Thermal fluctuations around classical crystalline ground states
The case of bounded fluctuations

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Abstract

We study low–temperature non Gaussian thermal fluctuations of a system of classical particles around a (hypothetical) crystalline ground state. These thermal fluctuations are described by the behaviour of a system of long range interacting charged dipoles at high–temperature and high–density. For the case of uniformly bounded fluctuations, the low–temperature linked cluster expansion describing the contribution to the free energy is derived and analysed. Finally some nonperturbative results on the existence and independence of boundary conditions of the Gibbs states for the associated dipole systems are obtained.

Key words: crystalline ground states, low temperature expansion, long range dipole systems, thermal fluctuations.

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Chapter 1

Introduction

The question why and how crystals form at low temperature belong to the major open problems in theoretical physics [1,2,18].

Considering a system of \( N \) classical particles described by some Hamiltonian function \( H \), we would like to know that the ground state configurations, which correspond to the local minima of \( H \), are very regular and that under a small perturbation obtained by coupling this \( N \)-particle system to a heat bath at temperature \( T_r \), the typical particle configurations for small values of \( T_r \) do not fluctuate much away from the crystallic ground state configuration. It is clear that certain surface effects could destroy this naive picture and therefore one has to pass to the thermodynamic limit which corresponds to letting \( N \uparrow \infty \) while keeping the density of particles fixed. The problem of verifying the validity of the above picture is still unsolved in general, and in the situation where the system is located in three dimensional space, which is most interesting from a physical point of view, there are very few results. However some progress has been made in lower dimensions both for finite systems (\( N < \infty \)) and in the thermodynamic limit (\( N \uparrow \infty \)). The case of one space dimension seems to be fairly well understood [3,4,6,7,20], but see [36]. For the case of a two-dimensional space our understanding is more restricted [8,9,10] and in higher dimensions only very few results are known [5,24]. In one and two dimensions also models with quasicrystalline behaviour at zero temperature [11,12] have been studied. Quite recently a quantum mechanical model showing crystallization has been discussed [13,14]. For a very readable survey of current insight into the crystal problem we refer the reader to [15].

The present contribution is devoted to the analysis of the crystal problem in three dimensional space. We select a special class of interactions for which the analysis of the thermodynamical limit of the free energy density describing fluctuations of a system at
low temperature around the hypothetical crystalline configuration, which minimizes the relative potential energy, is possible by relatively simple and standard methods. As we will see, the condition for the minimizing potential energy configurations can be expressed mathematically as a condition of positive definiteness of the Hessian matrix for the corresponding potential function. This enables us to rewrite the higher order contributions of the Taylor expansion around a crystalline, energy minimizing configuration in terms of certain Gaussian integrals. In this picture, non Gaussian fluctuations around the crystalline structure can be described by a highly nonlinear interacting system of dipoles in which the potential describing the interaction between the dipoles in the dipole gas framework decays rather slowly, but the interaction energy is integrable. A similarity with the corresponding problems of lattice systems may be seen from this picture.

The continuous and the lattice dipole systems with long range like interactions have been studied intensively only recently and a variety of deep results describing their high and low temperature properties have been derived rigorously.

We expect that some of the results obtained in [16,17,18,19,20] can be applied to the dipole systems which we put in evidence in our study of the formation of crystals in the three-dimensional space.

Restricting further the class of admissible potentials we consider a class of potentials which leads to bounded Taylor remainders for the corresponding expansions around crystalline ground state. For such potentials the associated dipole system describing fluctuations can be interpreted as a grand canonical ensemble gas of charged dipoles living on a Bravais lattice $\Omega_\infty$ and in thermal equilibrium at temperature $T_r^{-1}$ where $T_r$ is the temperature of the real system. Thus the low temperature behaviour of a real system is described by the high temperature behaviour of the corresponding charged dipole system. The activity of the associated dipole system is given by $-\frac{1}{kT}$ where $k$ is the Boltzmann constant and thus the low temperature behaviour of the real system is described by the high temperature/high density limit of the corresponding dipole system. Section 3 of the present paper is devoted to the study of the thermodynamic limit for the corresponding dipole systems using some basic tools of statistical mechanics, e.g. linked cluster expansion and Kirkwood–Salsburg identities [22,23]. Although most of the results established there are valid for an ensemble of dipoles of arbitrary sizes we shall restrict ourselves to the study of restricted ensemble consisting of dipoles of a uniformly bounded size. This cutoff is necessary for obtaining a finite contribution to the free energy density of the system we consider. The restriction to an ensemble of uniformly bounded dipole is equivalent to the restriction of an admissible size of possible deviations of real particles configurations from crystalline configurations. From the Gibbs measure point of view this means that we have restricted ourselves to the
contribution to the free energy density coming from locally finite configurations with uniformly bounded (at large distances) deviations from the (hypothetical) crystalline ground state. The problem of large deviations which we called large fluctuation problem is the main topic of a forthcoming, second part of this work [34]. An additional discussion of the meaning of the restriction to the bounded dipole case is included in Section 4, where also a discussion of the compatibility of our assumptions on the interaction potential paper can be found.
Chapter 2

Expansion around a crystalline ground state. The finite volume case.

Let us consider a system composed of \( n \) classical particles with masses equal to 1 (for simplicity) and enclosed in the bounded region \( \Lambda_N = \{ x \in \mathbb{R}^3 \mid |x^i| \leq N \text{ for } i = 1, 2, 3 \} \). The phase space coordinates of the system will be denoted by \((p,x)_n \equiv ((p_1,x_1),\ldots,(p_n,x_n))\), \( p_i \in \mathbb{R}^3, x_i \in \Lambda_N \). The particles interact through two-body potential forces described by the potentials \( V \). The class of potential for which our analysis applies will be determined by imposing certain conditions which will be listed below. A preliminary discussion of the compatibility of these hypotheses is given in section 4 of the present paper.

Hypothesis 0

The potential \( V \) is central, i.e. there exists a real-valued function \( \Phi \) on \( \mathbb{R}_1^+ \) such that \( V(x) = \Phi(|x|) \). The function \( \Phi \) has compact support and is of class at least \( C^3 \). The potential \( V \) is stable in the thermodynamical sense, i.e.,

\[
\exists B > 0, \forall n : \quad \mathcal{E}((x)_n) \equiv \sum_{1 \leq i < j \leq n} V(x_i - x_j) \geq -nB. \tag{2.1}
\]

The canonical (Maxwell-Boltzmann ensemble) partition function of the system at (inverse) temperature \( \beta > 0 \) reads:

\[
Z_N^n(\beta) = \int_{(R^3 \times \Lambda_N)^n} \prod_{i=1}^n dp_i dx_i \exp[-\beta \mathcal{E}((p,x)_n)], \tag{2.2}
\]

where the energy function is

\[
\mathcal{E}((p,x)_n) \equiv \sum_{i=1}^n \frac{p_i^2}{2} + \sum_{i \neq j=1}^n V(x_i - x_j). \tag{2.3}
\]
Integrating out the momenta we obtain:

\[
Z^N_n(\beta) = \left( \frac{2\pi}{\beta} \right)^{3n/2} \int_{\Lambda^N_n} \otimes_{i=1}^n dx_i \exp[-\beta E((x)_n)].
\] (2.4)

It is natural to try to apply the saddle point method to the study of the low temperature \((\beta \uparrow \infty)\) behaviour of the canonical partition function \(Z^N_n(\beta)\). The classical Laplace theorem tells us that if the minima of the function \(E((x)_n)\) are well separated then the following asymptotic formula is valid:

\[
Z^N_n(\beta)_{\beta \uparrow \infty} \sim \sum_{X_{\min}^n} e^{-\beta E(X_{\min}^n)} \int_{\Lambda^N_n} \prod_{i=1}^n \exp[-\beta \frac{1}{2} ((x_n) - X_{\min}^n), [D^2 E((x)_n - X_{\min}^n))] \cdot \exp[-\beta R(X_{\min}^n, (x)_n)] \otimes_{i=1}^n dx_i.
\] (2.5)

where we have denoted by \(X_{\min}^n = (x_1^m, ..., x_n^m)\) the minimizing configuration for the energy function \(E\), and the contribution coming from the first factor i.e. from \(e^{-\beta E(X_{\min}^n)}\), dominates as \(\beta \uparrow \infty\).

The zero temperature crystal problem in this picture amounts to answering the question whether the energy function \(E\) has a minimum at an (almost) regular configuration \(X_{\min}^n = (x_1^m, ..., x_n^m)\). In the finite volume situation we do not expect that the minimizing configuration \(X_{\min}^n\) forms a completely regular structure, because of surface effects. To avoid such problems we therefore pass to the thermodynamic limit, i.e., we consider the limit \(N \uparrow \infty\), keeping the density \(\rho = n/(2N)^3\) fixed. It is expected that there exists a certain regime of values and \(\rho\) in which the limiting minimizing configurations \(X_{\min}^\infty = (x_1^m, ..., x_n^m)\) are quite regular globally. A particularly interesting situation is the one where the (hypothetical) energy density minimizing configuration \(X_{\min}^\infty\) forms a Bravais lattice in \(R^3\).

Let us recall that a Bravais lattice \(\Omega_{\infty}\) in \(R^3\) is defined by three linearly independent vectors \(\vec{a}_1, \vec{a}_2, \vec{a}_3 \in R^3\) such that

\[
\Omega_{\infty} \equiv \{ n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \mid n_1, n_2, n_3 \in Z \}
\]

\[\text{(1)}\]

To deal with the case \(N = \infty\) it is convenient to use the energy density function

\[
\epsilon_{\rho}((x)_\infty) = \lim_{N \uparrow \infty} \frac{E((x)_n)}{(2N)^3 \rho - \text{fixed}}
\]

provided it exists.
Let us set $\Omega_N = \Lambda_N \cap \Omega_\infty$. Assuming $n = |\Omega_N|$ we can, by suitably relabeling and changing the variables, rewrite the energy function of $n$-particles in the following way:

$$E((x)_n) = \frac{1}{2} \sum_{\lambda, \mu \in \Omega_N, \lambda \neq \mu} V(\lambda - \mu + y_\lambda - y_\mu)$$

where the variables $y_\lambda$ measure the deviation of the $\lambda$ particle from the lattice point $\lambda \in \Omega_N$. This can be further represented as:

$$E((x)_n) = E^{cr}(\Omega_N) + E^{dev}(\Omega_N \mid \{y_\lambda\})$$

where

$$E^{cr}(\Omega_N) = \frac{1}{2} \sum_{\lambda \neq \mu} V(\lambda - \mu)$$

is the energy of the crystalline configuration $\Omega_N$ and

$$E^{dev}(\Omega_N \mid \{y_\lambda\}) = E((x)_n) - E^{cr}(\Omega_N)$$

measures the energy deviation of the real configuration $(x)_n$ from the energy of the crystalline configuration $\Omega_N$.

The crystalline energy $E^{cr}$ depends only on the parameters $\vec{a}_1, \vec{a}_2, \vec{a}_3$ spanning our Bravais lattice. Therefore one can easily find an equation on $\vec{a}_1, \vec{a}_2, \vec{a}_3$ that yields a stationary point for the crystalline energy $E^{cr}(\Omega_N)$ (see e.g., [21]). As an example, in the case of central potential forces described by the function $\Phi$ as in Hypothesis 0 the corresponding equation reads:

$$\sum_{n \in \mathbb{Z}^3} \frac{n^i n^j \Phi(|\lambda|)}{|\lambda|} = 0, \quad i, j = 1, 2, 3,$$

which is a set of 9 equations with 9 unknowns. This equation, together with the condition that the relevant Hessian is positive, then gives a local minimum for $E^{cr}(\Omega_N)$. 
We find that for technical reasons it is more convenient to work with a periodic version of the given finite Bravais lattice, henceforth we shall understand under $\Omega_N$ this periodic version.

The following hypothesis plays a crucial role in the present attempt to understand the formation of crystals in the low-temperature/high density region in three dimensional space.

Hypothesis 1

(H1$\alpha$). There exists a number $\rho_{cr} > 0$ such that for all $\rho \geq \rho_{cr}$ there exists a Bravais lattice solutions $\Omega_N$ of the minimizing problem for the corresponding $E^{cr}(\Omega_N)$. Moreover this holds uniformly in $N$ at least for sufficiently large $N$.

(H1$\beta$). The deviation energy function $E^{dev}(\Omega_N | \{y_n\}_{\lambda \in \Omega_N})$ has a stationary point at $\{y_\lambda = 0, \lambda \in \Omega_N\}$ which is a local minimum for sufficiently large values of $N$.

Part $\beta$ of Hypothesis 1 can be derived from the condition.

$$0 < (y, [D^2V]y) \equiv \frac{1}{2} \sum_{\lambda,\mu \in \Omega_N} (y_\lambda - y_\mu, [D^2V](\lambda - \mu)(y_\lambda - y_\mu))$$ (2.11)

where $[D^2V](\lambda - \mu)$ is the Hessian of $V$ evaluated at the lattice point $(\lambda - \mu)$, see e.g., [21].

Condition (2.11) can be used to deduce the existence of a certain functional integral representation of the quantities of interest. For this reason we define the matrix:

$$A_N(\lambda, \mu) = \begin{cases}
2 \sum_{\eta \in \Omega_N, \lambda \neq \eta} [D^2V](\lambda - \eta) & \text{if } \lambda = \mu \\
-[D^2V](\lambda - \mu) & \text{if } \lambda \neq \mu.
\end{cases}$$ (2.12)

Then we have the following equality:

$$\frac{1}{2} \sum_{\lambda,\mu \in \Omega_N} (y_\lambda - y_\mu, [D^2V](\lambda - \mu)(y_\lambda - y_\mu)) = \sum_{\lambda,\mu \in \Omega_N} (y_\lambda, A_N(\lambda, \mu)y_\mu)$$ (2.13)

From the hypothesis H1$\beta$ it follows that the matrix $A_N$ is strictly positive definite on the space $\mathbb{R}^{3|\Omega_N|}$ (with $|\Omega_N|$ the number of points in $\Omega_N$). On the Borel $\sigma$-algebra of sets of $\mathbb{R}^{3|\Omega_N|}$ we can therefore define the Gaussian measure $\mu^0_N$ with mean equal to zero and covariance matrix $C_N(\lambda, \mu) = A_N^{-1}(\lambda, \mu)$ equal to the inverse of the matrix $A_N(\lambda, \mu)$, i.e.,

$$\int_{\mathbb{R}^{3|\Omega_N|}} d\mu^0_N(y_1, ..., y_{|\Omega_N|}) \exp[i \sum_{\lambda \in \Omega_N} (\alpha_\lambda, y_\lambda)] = E^0_N(e^{i(\tilde{\alpha}, \tilde{y})}) = \exp[-\frac{1}{2}(\alpha, A_N^{-1}\alpha)] = \exp[-\frac{1}{2}(\alpha, C_N\alpha)]$$ (2.14)
\[
\tilde{\alpha} = (\alpha_1, ..., \alpha_{|\Omega_N|}),
\]
\[
(\tilde{\alpha}, \tilde{y}) = \sum_{\lambda \in \Omega_N} (\alpha_{\lambda}, y_{\lambda}),
\]
\[
(\tilde{\alpha}, C_N \tilde{\alpha}) = \sum_{\lambda \in \Omega_N} (\alpha_{\lambda}, \sum_{\mu \in \Omega_N} C_N(\lambda, \mu) \alpha_{\mu}),
\]
and similarly for \((\tilde{\alpha}, A_N^{-1} \tilde{\alpha})\). From the periodic lattice \(\Omega_N\) and the infinitely extended lattice \(\Omega_\infty\) we form the corresponding dual lattices \(\Gamma_N\) and \(\Gamma_\infty\) respectively. The corresponding dual groups or Brillouin zones are denoted by \(\hat{\Omega}_N\) and \(\hat{\Omega}_\infty\) respectively and are defined by \(\hat{\Omega}_N = [-N, N]^3/\Gamma_N\), \(\hat{\Omega}_\infty = \mathbb{R}^3/\Gamma_\infty\). We have:

\[
\frac{1}{2} \sum_{\lambda, \mu \in \Omega_N, \lambda \neq \mu} (y_\lambda - y_\mu, [D^2V](\lambda - \mu)(y_\lambda - y_\mu)) = \sum_{p \in \Omega_N} \overline{\hat{y}_N(p)}(\hat{A}_N(0) - \hat{A}_N(p))\hat{y}_N(p),
\]

where

\[
\hat{A}_N(p) \equiv \sum_{\lambda \in \Omega_N, \lambda \neq 0} [D^2V](\lambda)e^{ip\lambda}
\]

and

\[
\hat{y}_N(p) \equiv \sum_{\lambda \in \Omega_N} y_\lambda e^{ip\lambda}.
\]

For the infinitely extended lattice \(\Omega_\infty\) the corresponding formulae are:

\[
\frac{1}{2} \sum_{\lambda, \mu \in \Omega_\infty, \lambda \neq \mu} (y_\lambda - y_\mu, [D^2V](\lambda - \mu)(y_\lambda - y_\mu)) = \int_{\Omega_\infty} \overline{\hat{y}(p)}(\hat{A}_\infty(0) - \hat{A}_\infty(p))\hat{y}(p)dp,
\]

where

\[
\hat{y}(p) = \sum_{\lambda \in \Omega_\infty} y_\lambda e^{ip\lambda}
\]

and

\[
\hat{A}_\infty(p) = \sum_{\lambda \in \Omega_\infty, \lambda \neq 0} [D^2V](\lambda)e^{ip\lambda}
\]
We remark that, due to the compact support of \( D^2V(\lambda) \) and the fact that \( \Omega_N \) is compact, \( \hat{A}_N(p) \) is well-defined, and is the pointwise limit of \( \hat{A}_N(p) \) as \( N \to \infty \). Similarly, the right hand side of (2.22) is well-defined for all \( y \in L_2(\Omega_\infty) \). Hence the equalities (2.21), established first for a dense subset of \( L_2(\Omega_\infty) \), extend to the whole of \( L_2(\Omega_\infty) \).

Let us define the functional \( \mathcal{E}_{\Omega_\infty}^{\text{dev}} \) on the dense subset of \( L_2(\Omega_\infty) \) consisting of sequences \( \{y_\lambda\}_\lambda \), \( \lambda \in \Omega_\infty \) with compact support, by the formula (2.9) with \( N = \infty \), i.e., by

\[
\mathcal{E}_{\Omega_\infty}^{\text{fl}}(\Omega_\infty \mid \{y_\lambda\}_{\lambda \in \Omega_\infty}) \equiv \frac{1}{2} \sum_{\lambda, \mu \in \Omega_\infty, \lambda \neq \mu} [V(\lambda - \mu + y_\lambda - y_\mu) - V(\lambda - \mu)] .
\]

Then we have, using formula (2.20), the following:

**Lemma 2.1** Assume that the point \( \{y_\lambda = 0\} \), \( \lambda \in \Omega_\infty \) is a stationary point of \( \mathcal{E}_{\Omega_\infty}^{\text{dev}} \). Then it is a local minimum for \( \mathcal{E}_{\Omega_\infty}^{\text{dev}} \) if \( \hat{A}_N(0) - \hat{A}_\infty(p) \) is a positive definite matrix for all \( p \in \hat{\Omega}_\infty \). The corresponding statements hold for \( \mathcal{E}_{\Omega_N}^{\text{dev}} \) i.e., if \( \{y_\lambda\}, \lambda \in \Omega_N \) is a stationary point for \( \mathcal{E}_{\Omega_N}^{\text{fl}} \) then it is a local minimum if \( \hat{A}_N(0) - \hat{A}_N(p) \) is a positive definite matrix for all \( p \in \hat{\Omega}_N \).

By Fourier analysis, similarly as above, we find the following representation for the inverse matrices \( (A_N(\lambda, \mu))^{-1} \) and \( A_\infty(\lambda, \mu) \).

\[
C_N(\lambda - \mu) \equiv (A_N)(\lambda, \mu) = \sum_{p \in \hat{\Omega}_N} e^{ip(\lambda - \mu)}(\hat{A}_N(0) - \hat{A}_N(p))^{-1}
\]

and

\[
C_\infty(\lambda - \mu) \equiv (A_\infty^{-1})(\lambda, \mu) = \int_{\Omega_\infty} e^{ip(\lambda - \mu)}(\hat{A}_\infty(0) - \hat{A}_\infty(p))^{-1} dp.
\]

The following hypothesis will play an essential role in the following analysis.

**Hypothesis 2**

(H2α). There exists a constant \( c \), independent of \( N \), such that \( \hat{A}_N(p) - \hat{A}_N(0) \geq cp^2 + 0_N(p^2) \) as \( p \to 0 \).

(H2β). \( \hat{A}_N(p) = \hat{A}_N(0) \) iff \( p = 0 \).

Hypothesis 2 ensures that the functions \( C_N(\lambda - \mu) \) and \( C_\infty(\lambda - \mu) \) are well-defined and moreover \( C_\infty(\lambda - \mu) \) decays at least as \( \frac{1}{|\lambda - \mu|} \) for \( |\lambda - \mu| \to \infty \). The set of potentials for which (H2α) and (H2β) are satisfied is surprisingly rich, we refer to the work [21] and to section 4 of the present paper.
The previously introduced Gaussian measure $d\mu^0_N$ has the following density with respect to the Lebesgue measure

$$
\frac{d\mu^0_N}{\otimes_{\lambda \in \Omega^N} dy_\lambda} = \det\left(\frac{1}{2\pi} A_N(\lambda, \mu)\right)_{\lambda, \mu \in \Omega^N}^{-\frac{1}{2}} \exp\left[-\frac{1}{2} \sum_{\lambda, \mu \in \Omega^N} (y_\lambda, A_N(\lambda, \mu)y_\mu)\right] \tag{2.27}
$$

Expanding around the minimizing configuration $\Omega_N$, using the Gaussian measure integration $E^0_N$ and making a simple change of variables, we can represent the canonical partition function $Z_n^N$ in the following way:

$$
Z_n^N(\beta) = (2\pi)^{3n/2} \beta^{-3n} \cdot Z^{cr}(\Omega_N) \cdot z_N \cdot Z^{fl}_N(\beta), \tag{2.28}
$$

where we have introduced

- the crystalline partition function:

$$
Z^{cr}_\beta(\Omega_N) \equiv \exp\left[-\beta \mathcal{E}^{cr}(\Omega_N)\right] \tag{2.29}
$$

- the fluctuation partition function:

$$
Z^{fl}_N(\beta) \equiv E^0_N(\chi(|y_\lambda| \leq N)_{\lambda \in \Omega^N} \exp[-\beta \mathcal{R}(\Omega_N \mid \{\frac{y_\lambda}{\sqrt{\beta}}\}_{\lambda \in \Omega^N}] \tag{2.30}
$$

where

$$
\mathcal{R}(\Omega_N \mid \{y_\lambda\}_{\lambda \in \Omega^N}) \equiv \mathcal{E}((x)_n)
$$

$$
-\frac{1}{2} \sum_{\lambda, \mu \in \Omega^N} (y_\lambda - y_\mu, D^2V(\lambda - \mu)(y_\lambda - y_\mu)) - \mathcal{E}^{cr}(\Omega_N) \tag{2.31}
$$

is the Taylor remainder of the Taylor expansion of the energy $\mathcal{E}((x)_n)$ of the real configuration $x_n$ around the local minimum given by $\Omega_N$

- the normalisation factor for the measure $\mu^0_N$:

$$
z_N \equiv \det\left(\frac{1}{2\pi} A_N(\lambda - \mu)_{\lambda, \mu \in \Omega^N}\right)^{1/2} \tag{2.32}
$$

The free energy density of a system enclosed within the region $\Lambda_N$ (with periodic boundary conditions) is defined by:

$$
\beta P_N(\beta) = \frac{1}{|\Lambda_N|} \ln Z^*_N(\beta) \tag{2.33}
$$
Substituting (2.28) into (2.33) we obtain:

\[ \beta P_N(\beta) = \frac{3 \ln 2\pi}{2} \rho - 3 \rho \ln \beta + \beta P^c_N(\Omega_N | \beta) + \beta \tilde{z}_N + \beta p_N(\beta) \] (2.34)

where

\[ P^c_N(\Omega_N | \beta) = \frac{1}{\beta | \Lambda_N |} \ln \exp[ - \beta \mathcal{E}^c(\Omega_N) ] = - \frac{\mathcal{E}^c(\Omega_N)}{| \Lambda_N |} \] (2.35)

is the crystalline free energy density;

\[ \tilde{z}_N \equiv \frac{1}{2 \beta | \Lambda_N |} \ln \det((A_N(\lambda, \mu))_{| \Omega_N |}^{2 \pi} \lambda, \mu \in \Omega_N) \] (2.36)

is a numerical constant and

\[ p_N(\beta) \equiv \frac{1}{\beta | \Lambda_N |} \ln \mathbf{E}_N^0[ \chi(\{| y_{\lambda} \leq N \}_{\lambda \in \Omega_N}) \exp[ - \beta \mathcal{R}(\Omega_N | \{ y_{\lambda}/\sqrt{\beta} \}) ]] \] (2.37)

is the free energy density of nongaussian fluctuations around \( \Omega_N \).

A simple Fourier analysis is used to control the thermodynamic limit of the quantity \( \tilde{z}_N \).

We have

\[ \tilde{z}_N = \frac{1}{2 \beta | \Lambda_N |} \ln \det((A_N(\lambda, \mu))_{| \Omega_N |}^{2 \pi} \lambda, \mu \in \Omega_N) \]

\[ = \frac{1}{2 \beta | \Lambda_N |} \sum_{p \in \hat{\Omega}_N} \text{tr} \ln(\hat{A}_N(0) - \hat{A}_N(p)). \] (2.38)

As \( N \to \infty \) this tends to:

\[ z_\infty = \frac{1}{2 \beta | \Lambda |} \int_d dp \ln[\hat{A}_\infty(0) - \hat{A}_\infty(p)], \] (2.39)

which is finite, e.g., under the assumption (H2\( \alpha \)).

The most difficult element of our analysis concerns the problem of the existence of the thermodynamic limit of the free energy density of fluctuations around a crystalline ground state. Taking into account the formula

\[ \mathcal{R}(\Omega_N | \{ y_{\lambda}/\sqrt{\beta} \}_{\lambda \in \Omega_N}) = \sum_{\lambda, \mu \in \Omega_N} \mathcal{R}_\Omega(\lambda - \mu | y_{\lambda}/\sqrt{\beta}), \] (2.40)

where

\[ \mathcal{R}_\Omega(\lambda - \mu | y_{\lambda}/\sqrt{\beta}) \equiv V(\lambda + \beta^{-1/2} y_{\lambda} - \mu - \beta^{-1/2} y_{\mu}) \]

\[ - V(\lambda - \mu) - \frac{1}{2} (y_{\lambda} - y_{\mu})^2 D^2 V(\lambda - \mu)(y_{\lambda} - y_{\mu}/\sqrt{\beta}), \] (2.41)
we see that in the field theoretical picture given by the Gaussian integral representation (2.30) the partition function $Z^f_N$ can be viewed as the partition function of a gas of dipoles that sit on the lattice $\Omega_N$ and interact by a nonpolynomial and in general nonlocal potential given by (2.40). With some additional simplifying assumptions the problem of the thermodynamic limit of the free energy density and also for the corresponding Gibbs states describing the associated dipole systems will be studied in the next section by an application of techniques of statistical mechanics e.g. linked cluster expansion and analysis of the Kirkwood-Salzburg identities.
Chapter 3

Infinite volume limit. Bounded dipole length case.

In this section we shall discuss the thermodynamic limits of the free energy density and the Gibbs states of the associated dipole systems describing bounded fluctuations of the real configurations around the crystalline ground state given by a Bravais lattice $\Omega_{\infty}$.

3.1 A convergent expansion for the dipole partition function

In order to simplify the analysis as much as possible the following additional hypothesis will be introduced.

**Hypothesis 3.** There exists a family $(d\mu_\lambda)_{\lambda \in \mathbb{R}}$ of complex measures on $\mathbb{R}^3$ such that the following representation for the corresponding Taylor remainders defined by (2.42) hold for all $\lambda - \mu$:

$$R_{\Omega_N}(\lambda - \mu | x) = \int_{\mathbb{R}^3} d\mu_{\lambda - \mu}(\alpha) e^{i\alpha x}. \quad (3.1)$$

In addition we assume that $d\bar{\mu}_\lambda(\alpha) = d\mu_\lambda(-\alpha)$ so that $R_{\Omega_N}(\lambda - \mu | x)$ is real. We also make the following additional assumptions on the measure appearing in (3-1)$^1$.

(H3$\alpha$). $\int d|\mu_\lambda| |(\alpha)| |\alpha|^n < \infty$, for all $\lambda$ and all $n \in \mathbb{N}^+$

(H3$\beta$). $\int d|\mu_\lambda| |(\alpha)| e^{A|\alpha|^2}$, for some $A > 0$, and all $\lambda \in \Omega_{\infty}$. $A$ has to be sufficiently large (see below).

(H3$\gamma$). For all $\lambda$, $\text{supp } d\mu_\lambda$ is compact in $\mathbb{R}^3$.

The following trivial chain of implications holds: (H3$\gamma$) $\Rightarrow$ (H3$\beta$) $\Rightarrow$ (H3$\alpha$). Which one of the hypothesis $\alpha, \beta$ and $\gamma$ is needed depends on the particular situation we investigate (see below).

As a preliminary step in our analysis we remove the characteristic function restricting the

$^1$In fact we need only the existence of the first moments (see Proposition 3-2 below)
possible values of the size of fluctuations \( \{y_\lambda\} \) in (2.30) defining

\[
Z^d_N \equiv E_N^0(\exp[-\beta R(\Omega_N \mid \{\beta^{-1/2}y_\lambda\}_{\lambda \in \Omega_N})]).
\]  

(3.2)

Using the formula

\[
E_N^0(\prod_{j=1}^n(e^{i\beta^{-1/2}y_\lambda \cdot e^{-i\beta^{-1/2}y_\mu}}) = \exp[-\frac{1}{\beta^2} \sum_{1 \leq i,j \leq n} V_N(\lambda_i \mu_i \mid \lambda_j \mu_j)]
\]

(3.3)

where

\[
V_N(\lambda_i \mu_i \mid \lambda_j \mu_j) \equiv \alpha_i(C_N(\lambda_i \lambda_j) + C_N(\mu_i \mu_j) - C_N(\lambda_i \mu_j) - C_N(\mu_j \lambda_i))
\]

(3.4)

and taking into account H4 and H6 we obtain the following expansion of \( Z^d_N \):

\[
Z^d_N = \sum_{n \geq 0} \frac{(-\beta)^n}{n!} \sum_{\lambda_i, \mu_i \in \Omega_N \mid \lambda_i - \mu_i \leq R} \int \otimes_{l=1}^n d\mu_{\lambda_i - \mu_i}(\alpha_i)
\]

\[
\exp[-\frac{1}{\beta} \sum_{1 \leq i,j \leq n} V_N(\alpha_i \lambda_i \mu_i \mid \alpha_j \lambda_j \mu_j)].
\]

(3.5)

From the very simple inequality

\[
|E_N^0(\exp[i \sum_\lambda \alpha_\lambda y_\lambda]| \leq 1
\]

(3.6)

we deduce the following estimate on \( Z^d_N \):

\[
Z^d_N \leq \exp[\mid \beta \mid \mu^* \mid \tilde{D}_N(1) \mid]
\]

(3.7)

where

\[
\mu^* \equiv \sup_{\lambda \in \Omega_\infty} \{ \int \mid \mu_\lambda \mid \},
\]

and \( \mid \tilde{D}_N(1) \mid \) is the cardinality of the set \( \Omega_N \times \Omega_N \). Estimate (3.7) shows that the expansion (3.6) is absolutely convergent for any \( \beta > 0 \). For the dipole free energy density \( p^d_N(\beta) \equiv |\tilde{D}_N(1)|^{-1} \ln Z^H_N \) we obtain the upper bound:

\[
p^d_N(\beta) \leq \beta \mu^*
\]

(3.8)

uniformly in \( N \).

Although some of the results below hold for a dipole systems described by the dipole
partition function (3-3) it follows from the estimate (3.8) that in order to ensure the finiteness of the limit
\[ \lim_{\Lambda N} \frac{1}{\ln Z_N^d} \]
(see for (2.37)): without further assumptions on the interaction potential \( V \) we have to restrict the admissible length of dipoles. Let \( R \) be some fixed positive number. Then we define a bounded length dipole system by the following partition function
\[ Z_{bd}^d(\beta) \equiv E_N^0(\exp -\beta R_N^\mu(\Omega_N | \{\beta \frac{1}{2} y_{\lambda}\})) \]  (3.9)
where the restricted Taylor remainder \( R_N^\mu \) is given by:
\[ R_N^\mu(\Omega_n | \{\beta \frac{1}{2} y_{\lambda}\}) \equiv \sum_{\lambda, \mu} R_N(\lambda - \mu | \frac{y_{\lambda} - y_{\mu}}{\sqrt{\beta}}) \]  (3.10)
From now on an allowed maximal size of dipole given by a number \( R \) will be fixed. The following sort of stability also comes from estimate (3.7) in a simple way:
\[ \sum_{1 \leq i \neq j \leq n} V_N(\alpha_i \lambda_i \mu_i | \lambda_j \mu_j \alpha_j) \geq -2 \sum_{i=1}^n \alpha_i(C_N(0) - C_N(\lambda_i - \mu_i)) \alpha_i. \]  (3.11)
The expansion like (3.6) for \( Z_{bd}^d \) has the interpretation as a grand canonical partition function of a system of dipoles of length bounded by \( R \) on the lattice \( \Omega_N \) in the thermal equilibrium at inverse temperature \( 1/\beta \). Because of the crucial stability estimate (3.11) the standard tools of classical statistical mechanics, such as cluster expansions, Kirkwood-Salzburg type analysis [22] can be used to study the corresponding thermodynamical limit.
In order to simplify our notation the following abbreviations will be used:
\[ D_N^R(K) \equiv D_N^R(1) \times \ldots \times D_N^R(K) \]  (3.12)
\[ = \{ (\lambda_1, \mu_1, \alpha_1), \ldots, (\lambda_K, \mu_K, \alpha_K) | \lambda_i, \mu_i \in \Omega_N, | \lambda_i - \mu_i | \leq R, \alpha_i \in R^3 \} \equiv K\text{-dipoles configuration space.} \]
Furthermore we denote by
\[ \tilde{D}_N^R(K) = \tilde{D}_N^R(1) \times \ldots \times \tilde{D}_N^R(K) \]  (see (3.10))
the \( K\text{-dipoles restricted configuration space.} \)
For a generic \( \omega \in D_N^R(K) \) the following abbreviations will also be employed
\[ \omega = ((\lambda_1, \mu_1, \alpha_1), \ldots, (\lambda_n, \mu_n, \alpha_n)) \equiv (\lambda, \mu, \alpha)_n, D_N^R(1) \ni (\lambda_i, \mu_i, \alpha_i) \equiv d(i). \]  (3.14)
\[ \int d_N^R(i) \ldots \equiv \sum_{\lambda_i, \mu_i \in \Omega_N} \int d\mu_{\lambda_i - \mu_i}(\alpha_i) \]  
(3.15)

\[ \int d_N^R(1, \ldots, n) \ldots = \int d_N^R(n) \ldots \int d_N^R(1) \ldots \]  
(3.16)

\[ \int d_\infty^R(i) \ldots = \sum_{\lambda_i, \mu_i \in \Omega_\infty} \int d\mu_{\lambda_i - \mu_i}(\alpha_i) \ldots \]  
(3.17)

\[ \mathcal{E}_N((\alpha, \lambda, \mu)_n) \equiv \sum_{1 \leq i, j \leq n} V_N(\alpha_i, \lambda_i, \mu_i \mid \alpha_j \lambda_j \mu_j) \]  
(3.18)

\[ \mathcal{E}_\infty((\alpha, \lambda, \mu)_n) \equiv \sum_{1 \leq i, j \leq n} V_\infty(\alpha_i \lambda_i \mu_i \mid \alpha_j \lambda_j \mu_j) \]  
(3.19)

\[ \mathcal{E}_N((\alpha, \lambda, \mu)_n \mid (\alpha', \lambda', \mu')_m) \equiv \mathcal{E}_N((\alpha, \lambda, \mu)_n) - \mathcal{E}_N((\alpha, \lambda, \mu)_n) - \mathcal{E}_N((\alpha', \lambda', \mu')_m) \]  
(3.20)

and similarly for \( \mathcal{E}_\infty \).

Hence we can rewrite (3.6) for \( Z_N^{bd} \) in the following way

\[ Z_N^{bd} = \sum_{n \geq 0} \left( \frac{-\beta}{n!} \right)^n \int d_N^R(1, \ldots, n) \exp\left[ -\frac{1}{\beta} \mathcal{E}_N(d(1), \ldots, d(n)) \right] \]  
(3.21)

3.2 The linked cluster expansion for the free energy density.

Using a well known trick of Mayer [22,23] we can derive the linked cluster expansion for the free energy density for a finite volume system. For this purpose we write

\[ \exp\left[ -\frac{1}{\beta} \mathcal{E}_N(d(1), \ldots, d(n)) \right] = \prod_{i=1}^{n} V_N(i) \prod_{1 \leq i \neq j \leq n} \exp\left[ -\frac{1}{\beta} V_N(d(i) \mid d(j)) \right] \]  
(3.22)

\[ = \prod_{i=1}^{n} V_N(i) \prod_{1 \leq i \neq j \leq n} \left[ (\exp -\frac{1}{\beta} V_N(d(i) \mid d(j)) - 1) + 1 \right] \]

\[ = \prod_{i=1}^{n} V_N(i) \sum_{\Gamma \subset \{1, \ldots, n\}} \mathcal{M}(d(i \in \Gamma)) \]

where

\[ \mathcal{M}(d(i \in \Gamma)) \equiv \prod_{i,j \in \Gamma} \left( \exp\left[ -\frac{1}{\beta} V_N(d(i) \mid d(j)) \right] - 1 \right) \]  
(3.23)
and

\[ V_N(i) \equiv \exp\left[-\frac{1}{\beta} \alpha_i^2 (C_N(0) - C_N(\lambda_i - \mu_i))\right] \] \hspace{1cm} (3.24)

is the corresponding vertex function.

We denote by \( \mathcal{G}^N_n \) the set of all connected linear \( n \)-graphs that can be built on the set \( \tilde{D}_R^N(n) \). Putting the expansion (3.23) into (3.22) and resumming we obtain the linked cluster expansion in the following standard form:

\[ Z_N^{bd} = \exp\left[ \sum_{n \geq 1} (-\beta)^n \cdot b^N_n \right] \] \hspace{1cm} (3.25)

where

\[ b^N_n = \sum_{\Gamma \in \mathcal{G}^N_n} b^N_n(\Gamma) \] \hspace{1cm} (3.26)

and the contribution \( b^N_n(\Gamma) \) from the graph \( \Gamma \in \mathcal{G}^N_n \) is given by

\[ b^N_n(\Gamma) = \frac{1}{|D^R_N|} \int d^R_N(1) \cdots \int d^R_N(n) \prod_{i \in \mathcal{L}(\Gamma)} \left[ \exp -\frac{1}{\beta} V_N(l) - 1 \right] \prod_{i \in \mathcal{V}(\Gamma)} V_N(i) \] \hspace{1cm} (3.27)

where we have denoted the set of lines of a given \( \Gamma \in \mathcal{G}^N_n \) by \( \mathcal{L}(\Gamma) \), by \( \mathcal{V}(\Gamma) \) the set of vertices and taking \( l \in \Gamma \) we denote by \( l_0 \) the initial and resp. by \( l_e \) the endpoint of \( l \) and then we define \( V_N(l) \equiv V_N(l_0 | l_e) \).

From the positive definiteness of \( C_N \) it follows that \( C_N(0) - C_N(\mu) \geq 0 \) for any \( \mu \in \Omega_N \) and uniformly in \( N \). Therefore we can estimate the vertex function contribution to (3.26) by:

\[ | \prod_{i \in \mathcal{V}(\Gamma)} V_N(i) | \leq 1. \]

Our first result for the dipole free energy density in the thermodynamic limit \( N \to \infty \) is the following.

**Proposition 3.1** Assume that the hypotheses H2, H3 and H3γ are all valid. Then:

\[ \forall_n \forall \Gamma \in \mathcal{G}^N_n, \lim_{N \to \infty} | b^N_n(\Gamma) | < \infty \text{ for any } \beta \in R_+ \setminus \{0\}. \] \hspace{1cm} (3.28)

**Proof:**

Any connected, linear \( n \)-graph \( \Gamma \subset \mathcal{G}_n \) contains at least one spanning tree \( \text{st}(\Gamma) \). Let \( | \mathcal{L}(\Gamma) | = k+s \), where \( k = n-1 \) is the number of lines forming \( \text{st}(\Gamma) \) and \( s = | \mathcal{L}(\Gamma) | - n + 1 \) is the number of lines in \( \Gamma\setminus \text{st}(\Gamma) \). The contribution coming from the line \( l \notin \text{st}(\Gamma) \) can be estimated by a ”sup argument”:

\[ \sup_l | \exp[\frac{1}{\beta} V_N(l)] - 1 | \leq 4\beta^{-1} C^* | \alpha_{l_0} - \alpha_{l_e} | \exp[\beta^{-1} 4\alpha_{l_0} \alpha_{l_e} C^*] \] \hspace{1cm} (3.29)
where
\[ C^* \equiv \sup_N (\sup_\mu \| C_N(\mu) \|) \quad (3.30) \]

Setting
\[ \alpha^* \equiv \sup_{\lambda \in 0_R} \sup \{|\alpha| | \alpha \in \text{supp} d\mu\} \quad (3.31) \]

it follows
\[ |b_n(\Gamma)| \leq E(\beta)^s b_n(\mid s\Gamma\mid) \quad (3.32) \]

where
\[ E = 4\beta^{-1}C^*\alpha^2 \exp[\beta^{-1}4\alpha^2C^*] \quad (3.33) \]

and
\[ b_n(\mid s\Gamma\mid) = \frac{1}{D_N(1)} \int d_R N(1) \mid (1, \ldots, n) \mid \prod_{i=1}^{n-1} \mid \exp\left[-\frac{1}{\beta}V(d(i) | d(i + 1))\right] - 1 \mid. \quad (3.34) \]

Proceeding further we obtain
\[ |b_n(\mid s\Gamma\mid)| \leq \frac{1}{D_N(1)}E^{(n-1)} \int |d_R N(1, \ldots, n)| \prod_{i=1}^{n-1} V_N(d(i) | d(i + 1)|, \quad (3.35) \]

where now
\[ E' = \exp\left[\frac{4}{\beta}\alpha^2C^*\right]. \quad (3.36) \]

Let \( T_\rho \) be a translation by \( \rho \in \Omega_N \). Observing that the equality \( T_\rho V_N(\lambda, \mu, \alpha) \equiv V_N(\lambda + \rho, \mu + \rho, \alpha) = V_N(\lambda | \mu) \) holds, we can estimate
\[ \lim_{N \to \infty} \frac{1}{D_N(1)} \int |d_R N(1, \ldots, n)| \prod_{i=1}^{n-1} V_N(d(i) | d(i + 1)| \quad (3.37) \]

where
\[ \leq O(\beta) \sum_{\lambda_1 \in 0_R} \sum_{\lambda_2, \mu_2 \in \Omega_\infty} \sum_{\lambda_n, \mu_n} \sum_{|\lambda_2 - \mu_2| \leq R, |\lambda_n - \mu_n| \leq R} \int |d(\mu_\lambda - \mu_\lambda_1)| (\alpha_1) \int |d(\mu_\lambda_2 - \mu_\lambda_2)| (\alpha_2) \ldots \int |d(\mu_n - \mu_n)| (\alpha_n) \]

\[ \leq O'\left(\frac{1}{\beta}\right) \sum_{\lambda_1 \in 0_R} \sum_{|\lambda_2 - \mu_2| < R} \sum_{\lambda_2, \mu_2 \in \Omega_\infty} \{ \int |d(\mu_\lambda)| (\alpha_1) \int |d(\mu_\lambda_2 - \mu_\lambda_2)| (\alpha_2) V_\infty(0, \lambda_1, \alpha_1 | \alpha_2, \mu_2, \alpha_2) \}^{n-1} \]
where $O(\frac{1}{\beta})$ and $O'(\frac{1}{\beta})$ are numerical constants depending possibly of $R$ but not of $N$. We finish the proof if we show

$$\sum_{\lambda_1 \in \partial R} \sum_{\lambda_2, \mu_2 \in \Omega_\infty} \int d \mu \lambda_1 | (\gamma_1) d | \mu \lambda_2 - \mu_2 | (\gamma_2) |$$

(3.38)

This amounts to study the decay properties of $V_\infty(0, \lambda_1 | \lambda_2, \mu_2) = C_\infty(\lambda_2) - C_\infty(\mu_2) + C_\infty(\lambda_1 - \mu_2) - C_\infty(\lambda_1 - \lambda_2)$ as $| \lambda_2 | \uparrow \infty$. Let us define

$$\tilde{C}_\mu(\lambda) = C_\infty(\lambda) - C_\infty(\lambda - \mu).$$

(3.39)

Taking the Fourier transform of (3.40), using (2.21) and that $C_\infty(\lambda) = C_\infty(-\lambda)$ we obtain

$$\hat{\tilde{C}}_\mu(p) = (1 - \frac{1}{2} \cos p\mu)(A_\infty(0) - A_\infty(p))^{-1}.$$ (3.40)

From the hypothesis (H2$\beta$) it follows that $\hat{\tilde{C}}_\mu(p)$ stays bounded as $p \to 0$ whenever $\mu \neq 0$. Therefore by the Fourier-Tauberian theorem it follows that $\tilde{C}_\mu(\lambda)$ has to decay at least as $| \lambda |^{-3}$ as $| \lambda | \uparrow \infty$. Therefore taking $\mu' \neq 0$, we conclude that the function $\tilde{C}_{\infty, \mu}(\lambda) = \tilde{C}_\mu(\lambda) - \tilde{C}_\mu(\lambda - \mu')$ has to decay at least as fast as $| \lambda |^{-4}$ as $| \lambda | \uparrow \infty$ which is integrable over $R^3$. Let us apply this information to the problem (3.39). Using the definitions of $\tilde{C}_\infty$ and $\tilde{C}_{\infty, \mu}$

$$\sum_{\mu_1 \in \partial R} \sum_{\mu_2, \lambda_2 \in \Omega_\infty} \sum_{\alpha_1, \alpha_2} | V_\infty(0, \lambda_1 | \lambda_2, \mu_2, \alpha_2) |$$

(3.41)

$$\leq | \alpha_1 | \cdot | \alpha_2 | \cdot \sum_{\mu_1} \sum_{\mu_2, \lambda_2 \in \Omega_\infty} | \tilde{C}_{\infty, \mu_1}(\lambda_2) - \tilde{C}_{\infty, \mu_1}(\mu_2) |$$

$$\leq | \alpha_1 | \cdot | \alpha_2 | \cdot O''(1) \cdot \sum_{\lambda_2 \in \Omega_\infty} | \tilde{C}_{\infty, \mu}(\lambda_2) | < \infty$$

for some $\mu \neq 0$. \hfill \square

**Remark**

The above Prop. 3.1 can also be proven, essentially by the same method, replacing assumption H3$\gamma$ by H3$\beta$.

Let us define the virial coefficients $b^n_\infty(\Gamma)$ and the limit $N \uparrow \infty$ as the limit for $N \uparrow \infty$ of $b^n_N(\Gamma)$ as given by (3.28). Moreover by the translational invariance we impose the
restriction on \( \Gamma \) that at least one of its vertex has to be located at some \((0, \lambda)\) where \( \lambda \in O_R \). That the limit \( \lim_{N \to \infty} b^N(\Gamma) \) exists follows from the simple observation that for a fixed \( \Gamma \), the sequence \((b^N(\Gamma))_N\) is a Cauchy sequence in \( N \).

Let us remark that the limiting virial coefficient

\[
b^\infty(\Gamma) = \sum_{\mu_1 \in O_R} \int d\mu_1(\alpha_1) \int d^R(2, \ldots, n) \prod_{l \in \mathcal{L}(\Gamma)} \left[ \exp\left(-\frac{1}{\beta} V_\infty(l) - 1\right) \right] \times \prod_{i \in V(\Gamma)} V(i) \tag{3.42}
\]

are analytic functions in \( \frac{1}{\beta} \) for \( \beta \neq 0 \) and moreover \( \lim_{\beta \to \infty} b^\infty(\Gamma) = 0 \). From the Taylor expansion it follows that:

\[
\frac{d^M b^\infty(\Gamma)}{d\left(-\frac{1}{\beta}\right)^M} = \sum_{k_1, \ldots, k_{|\mathcal{L}(\Gamma)|} \geq 0} \sum_{r_1, \ldots, r_{|V(\Gamma)|} \geq 0} \frac{(-\frac{1}{\beta})^{\sum_{i=1}^{\mathcal{L}(\Gamma)} k_i + \sum_{j=1}^{|V(\Gamma)|} r_j}}{\prod_{i=1}^{\mathcal{L}(\Gamma)} k_i! \prod_{j=1}^{|V(\Gamma)|} r_j!} \tag{3.43}
\]

\[
\sum_{\mu_1 \in O_R} \int d\mu_1(\alpha_1) \int d^R(2, \ldots, n) \prod_{l \in \mathcal{L}(\Gamma)} V_\infty(l)^{k_l} \prod_{j=1}^{|V(\Gamma)|} V_\infty(j)^{r_j} \cdot \prod_{i \in V(\Gamma)} \left[ \exp\left(-\frac{1}{\beta} V_\infty(l) - (1 - \theta(k_l))\right) \right] \prod_{i \in V(\Gamma)} V(i)
\]

from which it follows that also

\[
\lim_{\beta \to \infty} \frac{d^M b^\infty(\Gamma)}{d\left(-\frac{1}{\beta}\right)^M} = 0 \quad (3.44)
\]

Since the total number of \( n \)-graphs \( \Gamma \) restricted as above is finite, we conclude that the virial coefficients \( b^\infty \) are analytic functions of \( \beta \) for \( \beta \neq 0 \) and moreover \( \lim_{\beta \to \infty} b^\infty(\beta) = 0 \) and also

\[
\lim_{\beta \to \infty} \frac{d^M b^\infty(\beta)}{d\left(-\frac{1}{\beta}\right)^M} = 0
\]
for any value of $M$.

A very convenient way to describe the virial coefficients in the limit $N \to \infty$ has been given by Brydges and Federbush [24]. We adopt their method to the case of the dipole systems to give the linked cluster expansion for $p_\infty(\beta)$. Towards this goal let us denote by $\Gamma_n$ the set of tree functions $\eta$, defined on the set $\{1, ..., n\}$, i.e., $\eta \in \Gamma_n \iff \eta : \{1, ..., n\} \to \{1, ..., n\}$ and $\eta(i) \leq i$ for any $i$. Denote by $(s)_{n-1} = (s_1, ..., s_{n-1}) \in [0, 1]^{\otimes n-1}$ a sequence of interpolating arguments and define corresponding interpolating energies by the following inductive process

\begin{equation}
\mathcal{E}_\infty((\lambda, \mu, \alpha)_n) \equiv \mathcal{E}_\infty((\lambda, \mu, \alpha)_n),
\end{equation}

\begin{equation}
\mathcal{E}_{\infty,i}(\lambda_1, \mu_1, \alpha_1) \equiv (1 - s_i)\mathcal{E}_\infty((\lambda, \mu, \alpha)_n | (\lambda_i, \mu_i, \alpha_i)) + s_i\mathcal{E}_{\infty,i-1}(\mathcal{E}_\infty((\lambda_1, \mu_1, \alpha_1)),
\end{equation}

\begin{equation}
\mathcal{E}_{\infty,n-1}(\lambda, \mu, \alpha)_n) \equiv \mathcal{E}^n_{\infty}((s)_{n-1}).
\end{equation}

Define a function $f(\eta, (s)_{n-1})$ by

\begin{equation}
\begin{cases}
  f(\eta, (s)_{n-1}) = \prod_{i=2}^{n-1} s_{i-1}s_{i-2}...s_{\eta(i)}, & \text{for } n \geq 2 \\
  f(\eta, s_1) = 1
\end{cases}
\end{equation}

where $s_{i-1}...s_{\eta(i)}$ is 1 if $\eta(i) = 1$. The n-th virial coefficient $b_n^\infty$ can be written in the following compact form

\begin{equation}
b_n^\infty(\beta) = \frac{1}{(-\beta)^{n-1}n} \sum_{\eta \in \Gamma_n} \int d(s)_{n-1} \int dR(\lambda, \mu, \alpha)_N \int d\mathcal{E}(d(i + 1)) | d(\eta(i)) \exp[\frac{1}{\beta} \mathcal{E}^n_{\infty}((s)_{n-1})]
\end{equation}

where

\begin{equation}
\int dR(\lambda, \mu, \alpha)_N = \sum_{\mu_1 \in \Omega_\infty} \int d\mu_1(\alpha_1) \sum_{\lambda_2, \mu_2 \in \Omega_\infty} | \lambda_2 - \mu_2 | \leq R
\end{equation}

The following estimate is well known (see [24])

\begin{equation}
\sum_{\eta \in \Gamma_n} \int d(s)_{n-1} f(\eta, (s)_{n-1}) \leq e^{n-1}
\end{equation}

The induction steps defined in (3.46) involve the convex sums of energies only, therefore the positive definiteness of the intermediate and final energy function is preserved in this process. This observation and estimate (3.50) lead to the following bound on the n-th virial coefficient

\begin{equation}
| b_n^\infty | \leq \frac{1}{| \beta |^{n-1} n} \parallel V_\infty \parallel_{1}^{n-1}
\end{equation}
where

\[ \| V_\infty \|_1 \equiv 0_R \sup_{\lambda \in R} (\int d | \mu_\lambda | (\alpha) | \alpha |) \]  

(3.51)

\[ \cdot \sup_{\lambda \in R} \left( \sum_{\lambda', \mu' \in \Omega_\infty} \int d | \mu_{\lambda' - \mu'} | (\alpha') | \alpha' | \| V_\infty(0, \lambda | \lambda', \mu') \| \right) \mid \lambda' - \mu' \leq R \]

where

\[ \tilde{V}_\infty(\lambda, \mu | \lambda', \mu') = C_\infty(\lambda - \lambda') + C_\infty(\mu - \mu') - C_\infty(\lambda - \mu') - C_\infty(\mu - \lambda'). \]  

(3.52)

In this way we have proved:

**Proposition 3.2** Assume hypotheses H2, H3 and H3\(\gamma\) are satisfied and moreover that \(\| V_\infty \|_1 < e^{-1}\), then the virial expansion

\[ P_\infty(\beta) = (-\beta) \cdot \sum_{n \geq 1} \frac{1}{n!} (s)_{n-1} \int d(s)_{n-1} \int d_R(\lambda, \mu, \alpha) \sum_{\eta \in T_n} f(\eta, (s)_{n-1}) \cdot \prod_{i=1}^{n-1} \mathcal{E}_\infty(d(i + 1) | d(\eta(i)) \exp[-\frac{1}{\beta} \mathcal{E}_\infty((s)_{n-1})] \right) \]

is absolutely convergent for any \(\beta \in C\) such that Re\(\beta > 0\).

**Remark**

Define the Borel transform \(\tilde{P}_\beta(\zeta)\) generating function for the virial coefficients by

\[ \tilde{P}_\beta(\xi) = \sum_{n \geq 1} \frac{(-\beta)^n \zeta^n b_\infty^n(\beta)}{n!} \]  

(3.54)

From the estimate (3.50) it follows that \(\tilde{P}_\beta(\zeta)\) is an entire analytic function on \(C\) in \(\zeta\), for any \(\beta \in R^+ \setminus \{0\}\). Therefore applying the inverse Borel transform to \(\tilde{P}_\beta\) we obtain a function \(P_\beta(z) = (B^{-1} \tilde{P}_\beta B^{-1})(z)\) for which an expansion in powers of \(z\) coincides with the virial expansion (3.54) for \(z = 1\) and moreover the expansion is a Borel summable as \(\beta \downarrow 0\):

\[ P_\beta(z) |_{z=1} = \sum_{n \geq 1} \frac{-(\beta)^n b_\infty^n(\beta)}{n!} + 0_N(\beta^{N+1}) \]  

(3.55)

with \(|0_N(\beta^{n+1})| \leq |C_N | \beta |^{N+1}\) for some constant \(C_N > 0\).

**Remark**

The Borel summability of the high-temperature expansion in the classical statistical mechanics has been studied in [26]. To prove Borel summability of the corresponding low
temperature expansion (3.54) one needs to expand the corresponding Mayer kernels in powers of $\beta^{-1}$ and then reformulate the whole expansion (3.54) in powers of $\beta^{-1}$.

### 3.3 The associated infinite volume Gibbs states.

In this section we shall construct the infinite volume Gibbs states describing dipole systems fulfilling all hypotheses H0 - H3 above. It is well known that the corresponding Gibbs states are determined by their correlation functions, see e.g. [22]. Therefore we concentrate on them in the following.

The finite volume correlation functions are given by:

$$\rho_N((\lambda, \mu, \alpha)_n) = (-\beta)^n E_N^\beta (\prod_{j=1}^n \exp[i\beta^{-1/2} \alpha_j (y_{\lambda_j} - y_{\mu_j})]) \quad (3.56)$$

where the expectation denoted as $E_N^\beta$ is defined as

$$E_N^\beta(-) = \frac{E^0_N(- \exp[-\beta R(\Omega_N \mid \{\beta^{-1/2} y_\lambda\}_{\lambda \in \Omega_N})])}{E^0_N(\exp[-\beta R(\Omega_N \mid \{\beta^{-1/2} y_\lambda\}_{\lambda \in \Omega_N})])} \quad (3.57)$$

To be more general we consider also the possible influence of the external dipole configurations on the thermodynamic limits of the corresponding Gibbs states. Towards this goal, let us consider a generic point $\omega \in (\Omega_\infty \times \Omega_\infty \times R^3)^\infty = \mathcal{D}_\rho(\infty)$, where $\mathcal{D}_\rho(\infty)$ is defined as a configuration of dipoles such that to every point $(\lambda, \mu) \in \Omega_\infty \times \Omega_\infty$ there is inserted at most $\rho$ dipoles with $\rho$ is some integer. It follows from the finite length dipole approximation that for every $\omega \in \mathcal{D}_\rho(\infty)$ there is only a finite number of dipoles that can share the same end point $\lambda \in \Omega_\infty$ and which contribute to the total energy in a nontrivial way.

The restriction of a given dipole configuration $\omega \in \Omega_\rho(\infty)$ to the set $(\Omega_\infty \times \Omega_\infty \times R^3)\setminus \{\Omega_N \times \Omega_N \times R\} \equiv \Sigma^C_N$ will be denoted by $\omega(N^C)$. The associated, finite volume, conditional Gibbs states are described by their conditional correlation functions $\rho_N^\omega$ which are defined for $\omega \in \Omega_\rho(\infty)$ by

$$\rho_N^\omega((\alpha, \lambda, \mu)_n) = (-\beta)^n \cdot E^0_\infty \left( \prod_{j=1}^n \exp[i\beta^{-1/2} \alpha_j (y_{\lambda_j} - y_{\mu_j})] \right) \cdot \exp -\beta \mathcal{R}(\Omega_N \mid \cdot) \cdot \exp -\beta \mathcal{F}_N(\omega(N^C)) \quad , \quad (3.58)$$

where

$$\mathcal{F}_N(\omega(N^C)) \equiv \sum_{(\lambda', \mu') \in \Sigma^C_N} \mathcal{R}(\lambda' - \mu' \mid y_{\lambda'} - y_{\mu'}) \quad (3.59)$$

gives the energy of a given configuration of dipoles $(\lambda, \mu, \alpha)_n$ inside $\Lambda_N$ with an external configuration $\omega(N^C)$ realizing a particular boundary condition. Due to the decay properties of $V_\infty$ and the assumption $\omega \in \mathcal{D}_\rho(\infty)$, the energy in (3.59) is finite.
The conditional partition function $Z_{N}^\omega$ used in (3.59) is given by the formula:

$$Z_{N}^\omega = \frac{E_{\infty}^0(e^{-\beta R(\Omega_N|\cdot)} e^{-\beta F_N(\omega(N_C))})}{E_{\infty}^0(e^{-\beta F_N(\omega(N_C))})}$$

(3.60)

Performing the following, (complex) shift transformation

$$y_\lambda - y_\mu \to y_\lambda - iC_\infty(y_\lambda - y_{\lambda_1}) - y_\mu - iC_\infty(y_\mu - y_{\mu_1})$$

(3.61)

in formula (3.59) and respectively

$$y_\lambda - y_\mu \to y_\lambda - iC_N(y_\lambda - y_{\lambda_1}) - y_\mu - iC_N(\mu - \mu_1)$$

(3.62)

in the formula (3.57) and calculating the corresponding Radon-Nikodym derivatives we obtain the following identities

$$\rho_N^\omega((\alpha, \lambda, \mu)_n) = (-\beta)^n \exp[\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))]
\cdot E_{N}^0(\prod_{j=2}^{n} e^{i\beta^2 \omega_j(y_{\lambda_j} - y_{\mu_j})} e^{-\beta R(\Omega_N|e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))})}
\exp - \beta F_N(\omega(N_C)|e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))}) - 1),$$

(3.63)

where

$$\mathcal{F}_N(\omega(N_C)|e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))} - 1) = \sum_{\lambda, \mu \in \Sigma_N^C \mid |\lambda - \mu| \leq R} \int d\gamma(\alpha'_\lambda - \mu) e^{i\lambda \cdot \gamma (\frac{y'_{\lambda} - y'}{\sqrt{\beta}})} (e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))} - 1)$$

and

$$\rho_N((\alpha, \lambda, \mu)_n) = (-\beta)^n \exp[\beta^{-1}\mathcal{E}_N(d(1)|\omega(N_C))]
\cdot E_{\infty}^0(\prod_{j=2}^{n} e^{i\beta^2 \omega_j(y_{\lambda_j} - y_{\mu_j})} e^{-\beta R(\Omega_N|e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))})}
\exp - \beta R(\Omega_N|e^{-\beta^{-1}\mathcal{E}_\infty(d(1)|\omega(N_C))}) - 1))$$

(3.64)

where

$$\mathcal{R}(\Omega_N|e^{-\beta^{-1}\mathcal{E}_N(d(1)|\omega(N_C))} - 1) \equiv \sum_{\lambda, \mu \in \Omega_N \mid |\lambda - \mu| \leq R} \int d\mu(\alpha_{\lambda - \mu} \cdot e^{i\lambda \cdot \gamma (\frac{y'_{\lambda} - y'}{\sqrt{\beta}})} (e^{-\beta^{-1}\mathcal{E}_N(d(1)|\omega(N_C))} - 1)$$

in which, after an expansion, we recognize the well known Kirkwood-Salzburg identities, see e.g. [22]. Using the method of a dual pair of Banach spaces as explained in [25], a large region of admissible $\beta$ will be determined in which the rigorous comparison analysis of (3.64) with (3.65) is possible.

For any $\xi > 0$ introduce a Banach space $E_{\xi}$ consisting of all sequences of functions $(f_n((\lambda, \mu, \alpha)_n)_{n=1,2,...})$ such that for any $n$, any $\lambda, \mu \in \Omega_{\infty}$ the functions $f_{\lambda,\mu}((\alpha)_n) \equiv$
\(f_n((\lambda, \mu, \alpha)_n)\) are measurable and such that the norm \(\| (f_n)_n \|_\xi = \sup_n \xi^{-n} \text{ess sup}(\lambda, \mu, \alpha)_n \mid f_n((\lambda, \mu, \alpha)_n)\) is finite. Several bounded linear operators will be defined to act in the space \(E_\xi\). The infinite volume Kirkwood-Salsburg operator \(K_\infty(\beta)\) is defined by

\[
(K_\infty((f_m)_m)_n((\lambda, \mu, \alpha)_n) \equiv \exp[-\frac{1}{\beta} \mathcal{E}_\infty((\lambda_1, \mu_1, \alpha_1) \mid (\lambda, \mu, \alpha)_n) \cdot \sum_{m \geq 0} \frac{1}{m!} \int d_{\infty}^R(\lambda', \mu', \alpha')_m \prod_{i=1}^{m} (\exp[-\frac{1}{\beta} \mathcal{E}_\infty((\lambda_1, \mu_1, \alpha_1) \mid (\lambda'_i, \mu'_i, \alpha'_i)) - 1]) \cdot f_{n+m-1}((\lambda, \mu, \alpha)_{n-1}^*, (\lambda', \mu', \alpha')_m)\]

where

\[(\lambda, \mu, \alpha)_{n-1}^* \equiv ((\lambda_2, \mu_2, \alpha_2), \ldots, (\lambda_n, \mu_n, \alpha_n)). \quad (3.66)\]

The finite volume, unconditional Kirkwood-Salsburg operator \(K_N\) is defined by:

\[
(K_N((f_m)_m)_n((\lambda, \mu, \alpha)_n) \equiv \exp[-\frac{1}{\beta} \mathcal{E}_N((\lambda_1, \mu_1, \alpha_1) \mid (\lambda, \mu, \alpha)_n) \cdot \sum_{m \geq 0} \frac{1}{m!} \int d_N^R(\lambda', \mu', \alpha')_m \prod_{i=1}^{m} (\exp[-\frac{1}{\beta} \mathcal{E}_N((\lambda_1, \mu_1, \alpha_1) \mid (\lambda'_i, \mu'_i, \alpha'_i)) - 1]) \cdot f_{n+m-1}((\lambda, \mu, \alpha)_{n-1}^*, (\lambda', \mu', \alpha')_m)\]

The energy factor operators are defined by:

\[
E_N^\infty((f_m)_m)_n((\lambda, \mu, \alpha)_n) \equiv \chi_N((\lambda, \mu)_n) \exp[-\frac{1}{\beta} \mathcal{E}_\infty((\lambda_1, \mu_1, \alpha_1) \mid \omega(N^c))] \\
\cdot (E_N \cdot f)_n((\lambda, \mu, \alpha)_n) \quad (3.68)
\]

where

\[
\chi_N((\lambda, \mu)_n) \equiv \begin{cases} 1 & (\lambda_i, \mu_i) \in \Omega_N \times \Omega_N \text{ for all } i \\ 0 & \text{otherwise} \end{cases} \quad (3.69)
\]

\[
E_N^N((f_m)_m)_n((\lambda, \mu, \alpha)_n) = \chi_N((\lambda, \mu)_n) \exp[-\frac{1}{\beta} \mathcal{E}_N((\lambda_1, \mu_1, \alpha_1) \mid (\lambda, \mu, \alpha)_n)] \cdot f_n((\lambda, \mu, \alpha)_n) \quad (3.70)
\]

\[
E_N((f_m)_m)_n((\lambda, \mu, \alpha)_n) = \chi_N((\lambda, \mu)_n) \exp[-\frac{1}{\beta} \mathcal{E}_\infty((\lambda_1, \mu_1, \alpha_1) \mid (\lambda, \mu, \alpha)_n)] \cdot f_n((\lambda, \mu, \alpha)_n) \quad (3.71)
\]

The projections \(\Pi_N\) are defined by

\[
\Pi_N((f_m)_m)_n((\lambda, \mu)_n) = \prod_{i=1}^{n} \chi_N((\lambda_i, \mu_i)) \cdot f_n((\lambda, \mu)_n) \quad (3.72)
\]
The finite volume conditional Kirkwood-Salsburg operator $K^\omega_N$ is defined as follows:

\[ K^\omega_N = E^\omega_N \cdot K_\infty \cdot \Pi_N. \] (3.73)

For further use we also define the operator $\tilde{K}_\infty$ through the relation

\[ K_\infty = E_N \cdot \tilde{K}_\infty. \] (3.74)

Also the finite volume version of $\tilde{K}_\infty$ is defined by

\[ K_N = E^N_N \cdot \tilde{K}_N. \] (3.75)

From the positive definiteness of $V_\infty$ it follows that we can split the set \((\Omega_\infty \times \Omega_\infty \times \mathbb{R}^3)^\otimes n\) as \(\bigcup_{j=1}^{n} \sum_j \), where \(\sum_j = \{(\lambda, \mu, \alpha)_n \in (\Omega_\infty \times \Omega_\infty \times \mathbb{R}^3)^\otimes n \mid \sum_{i \neq j} V_\infty(\lambda_i, \mu_i, \alpha_i \mid \lambda_j, \mu_j, \alpha_j) \geq -2 \sum_{i=1}^{n} \alpha_i^2 (C_N(0) - C_N(\lambda_i - \mu_i))\} \). Let then \(\eta_j^n\) denote the characteristic function of \(\sum_j \) and let \(\theta_j^n = \eta_j^n / \sum_{j=1}^{n} \eta_j^n\). Let \(S^n_k\) be defined on functions of \(n\)-variables \((\lambda, \mu, \alpha)_n\) as the circular permutations of \(k\)-steps on the complex arguments \((\lambda, \mu, \alpha)_n\) of these functions.

Then the index juggling operator \(J_\infty\) is defined as

\[ J_\infty((f_m)_m)_n((\lambda, \mu, \alpha)_n) = \sum_{k=1}^{n} S^n_k((\theta_j^n((\lambda, \mu, \alpha)_n) f_n((\lambda, \mu, \alpha)_n) \] (3.76)

In a similar way we define the Ruelle index juggling operator \(J_N\) which selects a labelling of coordinates in such a way that \(E_N((\lambda_1, \mu_1, \alpha_1) \mid (\lambda_n, \mu_n, \alpha_n)) \geq 0\).

Finally the following vectors are defined

\[ \alpha^\omega_N = (\exp [-\frac{1}{\beta} E_\infty((\lambda_1, \mu_1, \alpha_1) \mid (\lambda, \mu, \alpha)_1 \cup \omega(N^c)), 0, ...]) \] (3.77)

\[ \alpha_N = (\exp [-\frac{1}{\beta} E_N((\lambda_1, \mu_1, \alpha_1) \mid (\lambda_1, \mu_1, \alpha_1)), 0, ...]). \] (3.78)

With this notation the equalities (3.64) and (3.65) can be rewritten in the following way

\[ ((\rho^\omega_N)_n) = (-\beta)(\Pi_N \cdot J_\infty K^\omega_N \cdot \Pi_N)((\rho^\omega_N)_n) + (-\beta)\Pi_N \alpha^\omega_N \] (3.79)

and respectively

\[ ((\rho_N)_n) = -\beta(\Pi_N \cdot J_N \cdot K_N \Pi_N)((\rho_N)_n) - \beta\Pi_N \alpha_N. \] (3.80)

We expect that the infinite volume limits \(((\rho_\infty)_n)\) of \(((\rho_N)_n)\) should fulfill the following, infinite-volume Kirkwood-Salsburg identities:

\[ ((\rho_\infty)_n) = -\beta J_\infty K_\infty((\rho_\infty)_n) - \beta \alpha_\infty^\phi \] (3.81)
and in fact we will show this for the infinite volume limits of the conditional correlation functions, providing they exist.

The rigorous, comparison analysis of the identities (3.80), (3.81) and (3.82), based on the use of methods of the dual pair of Banach spaces as explained in [25] will be presented below. The conclusions obtained in this way seem to be much richer then the contraction map principle (see, i.e., [22]) ordinary used for such an analysis.

It is necessary to introduce the additional (technical) hypothesis for making our analysis complete.

**Hypothesis 4**

(H4) There exists a number \( \xi_* \), possibly depending on \( \rho \) and \( R \) such that for any \( \xi > \xi_* \) the family \( (\rho_N^\xi((\lambda,\mu,\alpha)_n))_N \) is weakly \( \ast \) precompact in the space \( E_\xi \) for any \( \omega \in D_{\rho}(\infty) \).

Note that for the case \( \omega = \phi \) and for the correlation functions (3.57) H4 is fulfilled due to estimate (3.7) and the Banach-Aloglou theorem. For a general \( \omega \in D_{\rho}(\infty) \) the necessary estimates are still to be proved.

To formulate the main result of our analysis let us define \( \sigma_\xi(I_\infty K_\infty) \) the spectral set of the operator \( J_\infty K_\infty(\beta) \) in the corresponding space \( E_\xi \) (see below) and let us define the set \( H_\xi \) as:

\[
H_\xi \equiv \{ \beta \in C \mid \text{Re}\beta > 0; \ |\beta| < \xi \text{ and } (-\beta)^{-1} \notin \sigma_\xi(J_\infty K_\infty(\beta)) \}
\]  

(3.82)

**Theorem 3.3** Let us assume that the hypotheses H0-H3, H3\(\gamma \) and H4 are all valid.

Then there exists a number \( \xi_* \) (possibly depending of \( \rho \) and \( R \)) such that for any \( \beta \in H_{\xi_*} \) there exists a unique thermodynamic limit \( \rho_\infty^\beta \) of \( \rho_N^\xi((\lambda,\mu,\alpha)_n) \) which does not depend in particular on \( \omega \in D_{\rho}(\infty) \) and is equal to the thermodynamic limit \( \rho_\infty \) of \( (\rho_N((\lambda,\mu,\alpha)_n)) \) which also exists as a unique limit as \( N \uparrow \infty \). The limits should be understood as limits in the locally uniform, componentwise topology of the space \( E_\xi \). The limiting correlation functions \( \rho_\infty \) depend analytically on \( \beta \), provided \( \beta \in H_{\xi_*} \), they are translationally invariant and posses a cluster decomposition property with respect to the translations of \( \Omega_\infty \times \Omega_\infty \).

Before passing to the proof of this theorem let us note some simple consequences which seem to be relevant for the discussion of the problem of the convergence of the linked cluster expansion worked out in this section. For this goal let us define

\[
C(\beta) \equiv \sup_{\lambda \in O_R} (\sup\{|\alpha|; \alpha \in \text{supp} d\mu_\lambda\} \cdot |O_R|)
\]

(3.83)
and
\[
C'(\beta) \equiv \sup_N \sup_{\lambda \in O_R} (| \sup \{| \alpha | | \alpha \in \text{supp } d\mu_\lambda \} \cdot | O_R |)
\]
(3.84)

\[
\left( \int d^R \sup \{ | (\lambda', \mu', \mu') | | \exp \left[ -\frac{1}{\beta} \mathcal{E}_N ((0, \lambda, \alpha) \cdot (\lambda', \mu', \alpha')) - 1 \right] \} \right).
\]

It follows from our hypothesis that these quantities are finite (see the proof of Prop. 3.1). Let us also define

\[
H_{\xi}^C \equiv \{ \beta \in C \mid \text{Re} \beta > 0 \text{ and } | \beta | \leq \min \{ | \xi |, C^{-1}(\beta)e^{-1} < 1 \} \}
\]
(3.85)

and

\[
H_{\xi}^{C'} \equiv \{ \beta \in C \mid \text{Re} \beta > 0 \text{ and } | \beta | \leq \min \{ | \xi |, C'(\beta)e^{-1} < 1 \} \}.
\]
(3.86)

**Corollary 3.4** Let us assume that all the assumptions of Theorem 3-3 are fulfilled. Then

\[ H_{\xi}^C \subset H_{\xi}(\beta) \text{ and } H_{\xi}^{C'} \subset H_{\xi}(\beta), \]

therefore all conclusions of Theorem 3-3 are true for \( \beta \in H_{\xi} \) (respectively \( \beta \in H_{\xi}^{C'} \)).

**Proof:**

It is very easy to check that for \( \beta \in H_{\xi}^C \) the corresponding Kirkwood-Salsburg operator

\[-\beta I_{\infty}K_{\infty} \text{ is a contraction of the corresponding space } E_{\xi} \text{ and therefore } -\beta^{-1} \notin \sigma_\xi(J_{\infty}K_{\infty}).\]

The same argument applies for the corresponding Kirkwood-Salsburg operator \( J_{N}K_{N} \) as well. \( \square \)

Another corollary of Theorem 3-3 can be formulated as follows. Let us define the conditional, finite-volume free energy density \( p_N^\omega \) as:

\[
p_N^\omega = \frac{1}{| D_N(1) |} \ln Z_N^\omega
\]
(3.87)

Then

**Corollary 3.5** Assume that all hypotheses of Theorem 3-3 hold. Then for any \( \omega \in D_c(\infty) \) the unique thermodynamic limit \( p_\infty(\beta) = \lim_{N \uparrow \infty} p_N^\omega(\beta) = \lim_{N \uparrow \infty} p_N^\phi \) exists, provided \( \beta \in H_{\xi} \). Moreover the map \( H_{\xi} \ni \beta \rightarrow p_\infty(\beta) \) is analytic.

**Proof of Theorem 3.3:**

The Banach space \( E_{\xi} \) is the dual of the Banach space \( \ast E_{\xi} \) which is formed from all
sequences \((\psi_n((\lambda, \mu, \alpha)_n))\) of functions defined on \((\Omega_\infty \times \Omega_\infty \times \mathbb{R}^3)^n\) measurable in the charge coordinates \(\alpha\) and such they have a finite norm \(* \| \|_\xi \) given by:

\[
* \| (\psi_n)_n \|_\xi = \sum_{n \geq 0} \xi^n \int d^{R_\infty} |(\lambda, \mu, \alpha) | \| \psi_n((\lambda, \mu, \alpha)_n) | .
\]

(3.88)

Define in the space \(E_\xi\) (for suitable \(\xi\) to be chosen later on) the following linear operators

\[
(*\tilde{K}_\infty((\psi_m)_m))_n((\lambda, \mu, \alpha)_n) = \sum_{l=0}^n \frac{1}{l!} \int d^{R_\infty} (\lambda', \mu', \alpha')
\]

\[
\prod_{i=1}^l \left[ \exp\left( -\frac{1}{\beta} E^{\infty}((\lambda_i, \mu_i, \alpha_i) | (\lambda', \mu', \alpha')) \right) - 1 \right]
\]

\[
\psi_{n+1-l}((\lambda', \mu', \alpha'), (\lambda_{l+1}, \mu_{l+1}, \alpha_{l+1}), \ldots (\lambda_n, \mu_n, \alpha_n))
\]

and

\[
(*\tilde{K}_N((\psi_m)_m))_n((\lambda, \mu, \alpha)_n) = \sum_{l=0}^n \frac{1}{l!} \int d^{N} (\lambda', \mu', \alpha')
\]

\[
\prod_{i=1}^l \left[ \exp\left( -\frac{1}{\beta} E^{N}((\lambda_i, \mu_i, \alpha_i) | (\lambda', \mu', \alpha')) \right) - 1 \right]
\]

\[
\psi_{n-1-l}((\lambda', \mu', \alpha'), (\lambda_{l+1}, \mu_{l+1}, \alpha_{l+1}), \ldots (\lambda_n, \mu_n, \alpha_n)).
\]

Calculating the corresponding dual operators to the operators \(*\tilde{K}_\infty\) and \(*\tilde{K}_N\) we arrive at the following equalities

\[(*\tilde{K}_\infty)^* = \tilde{K}_\infty \quad \text{and} \quad (*\tilde{K}_N)^* = \tilde{K}_N.\]

(3.91)

From the estimates

\[\| \tilde{K}_\infty \|_\xi \leq \xi^{-1} \exp[\xi C(\beta)]\]

(3.92)

\[\| \tilde{K}_N \|_\xi \leq \xi^{-1} \exp[\xi C(\beta)]\]

(3.93)

the continuity of operators \(*\tilde{K}_\infty\) and \(*\tilde{K}_N\) in the space \(*E_\xi\) and for any \(\xi > 0\) follows.

Let us choose a value of \(\xi\) such that the family \((\rho_N^{\xi})_N \subset E_\xi\) is weakly-* precompact and let further \(\rho_N^{\xi}\) be any of the accumulation points. As a result of the fact that finite-component sequences of compactly supported functions in the space \(*E_\xi\) form a dense subspace and the local decay properties of \(E_\infty\) (respectively \(E_N\)) we easily see that:

\[*\Pi_N \cdot *K_\infty \cdot *E_\infty \cdot *J_N \cdot *\Pi_N \quad \text{strongly} \quad *K_\infty \cdot *J_\infty\]

(3.94)
and

\[ \Pi_N \cdot \ast K_N \cdot \ast J_N \cdot \ast \Pi_N \rightarrow \text{strongly} \ast K_{\infty} \cdot \ast J_{\infty} \]  

(3.95)

as \( N \uparrow \infty \) and where \( \ast \Pi_N, \ast E_N^\omega \) and \( \ast I_N, \ast I_N^\infty \) are the corresponding predual of the operators \( \Pi_N, E_N^\omega \) and \( J_N^\infty, J_N \) whose existence and form of action on the space \( \ast E_\xi \), can be easily determined from the very definitions (3.73), (3.69),(3.77) and remark after (3.77).

Taking into account that \( \alpha_N^\omega \rightarrow \alpha_\infty^\phi \) in the weak -* topology of \( E_\xi \) and the convergence (3.92) we conclude that any \( \rho_\infty^\omega \) must fulfill the identity:

\[ \rho_\infty^\omega = (-\beta)I_\infty K_\infty \rho_\infty^\omega - \beta \alpha_\infty^\phi. \]  

(3.96)

Therefore assuming that \( \beta \in H_\xi(\beta) \) we conclude for the existence of a unique thermodynamic limit \( \rho_\infty^\omega \) which does not depends of \( \omega \), provided \( \omega \in D_{\rho}(\infty) \) and moreover \( \rho_N^\omega \rightarrow \rho_\infty^\omega \) in the weak -* topology. The same reasoning applies to \( \rho_N \) as well with the conclusion that the corresponding thermodynamic limit \( \rho_\infty = \rho_\infty^\omega \). Standard application of the Mayer-Montroll identities (see i.e. [22], [26]) then improves the proven weak -* convergence \( \rho_N^\omega \rightarrow \rho_\infty^\omega \) to the locally uniform componentwise as stated in Theorem. The remaining assertions are easier and will not be proven here.

Effective applications of Theorem 3-3 amounts to the study of the spectral properties of the operator \( J_\infty K_\infty \) in the space \( E_\xi \). Using the ideas and methods of [27, 28] it can be proved that \( \sigma_\xi(\Pi(\Lambda)J_N K_N^\phi \Pi(\lambda)) \equiv \{ -\beta \in C \mid Z_N^f((-\beta)^{-1}) = 0 \} \). However the localisation and the flow of zeros of the partition function \( Z_N^f \) as \( N \uparrow \infty \) is outside the scope of the present paper. It is not known to the authors whether the region \( H(\beta) \) is close to the low temperature region.

It should be mentioned that in the physical literature the limit temperature \( T \uparrow \infty \) and \( Z \uparrow \infty \) has been studied before and is known as Vlasov limit in theory of plasma physics [29]. The Vlasov limiting region exactly corresponds to the low temperature behaviour of dipole systems studied by us. Whether one can extract from the Vlasow theory some relevant information to the dipole systems describing fluctuation from the crystalline ground states remains to be studied.
Chapter 4

Concluding remarks

In this section we shall clarify the meaning of the hypotheses that we stated in the course of our analysis and put our work in a certain perspective from which further possible developments and the meaning of the low temperature expansion introduced here become clearer.

First we shall discuss hypothesis $H3$. The Taylor remainder (2-41) can be written as follows

$$R_{\Omega N}(\lambda - \mu \mid \frac{y_\lambda - y_\mu}{\sqrt{\beta}}) = \int_0^1 dt \frac{(1-t^2)}{2!} [D^3V](\lambda + ty_\lambda - \mu - ty_\mu)(y_\lambda - y_\mu)^3$$  \hspace{1cm} (4.1)

Due to the geometry of $R^3$, even if $V$ has compact support the size of the fluctuations $y_\lambda$ can be arbitrary. The only restriction is that $\lambda + y_\lambda - \mu - y_\mu \in \text{supp } V$. This leads to the question whether the Taylor remainder (4.1) can be a bounded function in the variable $y_\lambda - y_\mu$. From the elementary estimate

$$|\lambda + y_\lambda - \mu - y_\mu| \geq ||\lambda - \mu| - |y_\lambda - y_\mu||$$

and the assumption that $V$ is central it follows that this can be realized. As an example let us take:

$$f_\varepsilon(x) = \begin{cases} \exp[-\frac{1}{|x|^2 + \varepsilon^2}] & \text{for } |x| < \varepsilon, \\ 0 & |x| \geq \varepsilon \end{cases}$$  \hspace{1cm} (4.2)

Then from (4.2) we obtain

$$|f_\varepsilon(\lambda - \mu + y_\lambda - y_\mu)| \leq \exp[-\frac{1}{\varepsilon^2 - ||\lambda - \mu| - |y_\lambda - y_\mu||^2}]$$

if $|\lambda - \mu + y_\lambda - y_\mu| \geq \varepsilon$ and $f_\varepsilon(\lambda - \mu + y_\lambda - y_\mu) = 0$ if $|\lambda - \mu + y_\lambda - y_\mu| \geq \varepsilon$. This forces an exponentially fast decay of $|f_\varepsilon(\lambda - \mu + y_\lambda - y_\mu)||y_\lambda - y_\mu|^3$ as $|y_\lambda - y_\mu| \uparrow \infty$ provided
\(\lambda, \mu\) are kept fixed.

The partition function (2.30) can be rewritten as:

\[
Z_{N}^{fl}(\beta) = Z_{N}^{bd}(\beta) \frac{Z_{N}^{fl}(\beta) Z_{N}^{d}(\beta)}{Z_{N}^{bd}(\beta) Z_{N}^{d}(\beta)} \tag{4.3}
\]

therefore the corresponding free energy density is

\[
p_{N}^{fl}(\beta) = \frac{1}{\beta |\Lambda_{N}|} \ln Z_{N}^{bd}(\beta) + \frac{1}{\beta |\Lambda_{N}|} \ln Z_{N}^{fl}(\beta) \times \frac{1}{\beta |\Lambda_{N}|} \ln Z_{N}^{d}(\beta) \tag{4.4}
\]

The results of section 3 enables us to control rigorously

\[
\lim_{N \to \infty} \frac{1}{\beta |\Lambda_{N}|} \ln Z_{N}^{bd}(\beta) \equiv p_{\infty}^{fl}(\beta) \tag{4.5}
\]

which we call small fluctuations contribution to \(\lim_{N \to \infty} p_{N}^{fl}(\beta) \equiv p_{\infty}^{fl}(\beta)\) provided it exists. It is reasonable to expect that

\[
\lim_{N \to \infty} \frac{1}{\beta |\Lambda_{N}|} \ln \frac{Z_{N}^{fl}(\beta)}{Z_{N}^{d}(\beta)} = 0 \tag{4.6}
\]

therefore the only (but highly nontrivial) problem to solve is to show (with some additional hypothesis on \([D^{2}V]\)) the existence of the limit

\[
\lim_{N \to \infty} \frac{1}{\beta |\Lambda_{N}|} \ln \frac{Z_{N}^{d}(\beta)}{Z_{N}^{bd}(\beta)} \equiv p_{\infty}^{fl}(\beta) \tag{4.7}
\]

This limit be called large fluctuations free energy density. The superstability like hypothesis on \([D^{2}V]\) can produce a probability like estimates that make the appearance of very large dipoles very unprobable and this might be sufficient for the proof of the existence of \(p_{\infty}^{fl}(\beta)\).

Let \(\mu^{\beta}\) be the corresponding canonical Gibbs ensemble measure for the corresponding real system of particles at inverse temperature \(\beta\) and with the density \(\rho\). Assume that the lattice \(\mathcal{L}\) is the ground state configuration. We will say that the local finite configuration \(\omega\) is an almost \(\mathcal{L}\)-crystalline configuration iff for sufficiently \(N_{\omega} > 0\) a map

\[
l_{\omega}^{\mathcal{L}} : \omega_{\Lambda}^{R^{3}}[\Lambda - N_{\omega}, N_{\omega}] \to \mathcal{L}\setminus \omega_{N}
\]

(where \(\omega_{\Lambda}\) is the restriction of \(\omega\) to the set \(\Lambda\)) defined by:

\[
l_{\omega}^{\mathcal{L}}(x_{i}) = l^{\omega}(i)
\]

where: \(l^{\omega}(i) = \lambda\) if there exists only one \(l \in \mathcal{L}\) such that \(|x_{i} - \lambda| = \min\{|x_{i} - \lambda| \mid \lambda' \in \mathcal{L}\}\) and if there are several such \(\lambda \in \mathcal{L}\) on which the minimum of \(|x_{i} - \lambda'| \mid \lambda' \in \mathcal{L}\) is achieved the \(\lambda\) is choosen to be the first of them in the natural lexicographic order given to \(\mathcal{L}\).
exists and is bijective.

A Borel subset \( \Xi \) of the space of all locally finite configurations is called uniformly \( \mathcal{L} \)-crystalline iff there exists \( N(\Xi) \equiv \sup_{\omega \in \Xi} N_\omega < \infty \). If we suppose that for sufficiently small \( \frac{1}{\beta} \) the Gibbs measure \( \mu^\beta \) is supported by some uniformly crystalline subset then of course the problem of large fluctuations will be overcomed by a suitable relabeling procedura. However at present only a very limited knowledge on the support properties of the corresponding Gibbs measures is available, which is not sufficient for solving this problem.

Now we turn to the discussion of H1. In [32,33] Katz and Duneau have showed that the set of smooth central potentials with compact support that leads to an energy function \( \mathcal{E}(\( (x)_n \)) \) possessing Morse function properties is residual in the space of \( C^\infty(\mathbb{R}^+, \mathbb{R}) \) functions equipped with the Whitney topology. Moreover they showed that the Morse character of \( \mathcal{E}(\( (x)_n \)) \) is precisely the necessary and sufficient condition for having variations of potentials which gives rise to a continuous trajectory of equilibria, preserving the crystalline symmetries of the starting equilibrium configurations. The abstract results of [32,33] substantiate our motivation for imposing Hypothesis 1 onto our scheme.

That the set of potentials for which H2 holds is large is expressed in the following proposition.

**Proposition 4.1** The set of potentials \( \Phi \in C^\infty(\mathbb{R}^+, \mathbb{R}) \) for which H2 is true, is an non-void open set in the Whitney topology.

It would of course be interesting to produce explicit examples satisfying all assumptions we made, in particular the uniformity in N involved in H1, H2.

Some preliminary results on this problem are contained in [21] and a more complete discussion of this problem is now in preparation [34].

Another important question concerns the stability of the crystalline symmetry in the low temperature region in the following sense. In the Pirogov-Sinai theory [35] powerful probabilistic arguments are worked out to show that the corresponding pure phases do not fluctuate much around the ground state configuration in the low temperature region (This is expressed as follows: The probability of the occurrence a large contour \( \Gamma \) with length \( |\Gamma| \) is less then \( \exp(-\beta |\Gamma|) \). It is an important problem to develop systematically methods which show that the typical configurations of a real system (in the thermodynamic limit) in low temperature thermal equilibrium do not fluctuate much around the corresponding crystalline ground state configuration. But an even more important and harder problem is
to introduce an equivalent notion of the Peierls stability condition of ‘small’ perturbations of the ground state which leads to stability of crystalline symmetry in the low temperature region for the corresponding Gibbs state.
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