Journal of Applied Mathematics and Physics, 2022, 10, 1762-1784
https://www.scirp.org/journal/jamp
ISSN Online: 2327-4379
ISSN Print: 2327-4352

A Cluster Expansion Free Method for Computing Higher Derivatives of the Free Energy and Estimating the Error between the Finite and Infinite Volume Free Energy

Assane Lo

University of Wollongong, Dubai and Wollongong, Australia
Email: assanelo@uowdubai.ac.ae

How to cite this paper: Lo, A. (2022) A Cluster Expansion Free Method for Computing Higher Derivatives of the Free Energy and Estimating the Error between the Finite and Infinite Volume Free Energy. *Journal of Applied Mathematics and Physics*, **10**, 1762-1784.
https://doi.org/10.4236/jamp.2022.105123

Received: April 18, 2022
Accepted: May 28, 2022
Published: May 31, 2022

Abstract

The theory of phase transitions is one of the branches of statistical physics in which smoothness and continuity play an important role. In fact, phase transitions are characterized mathematically by the degree of non-analyticity of the thermodynamic potentials associated with the given system. In this paper, we propose a method that is not based on cluster expansions for computing the higher derivatives of the free energy and estimating the error between the finite and infinite volume free energy in certain continuum gas models. Our approach is suitable for a direct proof of the analyticity of the pressure or free energy in certain models of Kac-type. The methods known up to now strongly rely on the validity of the cluster expansion. An extension of the method to classical lattice gas models is also discussed.

Keywords

Witten Laplacians, Analyticity, Free Energy, Kac-Models

1. Introduction

The estimation of the error between the infinite and finite volume limit of the free energy in the continuum gas case is generally obtained under the condition of validity of the cluster expansion on the Hamiltonian. See [1] [2] [3] [4] [5] and references therein. The cluster expansion is the main tool for implementing renormalization arguments in Statistical Physics. It provides a method for calculating the logarithm of the partition function. However, it is only valid under certain assumptions on the Hamiltonian. In Section 2, we will discuss a direct nonpertubative method for computing the higher derivatives of the free energy in certain high dimensional classical unbounded models of Kac-type. Our method will provide a new framework for investigating the analyticity of the pressure or free energy.

There are several different thermodynamic potentials that can be used to describe the behavior and stability of a statistical mechanical system at equilibrium depending on the type of constraints imposed on the system. For a system which is isolated, the internal energy will be a minimum for the equilibrium state. However, if we couple the system thermally, mechanically, or chemically, other thermodynamic potentials will be minimized at equilibrium. The energy which is stored and retrievable in the form of work is called the free energy. It is generally given by the logarithm of the partition function divided by the volume of the region Λ containing the system. When the system becomes large $\Lambda \uparrow \mathbb{R}^d$ or $\Lambda \uparrow \mathbb{Z}^d$, this limit will actually result in a thermodynamic function. It is well known that any singularities for these thermodynamic functions will correspond to a change of phase of the system [6] [7]. Thus, investigating this thermodynamic limit has led to a long-standing standing problem of computing the error terms between the finite and infinite volume of pressure or free energy. Satisfactory results have been obtained in some special cases where the validity of the cluster expansion is taken for granted [1] [2] [3] [4] [5]. In Section 3, we will propose a method for estimating the error between the infinite and finite volume limit of the free energy in the continuum gas case without using cluster expansions. We shall also point out a direction for extending the result to a wider class of lattice gas cases. Similar results were obtained in [8]. However, the authors considered a one dimensional lattice system of unbounded real valued spins with a quadratic finite range interaction. The extension of their result to higher dimensional more general interactions was mentioned as an open problem. Our method provides a new paradigm for solving this question.

2. On the Derivatives of the Free Energy

Recall that the most famous result on the analyticity of the pressure is the circle theorem of Lee and Yang [9]. The Lee-Yang theorem theorem and its variants depend on the ferromagnetic character of the interaction. There are various other way of proving the infinite differentiability or the analyticity of the free energy for (ferromagnetic and non ferromagnetic) systems at high temperatures, or at low temperatures, or at large external fields. Most of these take advantage of a sufficiently rapid decay of correlations and/or cluster expansion methods. Related references are Bricmont, Lebowitz and Pfister [10], Dobroshin [11], Dobroshin and Sholsman [12] [13], Duneau *et al.* [14] [15] [16], Glimm and Jaffe [17] [18], Israel [19], Kotecky and Preiss [20], Kunz [21], Lebowitz [22] [23], Malyshev [24], Malychev and Milnos [25] and Prakash [26], S. Ott [27]. We will discuss a new method based on a convolution formula for the derivatives of the pressure. The only known exact formula of the pressure was obtained by M. Kac and J.M. Luttinger [28]. Kac-Luttinger formula has a limit of validity and is a representation of the free energy in terms of irreducible distribution functions. Along the same line, our formula is based on the Helfer-Sjostrand representation of the covariance of two functions in terms of the Witten-Laplacians on one-forms [29] [30] [31]. Recall that for a given C^∞-function Φ, the written-Laplacians on 0 and 1 forms are respectively given by

$$\mathbf{W}_\Phi^{(0)} = \left(-\Delta + \frac{|\nabla\Phi|^2}{4} - \frac{\Delta\Phi}{2}\right) \tag{1}$$

and

$$\mathbf{W}_\Phi^{(1)} = -\Delta + \frac{|\nabla\Phi|^2}{4} - \frac{\Delta\Phi}{2} + \mathbf{Hess}\Phi \tag{2}$$

These operators were first introduced by Edward Witten [32] in 1982 in the context of Morse theory for the study of some topological invariants of compact Riemannian manifolds. In 1994, Bernard Helffer and Jöhannes Sjostrand [29] introduced two elliptic differential operators

$$A_\Phi^{(0)} := -\Delta + \nabla\Phi\cdot\nabla \tag{3}$$

and

$$A_\Phi^{(1)} := -\Delta + \nabla\Phi\cdot\nabla + \mathbf{Hess}\Phi \tag{4}$$

sometimes called Helffer-Sjostrand operators serving to get direct methods for the study of integrals and operators in high dimensions of the type that appear in Statistical Mechanics and Euclidean Field Theory. In 1996, Jöhannes Sjostrand [33] observed that these so called Helffer-Sjostrand operators are in fact equivalent to Witten's Laplacians. Since then, there has been significant advances in the use of these Laplacians for the study of the thermodynamic behavior of quantities related to the Gibbs measure $Z^{-1}\mathrm{e}^{-\Phi}\mathrm{d}\mathbf{x}$. Helffer and Sjostrand used the Witten-Laplacians to derive an exact formula for the covariance of two functions. This formula is in some sense a stronger version of the Brascamp-Lieb inequality [34]. The formula may be written as:

$$\mathbf{cov}(f,g) = \int \left(A_\Phi^{(1)^{-1}}\nabla f\cdot\nabla g\right)\mathrm{e}^{-\Phi(\mathbf{x})}\mathrm{d}\mathbf{x}. \tag{5}$$

To understand the idea behind the formula mentioned above, let us denote by $\langle f\rangle$ the mean value of f with respect to the measure $\mathrm{e}^{-\Phi(\mathbf{x})}\mathrm{d}\mathbf{x}$, the covariance of two functions f and g is defined by

$$\mathbf{cov}(f,g) = \left\langle \left(f-\langle f\rangle\right)\left(g-\langle g\rangle\right)\right\rangle. \tag{6}$$

If one wants to have an expression of the covariance in the form

$$\mathbf{cov}(f,g) = \langle \nabla g\cdot\mathbf{w}\rangle_{L^2\left(\mathbb{R}^n,\mathbb{R}^n;\mathrm{e}^{-\Phi}\mathrm{d}x\right)}, \tag{7}$$

for a suitable vector field $\mathbf{w}$, we get, after observing that $\nabla g = \nabla\left(g-\langle g\rangle\right)$,

$$\mathbf{cov}(f,g) = \int \left(g-\langle g\rangle\right)(\nabla\Phi-\nabla)\cdot\mathbf{w}\mathrm{e}^{-\Phi(x)}\mathrm{d}x. \tag{8}$$

This leads to the question of solving the equation

$$f - \langle f \rangle = (\nabla\Phi - \nabla)\cdot \mathbf{w}. \tag{9}$$

Now trying to solve this above equation with $\mathbf{w} = \nabla u$, we obtain the equation

$$\left.\begin{aligned} f - \langle f \rangle &= A_\Phi^{(0)} u \\ \langle u \rangle &= 0. \end{aligned}\right\} \tag{10}$$

Assuming for now the existence of a smooth solution, we get by differentiation of this above equation:

$$\nabla f = A_\Phi^{(1)} \nabla u \tag{11}$$

and the formula is now easy to see.

In [35], Marc Kac considered two dimensional bounded models whose Hamiltonians are of the form

$$H_{\Lambda,\gamma}\left(\sigma_\Lambda / \sigma_{\Lambda^c}\right) = -\frac{1}{2}\sum_{i,j\in\Lambda} J_\gamma(i,j)\sigma_i\sigma_j - \sum_{i\in\Lambda,\, j\in\Lambda^c} J_\gamma(i,j)\sigma_i\sigma_j, \tag{12}$$

where Λ is a finite subset of $\mathbb{Z}^2$, $\sigma_\Lambda = (\sigma_i)_{i\in\Lambda} \in \{-1,1\}^\Lambda$ with boundary condition $\sigma_{\Lambda^c} = (\sigma_i)_{i\in\Lambda^c}$.

Marc Kac showed in that when $J(r) = \mathrm{e}^{-|r|}$, this model may be studied through the transfer operator

$$K_\gamma^m = \mathrm{e}^{-\frac{1}{2}\gamma q(\mathbf{x})}\mathrm{e}^{\gamma\Delta_m}\mathrm{e}^{-\frac{1}{2}\gamma q(\mathbf{x})}, \tag{13}$$

where

$$\gamma q(\mathbf{x}) = \frac{1}{2}\tanh\left(\frac{\gamma}{2}\right)\sum_{i=1}^m x_i^2 - \sum_{i=1}^m \ln\cosh\left[\sqrt{\frac{\gamma\beta}{2}}\left(x_i + x_{i+1}\right)\right], \tag{14}$$

with the convention $x_{m+1} = x_1$. He proved that when γ approaches 0, the behavior of the system only depends on the Kac potential

$$q(\mathbf{x}) = \sum_{i=1}^m \frac{x_i^2}{4} - \sum_{i=1}^m \ln\cosh\left[\sqrt{\frac{\beta}{2}}\left(x_i + x_{i+1}\right)\right]. \tag{15}$$

Thus by reducing the two dimensional problem into a one dimensional problem, M. Kac showed that the critical temperature occurs at $\beta_c = \frac{1}{4}$.

The d-dimensional mean field Kac Hamiltonian

$$\Phi(\mathbf{x}) = \frac{\mathbf{x}^2}{2} + g(\mathbf{x}), \tag{16}$$

where $g(\mathbf{x}) = -2\sum_{i\sim j}\ln\cosh\left[\sqrt{\frac{\beta}{2}}\left(x_i + x_j\right)\right]$ is a smooth function with bounded derivatives. Observe that this result of Marc Kac is the motivation behind the types of Hamiltonian that we use in this paper.

In the generalized framework, we shall consider systems where each component is located at a site *i* of a crystal lattice $\mathbb{Z}^d$; and is described by a continuous real parameter $x_i \in \mathbb{R}$. A particular configuration of the total system will be characterized by an element $\mathbf{x}=(x_i)_{i\in\Lambda}$ of the product space $\Omega=\mathbb{R}^\Lambda$. This set is called the configuration space or phase space.

We shall denote by $\Phi=\Phi^\Lambda$ the Hamiltonian which assigns to each configuration $\mathbf{x}\in\mathbb{R}^\Lambda$ a potential energy $\Phi(\mathbf{x})$: The probability measure that describes the equilibrium of the system is then given by the Gibbs measure

$$\mathrm{d}\mu^\Lambda(\mathbf{x})=Z_\Lambda^{-1}\mathrm{e}^{-\Phi(\mathbf{x})}\mathrm{d}\mathbf{x}. \tag{17}$$

$Z>0$ is a normalization constant,

$$Z=Z_\Lambda=\int_{\mathbb{R}^\Lambda}\mathrm{e}^{-\Phi(\mathbf{x})}\mathrm{d}\mathbf{x} \tag{18}$$

For any finite domain Λ of $\mathbb{Z}^d$; we shall consider a Hamiltonian of the phase space $\Omega=\mathbb{R}^\Lambda$ satisfying:

1) $\lim\limits_{|\mathbf{x}|\to\infty}|\nabla\Phi(\mathbf{x})|=\infty$,

2) For some *M*, any $\partial^\alpha\Phi$ with $|\alpha|=M$ is bounded on $\mathbb{R}^\Lambda$,

3) For $|\alpha|\ge 1$, $|\partial^\alpha\Phi(\mathbf{x})|\le C_\alpha\left(1+|\nabla\Phi(\mathbf{x})|^2\right)^{1/2}$ for some $C_\alpha>0$,

4) There exist $w>0, C>0$ such that $\mathbf{x}\cdot\nabla\Phi\ge C|\mathbf{x}|^{1+w}$ for all $|\mathbf{x}|\ge\frac{1}{C}$.

Here and in what follows, $\alpha=(\alpha_i)_{i=1,\cdots,m}\in\mathbb{Z}_+^{|\Lambda|}$ shall denote a multiindex. We set $|\alpha|=\sum_{i=1}^m\alpha_i$, $\alpha!=\alpha_1!\cdots\alpha_m!$. If $\beta=(\beta_i)_{i=1,\cdots,m}\in\mathbb{Z}_+^{|\Lambda|}$ and $\beta_j\le\alpha_j$ for all $j=1,\cdots,m$, then we write $\beta\le\alpha$. For $\alpha,\beta\in\mathbb{Z}_+^{|\Lambda|}$ such that $\beta\le\alpha$, we put $\binom{\alpha}{\beta}=\frac{\alpha!}{\beta!(\alpha-\beta)!}$. If $\alpha=(\alpha_i)_{i=1,\cdots,m}\in\mathbb{Z}_+^{|\Lambda|}$ and $x\in\mathbb{R}^d$ we write $x^\alpha=\prod_{i=1}^m x^{\alpha_i}$, and $\partial^\alpha=\partial^{\alpha_1}/\partial x_1^{\alpha_1}\cdots\partial^{\alpha_m}/\partial x_m^{\alpha_m}$. The Hessian of the Hamiltonian Φ will be denoted by $\mathbf{Hess}\Phi$. Finally, if *i* and *j* are two nearest neighbor sites in $\mathbb{Z}^d$ we write $i\sim j$.

2.1. The n^{th} Derivative of the Free Energy

We consider the Hamiltonian given by

$$\Phi^\beta(\mathbf{x})=\Phi_\Lambda(\mathbf{x})-\beta g(\mathbf{x}), \tag{19}$$

where β is a thermodynamic parameter (temperature or magnetic field), and *g* satisfying

$$|\partial^\alpha\nabla g|\le C_\alpha,\ \forall\alpha\in\mathbb{N}^{|\Lambda|}. \tag{20}$$

We shall assume that there exist β_0 and β_1 such that $\Phi^\beta(\mathbf{x})$ satisfies the assumptions 1 - 4 for all $\beta\in[\beta_0,\beta_1]$.

The finite volume pressure or free energy of the system is defined by

$$P_\Lambda(\beta)=\frac{1}{|\Lambda|}\ln\left[\int_{\mathbb{R}^\Lambda}\mathrm{d}\mathbf{x}\mathrm{e}^{-\Phi^\beta(\mathbf{x})}\right]. \tag{21}$$

We will be interested in the *k*-times differentiability of the free energy in the thermodynamic limit given by

$$P(\beta)=\lim_{|\Lambda|\to\infty}P_\Lambda(\beta). \tag{22}$$

We will use the following notations:

$$Z_{\Lambda}(\beta)=\int_{\mathbb{R}^{\Lambda}} e^{-\Phi^{\beta}(\mathbf{x})}d\mathbf{x}, \tag{23}$$

$$\langle\cdot\rangle_{\Lambda,\beta}=Z_{\Lambda}^{-1}(\beta)\int_{\mathbb{R}^{\Lambda}}\cdot e^{-\Phi^{\beta}(\mathbf{x})}d\mathbf{x}. \tag{24}$$

Observe that for an arbitrary suitable function $f(\beta)$

$$\frac{\partial}{\partial\beta}\langle f(\beta)\rangle_{\Lambda,\beta}=\langle f'(\beta)\rangle_{\Lambda,\beta}+\mathbf{cov}(f,g). \tag{25}$$

Now using the Helffer-Sjostrand formula, we have

$$\frac{\partial}{\partial\beta}\langle f(\beta)\rangle_{\Lambda,\beta}=\langle f'(\beta)\rangle_{\Lambda,\beta}+\left\langle A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla f)\cdot\nabla g\right\rangle_{\Lambda,\beta}. \tag{26}$$

Denote by $\mathcal{A}_g$ the operator $A_{\Phi^{\beta}}^{(1)^{-1}}(\cdot)\cdot\nabla g$ *i.e.*

$$\mathcal{A}_g f:=A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla f)\cdot\nabla g \tag{27}$$

Thus,

$$\frac{\partial}{\partial\beta}\langle f(\beta)\rangle_{\Lambda,\beta}=\left\langle\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)f\right\rangle_{\Lambda,\beta}. \tag{28}$$

The linear operator $\frac{\partial}{\partial\beta}+\mathcal{A}_g$ will be denoted by $\mathcal{H}_g$.

$$\mathcal{H}_g:=\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)f. \tag{29}$$

Observe that each $\beta\in[\beta_0,\beta_1]$ is associated with a unique C^{∞}-solution, $f(\beta)$ of the equation

$$A_{\Phi_{\Lambda}^{\beta}}^{(0)}f(\beta)=g-\langle g\rangle_{\Lambda,\beta},\ \langle f(\beta)\rangle_{\Lambda,\beta}=0. \tag{30}$$

Hence, $A_{\Phi_{\Lambda}^{t}}^{(1)}\mathbf{v}^{\beta}=\nabla g$ where $\mathbf{v}^{\beta}=\nabla f(\beta)$. Notice that the map $\beta\mapsto\mathbf{v}^{\beta}$ is well defined and $\{\mathbf{v}^{\beta}:\beta\in[\beta_0,\beta_1]\}$, is a family of smooth solutions on $\mathbb{R}^{\Lambda}$.

Under the notation above, we have the following Lemma:

Lemma 1. *Let g be a smooth function with bounded derivatives and assume that there exist* β_0 *and* β_1 *such* $\Phi^{\beta}(\mathbf{x})=\Phi_{\Lambda}(\mathbf{x})-\beta g(\mathbf{x})$ *satisfies the assumptions* 1 - 4 *for all* $\beta\in[\beta_0,\beta_1]$. *Then for all* $n\geq 1$, *the* n^{th} *derivative of the finite volume pressure is given by*

$$P_{\Lambda}^{(n)}(\beta)=(n-1)!\frac{\langle\mathcal{A}_g^{n-1}g\rangle_{\Lambda,\beta}}{|\Lambda|}, \tag{31}$$

where $\mathcal{A}_g^{n-1}g$ *is the composition of the operator* $\mathcal{A}_g g(\cdot)$ $n-1$ *times.*

Proof. First put $\theta_{\Lambda}(\beta)=|\Lambda|P_{\Lambda}(\beta)$. We then have

$$\theta_{\Lambda}'(\beta)=\langle g\rangle_{\Lambda,\beta}=\left\langle\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)^0 g\right\rangle_{\Lambda,\beta}=\langle\mathcal{H}_g^0 g\rangle_{\Lambda,\beta} \tag{32}$$

$$\theta_{\Lambda}''(\beta)=\frac{\partial}{\partial\beta}\langle g\rangle_{\Lambda,\beta}=\left\langle A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right\rangle_{\Lambda,\beta} \tag{33}$$

$$=\left\langle\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)g\right\rangle_{\Lambda,\beta}; \tag{34}$$

$$\theta'''_{\Lambda}(\beta) = \frac{\partial}{\partial\beta}\left\langle A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right\rangle_{\Lambda,\beta}$$
$$= \left\langle \frac{\partial}{\partial\beta}A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right\rangle_{\Lambda,\beta} + \left\langle\left(A_{\Phi^{\beta}}^{(1)^{-1}}\nabla\left(A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right)\right)\cdot\nabla g\right\rangle_{\Lambda,\beta} \tag{35}$$

$$= \left\langle\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)^2 g\right\rangle_{\Lambda,\beta}. \tag{36}$$

By induction it is easy to see that

$$\theta_{\Lambda}^{(n)}(\beta) = \left\langle\left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)^{n-1} g\right\rangle_{\Lambda,\beta} = \left\langle\mathcal{H}_g^{n-1}g\right\rangle_{\Lambda,\beta},\ (\forall n\geq 1). \tag{37}$$

Next, observe that

$$\mathcal{H}_g g = A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g = \mathcal{A}_g g \tag{38}$$

$$\mathcal{H}_g^2 g = \frac{\partial}{\partial\beta}\nabla f\cdot\nabla g + \left(A_{\Phi^{\beta}}^{(1)^{-1}}\nabla\left(A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right)\right)\cdot\nabla g \tag{39}$$

where f satisfies the equation $\nabla f = A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)$. With $\mathbf{v}^{\beta} = \nabla f$, we have

$$\frac{\partial}{\partial\beta}\nabla f = \frac{\partial\mathbf{v}^{\beta}}{\partial\beta} = A_{\Phi^{\beta}}^{(1)^{-1}}\left(\mathbf{Hess}g\mathbf{v}^{\beta} - \nabla g\cdot\nabla\mathbf{v}^{\beta}\right). \tag{40}$$

$$\mathcal{H}_g^2 g = A_{\Phi^{\beta}}^{(1)^{-1}}\left[\mathbf{Hess}g\mathbf{v}^{\beta} - \nabla g\cdot\nabla\mathbf{v}^{\beta} + \nabla\left(A_{\Phi^{\beta}}^{(1)^{-1}}(\nabla g)\cdot\nabla g\right)\right]\cdot\nabla g$$
$$= A_{\Phi^{\beta}}^{(1)^{-1}}2\nabla\left(A_g g\right)\cdot\nabla g = 2\mathcal{A}_g^2 g. \tag{41}$$

We will now prove by induction that

$$\mathcal{H}_g^{n-1}g = (n-1)!\mathcal{A}_g^{n-1}g \text{ for } n\geq 1. \tag{42}$$

We have already checked the result is true for $n = 1,2,3$. For induction, assume that

$$\mathcal{H}_g^{n-1}g = (n-1)!\mathcal{A}_g^{n-1}g. \tag{43}$$

if n is replaced by $\tilde{n}\leq n$.

$$\mathcal{H}_g^{n-1}g = \left(\frac{\partial}{\partial\beta}+\mathcal{A}_g\right)\left((n-1)!\mathcal{A}_g^{n-1}g\right) \tag{44}$$

$$= (n-1)!\left(\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-1}g + \mathcal{A}_g^{n}g\right). \tag{45}$$

Now

$$\mathcal{A}_g^{n-1}g = \left[A_{\Phi^{\beta}}^{(1)^{-1}}\nabla\left(\mathcal{A}_g^{n-2}g\right)\right]\cdot\nabla g = \nabla\varphi_n\cdot\nabla g \tag{46}$$

where $\nabla\varphi_n = \left[A_{\Phi^{\beta}}^{(1)^{-1}}\nabla\left(A_g^{n-2}g\right)\right]$. We obtain,

$$\frac{\partial}{\partial\beta}\nabla\varphi_n = A_{\Phi^{\beta}}^{(1)^{-1}}\left(\frac{\partial}{\partial\beta}\nabla\mathcal{A}_g^{n-2}g + \mathbf{Hess}g\nabla\varphi_n - \nabla g\cdot\nabla\left(\nabla\varphi_n\right)\right). \tag{47}$$

Hence,

$$\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-1}g=\frac{\partial}{\partial\beta}\nabla\varphi_n\cdot\nabla g \tag{48}$$

$$=\left[A_{\Phi^\beta}^{(1)^{-1}}\left(\frac{\partial}{\partial\beta}\nabla\mathcal{A}_g^{n-2}g+\mathbf{Hess}g\nabla\varphi_n-\nabla g\cdot\nabla\left(\nabla\varphi_n\right)\right)\right]\cdot\nabla g \tag{49}$$

$$=\left[A_{\Phi^t}^{(1)^{-1}}\left(\frac{\partial}{\partial\beta}\nabla\mathcal{A}_g^{n-2}g+\nabla\left(\nabla\varphi_n\cdot\nabla g\right)\right)\right]\cdot\nabla g \tag{50}$$

$$=\mathcal{A}_g\left[\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-2}g+\mathcal{A}_g\left(\mathcal{A}_g^{n-2}g\right)\right] \tag{51}$$

$$=\mathcal{A}_g\mathcal{H}_g\left(\mathcal{A}_g^{n-2}g\right)=\mathcal{A}_g\mathcal{H}_g\left(\frac{1}{(n-2)!}\mathcal{H}_g^{(n-2)}g\right) \tag{52}$$

$$=\frac{1}{(n-2)!}\mathcal{A}_g\mathcal{H}_g^{(n-1)}g \tag{53}$$

$$=\frac{1}{(n-2)!}\mathcal{A}_g\left((n-1)!\mathcal{A}_g^{n-1}g\right) \tag{54}$$

$$=(n-1)\mathcal{A}_g^n g. \tag{55}$$

Thus,

$$\mathcal{H}_g^n g=(n-1)!(n-1+1)\mathcal{A}_g^n g=n!\mathcal{A}_g^n g. \tag{56}$$

The result follows. ■

Next, we propose to find a formula of $P_\Lambda^{(n)}(\beta)$ that only involves $\Phi^\beta(\mathbf{x})$ and $g(\mathbf{x})$.

Proposition 2. *Let g be a smooth function with bounded derivatives and assume that there exist β_0 and β_1 such $\Phi^\beta(\mathbf{x})=\Phi_\Lambda(\mathbf{x})-\beta g(\mathbf{x})$ satisfies the assumptions* 1 - 4 *for all $\beta\in[\beta_0,\beta_1]$. Then for all $n\ge1$, we have the following formula for computing the n^{th} derivative $P_\Lambda^{(n)}(\beta)$ of the free energy.*

$$\sum_{k=0}^{n-1}\frac{\langle g^k\rangle_{\Lambda,\beta}}{k!}\frac{P_\Lambda^{(n-k)}(\beta)}{(n-k-1)!}=\frac{1}{(n-1)!}\frac{\langle g^n\rangle_{\Lambda,\beta}}{|\Lambda|},\ n\ge1. \tag{57}$$

Observe that the derivatives of all orders $P_\Lambda^{(n)}(\beta)$ can be computed by recursion.

Proof. First observe that

$$\left\langle g^p\mathcal{A}_g h\right\rangle_{\Lambda,\beta}=\left\langle g^p A_{\Phi^\beta}^{(1)^{-1}}\nabla h\cdot\nabla g\right\rangle_{\Lambda,\beta} \tag{58}$$

$$=\frac{1}{p+1}\left\langle A_{\Phi^\beta}^{(1)^{-1}}\nabla h\cdot\nabla g^{p+1}\right\rangle_{\Lambda,\beta} \tag{59}$$

$$=\frac{1}{p+1}\mathbf{cov}\left(g^{p+1},h\right) \tag{60}$$

$$=\frac{1}{p+1}\left[\left\langle g^{p+1}h\right\rangle_{\Lambda,\beta}-\left\langle g^{p+1}\right\rangle_{\Lambda,\beta}\langle h\rangle_{\Lambda,\beta}\right],\ p=0,1,\cdots \tag{61}$$

Setting $k=p+1$ and $h=\mathcal{A}_g^{n-k-1}g$, yields

$$\left\langle g^{k}\right\rangle_{\Lambda,\beta}\left\langle \mathcal{A}_{g}^{n-k-1}g\right\rangle_{\Lambda,\beta}=\left\langle g^{k}\mathcal{A}_{g}^{n-k-1}g\right\rangle_{\Lambda,\beta}-k\left\langle g^{k-1}\mathcal{A}_{g}^{n-k}g\right\rangle_{\Lambda,\beta}. \tag{62}$$

Now dividing by $k!$, summing over k and noticing that on the right hand side one obtains a telescoping sum, yields

$$\sum_{k=0}^{n-1}\frac{\left\langle g^{k}\right\rangle_{\Lambda,\beta}\left\langle \mathcal{A}_{g}^{n-k-1}g\right\rangle_{\Lambda,\beta}}{k!}=\frac{1}{(n-1)!}\left\langle g^{n}\right\rangle_{\Lambda,\beta}. \tag{63}$$

Now using Lemma 1, we have

$$\left\langle \mathcal{A}_{g}^{n-k-1}g\right\rangle_{\beta,\Lambda}=\frac{|\Lambda|P_{\Lambda}^{(n-k)}(\beta)}{(n-k-1)!}. \tag{64}$$

Hence,

$$\sum_{k=0}^{n-1}\frac{\left\langle g^{k}\right\rangle_{\Lambda,\beta}}{k!}\frac{P_{\Lambda}^{(n-k)}(\beta)}{(n-k-1)!}=\frac{1}{(n-1)!}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta}}{|\Lambda|},\quad n\geq 1. \tag{65}$$

■

2.2. Towards a Direct Method for the Analyticity of the Free Energy

Proposition 3. *Let g be a smooth function satisfying* (20) *and assume that there exist* β_0 *and* β_1 *such* $\Phi^{\beta}(\mathbf{x})=\Phi_{\Lambda}(\mathbf{x})-\beta g(\mathbf{x})$ *satisfies the assumptions* 1 - 4 *for all* $\beta\in[\beta_0,\beta_1]$. *If*

$$\lim_{n\to\infty}\left|\frac{\left\langle g^{n+1}\right\rangle_{\Lambda,\beta^*}}{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}}\right|<\infty\quad\forall\beta^*\in[\beta_0,\beta_1], \tag{66}$$

then for any $\Lambda\subset\mathbb{Z}^d$, the finite volume pressure $P_{\Lambda}(\beta)$ is analytic on $[\beta_0,\beta_1]$.

Proof. Let β^* be an arbitrary point on $[\beta_0,\beta_1]$. Putting $\beta=\beta^*$ in the result of proposition 2, we get

$$\sum_{k=0}^{n-1}\frac{\left\langle g^{k}\right\rangle_{\Lambda,\beta^*}}{k!}\frac{(n-k)P_{\Lambda}^{(n-k)}(\beta^*)}{(n-k)!}=\frac{1}{(n-1)!}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}}{|\Lambda|},\quad n\geq 1. \tag{67}$$

$$\Leftrightarrow$$

$$\sum_{k=0}^{n}\frac{\left\langle g^{k}\right\rangle_{\Lambda,\beta^*}}{k!}\frac{(n-k)P_{\Lambda}^{(n-k)}(\beta^*)}{(n-k)!}=\frac{1}{(n-1)!}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}}{|\Lambda|},\quad n\geq 1. \tag{68}$$

Now multiply both sides of the equation by $(\beta-\beta^*)^n$ to get

$$\begin{aligned}&\sum_{k=0}^{n}\frac{\left\langle g^{k}\right\rangle_{\Lambda,\beta^*}(\beta-\beta^*)^{k}}{k!}\frac{(n-k)P_{\Lambda}^{(n-k)}(\beta^*)}{(n-k)!}(\beta-\beta^*)^{n-k}\\&=\frac{1}{(n-1)!}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}(\beta-\beta^*)^{n}}{|\Lambda|}=\frac{1}{|\Lambda|}\frac{n\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}(\beta-\beta^*)^{n}}{n!}.\end{aligned} \tag{69}$$

Put

$$G_n^{\Lambda}(\beta):=\int_{\mathbb{R}^{\Lambda}}g^{n}(\mathbf{x})\mathrm{e}^{-\Phi^{\beta}(X)}\mathrm{d}\mathbf{x}. \tag{70}$$

If

$$\lim_{n\to\infty}\left|\frac{\left\langle g^{n+1}\right\rangle_{\Lambda,\beta^*}}{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}}\right| = \lim_{n\to\infty}\left|\frac{G_{n+1}^{\Lambda}\left(\beta^*\right)}{G_{n}^{\Lambda}\left(\beta^*\right)}\right| < \infty, \tag{71}$$

then the power series $\sum_{n=0}^{\infty}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{(n-1)!}$ and $\sum_{n=0}^{\infty}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!}$ have infinite radius of convergence. Summing with respect to n, we obtain the Cauchy product

$$\begin{aligned}&\left(\sum_{n=0}^{\infty}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!}\right)\left(\sum_{n=0}^{\infty}\frac{nP_{\Lambda}^{(n)}\left(\beta^*\right)}{n!}\left(\beta-\beta^*\right)^n\right)\\ &=\frac{1}{|\Lambda|}\sum_{n=0}^{\infty}\frac{n\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!},\ \text{for } \beta\neq\beta^*.\end{aligned} \tag{72}$$

$$\sum_{n=0}^{\infty}\frac{nP_{\Lambda}^{(n)}\left(\beta^*\right)}{n!}\left(\beta-\beta^*\right)^n=\frac{1}{|\Lambda|}\frac{\sum_{n=0}^{\infty}\frac{n\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!}}{\sum_{n=0}^{\infty}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!}},\ \beta\neq\beta^*. \tag{73}$$

Multiplying both sides of this last equation by $\left(\beta-\beta^*\right)^{-1}$, we get

$$\begin{aligned}\sum_{n=0}^{\infty}\frac{nP_{\Lambda}^{(n)}\left(\beta^*\right)}{n!}\left(\beta-\beta^*\right)^{n-1}&=\frac{1}{|\Lambda|}\frac{\sum_{n=0}^{\infty}\frac{n\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^{n-1}}{n!}}{\sum_{n=0}^{\infty}\frac{\left\langle g^{n}\right\rangle_{\Lambda,\beta^*}\left(\beta-\beta^*\right)^n}{n!}}\\ &=\frac{1}{|\Lambda|}\frac{\sum_{n=0}^{\infty}\frac{nG_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^{n-1}}{n!}}{\sum_{n=0}^{\infty}\frac{G_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^n}{n!}},\ \beta\neq\beta^*.\end{aligned} \tag{74}$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}}{\mathrm{d}\beta}\sum_{n=0}^{\infty}\frac{P_{\Lambda}^{(n)}\left(\beta^*\right)}{n!}\left(\beta-\beta^*\right)^n=\frac{1}{|\Lambda|}\frac{\frac{\mathrm{d}}{\mathrm{d}\beta}\sum_{n=0}^{\infty}\frac{G_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^n}{n!}}{\sum_{n=0}^{\infty}\frac{G_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^n}{n!}}. \tag{75}$$

Now integrating both sides, we obtain

$$\begin{aligned}\sum_{n=0}^{\infty}\frac{P_{\Lambda}^{(n)}\left(\beta^*\right)}{n!}\left(\beta-\beta^*\right)^n&=\frac{1}{|\Lambda|}\ln\left(\left|\sum_{n=0}^{\infty}\frac{G_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^n}{n!}\right|\right)+C_{\Lambda}\\ &=\frac{1}{|\Lambda|}\ln\left(\left|1+\sum_{n=1}^{\infty}\frac{G_{n}^{\Lambda}\left(\beta^*\right)\left(\beta-\beta^*\right)^n}{n!}\right|\right)+C_{\Lambda}.\end{aligned} \tag{76}$$

Now taking limit when $\beta \to \beta^*$, on both sides of this last equation, we see that $C_\Lambda = 0$. Thus

$$\sum_{n=0}^{\infty} \frac{P_\Lambda^{(n)}(\beta^*)}{n!}(\beta-\beta^*)^n = \frac{1}{|\Lambda|}\ln\left(\left|\sum_{n=0}^{\infty} \frac{G_n^\Lambda(\beta^*)(\beta-\beta^*)^n}{n!}\right|\right) \tag{77}$$

Now observe that

$$\frac{\mathrm{d}^{(n)}}{\mathrm{d}\beta^n}\left[Z_\Lambda(\beta)\right] = Z_\Lambda^{(n)}(\beta) = G_n^\Lambda(\beta). \tag{78}$$

$$\lim_{n\to\infty}\left|\frac{G_{n+1}^\Lambda(\beta^*)}{G_n^\Lambda(\beta^*)}\right| < \infty \left(\text{uniformly in } \beta^*\right) \Rightarrow \left|\frac{G_{n+1}^\Lambda(\beta^*)}{G_n^\Lambda(\beta^*)}\right| \text{ is bounded.} \tag{79}$$

There exists $a > 0$ such that

$$\left|\frac{G_{n+1}^\Lambda(\beta^*)}{G_n^\Lambda(\beta^*)}\right| \le a \ \text{ for all } n. \tag{80}$$

By iteration, we obtain

$$\left|\frac{G_{n+1}^\Lambda(\beta^*)}{Z_\Lambda(\beta^*)}\right| \le a^{n+1}. \tag{81}$$

Hence,

$$\left|G_n^\Lambda(\beta^*)\right| \le Ma^n \tag{82}$$

where

$$M =: \sup_{\beta^* \in [\beta_0, \beta_1]} Z_\Lambda(\beta^*). \tag{83}$$

Thus, there exists positive constants a and M such that

$$\left|\frac{\mathrm{d}^{(n)}}{\mathrm{d}\beta^n}\left[Z_\Lambda(\beta^*)\right]\right| \le Ma^n \quad \forall \beta^* \in [\beta_0, \beta_1]. \tag{84}$$

We conclude that $Z_\Lambda(\beta)$ is analytic on $[\beta_0, \beta_1]$ and

$$Z_\Lambda(\beta) = \sum_{n=0}^{\infty} \frac{Z_\Lambda^{(n)}(\beta^*)(\beta-\beta^*)^n}{n!} = \sum_{n=0}^{\infty} \frac{G_n^\Lambda(\beta^*)(\beta-\beta^*)^n}{n!}, \tag{85}$$

for all β in some neighborhood of β^*. Now using Equation (57), we obtain

$$\sum_{n=0}^{\infty} \frac{P_\Lambda^{(n)}(\beta^*)}{n!}(\beta-\beta^*)^n = \frac{1}{|\Lambda|}\ln\left(Z_\Lambda(\beta)\right) = P_\Lambda(\beta) \tag{86}$$

for all β in some neighborhood of $\beta^* \in [\beta_0, \beta_1]$. ■

Remark 4. *Observe that the left-hand side of Equation* (57) *in proposition* 2 *is a circular convolution equation of the sequences* $\left\{\frac{\langle g^k\rangle_{\Lambda,\beta}}{k!}\right\}_k$ *and* $\left\{\frac{kP_\Lambda^{(k)}(\beta)}{k!}\right\}$.

Thus a suitable deconvolution may give a more exact formula for the derivatives *of the pressure. This issue will be investigated further to extend the result to the infinite volume case* ($\lim_{\Lambda\to\mathbb{Z}^d} P_\Lambda^{(n)}(\beta)$). *One may also use equation* (57) *to obtain a more precise estimate of the truncated correlations.*

3. Estimating the Error in the Thermodynamic Limit: The Continuum Gas Case

We shall consider the usual continuum gas model composed of N particles confined in a box $\Lambda_\ell = \left(\frac{-\ell}{2},\frac{\ell}{2}\right]^d \subset \mathbb{R}^d$ with $\ell > 0$. The state of such a system is given by the collection $\left(p_j, q_j\right)_{j=1,\cdots,N}$ of the momentum $p_j \in \mathbb{R}^d$ and the position $q_j \in \Lambda_\ell$ of each particle. The configuration space or set of microstate spaces is $\Omega_{\Lambda_\ell;N} = \left(\mathbb{R}^d \times \Lambda_\ell\right)^N$.

The usual Hamiltonian giving the sum of the kinetic and potential energy is

$$\Phi\left(p_1, q_1, \cdots, p_N, q_N\right) = \sum_{j=1}^{N} \frac{\left\|p_j\right\|_2^2}{2m} + \sum_{1\le i<j\le N} V\left(q_j - q_i\right), \tag{87}$$

where m is the mass of each particle and the potential V determines the contribution to the total energy resulting from the interaction between the i^{th} and the j^{th} particles generally assumed to depend only on the distance, $\left\|q_j - q_i\right\|_2$ between the particles. It is well known that in the canonical ensemble distribution, the momenta have no effect on the probability of events depending only on the position.

Thus, we shall consider Hamiltonians is of the form

$$\Phi_\Lambda^N(\mathbf{q}) = \sum_{1\le i<j\le N} V\left(q_j - q_i\right),\ \mathbf{q} = \left(q_1, \cdots, q_N\right) \in \Lambda_\ell^N. \tag{88}$$

over the configuration space $\Omega_{\Lambda_\ell;N} = \Lambda^N \left(\Lambda = \Lambda_\ell\right)$, where $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ and $\rho := \frac{N}{|\Lambda|}$ is the particle density assumed to be constant. We shall also assume that the particles interact via a stable pair potential. *i.e.*, there exists K positive such that

$$\sum_{1\le i<j\le N} V\left(q_j - q_i\right) \ge -KN, \tag{89}$$

for all N and all configuration $\mathbf{q} = \left(q_1, \cdots, q_N\right) \in \Lambda^N$.

The probability measure that describes the equilibrium of the system is then given by the Gibbs measure

$$\mathrm{d}\mu^\Lambda(\mathbf{q}) = Z_{\beta,\Lambda,N}^{-1} \mathrm{e}^{-\beta\Phi_\Lambda^N(\mathbf{q})} \mathrm{d}\mathbf{q}. \tag{90}$$

$Z_{\beta,\Lambda,N}^{-1} > 0$ is the canonical partition function of the system and is given by ,

$$Z = Z_{\beta,\Lambda,N} = \frac{1}{N!} \int_{\Lambda^N} \mathrm{e}^{-\beta\Phi_\Lambda^N(\mathbf{q})} \mathrm{d}\mathbf{q}. \tag{91}$$

$\beta > 0$ is a thermodynamic parameter representing the inverse temperature. Note that here, we are using a zero boundary condition Hamiltonian. *i.e.*, we are assuming that there are no particles outside of $\Lambda = \Lambda_\ell$.

The finite volume free energy is given by

$$f_{\beta,\Lambda}(N) = \frac{-1}{\beta|\Lambda|}\ln\left(Z_{\beta,\Lambda,N}\right), \text{ where } |\Lambda| = \ell^d \text{ is the volume of } \Lambda. \tag{92}$$

In the thermodynamic limit, $|\Lambda|, N \to \infty$ but the density $\rho := \frac{N}{|\Lambda|}$ remains constant. The infinite volume free energy obtained by taking the thermodynamic limit is potentially dependent on the density ρ and is given by

$$f_\beta(\rho) = \lim_{\substack{|\Lambda|, N\to\infty \\ \frac{N}{|\Lambda|}=\rho=const}} f_{\beta,\Lambda}(N). \tag{93}$$

In [1], the authors showed that given the validity of the cluster expansion, this limit exists and is given by

$$f_\beta(\rho) = \frac{1}{\beta}\left[\rho(\ln\rho - 1) - \sum_{n\geq 1}\frac{\beta_n \rho^{n+1}}{n+1}\right], \tag{94}$$

where

$$\beta_n = \frac{1}{n!}\sum_{\substack{g\in\mathcal{B}_{n+1} \\ \{1\}\in V(g)}} \int_{\mathbb{R}^{dn}} \prod_{\{i,j\}\in E(g)} \left(\mathrm{e}^{-\beta V(q_i - q_j)} - 1\right)\mathrm{d}q_2 \cdots \mathrm{d}q_{n+1}, \; q_1 := 0, \tag{95}$$

where $V:\mathbb{R}^d \to \mathbb{R}\cup\{\infty\}$, $\mathcal{B}_{n+1}$ is the set of 2-connected graphs g on $(n+1)$ vertices and $E(g)$ is the set of edges of the graph g. In [2], the terms contributing to the finite volume correction of the free energy are computed. More precisely, the author showed that there exists a constant $\kappa = \kappa(\beta, B) > 0$, independent of N and Λ, such that if

$$\rho\int_{\mathbb{R}^d}\left|\mathrm{e}^{-\beta V(\mathbf{q})} - 1\right|\mathrm{d}\mathbf{q} < \kappa \text{, then} \tag{96}$$

$$\left|\frac{1}{|\Lambda|}\ln\left(Z_{\beta,\Lambda,N}\right) - \beta f_\beta(\rho)\right| \leq \frac{C_\rho}{|\Lambda|}, \text{ for some } C_\rho > 0. \tag{97}$$

Recall that again here, the proof of this result heavily relies of the validity of the cluster expansion.

In this paper, we propose a method for estimating the error without using cluster expansions under a lower regularity assumption of the interaction. Put

$$\xi(N) = -\ln\left(\int_{\Lambda^N}\mathrm{e}^{-\beta\Phi_\Lambda^N(\mathbf{q})}\mathrm{d}\mathbf{q}\right) \tag{98}$$

We first need the following classical Lemma.

Lemma 5. ([36]) *Let D a given fixed positive constant D, and* $\xi(N)$ *be a sequence of real numbers satisfying*

$$|\xi(N+M) - \xi(N) - \xi(M)| \leq D, \text{ for each } N \text{ and } M \in \mathbb{N}. \tag{99}$$

The limit of the sequence $\frac{\xi(N)}{N}$ *exists and*

$$\left|\frac{\xi(N)}{N} - \lim_{N\to\infty}\frac{\xi(N)}{N}\right| \leq \frac{D}{N}. \tag{100}$$

Proof. Let

$$a(N)=\frac{\xi(N)}{N}. \tag{101}$$

Using

$$\left|\xi(N+M)-\xi(N)-\xi(M)\right|\le D,\ \text{for each } N \text{ and } M\in\mathbb{N}, \tag{102}$$

we have

$$\left|a(N+M)-\frac{N}{N+M}a(N)-\frac{M}{N+M}a(M)\right|\le\frac{D}{N+M}. \tag{103}$$

In particular, for $M=N$, we get

$$\left|a(2N)-a(N)\right|\le\frac{D}{2N}. \tag{104}$$

and by iteration:

$$\left|a\left(2^{k+1}N\right)-a\left(2^{k}N\right)\right|\le\frac{D}{2^{k}N} \tag{105}$$

$\Rightarrow a^*(N):=\lim_{k\to\infty}a\left(2^kN\right)$ exists and

$$\left|a^*(N)-a(N)\right|\le\frac{D}{N}. \tag{106}$$

Now replacing N and M in (103) by 2^kN and 2^kM respectively, and taking the limit as $k\to\infty$ yields

$$a^*(N+M)=\frac{N}{N+M}a^*(N)+\frac{M}{N+M}a^*(M). \tag{107}$$

Next, we define $\xi^*(N):=Na^*(N)$ and rewrite (106) as

$$\xi^*(N+M)=\xi^*(N)+\xi^*(M). \tag{108}$$

This implies

$$a^*(N)=a^*(1). \tag{109}$$

The result follows from (106) and (109). ■

Proposition 6. *Assume that the interaction $V:\mathbb{R}^d\to\mathbb{R}\cup\{\infty\}$ is stable and that there exists a differentiable function $\psi:\mathbb{R}\to\mathbb{R}$ with bounded first derivative satisfying $\psi(0)=0$ such that*

$$V(\mathbf{x})\le\psi\left(\|\mathbf{x}\|_2\right),\ \forall\,\mathbf{x}\in\mathbb{R}^d. \tag{110}$$

There exist $\ell_0>0$ and $N_0\in\mathbb{N}$ such that

$$\left|f_{\beta,\Lambda}(N)-f_\beta(\rho)\right|\le\frac{2\|\psi'\|_\infty\sqrt{d}}{\rho|\Lambda|}\ \text{for } \ell\ge\ell_0 \text{ and } N\ge N_0. \tag{111}$$

Remark 7. *Note that compared to Theorem* 2.1 *in* [2] *this result does not use the cluster expansion at all. We only need a lower regularity assumption of the type used in* [37] *and* [1]. *Moreover, the result provides an explicit expression of the constant $\hat{C}(\rho)$ in the right-hand side.*

Proof. Put

$$\xi(N) = -\ln\left(\int_{\Lambda^N} \mathrm{e}^{-\beta\Phi_\Lambda^N(\mathbf{q})}\mathrm{d}\mathbf{q}\right) \tag{112}$$

$$\Phi_\Lambda^N(\mathbf{q}) = \sum_{1\le i<j\le N} V\left(q_j - q_i\right) \tag{113}$$

$$\le \sum_{1\le i<j\le N} \psi\left(\left\|\left(q_j - q_i\right)\right\|_2\right) \tag{114}$$

$$= \sum_{1\le i<j\le N} \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\psi\left(s\left\|\left(q_j - q_i\right)\right\|_2\right)\mathrm{d}s \tag{115}$$

$$= \sum_{1\le i<j\le N} \left\|\left(q_j - q_i\right)\right\|_2 \int_0^1 \psi'\left(s\left\|\left(q_j - q_i\right)\right\|_2\right)\mathrm{d}s \tag{116}$$

$$\le \left\|\psi'\right\|_\infty \sum_{j=1}^N \sum_{i<j} \left\|\left(q_j - q_i\right)\right\|_2, \tag{117}$$

$$\le \left\|\psi'\right\|_\infty \sum_{j=1}^N \sum_{i<j} \sqrt{d}\,\ell,\ \ \forall\left(q_1,\cdots,q_N\right)\in\Lambda_\ell^N \tag{118}$$

$$= \left\|\psi'\right\|_\infty \sqrt{d}\,\ell \sum_{j=1}^N (j-1) \tag{119}$$

$$= \left\|\psi'\right\|_\infty \sqrt{d}\,\frac{1}{2}N(N-1)\ell. \tag{120}$$

For $\delta > 0$ and $\varepsilon \in [0,1]$, define

$$\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta) := \left(1-\varepsilon\mathrm{e}^{-\delta\ell N^2}\right)\Phi_\Lambda^{N+M}(\mathbf{q}) + \varepsilon\mathrm{e}^{-\delta\ell N^2}\left[\Phi_\Lambda^N \oplus \Phi_\Lambda^M(\mathbf{q})\right] \tag{121}$$

where

$$\Phi_\Lambda^N \oplus \Phi_\Lambda^M(\mathbf{q}) := \Phi_\Lambda^N\left(\mathbf{q}_N\right) + \Phi_\Lambda^M\left(\mathbf{q}_M\right) \text{ with } \mathbf{q} = \left(\mathbf{q}_N,\mathbf{q}_M\right)\in\Lambda^{N+M}. \tag{122}$$

We have

$$\begin{aligned}&\frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\right)\\ &= \frac{\beta\mathrm{e}^{-\delta\ell N^2}\int_{\Lambda^{N+M}}\left[\Phi_\Lambda^{N+M}(\mathbf{q}) - \Phi_\Lambda^N\oplus\Phi_\Lambda^M(\mathbf{q})\right]\mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}}{\int_{\Lambda^{N+M}}\mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}}.\end{aligned} \tag{123}$$

Now using the stability condition and $\Phi_\Lambda^N(\mathbf{q}) \le \left\|\psi'\right\|_\infty \frac{\sqrt{d}}{2}N(N-1)\ell$ for all N, we have

$$\left[\Phi_\Lambda^{N+M}(\mathbf{q}) - \Phi_\Lambda^N\oplus\Phi_\Lambda^M(\mathbf{q})\right]$$

$$\ge -K(N+M) \tag{124}$$

$$-\left\|\psi'\right\|_\infty \frac{\sqrt{d}}{2}\ell\left[N(N-1)+M(M-1)\right], \tag{125}$$

and

$$\left[\Phi_\Lambda^{N+M}(\mathbf{q}) - \Phi_\Lambda^N\oplus\Phi_\Lambda^M(\mathbf{q})\right] \tag{126}$$

$$\leq \|\psi'\|_\infty \frac{\sqrt{d}}{2}(N+M)(N+M-1)\ell + K(N+M). \tag{127}$$

Thus,

$$\left|\Phi_\Lambda^{N+M}(\mathbf{q}) - \Phi_\Lambda^N \oplus \Phi_\Lambda^M(\mathbf{q})\right| \tag{128}$$

$$\leq \|\psi'\|_\infty \frac{\sqrt{d}}{2}(N+M)(N+M-1)\ell + K(N+M) \tag{129}$$

$$= (M+N)\left[CN\ell + CM\ell + K - C\right], \left(\text{where } C = \|\psi'\|_\infty \frac{\sqrt{d}}{2}\right) \tag{130}$$

$$\leq 2N(2CN\ell + K - C) \ (\text{with } M \leq N) \tag{131}$$

$$= 4CN^2\ell\left(\frac{K-C}{2CN\ell} + 1\right) \tag{132}$$

It then follows from (123) that

$$\left|\frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\right)\right| \leq 4\beta C\ell N^2 \mathrm{e}^{-\delta\ell N^2}\left(\frac{K-C}{2CN\ell}+1\right). \tag{133}$$

Observe that

$$\lim_{\substack{\ell\to\infty \\ N\to\infty}} \ell N^2 \mathrm{e}^{-\delta\ell N^2}\left(\frac{K-C}{2CN\ell}+1\right) = 0 \ \text{ for all } 0<\delta\leq 1. \tag{134}$$

Hence, there exist $\ell_0 > 0$ and $N_0 \in \mathbb{N}$ such that

$$\ell N^2 \mathrm{e}^{-\delta\ell N^2}\left(\frac{K-C}{2CN\ell}+1\right) < 1 \ \text{ for } \ell \geq \ell_0 \text{ and } N \geq N_0. \tag{135}$$

Thus,

$$\left|\frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\right)\right| \leq 4\beta C, \ \text{ for } \ell \geq \ell_0 \text{ and } N \geq N_0. \tag{136}$$

Next, we integrate with respect to $\varepsilon \in [0,1]$ to get

$$\begin{aligned} &\left|\int_0^1 \frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\mathrm{d}\varepsilon\right)\right| \\ &\leq \int_0^1 \left|\frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\mathrm{d}\varepsilon\right)\right| \leq 4\beta C \end{aligned} \tag{137}$$

$$\Rightarrow$$

$$\lim_{\delta\to 0^+}\left|\int_0^1 \frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\Phi_\Lambda^{(N,M)}(\mathbf{q},\varepsilon,\delta)}\mathrm{d}\mathbf{q}\mathrm{d}\varepsilon\right)\right| \leq 4\beta C \tag{138}$$

$$\Leftrightarrow$$

$$\left|\int_0^1 \frac{\partial}{\partial\varepsilon}\ln\left(\int_{\Lambda^{N+M}} \mathrm{e}^{-\beta\left[(1-\varepsilon)\Phi_\Lambda^{N+M}(\mathbf{q})+\varepsilon\left[\Phi_\Lambda^N\oplus\Phi_\Lambda^M(\mathbf{q})\right]\right]}\mathrm{d}\mathbf{q}\mathrm{d}\varepsilon\right)\right| \leq 4\beta C \tag{139}$$

$$\Leftrightarrow$$

$$\left|\xi(N+M) - \xi(N) - \xi(M)\right| \leq D \tag{140}$$

where

$$D = 2\beta \|\psi'\|_\infty \sqrt{d}. \tag{141}$$

The result follows from Lemma 5. ■

The result of Proposition 6 may be extended to the case where ψ is given by $\psi(t) = a_1 t + a_2 t^2 + \cdots + a_m t^m$, with $a_i \geq 0\ (i = 1, \cdots, m-1)$ and $a_m > 0$. Indeed,

$$\left\|\left(q_j - q_i\right)\right\|_2^n \leq d^{\frac{n}{2}} \ell^n,\ \forall \left(q_1, \cdots, q_N\right) \in \Lambda_\ell^N \tag{142}$$

Hence,

$$\begin{aligned}
\Phi_\Lambda^N(\mathbf{q}) &\leq \sum_{1 \leq i < j \leq N} \psi\left(\left\|\left(q_j - q_i\right)\right\|_2\right) \\
&= \sum_{j=1}^{N} \sum_{i<j} \left(a_1 \left\|\left(q_j - q_i\right)\right\|_2 + a_2 \left\|\left(q_j - q_i\right)\right\|_2^2 + \cdots + a_m \left\|\left(q_j - q_i\right)\right\|_2^m\right) \\
&\leq \sum_{j=1}^{N} \sum_{i<j} \left(a_1 d^{\frac{1}{2}} \ell + a_2 d \ell^2 + \cdots + a_m d^{\frac{m}{2}} \ell^m\right) \\
&= \frac{1}{2} N(N-1) \left(a_1 d^{\frac{1}{2}} \ell + a_2 d \ell^2 + \cdots + a_m d^{\frac{m}{2}} \ell^m\right) \\
&= \frac{1}{2} N(N-1) \ell^m \alpha(\ell),
\end{aligned} \tag{143}$$

where

$$\alpha(\ell) = \left(a_1 d^{\frac{1}{2}} \ell^{-m+1} + a_2 d \ell^{-m+2} + \cdots + a_m d^{\frac{m}{2}}\right) \to a_m d^{\frac{m}{2}} \text{ as } \ell \to \infty. \tag{144}$$

Now repeating the argument of the proof of Proposition 6 with

$$\Phi_\Lambda^{(N,M)}(\mathbf{q}, \varepsilon, \delta) := \left(1 - \varepsilon \mathrm{e}^{-\delta \ell^m N^2}\right) \Phi_\Lambda^{N+M}(\mathbf{q}) + \varepsilon \mathrm{e}^{-\delta \ell^m N^2} \left[\Phi_\Lambda^N \oplus \Phi_\Lambda^M(\mathbf{q})\right], \tag{145}$$

we obtain the following result

Proposition 8. *Assume that the interaction* $V : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$ *is stable and that there exists a polynomial function*

$$\psi(t) = a_0 + a_1 t + a_2 t^2 + \cdots + a_m t^m \tag{146}$$

with $a_i \geq 0\ (i = 1, \cdots, m-1)$ *and* $a_m > 0$ *such that*

$$V(x) \leq \psi\left(\|x\|_2\right),\ \forall x \in \mathbb{R}^d. \tag{147}$$

There exist $\ell_0 > 0$ *and* $N_0 \in \mathbb{N}$ *such that*

$$\left|f_{\beta,\Lambda}(N) - f_\beta(\rho)\right| \leq \frac{4 a_m d^{\frac{m}{2}}}{\rho |\Lambda|} \text{ for } \ell \geq \ell_0 \text{ and } N \geq N_0. \tag{148}$$

4. The Lattice Gas Case

We will indeed consider systems where each component is located at a site i of a crystal lattice $\Lambda \subset \mathbb{Z}^d$; and is described by a continuous real parameter $x_i \in \mathbb{R}$. A particular configuration of the total system will be characterized by an element $\mathbf{x} = (x_i)_{i \in \Lambda}$ of the product space $\Omega = \mathbb{R}^\Lambda$.

We shall denote by $\Phi = \Phi^\Lambda$ the Hamiltonian which assigns to each configuration $\mathbf{x} \in \mathbb{R}^{\Lambda}$ a potential energy $\Phi^{\Lambda}(\mathbf{x})$: The probability measure that describes the equilibrium of the system is then given by the Gibbs measure

$$\mathrm{d}\mu^{\Lambda,\beta}(\mathbf{x}) = Z_{\Lambda}^{-1} \mathrm{e}^{-\beta\Phi^{\Lambda}(\mathbf{x})} \mathrm{d}\mathbf{x}.$$

$Z_{\Lambda,\beta} > 0$ is a normalization constant,

$$Z = Z_{\Lambda,\beta} = \int_{\mathbb{R}^{\Lambda}} \mathrm{e}^{-\beta\Phi^{\Lambda}(\mathbf{x})} \mathrm{d}\mathbf{x}.$$

$$f_{\beta,\Lambda} = \frac{-1}{\beta|\Lambda|} \ln\left(Z_{\Lambda,\beta}\right), \text{ where } |\Lambda| = \text{the number of sites in } \Lambda.$$

The thermodynamic limit is taken in the sense of $|\Lambda| \to \infty$.

$$f_{\beta} := \lim_{|\Lambda|\to\infty} f_{\beta,\Lambda}$$

As in [38], we shall make the following assumptions on Φ^{Λ}.

1) Φ^{Λ} is measurable.

2) Strong Regularity. There exists a bounded function W

$$|W(\mathbf{x})| \le C \text{ for all } \mathbf{x} \tag{149}$$

such that if Λ_1 and Λ_2 are disjoint finite subsets of $\mathbb{Z}^d$ and $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \mathbb{R}^{\Lambda_1} \times \mathbb{R}^{\Lambda_2}$ is a configuration in $\mathbb{R}^{\Lambda_1 \cup \Lambda_2}$,

$$\Phi^{\Lambda_1\cup\Lambda_2}(\mathbf{x}) = \Phi^{\Lambda_1}(\mathbf{x}_1) + \Phi^{\Lambda_2}(\mathbf{x}_2) + W(\mathbf{x}). \tag{150}$$

Put

$$\xi(N) = -\ln\left(\int_{\mathbb{R}^{\Lambda}} \mathrm{e}^{-\beta\Phi^{\Lambda}(\mathbf{x})} \mathrm{d}\mathbf{x}\right),$$

where N is the number of sites in Λ. (Assuming that each site houses one component)

Let Λ_1 and Λ_2 be disjoint finite subsets of $\mathbb{Z}^d$ and denote by N_1 and N_2 their number of sites, respectively.

For $\varepsilon \in [0,1]$, define

$$\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x}) := (1-\varepsilon)\Phi^{\Lambda_1\cup\Lambda_2}(\mathbf{x}) + \varepsilon\left[\Phi^{\Lambda_1} \oplus \Phi^{\Lambda_2}(\mathbf{x})\right] \tag{151}$$

where $\Phi^{\Lambda_1} \oplus \Phi^{\Lambda_2}(\mathbf{x}) = \Phi^{\Lambda_1}(\mathbf{x}_1) + \Phi^{\Lambda_2}(\mathbf{x}_2)$, $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \mathbb{R}^{\Lambda_1} \times \mathbb{R}^{\Lambda_2}$ is a configuration in $\mathbb{R}^{\Lambda_1\cup\Lambda_2}$.

$$\begin{aligned} \Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x}) &= (1-\varepsilon)\Phi^{\Lambda_1\cup\Lambda_2}(\mathbf{x}) + \varepsilon\left[\Phi^{\Lambda_1} \oplus \Phi^{\Lambda_2}(\mathbf{x})\right] \\ &= \Phi^{\Lambda_1}(\mathbf{x}_1) + \Phi^{\Lambda_2}(\mathbf{x}_2) + (1-\varepsilon)W(\mathbf{x}) \\ &= \Phi^{\Lambda_1\cup\Lambda_2}(\mathbf{x}) - \varepsilon W(\mathbf{x}). \end{aligned} \tag{152}$$

$$\frac{\partial}{\partial\varepsilon} \ln\left(\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}\right) = \frac{\beta\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} W(X)\, \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}}{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}} \tag{153}$$

$$\left|\frac{\partial}{\partial\varepsilon} \ln\left(\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}\right)\right| \le \frac{\beta\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} |W(\mathbf{x})|\, \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}}{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})} \mathrm{d}\mathbf{x}} \le C\beta. \tag{154}$$

Next, we integrate with respect to $\varepsilon \in [0,1]$ to get

$$\left|\xi(N+M)-\xi(N)-\xi(M)\right| \le \mathbf{b}\|W\|_{\infty}, \tag{155}$$

where N and M are the number of sites is Λ_1 and Λ_2 respectively.

Using Lemma 5, we obtain

Proposition 9. *If the Hamiltonian* Φ^{Λ} *is measurable and strongly regular in the sense of Assumption* 2, *then there exists a positive constant* C *such that*

$$\left|f_{\beta,\Lambda}-f_{\beta}\right| \le \frac{C}{|\Lambda|} \tag{156}$$

Remark 10. *In the case where the Hamiltonian is regular in the sense of* [38]. *i.e., there exists a decreasing positive function* Ψ *on the natural integers such that*

$$\sum_{i\in Z^d} \Psi(|i|) < \infty. \tag{157}$$

Furthermore, if Λ_1 *and* Λ_2 *are disjoint finite subsets of* $\mathbb{Z}^d$ *and* $\mathbf{x}=(\mathbf{x}_1,\mathbf{x}_2)\in\mathbb{R}^{\Lambda_1}\times\mathbb{R}^{\Lambda_2}$ *is a configuration in* $\mathbb{R}^{\Lambda_1\cup\Lambda_2}$,

$$\Phi^{\Lambda_1\cup\Lambda_2}(\mathbf{x}) = \Phi^{\Lambda_1}(\mathbf{x}_1)+\Phi^{\Lambda_2}(\mathbf{x}_2)+W(\mathbf{x}), \tag{158}$$

where W *is not necessarily bounded but satisfies*

$$|W(\mathbf{x})| \le \sum_{i\in\Lambda_1}\sum_{j\in\Lambda_2}\frac{\Psi(|j-i|)}{2}\left(x_i^2+x_j^2\right). \tag{159}$$

Using the logarithmic derivative approach as above, we have

$$\begin{aligned}
&\left|\frac{\partial}{\partial\varepsilon}\ln\left(\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}} \mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}\right)\right| \\
&\le \frac{\beta\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}|W(\mathbf{x})|\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}}{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}} \\
&\le \beta\sum_{i\in\Lambda_1}\sum_{j\in\Lambda_2}\frac{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}\frac{\Psi(|j-i|)}{2}\left(x_i^2+x_j^2\right)\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}}{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}} \\
&= \beta\sum_{i\in\Lambda_1}\sum_{j\in\Lambda_2}\left\langle g_{ij}\right\rangle_{\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}},
\end{aligned} \tag{160}$$

where

$$g_{ij} = \frac{\Psi(|j-i|)}{2}\left(x_i^2+x_j^2\right), \tag{161}$$

and

$$\langle\cdot\rangle_{\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}} := \frac{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}\cdot\,\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}}{\int_{\mathbb{R}^{\Lambda_1\cup\Lambda_2}}\mathrm{e}^{-\beta\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}(\mathbf{x})}\mathrm{d}\mathbf{x}}. \tag{162}$$

To estimate $\left\langle g_{ij}\right\rangle_{\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}}$, *one may use the Witten-Laplacian formalism* [8] [29] [31] [33] *under additional assumptions on the Hamiltonian. Indeed, let* $\mathbf{v}$ *be the solution of*

$$\nabla g_{ij} = \left(-\boldsymbol{\Delta} + \nabla \Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)} \cdot \nabla\right)\mathbf{v} + \mathbf{Hess}\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}\mathbf{v}, \tag{163}$$

Under the existence of solution assumptions on Φ^{Λ} (*see* [29] *and* [30]), *one can see that* $\mathbf{v}$ *is also a solution of the system*

$$g_{ij} = \langle g_{ij} \rangle_{\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}} + \mathbf{v} \cdot \nabla \Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)} - div\mathbf{v}. \tag{164}$$

It turns out that if 0 *is a critical point of* Φ^{Λ} *for all* Λ *then*

$$\langle g_{ij} \rangle_{\Phi_{\varepsilon}^{(\Lambda_1,\Lambda_2)}} = div\mathbf{v}(0). \tag{165}$$

The problem is now reduced to find suitable estimate for $\mathrm{div}\mathbf{v}(0)$. *This will be the topic of further investigation. Some possible ideas may be found in* [6] *and* [29].

5. Conclusion

We took advantage of the Witten Laplacian formalism to provide a direct (cluster expansion-free method) for calculating the higher derivatives of the free energy. The discrete convolution formula obtained in Proposition 2 gives an implicit relationship between the higher derivatives of the free energy and the moments of the source term g in the form of a discrete convolution. We used the Cauchy formula for the product of two series to determine the convergence of the power series of the free energy with respect to the corresponding thermodynamic parameter. However, we believe that a more appropriate discrete deconvolution transform may result in a better formula of the n^{th} derivative of the free energy. This issue is currently being investigated. The approach taken in this paper provides a framework for dealing with one of the limitations mentioned in [8]. Indeed, the results in [8] are restricted to unbounded one dimensional models with quadratic interactions. The authors pointed out that the extension of their results about the decay of correlations and mixing properties to more general interactions is left as an open problem. Because of the relationship that exists between the higher derivatives of the free energy and the truncated correlations, our formula may be used to provide an extension of the results obtained in [8].

Acknowledgements

I would like to express my special thanks of gratitude to Dr. Haru Pinson and Prof. Thomas Kennedy at the University of Arizona.

Availability of Data

The author confirms that the data supporting the results of this paper are available within the article and the references.

Funding and/or Conflicts of interests/Competing interests

- The author declares that this work is original and has not been published elsewhere nor is it currently under consideration for publication elsewhere.

- The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
- The author is affiliated with the University of Wollongong Network. However, this research is fully independent and is not funded by any agency.

References

[1] Pulvirenti, E. and Tsagkarogiannis, D. (2012) Cluster Expansion in the Canonical Ensemble. *Communications in Mathematical Physics*, **316**, 289-306. https://doi.org/10.1007/s00220-012-1576-y

[2] Pulvirenti, E. and Tsagkarogiannis, D. (2015) Finite Volume Corrections and Decay of Correlations in the Canonical Ensemble. *Journal of Statistical Physics*, **159**, 1017-1039. https://doi.org/10.1007/s10955-015-1207-z

[3] Cammarota, C. (1982) Decay of Correlations for Infinite Range Interactions in Unbounded Spin Systems. *Communications in Mathematical Physics*, **85**, 517-528. https://doi.org/10.1007/BF01403502

[4] Kotecky, R. (2006) Cluster Expansion. In: Francoise, J.-P., Naber, G.L. and Tsou, S.T., Eds., *Encyclopedia of Mathematical Physics*, Vol. 1, Elsevier, Oxford, 531-536.

[5] Ueltschi, D. (2004) Cluster Expansions and Correlation Functions. *Moscow Mathematical Journal*, **4**, 511-522. https://doi.org/10.17323/1609-4514-2004-4-2-511-522

[6] Minlos, R.A. (2000) Introduction to Mathematical Statistical Physics. American Mathematical Society, Providence. https://doi.org/10.1090/ulect/019

[7] Gallavotti, G. (1999) Statistical Mechanics: A Short Treatise. Springer Verlag, Berlin. https://doi.org/10.1007/978-3-662-03952-6

[8] Kwon, Y. and Menz, G. (2019) Decay of Correlations and Uniqueness of the Infinite-Volume Gibbs Measure of the Canonical Ensemble of 1d-Lattice Systems. *Journal of Statistical Physics*, **176**, 836-872. https://doi.org/10.1007/s10955-019-02324-1

[9] Yang, C.N. and Lee, T.D. (1952) Statistical Theory of Equations of State and Phase Transition I. Theory of Condensation. *Physical Review*, **87**, 404-409. https://doi.org/10.1103/PhysRev.87.404

[10] Bricmont, J., Lebowitz, J.L. and Pfister, C.E. (1980) Low Temperature Expansion for Continuous Spin Ising Models. *Communications in Mathematical Physics*, **78**, 117-135. https://doi.org/10.1007/BF01941973

[11] Dobrushin, R.L. (1986) Induction on Volume and No Cluster Expansion. In: Mebkhout, M. and Seneor, R., Eds., *VIII International Congress on Mathematical Physics*, World Scientific, Singapore, 73-91.

[12] Dobrushin, R.L. and Sholsmann, S.B. (1985) Completely Analytical Gibbs Fields. In: Fritz, J., Jaffe, A. and Szasz, D., Eds., *Statistical Mechanics and Dynamical Systems*, Birkhauser, Boston, 371-403. https://doi.org/10.1007/978-1-4899-6653-7_21

[13] Dobrushin, R.L. and Sholsmann, S.B. (1987) Completely Analytical Interactions: Constructive Description. *Journal of Statistical Physics*, **46**, 983-1014. https://doi.org/10.1007/BF01011153

[14] Duneau, M., Iagolnitzer, D. and Souillard, B. (1973) Decrease Properties of Truncated Correlation Functions and Analyticity Properties for Classical Lattice and Continuous Systems. *Communications in Mathematical Physics*, **31**, 191-208. https://doi.org/10.1007/BF01646265

[15] Duneau, M., Iagolnitzer, D. and Souillard, B. (1974) Strong Cluster Properties for Classical Systems with Finite Range Interaction. *Communications in Mathematical Physics*, **35**, 307-320. https://doi.org/10.1007/BF01646352

[16] Duneau, M., Iagolnitzer, D. and Souillard, B. (1975) Decay of Correlations for Infinite Range Interactions. *Journal of Mathematical Physics*, **16**, 1662-1666. https://doi.org/10.1063/1.522734

[17] Glimm, J. and Jaffe, A. (1985) Expansion in Statistical Physics. *Communications on Pure and Applied Mathematics*, **38**, 613-630. https://doi.org/10.1002/cpa.3160380511

[18] Glimm, J. and Jaffe, A. (1981) Quantum Physics. A Functional Integral Point of View. Springer, New York. https://doi.org/10.1007/978-1-4684-0121-9

[19] Israel, R.B. (1976) High Temperature Analyticity in Classical Lattice Systems. *Communications in Mathematical Physics*, **50**, 245-257. https://doi.org/10.1007/BF01609405

[20] Kotecky, R. and Preiss, D. (1986) Cluster Expansions for Abstract Polymers Models. *Communications in Mathematical Physics*, **103**, 491-498. https://doi.org/10.1007/BF01211762

[21] Kunz, H. (1978) Analyticity and Clustering Proporties of Unbounded Spin Systems. *Communications in Mathematical Physics*, **59**, 53-69. https://doi.org/10.1007/BF01614154

[22] Lebowitz, J.L. (1972) Bounds on the Correlations and Analyticity Properties of Ising Spin Systems. *Communications in Mathematical Physics*, **28**, 313-321. https://doi.org/10.1007/BF01645632

[23] Lebowitz, J.L. (1975) Uniqueness, Analyticity and Decay Properties of Correlations in Equilibrium Systems. *International Symposium on Mathematical Problems in Theoretical Physics*, Kyoto, 23-29 January 1975, 68-80. https://doi.org/10.1007/BFb0013358

[24] Malyshev, V.A. (1980) Cluster Expansions in Lattice Models of Statistical Physics and the Quantum Theory of Fields. *Russian Math Surveys*, **35**, 23-53. https://doi.org/10.1070/RM1980v035n02ABEH001622

[25] Malyshev, V.A. and Milnos, R.A. (1985) Gibbs Random Fields: The Method of Cluster Expansions. Nauka, Moscow. (In Russian)

[26] Prakash, C. (1983) High Temperature Differentiability of Lattice Gibbs States by Dobrushin Uniqueness Techniques. *Journal of Statistical Physics*, **31**, 169-228. https://doi.org/10.1007/BF01010929

[27] Ott, S. (2020) Weak Mixing and Analyticity of the Pressure in the Ising Model. *Communications in Mathematical Physics*, **377**, 675-696. https://doi.org/10.1007/s00220-019-03606-1

[28] Kac, M. and Luttinger, J.M. (1973) A Formula for the Pressure in Statistical Mechanics. *Journal of Mathematical Physics*, **14**, 583. https://doi.org/10.1063/1.1666362

[29] Helffer, B. and Sjostrand, J. (1994) On the Correlation for Kac-Like Models in the Convex Case. *Journal of Statistical Physics*, **74**, 147-187. https://doi.org/10.1007/BF02186817

[30] Jon, J. (2000) On Spectral Properties of Witten-Laplacians, Their Range of Projections and Brascamp-Lieb Inequality. *Integral Equations Operator Theory*, **36**, 288-324. https://doi.org/10.1007/BF01213926

[31] Bodineau, T. and Helffer, B. (1999) The Log-Sobolev Inequality for Unbounded

Spin Systems. *Journal of Functional Analysis*, **166**, 168-178. https://doi.org/10.1006/jfan.1999.3419

[32] Witten, E. (1982) Supersymmetry and Morse Theory. *Journal of Differential Geometry*, **17**, 661-692. https://doi.org/10.4310/jdg/1214437492

[33] Sjostrand, J. (1996) Correlation Asymptotics and Witten Laplacians. *Algebra and Analysis*, **8**, 160-191.

[34] Brascamp, H. and Lieb, E.H. (1976) On Extensions of the Brunn-Minkowski and Prekopa-Leindler Theorems Including Inequalities for Log Concave Functions, and with Application to the Diffusion Equation. *Journal of Functional Analysis*, **22**, 366-389. https://doi.org/10.1016/0022-1236(76)90004-5

[35] Kac, M. (1966) Mathematical Mechanism of Phase Transitions. Gordon & Breach, New York.

[36] Ruelle, D. (1969) Statistical Mechanics, Mathematical Physics Monograph Series. Benjamin, New York.

[37] Fischer, M. and Lebowitz, J. (1970) Asymptotic Free Energy of a System with Periodic Boundary Conditions. *Communications in Mathematical Physics*, **19**, 251-272. https://doi.org/10.1007/BF01646633

[38] Ruelle, D. (1976) Probability Estimates for Continuous Spin Systems. *Communications in Mathematical Physics*, **50**, 189-194. https://doi.org/10.1007/BF01609400