) = [v - 1 - (vx)^2] + v\delta_2 [v - 1 - vx] + p_3 (vx) [e^{vx + \frac{1}{2}\Gamma(vx)^2} - 1] - \frac{v^2}{2} \delta_3 \quad (F.2)
\]

From considerations on the virial series we expect a fixed point of eqs. (F.1) of the values of $x$ and $\Gamma$ given by eq. (4.4.7), $x^* = 2e^{-3/2}$ and $\Gamma^* = -1/4$.

The poles of $s(v)$ are the zeroes of the function $f(v)$

\[
f(v)_{x, \Gamma} = v - e^{vx + \frac{1}{2}\Gamma(vx)^2} \quad (F.3)
\]

At $(x^*, \Gamma^*)$ this function has the following properties, which we shall need for future use: $(f_*^{(0)}(v) = f(v)_{x^*, \Gamma^*})$:

\[
f_*^{(0)}(v^*) = f_*^{(1)}(v^*) = f_*^{(2)}(v^*) = v; \quad v^* = e^{3/2} \quad (F.4^a)
\]

\[
f_*^{(3)}(v^*) = 2e^{-3} \quad f_*^{(4)}(v^*) = 2e^{-9/2} \quad f_*^{(5)}(v^*) = -6e^{-6} \quad (F.4^b)
\]
Eq. (F.4a) says that at \((x^*,\Gamma^*)\) \(f(v)\) has three coinciding roots at \(v = v^* = e^{3/2}\) (compare \(n^*/x^*\) in eq. (4.4.5)). These roots we use to fix \(\hat{s}_2, p_3\) and \(\hat{s}_3\) as argued in section 4.4.

The 0th, 1st and 2nd derivatives of eq. (F.2) with respect to \(v\) at \(v = v^*\) (and \(x^*,\Gamma^*\)) give a left-hand side that is zero, and (after suitable multiplications) the following three equations:

\[
2e^{3/2} - 9 + e^{3/2} \hat{s}_2 [2e^{3/2} - 6] + 4p_3 [2e^{3/2} - 2] - e^{3/2} \hat{s}_3 = 0
\]

\[
e^{3/2} - 5 + e^{3/2} \hat{s}_2 [2e^{3/2} - 5] + 4p_3 [3e^{3/2} - 2] - e^{3/2} \hat{s}_3 = 0
\] (F.5)

\[-3 + e^{3/2} \hat{s}_2 [2e^{3/2} - 4] + 4p_3 [6e^{3/2} - 2] - e^{3/2} \hat{s}_3 = 0
\]

This leads to the solutions for \(\hat{s}_2, p_3\) and \(\hat{s}_3\):

\[
\hat{s}_2 = 1 - 5e^{-3/2} = -0.115651
\]

\[
p_3 = \frac{1}{4} e^{-3/2} = 0.055783 \quad (\hat{\beta}_3 = x^* p_3 = 3^{-9/2} = 0.011109)
\]

\[
\hat{s}_3 = 2 - 14e^{-3/2} + 23e^{-3} - 2e^{-9/2} = -0.000938
\] (F.6)

Substitution in eqs. (F.1) yields \(\dot{x} = \dot{\Gamma} = 0\), while \(\ddot{u} = 0\) for

\[
x^* = \frac{1}{1-x-\hat{s}_2} = \frac{1}{3} e^{3/2}
\] (F.7)

which is equivalent with the value of \(p^*/x^*\) given in eq. (4.4.5), as it should.

Since \(\frac{\delta x}{\delta \mu} = \frac{\delta \tau}{\delta \mu} = \frac{\delta u}{\delta \mu} = 0\), there is at the fixed point a zero eigenvalue (which is a result of scale invariance). Therefore we investigate the linearization matrix of \((x,\Gamma)\) only. For that purpose we need \(\frac{\delta \hat{s}_2}{\delta x}, \frac{\delta \hat{s}_2}{\delta \Gamma}, \text{ etc.}\), which can be calculated by differentiation of eq. (F.2) with respect to \(x\) and \(\Gamma\) first, and then take the 0th, 1st and 2nd
derivative with respect to \( v \) at \( v = v^* \) to get the conditions for 
\[
\left( \frac{\partial \hat{s}_2}{\partial \xi}, \frac{\partial \rho_3}{\partial \xi}, \frac{\partial \hat{s}_3}{\partial \xi} \right) \text{ and } \left( \frac{\partial \hat{s}_2}{\partial \Gamma}, \frac{\partial \rho_3}{\partial \Gamma}, \frac{\partial \hat{s}_3}{\partial \Gamma} \right)
\] respectively. The values for 
\[
\frac{\partial S(u)}{\partial \xi} \text{ and } \frac{\partial S(u)}{\partial \Gamma}
\] are irrelevant due to eq. (F.4\(^a\)), as before.

What we do need is the values of \( S(v^*), \frac{\partial S}{\partial v} (v^*) \) and \( \frac{\partial^2 S}{\partial v^2} (v^*) \). These are found by differentiation of eq. (F.2) with respect to \( v \), three, four and five times respectively and setting \( v = v^* \). With the use of eqs. (F.4\(^b\)) one finds:

\[
S(v^*) = 2e^{-3/2}, \quad \frac{\partial S}{\partial v} (v^*) = -\frac{11}{4} e^{-3}, \quad \frac{\partial^2 S}{\partial v^2} (v^*) = -\frac{29}{40} e^{-9/2} \quad (F.8)
\]

It is easy to see that differentiation of eq. (F.2) with respect to \( x \) and \( \Gamma \) (at \((x^*,\Gamma^*)\)) eventually gives rise to a linear equation for 
\[
\left( \frac{\partial \hat{s}_2}{\partial \xi}, \frac{\partial \rho_3}{\partial \xi}, \frac{\partial \hat{s}_3}{\partial \xi} \right) \text{ (} \xi = x, \Gamma \text{), which only differs in the inhomogeneous part,}
\]
depending on the values of eqs. (F.4\(^b\)), (F.6) and (F.8) and numerical factors.

The equation thus reads with \( \xi = (x, \Gamma) \) (compare eq. (F.5)):

\[
(A1)_{\xi} + e^{3/2} \frac{\partial \hat{s}_2}{\partial \xi} \left[ 2e^{3/2}x - 6 \right] + 4 \frac{\partial \rho_3}{\partial \xi} \left[ 2e^{3/2}x - 2 \right] - e^3 \frac{\partial \hat{s}_3}{\partial \xi} = 0
\]

\[
(A2)_{\xi} + e^{3/2} \frac{\partial \hat{s}_2}{\partial \xi} \left[ 2e^{3/2}x - 5 \right] + 4 \frac{\partial \rho_3}{\partial \xi} \left[ 3e^{3/2}x - 2 \right] - e^3 \frac{\partial \hat{s}_3}{\partial \xi} = 0 \quad (F.9)
\]

\[
(A3)_{\xi} + e^{3/2} \frac{\partial \hat{s}_2}{\partial \xi} \left[ 2e^{3/2}x - 4 \right] + 4 \frac{\partial \rho_3}{\partial \xi} \left[ 6e^{3/2}x - 2 \right] - e^3 \frac{\partial \hat{s}_3}{\partial \xi} = 0
\]

The answers for \((A)_{x}\) and \((A)_{\Gamma}\) are:

\[
(A1)_{x} = -2e^{3} + 10e^{3/2} - 2; \quad (A1)_{\Gamma} = 8
\]

\[
(A2)_{x} = -2e^{3} + \left(10\frac{1}{8}\right)e^{3/2} - 2; \quad (A2)_{\Gamma} = 12\frac{1}{2} \quad (F.10)
\]

\[
(A3)_{x} = -2e^{3} + \left(9\frac{7}{80}\right)e^{3/2} - 2; \quad (A3)_{\Gamma} = 25\frac{11}{20}
\]

With these inhomogeneous parts one is able to find the wanted
quantities, being:

\[
\frac{\delta s^2}{\delta x} = -\frac{29}{160} = -0.18250
\]
\[
\frac{\delta p^3}{\delta x} = \frac{29}{160} = 0.43250 \\
\frac{\delta s^3}{\delta x} = -2\frac{29}{80} + 12\frac{1}{5} e^{-3/2} - 2\frac{29}{80} e^{-3} = -0.007934
\]

and

\[
\frac{\delta s^2}{\delta \Gamma} = -\frac{9}{40} e^{-3/2} = 0.05204
\]
\[
\frac{\delta p^3}{\delta \Gamma} = -1\frac{11}{160} e^{-3/2} = -0.036470 \\
\frac{\delta s^3}{\delta \Gamma} = -\frac{9}{20} e^{-3/2} + \frac{4}{5} e^{-3} + 8\frac{11}{20} e^{-9/2} = 0.034403
\]

Substitution in the expressions for \( \frac{\delta x}{\delta x}, \frac{\delta x}{\delta \Gamma}, \frac{\delta \Gamma}{\delta x} \) and \( \frac{\delta \Gamma}{\delta \Gamma} \) yields the linearization matrix given by eq. (4.4.21) in section 4.4, and gives rise to the mean field exponents, eq. (4.4.22).
Summary

In chapter I we introduce a renormalization scheme for the fluid in the grand canonical description. It is formulated with the aid of a stochastic process that determines the decrease in the number of degrees of freedom, and is realized by weighted decimation followed by rescaling. The resulting flow equations are a hierarchy in terms of the pressure $p$, the chemical potential $\mu$ and $k$-particle potentials $\phi(\vec{r}_1, \ldots, \vec{r}_k)$. It involves the choice of $k$-particle decimation weights $s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)$ that determine the probability to remove a particle from a group of particles. In terms of these weights one is also able to derive a flow for the reduced probability densities.

Chapter II treats a truncation on the exact hierarchy of the flow equations. The resulting equations are formulated in terms of the chemical potential $\mu$ and the pair potential $\phi(r)$ only, called $(\mu, \phi)$-flow. This scheme involves the choice of the one- and two particle weights, $s_1$ and $s_2(r)$, which can be chosen such that the pair potential $\phi(r)$ is able to keep its core under renormalization. A numerical scheme has been developed to treat the integro-differential equations that are defined by the flow of the potentials and to search for the existence of fixed points of the flow. We indeed find a critical fixed point, having two relevant eigenvalues of the linearization matrix, which are related to the critical exponents.

The fixed point potential $\phi^*(r)$ has a shape that one expects for a fluid in a critical state, and depends moderately on the precise choice of the weights. The calculated critical exponents, however, show too much dependence on the free parameters that appear in the weights. Since this must be a consequence of the neglect of many particle terms, we formulate heuristically conditions for which weight this neglect can be justified.

In the search for a formulation of a systematic approach to the realization of $(\mu, \phi)$-flow, we meet several problems which are treated in chapter III. Under the assumption that it is possible to adjust $s(\vec{r}_1; \vec{r}_2, \ldots, \vec{r}_k)$ to make $\phi(\vec{r}_1, \ldots, \vec{r}_k) = 0$, we discuss whether this has consequences for the regularity of the weights and the flow near the critical point. Among other results we find that $(\mu, T)$-flow, flow of the chemical potential and the temperature alone, can be made regular.
only with the knowledge beforehand of the singularities in the pressure. Therefore it is not a useful scheme.

For \((\mu, \varphi)\)-flow we derive an equation which is a consequence of the match between the flow of the pressure as it follows from decimation, and the one that uses functional derivatives of the pressure with respect to \(\mu\) and \(\varphi(r)\). The last yields a flow for the pressure in terms of \(\dot{\mu}\) and \(\dot{\varphi}(r)\) in combination with the reduced probability densities. This match has its consequences for the freedom in choosing weights.

In chapter IV we start with a systematic calculation of the weights that set the higher particle potential flow zero. One is able to make a diagram expansion in powers of the fugacity \(z\) for the three particle weight \(s(\vec{r}_3; \vec{r}_1, \vec{r}_2)\) near the ideal gas limit. This weight enters in the flow of the pair potential \(\varphi(r)\). Since there appears to be a large freedom in choosing such a weight, we proceed with studying these parts of the flow that do not feel this freedom. We so arrive at a flow for scale invariant combinations of Mayer cluster diagrams and of the fugacity.

The simplest theory is to neglect all diagrams with loops, the Cayley tree approximation, which appears to have no critical fixed point. Inclusion of the simplest loop to all orders in the fugacity leads to the existence of a critical fixed point with (classical) mean field exponents. In that approximation one finds that the weights \(s(\vec{r}_1; \vec{r}_2, \vec{r}_k)\), which set \(\varphi(\vec{r}_1, \ldots, \vec{r}_k) = 0\), diverge for \(k \rightarrow \infty\), running via a deep minimum. This indicates that the production of many particle terms can have considerable impact on the calculation of the critical exponents.

Regularity of the \((\mu, \varphi)\)-flow is found to demand us to have knowledge of the roots of the singular fugacity-density relation \(z(n)\) in the complex \(n\)-plane. This means that strict constraining the flow to \(\mu\) and \(\varphi(r)\) misses its original aim to explain the singularities in the thermodynamic quantities at criticality. It is concluded that \((\mu, \varphi)\)-flow is incapable of giving a satisfactory description of a non classical fluid but that \((\mu, \varphi)\)-flow may serve as a starting point for a more systematic calculation of the many particle potentials in perturbative way.
Samenvatting

In hoofdstuk I introduceren we een renormalisatieschema voor het gas-vloeistof systeem beschreven in het groot kanonieke ensemble. Met behulp van een stochastisch proces bepalen we de reduktie in het aantal vrijheidsgraden. Dit wordt gerealiseerd door het proces van gewogen decimatie gevolgd door herschaling. De resulterende renormalisatievergelijkingen vormen een hierarchie voor de druk $p$, de chemische potentiaal $\mu$ en de $k$-deeltjespotentiaal $\psi(\vec{r}_1...\vec{r}_k)$. Deze bevatten $k$-deeltjes decimatiegewichten $s(\vec{r}_1;\vec{r}_2...\vec{r}_k)$ die de waarschijnlijkheid bepalen om één deeltje uit een groep van $k$-deeltjes te verwijderen. Met deze gewichten is het mogelijk renormalisatievergelijkingen af te leiden voor de gereduceerde waarschijnlijkheidsschichten.

Hoofdstuk II behandelt een benadering van de renormalisatievergelijkingen zoals die volgt door het afbreken van de exacte hierarchie. De resulterende vergelijkingen zijn geformuleerd met behulp van de chemische potentiaal $\mu$ en de paar-potentiaal $\psi(r)$, genaamd $(\mu,\psi)$-renormalisatie. Dit schema bevat de één- en twee decimatiegewichten $s_1$ en $s_2(r)$, die zo gekozen kunnen worden dat onder renormalisatie de paar-potentiaal haar harde kern kan behouden. Een numerieke methode is ontwikkeld om de integro-differentiaalvergelijkingen te behandelen, die gedefinieerd worden door de renormalisatievergelijkingen van de potentiaal en de vraag naar de aanwezigheid van een vast punt van die vergelijkingen. We vinden onderaand een kritiek vast punt, waarvan de lineairisatiematrix twee relevante eigenwaarden bezit, welke samenhangen met de kritieke exponenten.

De vaste puntspotentiaal $\psi^*(r)$ heeft de vorm die men verwacht voor een gas-vloeistof kritieke toestand, en hangt zwak af van de precieuze keuze voor de gewichten. De berekende kritieke exponenten blijken te veel af te hangen van de vrije parameters die in de gewichten voorkomen. Daar dit een gevolg moet zijn van het verwaarlozen van de veeldeeltjes-termen onderzoeken we op heuristische wijze voor welke keuze van de gewichten dit te rechtvaardigen is.

Onderzoek naar de mogelijkheid om te komen tot een systematische benadering voor de realisatie van $(\mu,\psi)$-renormalisatie levert enige problemen, die worden behandeld in hoofdstuk III. Aannemend dat het mogelijk is het gewicht $s(\vec{r}_1;\vec{r}_2...\vec{r}_k)$ zo aan te passen dat $\psi(\vec{r}_1...\vec{r}_k) = 0$. 

komen we tot een discussie van de gevolgen voor de regulariteit van deze gewichten en de renormalisatievergelijkingen dicht bij het kritieke punt. Als gevolg vinden we dat \((\mu, T)\)-renormalisatie, d.w.z. die van enkel de chemische potentiaal en de temperatuur, alleen reguler gemaakt kan worden met kennis vooraf van de singulariteiten in de druk. Derhalve is dit een onbruikbaar schema.

Voor \((\mu, \phi)\)-renormalisatie leiden we een vergelijking af die een uitvloeisel is van het doen overeenkomen van twee alternatieve renormalisatievergelijkingen voor de druk. De eerste is een direct gevolg van gewogen decimatie, terwijl de tweede gebruik maakt van de functionele afgeleiden van de druk naar \(\mu\) en \(\phi(r)\). Deze laatste leidt tot renormalisatie van de druk uitgedrukt in \(\mu\) en \(\phi(r)\), gecombineerd met de gereduceerde waarschijnlijkheidsdichtheden.

Ten gevolge hiervan wordt de vrijheid voor de keuze van de gewichten ingeperkt.

Hoofdstuk IV begint met een systematische berekening van de gewichten die de renormalisatie van de hogerepunts potentialen te niet doet. Het is mogelijk te komen tot een diagram ontwikkeling in machten van de fugaciteit \(z\) voor het drie-deeltjes gewicht \(s(\vec{r}_1; \vec{r}_2 \vec{r}_3)\) vlakbij de ideale gas limiet. Dit gewicht komt voor in de renormalisatievergelijking van de paar-potentiaal \(\phi(r)\). Daar er een grote vrijheid blijkt te bestaan in de keuze van zo'n gewicht, gaan we voort met juist drie delen van de renormalisatievergelijkinge bekijken, die deze vrijheid niet voelen. Hiermee komen we tot een renormalisatievergelijking voor schaal-invariante combinaties van Mayer cluster diagrammen en van de fugaciteit.

De meest simpele theorie is degene die alle diagrammen met "loops" verwaarloost, de zogenaamde "Cayley-tree" benadering. Deze blijkt geen aanleiding te geven tot het bestaan van een kritiek vast punt. Meenemen van het eenvoudigste "loop" diagram tot op alle ordes in de fugaciteit leidt tot vergelijkingen die een kritiek vast punt bezitten, met klassieke (mean field) exponenten. In deze benadering vindt men dat de gewichten \(s(\vec{r}_1; \vec{r}_2 \ldots \vec{r}_k)\), welke \(\phi(\vec{r}_1 \ldots \vec{r}_k) = 0\) maken, divergeren als functie van \(k\) voor \(k \to \infty\), via het doorlopen van een diep minimum. Dit duidt aan dat de veeldeeltjes-potentiaal in grote mate worden aangemaakt, wat stringente gevolgen kan hebben voor de berekening van de kritieke exponenten.
Regulariteit van de renormalisatievergelijkingen in \( \mu \) en \( \varphi(r) \) blijkt ons de eis op te leggen, kennis te hebben van alle wortels van de fugaciteit-dichtheid relatie \( z(n) \), in het complexe \( n \)-vlak. Dit betekent dat te strikte beperkingen van de renormalisatievergelijkingen tot \( \mu \) en \( \varphi(r) \) zijn doel voorbij schiet om de singulariteiten in de thermodynamische grootheden bij het kritische punt te verklaren. We concluderen dat \((\mu,\varphi)\)-renormalisatie niet in staat is een bevredigend beeld te geven van een niet klassieke vloeistof, maar dat deze zou kunnen dienen als aanzet tot een meer systematische berekening van de meerdeeltjes-potentialen op een perturbatieve manier.
STELLINGEN
behoorende bij het proefschrift
"Renormalization of the gas-liquid transition"

1. In een renormalisatie schema voor de gas-vloeistof overgang met behulp
van de procedure van gewogen decimatie is het wezenlijk meerdeeltjes-
potentialen in de berekeningen te betrekken.
(Dit proefschrift)

2. Voor de diffusie van een deeltje, beschreven door de Smoluchowski
vergelijking in een één dimensionale keten van putten, is het mogelijk
een tijdschaal te definiëren zodat de kans dat het deeltje zich in
één der putten bevindt bepaald wordt door een Master vergelijking
van het "hopping model" type.
(Doctoraalscriptie F. van Dieren)

3. Voor iedere binaire rij die met een teruggekoppeld schuifregister
geproduceerd kan worden geldt dat de correlatiefuncties van willekeurige
orde tweewaardig zijn.

4. Het testen van een algoritme voor het genereren van aselecte toevals-
egallen dient uiteindelijk in directe samenhang te geschieden met
het (fysische) probleem waarvoor men deze toevalsgetallen nodig heeft.

5. De door een voldoend sterk magneetveld teweeggebrachte faseovergang
in de triangulaire Ising antiferro magneet met oneindig sterke koppeling
is niet van het drie toestanden Potts type.

6. Het verschijnsel "zwakke universaliteit" in het Baxter model houdt niet in
dat de geschaalde distributiefunctie van de magnetisatie op de kritieke
lijn universeel is.

7. Fysisch gezien is het negentiende eeuwse experiment om een pianoklavier
meervoudig esafonisch in te delen, het meest geschikt.