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A UNIFORM CONVEXITY METHOD FOR ESTIMATING CORRELATIONS AND CALCULATING THE DERIVATIVES OF THE FREE ENERGY IN LATTICE GAS MODELS OF KAC TYPE

Abstract. In this paper, we propose a uniform convexity assumption that will lead to a direct proof of the decay of correlations. We also discuss its consequence on the log-Sobolev inequality along with a direct method for calculating the derivatives of the free energy in certain classical unbounded lattice models.

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1 Background introduction on the Witten–Laplacians

In 1982, Edward Witten published the paper [32] on supersymmetry and Morse theory; to relate some invariants of a Riemannian manifold $\mathbf{M}$ with some indices of a Morse function $\Phi \in C^\infty(\mathbf{M})$, he introduced the Witten derivative $\mathbf{d}_\Phi$ and the Witten coderivative $\mathbf{d}_\Phi^*$ by simply setting

$$\mathbf{d}_\Phi = \mathbf{e}^{-\frac{\Phi}{2}}\mathbf{d}\mathbf{e}^{\frac{\Phi}{2}} \text{ and } \mathbf{d}_\Phi^* = \mathbf{e}^{\frac{\Phi}{2}}\mathbf{d}^*\mathbf{e}^{-\frac{\Phi}{2}},$$

where $\mathbf{d}$ and $\mathbf{d}^*$ are the exterior derivative and exterior coderivative, respectively. The Witten Laplacian is then defined to be the associated second order operator

$$\mathbf{W}_\Phi = (\mathbf{d}_\Phi + \mathbf{d}_\Phi^*)^2 = \mathbf{d}_\Phi\mathbf{d}_\Phi^* + \mathbf{d}_\Phi^*\mathbf{d}_\Phi$$

acting on the exterior algebra bundle of the cotangent bundle of M as the standard Laplacian does.

Choosing a local orthonormal frame field $\mathbf{e}_1, \ldots, \mathbf{e}_d$ and denoting by $\mathbf{e}^1, \ldots, \mathbf{e}^d$ its dual coframe field, $\mathbf{d}$ and $\mathbf{d}^*$ could be easily represented in terms of the Riemannian connection $\boldsymbol{\nabla}$ as

$$\mathbf{d} = \mathbf{e}^i \wedge \boldsymbol{\nabla}_{e_i} \text{ and } \mathbf{d}^* = -\mathbf{i}(\mathbf{e}_j)\boldsymbol{\nabla}_{ej},$$

where $\mathbf{i}$ denotes the interior product. Here and in the rest of this section, we use the Einstein summation convention, namely, an index occurring twice in a product is to be summed from 1 up to the space dimension. Consequently, we have

$$\mathbf{d}_\Phi = \mathbf{e}^i \wedge \boldsymbol{\nabla}_{e_i} + \mathbf{e}^i\,\frac{\Phi_{;\,i}}{2} \text{ and } \mathbf{d}_\Phi^* = -\mathbf{i}(\mathbf{e}_j)\boldsymbol{\nabla}_{e_j} + \mathbf{i}(\mathbf{e}_j)\,\frac{\Phi_{;\,i}}{2},$$

where $\Phi_{;\,i_1 i_2 \cdots}$ denote the components of multiple covariant differentiation relative to the local frame field $\mathbf{e}_1, \ldots, \mathbf{e}_d$

$$\Phi_{;\,ij} = \boldsymbol{\nabla}_{\mathbf{e}_j}\nabla_{\mathbf{e_i}}\Phi - \nabla_{\nabla_{\mathbf{e}_j}\mathbf{e}_i}\Phi.$$

Since $\mathbf{e}^i \wedge \boldsymbol{\nabla}_{e_i}$ and $\mathbf{i}(\mathbf{e}_j)\boldsymbol{\nabla}_{ej}$ do not depend on the choice of the local orthonormal frame and coframe field, we may assume that $\mathbf{e}_1, \ldots, \mathbf{e}_d$ come from a normal coordinate centered at an arbitrary point and, consequently, have

$$\boldsymbol{\nabla}_{\mathbf{e}_j}\mathbf{e}^i \wedge = \boldsymbol{\nabla}_{\mathbf{e}_i}\mathbf{i}(\mathbf{e}_j) = 0.$$

Now, using the fact that

$$\mathbf{e}^i \wedge \mathbf{i}(\mathbf{e}_j) + \mathbf{i}(\mathbf{e}_j)\mathbf{e}^i \wedge = \delta_{ij},$$

we have

$$\mathbf{W}_\Phi^{(p)} = \boldsymbol{\Delta} - \frac{\Phi_{;\,i}\Phi_{;\,i}}{4} + \frac{\Phi_{;\,ij}}{2}\,(\mathbf{e}^i \wedge \mathbf{i}(\mathbf{e}_j) - \mathbf{i}(\mathbf{e}_j)\mathbf{e}^i \wedge).$$

In the case of $\mathbb{R}^n$, where covariant differentiation becomes a standard differentiation, the Witten Laplacian on 0-forms acting on a smooth function f gives

$$\mathbf{W}_\Phi^{(0)} f = -\boldsymbol{\Delta} f - \frac{\Phi_{x_i}\Phi_{x_i}}{4}\,f - \frac{\Phi_{x_i x_i}}{2}\,f = \Big(-\boldsymbol{\Delta} + \frac{|\boldsymbol{\nabla}\Phi|^2}{4} - \frac{\boldsymbol{\Delta}\Phi}{2} \Big) f.$$

The Witten Laplacian on one-forms acting on a one form

$$u = u^k(x)dx^k$$

gives

$$\mathbf{W}_\phi^{(1)} u = \boldsymbol{\Delta} u - \frac{\phi_{x_i}\phi_{x_i}}{4}\,u - \frac{\phi_{x_i x_i}}{2}\,u + 2\,\frac{\phi_{x_k x_i}}{2}\,dx^i \wedge \mathbf{i}_{\frac{\partial}{\partial x_k}} u.$$

Identifying one-forms with vector fields in $\mathbb{R}^n$, we obtain

$$\mathbf{W}_\Phi^{(1)}\mathbf{u} = \Big(-\boldsymbol{\Delta} + \frac{|\boldsymbol{\nabla}\Phi|^2}{4} - \frac{\boldsymbol{\Delta}\Phi}{2} \Big) \otimes \mathbf{u} + \mathbf{Hess}\,\Phi\mathbf{u}.$$

The tensor notation simply means that the operator $-\mathbf{\Delta} + \frac{|\mathbf{\nabla}\Phi|^2}{4} - \frac{\mathbf{\Delta}\Phi}{2}$ acts diagonally on each component of the vector field $\mathbf{u}$. Let us also point out that the identification between the forms and vectors fields is a common practice in Riemaniann geometry and is done via themetric tensor.

As first observed by Bernard Helffer and Johannes Sjötrand [16, 30], these Laplacians provide new methods for solving problems coming from Statistical Mechanics. The methods are generally based on the analysis of the differential operators

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

and

$$A_\Phi^{(1)} := A_\Phi^{(0)} \otimes Id + \mathbf{Hess}\,\Phi.$$

These two elliptic differential operators for which a Fredholm theory can be developed [18] are equivalent to Witten's Laplacians $W_\Phi^{(0)}$ and $W_\Phi^{(1)}$, respectively, where

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

and

$$\mathbf{W}_\Phi^{(1)} = \Big(-\mathbf{\Delta} + \frac{|\mathbf{\nabla}\Phi|^2}{4} - \frac{\mathbf{\Delta}\Phi}{2} \Big) \otimes \mathbf{I} + \mathbf{Hess}\,\Phi.$$

Indeed, it only suffices to observe that

$$W_\Phi^{(\,\cdot\,)} = e^{-\Phi/2} \circ A_\Phi^{(\,\cdot\,)} \circ e^{\Phi/2}$$

and the map

$$\begin{gathered} U_\Phi : L^2(\mathbb{R}^\Lambda) \to L^2(\mathbb{R}^\Lambda, e^{-\Phi} dx), \\ u \mapsto e^{\frac{\Phi}{2}} u. \end{gathered}$$

These operators are used to get direct methods for integrals of the type that appear in Statistical Mechanics and Euclidean Field Theory [1–4, 7]. As a simple illustration, suppose one is interested in the study of the mean value $\langle g \rangle_\Lambda$, where

$$\langle g \rangle_\Lambda = \int g \, d\mu_\Lambda$$

and

$$d\mu_\Lambda = \frac{e^{-\Phi}\, dx}{\int e^{-\Phi}\, dx}\,.$$

For a suitable smooth function g, one can first solve the equation

$$\mathbf{\nabla} g = (-\mathbf{\Delta} + \mathbf{\nabla}\Phi \cdot \mathbf{\nabla})\mathbf{v} + \mathbf{Hess}\,\Phi\mathbf{v},$$

where the solution $\mathbf{v}$ is a suitable C^∞-vector field and the operator $(-\mathbf{\Delta} + \mathbf{\nabla}\Phi \cdot \mathbf{\nabla})$ acts diagonally on each component of $\mathbf{v}$. Under certain assumptions on the Hamiltonian Φ, one can see that $\mathbf{v}$ is also a solution of the system

$$g = \langle g \rangle_\Lambda + \mathbf{v} \cdot \mathbf{\nabla}\Phi - \operatorname{div} \mathbf{v}.$$

It turns out that if $g(0) = 0$ and 0 is a critical point of Φ, then

$$\langle g \rangle_\Lambda = \operatorname{div} \mathbf{v}(0).$$

The study of the thermodynamic properties of the mean value is then reduced to estimating the derivatives of the solution $\mathbf{v}$.

Numerous techniques have been developed for the study of integrals associated to the equilibrium Gibbs state for certain unbounded spins systems [1–4, 15, 16, 24, 25, 30, 34]. One of the most striking result is the Helffer–Sjötrand formula which is an exact formula for the covariance of two functions in terms of the Witten Laplacian on one-forms leading to sophisticated methods for estimating the two-point correlation functions. This formula is in some sense a stronger and more flexible version of the Brascamp-Lieb inequality [5]. The formula can be written as

$$\mathbf{cov}\,(f,g) = Z^{-1} \int \big(A_\Phi^{(1)^{-1}} \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} g\big) e^{-\Phi(x)}\,dx,$$

where Z is a normalization constant.

To understand the idea behind the formula mentioned above, let us denote by $\langle f\rangle_\Lambda$ the mean value of f with respect to the measure

$$Z^{-1} e^{-\Phi(x)}\,dx,$$

the covariance of two functions f and g is defined by

$$\mathbf{cov}\,(f,g) = \Big\langle \big(f - \langle f\rangle_\Lambda\big)\big(g - \langle g\rangle_\Lambda\big)\Big\rangle.$$

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

$$\mathbf{cov}\,(f,g) = \big\langle \boldsymbol{\nabla} g \cdot \mathbf{w}\big\rangle_{L^2(\mathbb{R}^n,\mathbb{R}^n;e^{-\Phi}\,dx)}$$

(as in the case of the Brascamp–Lieb inequality) for a suitable vector field $\mathbf{w}$, after observing that $\boldsymbol{\nabla} g = \boldsymbol{\nabla}(g - \langle g\rangle)$ we get

$$\mathbf{cov}\,(f,g) = Z^{-1} \int \big(g - \langle g\rangle_\Lambda\big)(\boldsymbol{\nabla}\Phi - \boldsymbol{\nabla}) \cdot \mathbf{w} e^{-\Phi(x)}\,dx.$$

This leads to the question of solving the equation

$$f - \langle f\rangle_\Lambda = (\boldsymbol{\nabla}\Phi - \boldsymbol{\nabla}) \cdot \mathbf{w}.$$

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

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

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

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

and the formula is now easily seen.

2 Relevant unbounded models

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 $X = (x_i)_{i\in\Lambda}$ of the product space $\Omega = \mathbb{R}^\Lambda$. This set is called the configuration space or phase space.

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

$$d\mu^\Lambda(X) = Z_\Lambda^{-1} e^{-\Phi(X)}\,dX,$$

$Z > 0$ is a normalization constant,

$$Z = Z_\Lambda = \int_{\mathbb{R}^\Lambda} e^{-\Phi(X)}\,dX.$$

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

(1) $\lim_{|X|\to\infty} |\nabla\Phi(X)| = \infty$.

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

(3) For $|\alpha| \geq 1$,

$$|\partial^\alpha\Phi(X)| \leq C_\alpha\big(1 + |\nabla\Phi(X)|^2\big)^{1/2} \text{ for some } C_\alpha > 0.$$

(4) There exist $w > 0$, $C > 0$ such that

$$X \cdot \nabla\Phi \geq C|X|^{1+w} \text{ for all } |X| \geq \frac{1}{C}.$$

Here and in what follows, $\alpha = (\alpha_i)_{i=1,\dots,m} \in \mathbb{Z}_+^{|\Lambda|}$ denotes a multiindex. We set $|\alpha| = \sum\limits_{i=1}^m \alpha_i$, $\alpha! = \alpha_1!\cdots\alpha_m!$. If $\beta = (\beta_i)_{i=1,\dots,m} \in \mathbb{Z}_+^{|\Lambda|}$ and $\beta_j \leq \alpha_j$ for all $j = 1,\dots,m$, then we write $\beta \leq \alpha$. For $\alpha, \beta \in \mathbb{Z}_+^{|\Lambda|}$ such that $\beta \leq \alpha$, we put $\binom{\alpha}{\beta} = \frac{\alpha!}{\beta!\,(\alpha-\beta)!}$. If $\alpha = (\alpha_i)_{i=1,\dots,m} \in \mathbb{Z}_+^{|\Lambda|}$ and $X \in \mathbb{R}^d$, we write

$$X^\alpha = \prod_{i=1}^m x^{\alpha_i}$$

and

$$\partial^\alpha = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_m}}{\partial x_m^{\alpha_m}}.$$

The Hessian of the Hamiltonian Φ is denoted by $\mathbf{Hess}\,\Phi$. If i and j are two nearest neighbor sites in $\mathbb{Z}^d$, we write $i \sim j$. Finally, $d(i,j)$ denotes the Manhattan distance of two lattice sites $i, j \in \mathbb{Z}^d$.

Throughout this paper, we assume that the source function g satisfies

$$|\partial^\alpha \nabla g| \leq C_\alpha, \quad \forall\, \alpha \in \mathbb{N}^{|\Lambda|}. \tag{2.1}$$

3 Decay of correlations without using 1-dimensional Witten Laplacians

In [4, 15], the authors studied the existence of uniform logarithmic Sobolev inequalities by using Zegarlinski criterion. Because of the difficulty in having a uniform lower bound for the spectrum of the Witten Laplacian, they considered the models whose Hamiltonians are of the form

$$\Phi_\Lambda(X) = \sum_{j\in\Lambda}\phi(x_j) + \frac{\mathcal{J}}{2}\sum_{\substack{(\{i\}\cup\{k\})\cap\Lambda\neq\varnothing,\\ j\sim k}} |z_j - z_k|^2,$$

under the condition of strict convexity at ∞ on ϕ. The authors first discussed uniform estimates for a family of 1-dimensional Witten Laplacians and then explained how the result may be generalized to higher dimensions. In [4], Helffer and Bodineau gave a proof of the log–Sobolev inequality for similar models but under weaker assumptions on ϕ.

We consider classical continuous models whose Hamiltonians satisfy the assumptions (1)–(4) above. This is a generalized version of the type of Hamiltonians used in [4] and [15].

We discuss a direct method for proving uniform decay of correlations without using the one-dimensional cases as discussed in [4] and [15]. As a consequence, we give a proof of the logarithmic Sobolev inequality that does not use the one-dimensional Witten Laplacians. Our method is based on a weak uniform strict convexity on the Hamiltonian.

3.1 The decay of correlations

Definition. The lattice support, S_g of a function g on $\mathbb{R}^\Lambda$, is defined here to be the smallest subset Γ of $\Lambda \subset \mathbb{Z}^d$ for which g can be written as a function of x_j alone with $j \in \Gamma$. For instance, if $g = x_i$, $S_g = \{i\}$.

Lemma 3.1. *Suppose that there exist $\rho_\Lambda \geq 1$ and $\delta_0 > 0$ such that*

$$M\,\mathbf{Hess}\,\Phi M > \rho_\Lambda, \quad \textit{where } M \textit{ is the diagonal matrix } M = (e^{-\delta_0 d(i,S_g)})_{i\in\Lambda}.$$

Then

$$MA_\Phi^{(1)}M > \rho_\Lambda \geq 1.$$

Proof. It follows from Theorem 1.6 – [18] (see also [30]) that the operator

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

in the sense of the operator inequalities, i.e.,

$$A_\Phi^{(1)} - \mathbf{Hess}\,\Phi > 0.$$

Now, using classical results on the operator inequality (see [28]), we have

$$MA_\Phi^{(1)}M > M\,\mathbf{Hess}\,\Phi M > \rho_\Lambda. \qquad \square$$

Proposition 3.1. *Suppose that the Hamiltonian Φ satisfies the assumptions* (1)–(4) *above and there exist $\rho_\Lambda \geq 1$ and $\delta_0 > 0$ such that*

$$M\,\mathbf{Hess}\,\Phi M > \rho_\Lambda, \quad \textit{where } M \textit{ is the diagonal matrix } M = (e^{-\delta_0 d(i,S_g)})_{i\in\Lambda}.$$

Let gand h be smooth functions on $\mathbb{R}^\Gamma$, and $\mathbb{R}^{\Gamma'}$, where Γ and $\Gamma' \subsetneqq \Lambda$ with $\Gamma \cap \Gamma' = \varnothing$ denote, respectively, the support of g and h, and assume that g and h satisfy (2.1)*. Then*

$$|\mathbf{cov}\,(g,h)| < Ce^{-\delta_0 d(S_h,S_g)},$$

where C is a positive constant that does not depend on Λ, but possibly depends on the size of the supports of g and h.

Proof. There exists $c_1 > 0$ such that

$$A_\Phi^{(1)} \geq c_1.$$

Moreover, we have the Helffer–Sjötrand formula

$$\mathbf{cov}\,(g,h) = Z^{-1} \int\limits_{\mathbb{R}^\Lambda} \big(A_\Phi^{(1)^{-1}} \mathbf{\nabla} g \cdot \mathbf{\nabla} h\big) e^{-\Phi(x)}\,dx, \tag{3.1}$$

where

$$Z = \int\limits_{\mathbb{R}^\Lambda} e^{-\Phi(x)}\,dx.$$

Multiplying the equation

$$A_\Phi^{(1)} \mathbf{\nabla} f = \mathbf{\nabla} g$$

by M, we obtain

$$MA_\Phi^{(1)} \mathbf{\nabla} f = M\mathbf{\nabla} g \Longleftrightarrow MA_\Phi^{(1)} MM^{-1}\mathbf{\nabla} f = M\mathbf{\nabla} g.$$

Taking the inner product with $M^{-1}\mathbf{\nabla} f$ on both sides of this last equality and integrating with respect to $Z^{-1}e^{-\Phi}\,dx$, we obtain

$$\big\langle MA_\Phi^{(1)} MM^{-1}\mathbf{\nabla} f, M^{-1}\mathbf{\nabla} f\big\rangle_\Lambda = \big\langle M\mathbf{\nabla} g, M^{-1}\mathbf{\nabla} f\big\rangle_\Lambda.$$

Note that this inner product is well defined under the assumptions (1)–(4) above on the Hamiltonian. Now, using the fact that $M\,\mathbf{Hess}\,\Phi M > \rho_\Lambda \geq 1$, we have

$$\langle MA_\Phi^{(1)}MM^{-1}\nabla f, M^{-1}\nabla f\rangle_\Lambda \geq \rho_\Lambda \|M^{-1}\nabla f\|_\Phi^2.$$

Thus using the Cauchy–Schwartz inequality on the right-hand side, we get

$$\rho_\Lambda \|M^{-1}\nabla f\|_\Phi^2 \leq \|M\nabla g\|_\Phi \|M^{-1}\nabla f\|_\Phi,$$

where

$$\rho_\Lambda \geq 1 \;\text{ and }\; \|u\|_\Phi := \Big(Z^{-1} \int\limits_{\mathbb{R}^\Lambda} |u|^2 e^{-\Phi(x)}\,dx \Big)^{1/2}.$$

If $\|M^{-1}\nabla f\|_\Phi = 0$, then $A_\Phi^{(1)^{-1}}\nabla g = 0$ and the result follows. If $\|M^{-1}\nabla f\|_\Phi \neq 0$, then we have

$$\|M^{-1}\nabla f\|_\Phi \leq \|M\nabla g\|_\Phi.$$

Equivalently,

$$\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} e^{2\delta_0 d(i,S_g)} f_{x_i}^2 e^{-\Phi(x)}\,dx \leq \int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} e^{-2\delta_0 d(i,S_g)} g_{x_i}^2 e^{-\Phi(x)}\,dx. \tag{3.2}$$

Now, using the fact that $g_{x_i} = 0$ if $i \notin S_g$, $d(i,S_g) = 0$ if $i \in S_g$ and (2.1), we obtain

$$\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} e^{2\delta_0 d(i,S_g)} f_{x_i}^2 e^{-\Phi(x)}\,dx < ZC_g,$$

where C_g is a positive constant that depends only on the size of the support of g. Thus we finally get

$$Z^{-1}\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} e^{2\delta_0 d(i,S_g)} f_{x_i}^2 e^{-\Phi(x)}\,dx < C_g.$$

Now, we use formula (3.1) to get

$$\begin{aligned}
|\mathbf{cov}\,(g,h)| &= Z^{-1}\Big| \int\limits_{\mathbb{R}^\Lambda} \nabla f\cdot\nabla h e^{-\Phi(x)}\,dx \Big| \leq Z^{-1}\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} \big| f_{x_i}(x) e^{\delta_0 d(i,S_g)} e^{-\delta_0 d(i,S_g)} h_{x_i}\big| e^{-\Phi(x)}\,dx \\
&\leq Z^{-1}\int\limits_{\mathbb{R}^\Lambda} \Big(\sum_{i\in\Lambda} f_{x_i}^2(x) e^{2\delta_0 d(i,S_g)}\Big)^{1/2} \Big(\sum_{i\in S_h} h_{x_i}^2(x) e^{-2\delta_0 d(i,S_g)}\Big)^{1/2} e^{-\Phi(x)}\,dx \\
&\leq Z^{-1}\Big[\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in\Lambda} f_{x_i}^2(x) e^{2\delta_0 d(i,S_g)}\,d\mu^\Lambda(x)\Big]^{1/2} \Big[\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in S_h} h_{x_i}^2(x) e^{-2\delta_0 d(i,S_g)}\,d\mu^\Lambda(x)\Big]^{1/2} \\
&< \sqrt{C_g}\Big[Z^{-1}\int\limits_{\mathbb{R}^\Lambda} \sum_{i\in S_h} h_{x_i}^2(x)\,d\mu^\Lambda(x)\Big]^{1/2} e^{-\delta_0 d(S_h,S_g)} < \sqrt{C_g}\sqrt{C_h}\, e^{-\delta_0 d(S_h,S_g)}.
\end{aligned}$$

Here, C_g and C_h are independent of Λ. They depend only on the size of the support of g and h, respectively. □

One can see that our method in the proof given above allows us to avoid having ρ_Λ to be involved in the constant in the right-hand side. Thus we obtain the following mixing condition.

Corollary 3.1. *Suppose that the Hamiltonian Φ satisfies the assumptions* (1)–(4) *above and there exist $\rho_\Lambda \geq 1$ and $\delta_0 > 0$ such that*

$$M\,\mathbf{Hess}\,\Phi M > \rho_\Lambda, \;\text{ where } M \text{ is the diagonal matrix } M = (e^{-\delta_0 d(i,S_g)})_{i\in\Lambda}.$$

Let g and h be smooth functions on $\mathbb{R}^\Gamma$ and $\mathbb{R}^{\Gamma'}$, where Γ and $\Gamma' \subsetneqq \Lambda$ with $\Gamma\cap\Gamma' = \varnothing$ denote, respectively, the support of g and h, and assume that g and h satisfy (2.1). *Then*

$$|\mathbf{cov}\,(g,h)| \leq e^{-\delta_0 d(S_h,S_g)} \|\nabla g\|_\Phi \|\nabla h\|_\Phi. \tag{3.3}$$

Corollary 3.2. *Suppose that the Hamiltonian Φ satisfies the assumptions* (1)–(4) *above and there exist $\rho_\Lambda \geq 1$ and $\delta_0 > 0$ such that*

$$M \,\mathbf{Hess}\, \Phi M > \rho_\Lambda, \quad \text{where } M \text{ is the diagonal matrix } M = (e^{-\delta_0 d(i,S_g)})_{i\in\Lambda}.$$

Then

$$|\mathbf{cov}\,(x_i, x_j)| < Ce^{-\delta_0 d(i,j)},$$

where C is a positive constants that does not depend on Λ.

Proof. Take $g = x_i$ and $h = x_j$. □

3.2 Example of models satisfying the assumptions

Consider the cases, where the Hamiltonian is given by

$$\Phi^\Lambda(x) = \sum_{j\in\Lambda} \phi(x_j) + g(x),$$

where

- $x = (x_i)_{i\in\Lambda}$,
- $\phi \in C^2(\mathbb{R}, \mathbb{R})$ is a one particle phase on $\mathbb{R}$ with at least quadratic increase at ∞ as discussed in [4, 15],
- $g \in C^\infty(\mathbb{R}^\Gamma)$ $(\Gamma = S_g)$,
$$|\partial^\alpha \boldsymbol{\nabla} g| \leq C_\alpha, \quad \forall\, \alpha \in \mathbb{N}^{|\Lambda|}.$$
- If $C_g > 0$ is such that $|g_{x_i x_j}| \leq C_g$ and $\mathcal{K}_g = C_g(1 + |\Gamma|)$, we make the following assumption: there exists $\rho \geq 1$ such that the function $\widetilde{\phi}(t) := \phi(t) - \frac{\mathcal{K}_g}{2}\, t^2$ satisfies
$$\frac{d^2\widetilde{\phi}(t)}{dt^2} > \rho.$$

Let us now verify that

$$\Phi^\Lambda(x) = \sum_{j\in\Lambda} \phi(x_j) + g(x)$$

satisfies our main assumption, i.e., there exists $\rho_\Lambda \geq 1$ such that

$$M \,\mathbf{Hess}\, \Phi M > \rho_\Lambda, \text{ where } M = (e^{-\delta_0 d(i,S_g)})_{i\in\Lambda} \text{ for some } \delta_0 > 0.$$

The first and second derivatives of Φ^Λ give

$$\Phi^\Lambda_{x_i}(x) = \phi'(x_i) + g_{x_i}(x),$$
$$\Phi^\Lambda_{x_i x_j}(x) = \begin{cases} \phi''(x_i) + g_{x_i x_i}(x), & \\ g_{x_i x_j}(x) & \text{if } i \neq j. \end{cases}$$

Let $P = \operatorname{diag}(e^{-\xi d(i,S_g)})_{i\in\Lambda}$, $\xi > 0$. We have

$$\begin{aligned}
(P \,\mathbf{Hess}\, \Phi P x, x) &= \sum_{i\in\Lambda} \Big[(\phi''(x_i) + g_{x_i x_i}(x)) e^{-2\xi d(i,S_g)} x_i^2 + \sum_{j\in\Lambda,\, j\neq i} g_{x_i x_j}(x) e^{-\xi[d(i,S_g)+d(j,S_g)]} x_i x_j \Big] \\
&= \sum_{i\in\Lambda} \phi''(x_i) e^{-2\xi d(i,S_g)} x_i^2 + \sum_{i\in S_g} g_{x_i x_i}(x) x_i^2 + \sum_{i\in S_g} \sum_{j\in S_g,\, j\neq i} g_{x_i x_j}(x) x_i x_j \\
&\geq \sum_{i\in\Lambda} \phi''(x_i) e^{-2\xi d(i,S_g)} x_i^2 - C_g \sum_{i\in S_g} x_i^2 + \sum_{i\in S_g} \sum_{j\in S_g,\, j\neq i} g_{x_i x_j}(x) x_i x_j \\
&\geq \sum_{i\in\Lambda} \phi''(x_i) e^{-2\xi d(i,S_g)} x_i^2 - C_g \sum_{i\in\Lambda} x_i^2 + \sum_{i\in S_g} \sum_{j\in S_g,\, j\neq i} g_{x_i x_j}(x) x_i x_j \quad (S_g \subsetneq \Lambda).
\end{aligned}$$

There is Schur's Lemma (see [31]) stating that for each pair of sequence $(x_i)_{1\leq i\leq m}$ and $(y_j)_{1\leq j\leq n}$, we have the bound

$$\Big|\sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_iy_j\Big| \leq \sqrt{RC}\Big(\sum_{i=1}^{m}|x_i|^2\Big)^{1/2}\Big(\sum_{j=1}^{n}|y_j|^2\Big)^{1/2},$$

where R and C are the row sum and the column sum maxima defined by

$$R = \max_i \sum_{j=1}^{n}|c_{ij}| \ \text{ and } \ C = \max_j \sum_{i=1}^{m}|c_{ij}|.$$

Using this result, we have

$$\Big|\sum_{i\in S_g}\sum_{j\in S_g,\, j\neq i} g_{x_ix_j}(x)x_ix_j\Big| \leq \sqrt{R_\Lambda C_\Lambda}\sum_{i\in\Lambda} x_i^2,$$

where

$$R_\Lambda = \max_{i\in S_g}\sum_{j\in S_g}|g_{x_ix_j}(x)| \leq C_g|\Gamma| \ \text{ and } \ C_\Lambda = \max_{j\in\Lambda}\sum_{i\in S_g}|g_{x_ix_j}(x)| \leq C_g|\Gamma|.$$

Thus

$$\begin{aligned}(P\,\mathbf{Hess}\,\Phi P x, x) &\geq \sum_{i\in\Lambda}\phi''(x_i)e^{-2\xi d(i,S_g)}x_i^2 - C_g\sum_{i\in\Lambda}x_i^2 - C_g|\Gamma|\sum_{i\in\Lambda}x_i^2\\ &= \sum_{i\in\Lambda}\Big[\phi''(x_i)e^{-2\xi d(i,S_g)} - C_g(1+|\Gamma|)\Big]x_i^2, \ \ \forall\,\xi>0, \ \ \forall\, x\in\mathbb{R}^\Lambda.\end{aligned}$$

Hence

$$\begin{aligned}\lim_{\xi\to 0^+}(P\,\mathbf{Hess}\,\Phi P x, x) &\geq \sum_{i\in\Lambda}\big[\phi''(x_i) - \mathcal{K}_g\big]x_i^2, \ \ \forall\, x\in\mathbb{R}^\Lambda \ \ \text{(uniform limit)}\\ &> \rho\sum_{i\in\Lambda}x_i^2.\end{aligned}$$

Hence $\exists\,\delta_0>0$ such that

$$\xi\leq\delta_0 \Longrightarrow (P\,\mathbf{Hess}\,\Phi P x, x) > \rho\sum_{i\in\Lambda}x_i^2.$$

In particular, when $\xi=\delta_0$ with $M=(e^{-\delta_0 d(i,S_g)})_{i\in\Lambda}$, we have

$$(M\,\mathbf{Hess}\,\Phi P M x, x) > \rho\sum_{i\in\Lambda}x_i^2.$$

The result follows.

4 What about higher correlations?

Recall that

$$d_\Phi = e^{-\Phi/2}de^{\Phi/2} \ \text{ and } \ d_\Phi^* = e^{\Phi/2}d^*e^{-\Phi/2},$$

where d and d^* are the exterior derivative and exterior coderivative, respectively. The Witten Laplacian is then defined to be the associated second order operator

$$W_\Phi^{(k)} = (d_\Phi + d_\Phi^*)^2 = d_\Phi d_\Phi^* + d_\Phi^* d_\Phi.$$

acting on k-forms.

We now consider the operators $A_\Phi^{(k)}$ given by

$$A_\Phi^{(k)} = e^{\Phi/2}\circ W_\Phi^{(k)}\circ e^{-\Phi/2}$$

acting on the weighted spaces $L^2(\mathbb{R}^\Lambda, e^{-\Phi}\,dx, \Lambda^k\mathbb{R}^\Lambda)$ [18], the space of k-smooth forms with coefficients in $L^2(\mathbb{R}^\Lambda, e^{-\Phi}\,dx)$. The norm on this space is defined by

$$\Big\| \sum_{i_1<\cdots<i_k} f_{i_1\cdots i_k}\,dx^{i_1}\cdots dx^{i_k} \Big\|_\Phi = \Big(Z^{-1} \int\limits_{\mathbb{R}^\Lambda} \sum_{i_1<\cdots<i_k} f^2_{i_1\cdots i_k}(x) e^{-\Phi}\,dx \Big)^{1/2}.$$

If d_k denotes the differential k-form operator and d_k^* is its adjoint, we have

$$d_k A_\Phi^{(k)} = A_\Phi^{(k+1)} d_k. \tag{4.1}$$

This equality is a higher order version of $\nabla A_\Phi^{(0)} = A_\Phi^{(1)}\nabla$ which is obtained when identifying 0-forms with functions and 1-forms with vector fields.

Recall that under the assumption (1)–(4), the operators $A_\Phi^{(k)}$ are positive on $L^2(\mathbb{R}^\Lambda, e^{-\Phi}dx, \Lambda^k\mathbb{R}^\Lambda)$ $(k \geq 1)$ (see [18, Section 4.1]).

Proposition 4.1. *Let M^k be the multiplication operators on $L^2(\mathbb{R}^\Lambda, e^{-\Phi}\,dx, \Lambda^k\mathbb{R}^\Lambda)$:*

$$M^k \sum_{i_1<\cdots<i_k} f_{i_1\cdots i_k}\,dx^{i_1}\cdots dx^{i_k} := \sum_{i_1<\cdots<i_k} \delta(i_1,\dots,i_k) f_{i_1\cdots i_k}\,dx^{i_1}\cdots dx^{i_k},$$

where $\delta(i_1,\dots,i_k) = (e^{-\delta_0 d(\{i_1,\dots,i_k\},S_g)})_{i_1,\dots,i_k\in\Lambda}$ for some $\delta_0 > 0$ and $g \in C^\infty(\mathbb{R}^\Gamma)$ satisfying

$$|\partial^\alpha \boldsymbol{\nabla} g| \leq C_\alpha, \quad \forall\, \alpha \in \mathbb{N}^{|\Lambda|}.$$

Suppose that the Hamiltonian Φ satisfies the assumptions (1)–(4) above and there exist $\rho_k \geq 1$ and $\delta_0 > 0$ such that

$$M_k A_\Phi^{(k)} M_k > \rho_k \geq 1 \ \ (k \geq 1),$$

then

$$Z^{-1} \int\limits_{\mathbb{R}^\Lambda} \sum_{i_1<\cdots<i_k} f^2_{x_{i_1}\cdots x_{i_k}}(x) e^{2\delta_0 d(\{i_1,\dots,i_k\},S_g)} e^{-\Phi}\,dx \leq C_k, \tag{4.2}$$

where C_k is a positive constant independent of Λ.

Proof. The multiplication operator M_k defined on $L^2(\mathbb{R}^\Lambda, e^{-\Phi}\,dx, \Lambda^k\mathbb{R}^\Lambda)$ by

$$M_k \sum_{i_1<\cdots<i_k} f_{i_1\cdots i_k}\,dx^{i_1}\cdots dx^{i_k} := \sum_{i_1<\cdots<i_k} e^{-\delta_0 d(\{i_1,\dots,i_k\},S_g)} f_{i_1\cdots i_k}\,dx^{i_1}\cdots dx^{i_k}$$

is self-adjoint and invertible. Let f be a smooth solution of

$$A_\Phi^{(0)} f = g - \langle g\rangle_\Lambda \ \text{ in } \mathbb{R}^\Lambda.$$

Using $d_k A_\Phi^{(k)} = A_\Phi^{(k+1)} d_k$, we have

$$A_\Phi^{(k)} \nabla^k f = \nabla^k g,$$

where $\nabla^k u$ denotes the k-order Hessian of u [18]. Multiplying both sides by M_k and taking the inner product with $M_k^{-1}\nabla^k f$, we obtain

$$\big\langle M_k A_\Phi^{(k)} M_k M_k^{-1} \nabla^k f, M_k^{-1}\nabla^k f \big\rangle = \big\langle M_k \nabla^k g, M_k^{-1}\nabla^k f \big\rangle.$$

It then follows from the assumption $M_k A_\Phi^{(k)} M_k > \rho_k \geq 1$ and Cauchy–Schwartz inequality that

$$\|M_k^{-1}\nabla^k f\|_\Phi^2 \leq \rho_k \|M_k^{-1}\nabla^k f\|_\Phi^2 \leq \|M_k \nabla^k g\|_\Phi \|M_k^{-1}\nabla^k f\|_\Phi. \tag{4.3}$$

If $\|M_k^{-1}\nabla^k f\|_\Phi = 0$, then there is nothing to prove. However, if $\|M_k^{-1}\nabla^k f\|_\Phi \neq 0$, we have

$$\int_{\mathbb{R}^\Lambda} \sum_{i_1\cdots i_k} f^2_{x_{i_1}\cdots x_{i_k}}(x) e^{2\delta_0 d(\{i_1,\ldots,i_k\},S_g)} e^{-\Phi}\, dx$$
$$\leq \int_{\mathbb{R}^\Lambda} \sum_{i_1\cdots i_k} g^2_{x_{i_1}\cdots x_{i_k}}(x) e^{-2\delta_0 d(\{i_1,\ldots,i_k\},S_g)} e^{-\Phi}\, dx$$
$$= \int_{\mathbb{R}^\Lambda} \sum_{i_1\cdots i_k \in S_g} g^2_{x_{i_1}\cdots x_{i_k}}(x) e^{-2\delta_0 d(\{i_1,\ldots,i_k\},S_g)} e^{-\Phi}\, dx \leq C_{k,g}.$$

where $C_{k,g}$ is a positive constant that depends only on the support of g. □

The higher order correlation is defined as

$$\langle g_1, \ldots, g_k\rangle := \big\langle (g_1 - \langle g_1\rangle)\cdots(g_k - \langle g_k\rangle)\big\rangle. \tag{4.3}$$

Using the estimate above for the higher order Hessians of the solution f and following the same argument as in the proof of Proposition 3.1, we obtain

Proposition 4.2. *Let g_1, g_2, g_3 be smooth functions satisfying (2.1) with $S_{g_i} \cap S_{g_j} = \varnothing$ ($i,j = 1,2,3$; $i \neq j$), where S_{g_i} denotes the support of g_i. Suppose that the Hamiltonian Φ satisfies the assumptions* (1)–(4) *above and there exist $\rho_2 \geq 1$ and $\delta_0 > 0$ such that*

$$M_2 A_\Phi^{(2)} M_2 > \rho_2 \geq 1.$$

Then we have the following higher order correlations:

$$|\langle g_1, g_2, g_3\rangle| \leq C\Big[e^{-\delta_0 d(S_{g_2},S_{g_1})} + e^{-\delta_0 d(S_{g_3},S_{g_1})}\Big].$$

If $g_1 = x_i$, $g_2 = x_j$ and $g_3 = x_k$, we obtain

$$\Big|\Big\langle \big(x_i - \langle x_i\rangle\big)\big(x_j - \langle x_j\rangle\big)\big(x_k - \langle x_k\rangle\big)\Big\rangle\Big| \leq C\big[e^{-\delta_0 d(i,j)} + e^{-\delta_0 d(i,k)}\big].$$

Remark. Note that in the one-dimensional case, we obtain a stronger exponential decay in the sense that

$$d(i,j) \to \infty \Longrightarrow d(i,k) \to \infty.$$

Indeed, we have

$$i \leq j \leq k \Longrightarrow d(i,k) = d(i,j) + d(j,k) \geq d(i,j).$$

However, this is not the case in higher dimensions. Thus if $d > 1$, this exponential decay of the correlations is weaker in the sense that the decay occurs as you simultaneously pull the spins away from a fixed one.

5 Calculating the derivatives of the free energy

Phase transitions and critical points correspond to mathematical singularities in the thermodynamic potentials and other thermodynamic quantities which are related to appropriate derivatives of the free energy. For example, at the critical point of a ferromagnetic system, the spontaneous magnetization vanishes and the susceptibility diverges. It is therefore central to develop the methods for calculating derivatives of the free energy as a function of the thermodynamic parameter. The most famous result on the analyticity of the free energy is the circle theorem by Lee and Yang [33]. The Lee–Yang theorem and its variants depend on the ferromagnetic character of the interaction. There are various other ways of proving the infinite differentiability or the analyticity of the free energy for (ferromagnetic and non ferromagnetic) systems at high or low temperatures, or at large external fields. Most of them take advantage of a sufficiently rapid decay of correlations and/or cluster expansion methods. Here is a small sample of relevant references: Bricmont, Lebowitz and Pfister [6], Dobroshin [7], Dobroshin and Sholsman [8, 9], Duneau et al [10–12], Glimm and Jaffe [13, 14], Israel [17], Kotecky and Preiss [20], Kunz [21], Lebowitz [22,23], Malyshev [26], Malychev and Milnos [27] and Prakash [29]. To our knowledge, the only available exact formula of the free energy was obtained by M. Kac and J. M. Luttinger [19]. Kac–Luttinger formula has a limit of validity and is a representation of the free energy in terms of irreducible distribution functions. In this section of the paper, we derive a more explicit formula of the higher derivatives of the free energy that is suitable for applications. Our method is again based on the Witten–Laplacian formalism framework.

We consider the Hamiltonian given by

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

where β is a thermodynamic parameter (temperature or magnetic field) and g satisfies

$$|\partial^{\alpha} \boldsymbol{\nabla} g| \leq C_{\alpha}, \ \ \forall\, \alpha \in \mathbb{N}^{|\Lambda|}.$$

We assume that there exist positive β_0 and β_1 such that $\Phi^{\beta}(x)$ satisfies the assumptions (1)–(4) for all $\beta \in (\beta_0, \beta_1)$ (see [24] for more details).

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

$$P_{\Lambda}(\beta) = \frac{1}{|\Lambda|} \ln \Bigg[\int\limits_{\mathbb{R}^{\Lambda}} e^{-\Phi^{\beta}(x)}\, dx \Bigg].$$

We are interested in the k-times differentiability of the free energy in the thermodynamic limit given by

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

We use the following notations:

$$Z_{\Lambda,\beta} = \int\limits_{\mathbb{R}^{\Lambda}} e^{-\Phi^{\beta}(X)}\, dX,$$

$$\langle\, \cdot\, \rangle_{\beta,\Lambda} = Z_{\Lambda,\beta}^{-1} \int\limits_{\mathbb{R}^{\Lambda}} \cdot e^{-\Phi^{\beta}(X)}\, dX.$$

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

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

Now, using the Helffer–Sjötrand formula (3.1), we have

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

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

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

Thus

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

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

$$\mathcal{H}_g := \Big(\frac{\partial}{\partial \beta} + \mathcal{A}_g \Big) f.$$

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

$$\begin{cases} A^{(0)}_{\Phi^{\beta}_{\Lambda}} f(\beta) = g - \langle g \rangle_{L^2(\mu)}, \\ \langle f(\beta) \rangle_{L^2(\mu)} = 0. \end{cases}$$

Hence

$$A^{(1)}_{\Phi^{t}_{\Lambda}} \mathbf{v}^{\beta} = \boldsymbol{\nabla} g,$$

where $\mathbf{v}^\beta = \boldsymbol{\nabla} f(\beta)$. Notice that the map

$$\beta \mapsto \mathbf{v}^\beta$$

is well defined and

$$\left\{\mathbf{v}^\beta :\ \beta \in (\beta_0, \beta_1)\right\}$$

is a family of smooth solutions on $\mathbb{R}^\Lambda$.

Under the notation above, we have the following

Proposition 5.1. *Let g be a smooth function satisfying (2.1), and $\beta_0 > 0$ such that $\Phi^\beta(x) = \Phi_\Lambda(x) - \beta g(x)$ satisfies the assumptions (1)–(4) for all $\beta \in [0, \beta_0)$ (see [24, Section 7]). Then for all $n \geq 1$, the nth derivative of the finite volume pressure is given by*

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

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

Here, we give only an outline of the proof of this proposition without discussing the dependency and control of the solution on the parameter β. This issue has been discussed rigorously in [16] and [24] using a sophisticated bootstrap argument.

Proof. First, put

$$\theta_\Lambda(\beta) = |\Lambda| P_\Lambda(\beta),$$

we have

$$\begin{aligned}
\theta'_\Lambda(\beta) &= \langle g \rangle_{\beta,\Lambda} = \Big\langle \Big(\frac{\partial}{\partial \beta} + \mathcal{A}_g\Big)^0 g \Big\rangle_{\beta,\Lambda} = \langle \mathcal{H}^0_g g \rangle_{\beta,\Lambda}, \\
\theta''_\Lambda(\beta) &= \frac{\partial}{\partial \beta} \langle g \rangle_{\beta,\Lambda} = \big\langle A^{(1)^{-1}}_{\Phi^\beta} (\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g \big\rangle_{\beta,\Lambda} = \Big\langle \Big(\frac{\partial}{\partial \beta} + \mathcal{A}_g\Big) g \Big\rangle_{\beta,\Lambda}, \\
\theta'''_\Lambda(\beta) &= \frac{\partial}{\partial \beta} \big\langle A^{(1)^{-1}}_{\Phi^\beta} (\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g \big\rangle_{\beta,\Lambda} \\
&= \Big\langle \frac{\partial}{\partial \beta} A^{(1)^{-1}}_{\Phi^\beta} (\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g \Big\rangle_{\beta,\Lambda} + \Big\langle \Big(A^{(1)^{-1}}_{\Phi^\beta} \boldsymbol{\nabla}\big(A^{(1)^{-1}}_{\Phi^\beta}(\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g\big)\Big)\cdot \boldsymbol{\nabla} g \Big\rangle_{\beta,\Lambda} \\
&= \Big\langle \Big(\frac{\partial}{\partial \beta} + \mathcal{A}_g\Big)^2 g \Big\rangle_{\beta,\Lambda},
\end{aligned}$$

By induction, it is easy to see that

$$\theta^{(n)}_\Lambda(\beta) = \Big\langle \Big(\frac{\partial}{\partial \beta} + \mathcal{A}_g\Big)^{n-1} g \Big\rangle_{\beta,\Lambda} = \langle \mathcal{H}^{n-1}_g g \rangle_{\beta,\Lambda}, \quad \forall\, n \geq 1.$$

Next, observe that

$$\begin{aligned}
\mathcal{H}_g g &= A^{(1)^{-1}}_{\Phi^\beta} (\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g = \mathcal{A}_g g, \\
\mathcal{H}^2_g g &= \frac{\partial}{\partial \beta} \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} g + \Big(A^{(1)^{-1}}_{\Phi^\beta} \boldsymbol{\nabla}\big(A^{(1)^{-1}}_{\Phi^\beta}(\boldsymbol{\nabla} g)\cdot \boldsymbol{\nabla} g\big)\Big)\cdot \boldsymbol{\nabla} g,
\end{aligned}$$

because f satisfies the equation

$$\boldsymbol{\nabla} f = A_{\Phi^\beta}^{(1)^{-1}}(\boldsymbol{\nabla} g).$$

With $\mathbf{v}^\beta = \boldsymbol{\nabla} f$, we have

$$\frac{\partial}{\partial\beta}\nabla f = \frac{\partial \mathbf{v}^\beta}{\partial\beta} = A_{\Phi^\beta}^{(1)^{-1}}\big[(\mathbf{Hess}\, g)\mathbf{v}^\beta - \nabla g\cdot\nabla\mathbf{v}^\beta\big],$$

$$\mathcal{H}_g^2 g = A_{\Phi^\beta}^{(1)^{-1}}\Big[(\mathbf{Hess}\, g)\mathbf{v}^\beta - \nabla g\cdot\nabla\mathbf{v}^\beta + \nabla\big(A_{\Phi^\beta}^{(1)^{-1}}\nabla g\cdot\nabla g\big)\Big]\cdot\nabla g.$$

Now, observe that

$$\begin{aligned}\nabla(A_{\Phi^\beta}^{(1)^{-1}}\nabla g\cdot\nabla g) &= \nabla(\nabla f\cdot\nabla g) = \nabla(\mathbf{v}^\beta\cdot\nabla g)\\ &= (\mathbf{Hess}\, g)\mathbf{v}^\beta - \nabla g\cdot\nabla\mathbf{v}^\beta \ \ \text{(after expanding the gradient).}\end{aligned}$$

Thus

$$\begin{aligned}\mathcal{H}_g^2 g &= A_{\Phi^\beta}^{(1)^{-1}}\Big[\nabla\big(A_{\Phi^\beta}^{(1)^{-1}}\nabla g\cdot\nabla g\big) + \nabla\big(A_{\Phi^\beta}^{(1)^{-1}}\nabla g\cdot\nabla g\big)\Big]\cdot\nabla g\\ &= A_{\Phi^\beta}^{(1)^{-1}}\big[2\nabla\big(A_{\Phi^\beta}^{(1)^{-1}}\nabla g\cdot\nabla g\big)\big]\cdot\nabla g = 2A_{\Phi^\beta}^{(1)^{-1}}[A_g g]\cdot\nabla g = 2A_g^2 g\end{aligned}$$

We will now prove by induction that

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

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

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

If n is replaced by $\widetilde{n}\leq n$, then

$$\mathcal{H}_g^{n-1} g = \Big(\frac{\partial}{\partial\beta} + \mathcal{A}_g\Big)\big((n-1)!\,\mathcal{A}_g^{n-1} g\big) = (n-1)!\,\Big(\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-1} g + \mathcal{A}_g^{n} g\Big).$$

Now,

$$\mathcal{A}_g^{n-1} g = \big[A_{\Phi^\beta}^{(1)^{-1}}\boldsymbol{\nabla}(\mathcal{A}_g^{n-2} g)\big]\cdot\boldsymbol{\nabla} g = \boldsymbol{\nabla}\varphi_n\cdot\boldsymbol{\nabla} g,$$

where

$$\boldsymbol{\nabla}\varphi_n = \big[A_{\Phi^\beta}^{(1)^{-1}}\boldsymbol{\nabla}(A_g^{n-2} g)\big].$$

We obtain

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

Hence

$$\begin{aligned}\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-1} g &= \frac{\partial}{\partial\beta}\boldsymbol{\nabla}\varphi_n\cdot\boldsymbol{\nabla} g\\ &= \Big[A_{\Phi^\beta}^{(1)^{-1}}\Big(\frac{\partial}{\partial\beta}\boldsymbol{\nabla}\mathcal{A}_g^{n-2} g + (\mathbf{Hess}\, g)\boldsymbol{\nabla}\varphi_n - \boldsymbol{\nabla} g\cdot\boldsymbol{\nabla}(\boldsymbol{\nabla}\varphi_n)\Big)\Big]\cdot\boldsymbol{\nabla} g\\ &= \Big[A_{\Phi^t}^{(1)^{-1}}\Big(\frac{\partial}{\partial\beta}\boldsymbol{\nabla}\mathcal{A}_g^{n-2} g + \boldsymbol{\nabla}(\boldsymbol{\nabla}\varphi_n\cdot\boldsymbol{\nabla} g)\Big)\Big]\cdot\boldsymbol{\nabla} g\\ &= \mathcal{A}_g\Big[\frac{\partial}{\partial\beta}\mathcal{A}_g^{n-2} g + \mathcal{A}_g(\mathcal{A}_g^{n-2} g)\Big]\\ &= \mathcal{A}_g\mathcal{H}_g(\mathcal{A}_g^{n-2} g).\\ &= \mathcal{A}_g\mathcal{H}_g\Big(\frac{1}{(n-2)!}\,\mathcal{H}_g^{(n-2)} g\Big) \ \text{(from the induction hypothesis)}\\ &= \frac{1}{(n-2)!}\,\mathcal{A}_g\mathcal{H}_g^{(n-1)} g\\ &= \frac{1}{(n-2)!}\,\mathcal{A}_g\big((n-1)!\,\mathcal{A}_g^{n-1} g\big) \ \text{(still by the induction hypothesis)}\\ &= (n-1)\mathcal{A}_g^n g.\end{aligned}$$

Thus
$$\mathcal{H}_g^n g = (n-1)!\,(n-1+1)\mathcal{A}_g^n g = n!\,\mathcal{A}_g^n g.$$
The result follows. □

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

Proposition 5.2. *Let g be a smooth function satisfying (2.1) and assume that there exist β_0 and β_1 such that $\Phi^\beta(x) = \Phi_\Lambda(x) - \beta g(x)$ satisfies the assumptions (1)–(4) for all $\beta \in (\beta_0, \beta_1)$. Then for all $n \geq 1$, we have the following recursion formula to compute the nth derivative $P_\Lambda^{(n)}(\beta)$ of the free energy:*
$$\sum_{k=0}^{n-1} \frac{\langle g^k\rangle_{\Lambda,\beta}}{k!}\,\frac{P_\Lambda^{(n-k)}(\beta)}{(n-k-1)!} = \frac{1}{(n-1)!}\,\frac{\langle g^n\rangle_{\Lambda,\beta}}{|\Lambda|}\,,\quad n\geq 1. \tag{5.1}$$

Proof.
$$\langle A_g^{n-1} g\rangle_\Lambda = Z^{-1}\int\limits_{\mathbb{R}^\Lambda} \big(A_\Phi^{(1)^{-1}} \boldsymbol{\nabla} A_g^{n-2} g\cdot \boldsymbol{\nabla} g\big) e^{-\Phi(x)}\,dx = \mathbf{cov}\,(A_g^{n-2}g, g) = \langle g A_g^{n-2} g\rangle_\Lambda - \langle g\rangle_\Lambda \langle A_g^{n-2} g\rangle_\Lambda.$$

Now, denote by ζ_n^i the components of $A_\Phi^{(1)^{-1}}\boldsymbol{\nabla} A_g^{n-3} g$. We have
$$\begin{aligned}
\langle g A_g^{n-1} g\rangle_\Lambda &= Z^{-1}\int\limits_{\mathbb{R}^\Lambda} g\sum_{i\in\Lambda}\zeta_n^i g_{x_i} e^{-\Phi(x)}\,dx = Z^{-1}\int\limits_{\mathbb{R}^\Lambda}\sum_{i\in\Lambda}\zeta_n^i g g_{x_i} e^{-\Phi(x)}\,dx \\
&= Z^{-1}\int\limits_{\mathbb{R}^\Lambda}\sum_{i\in\Lambda}\zeta_n^i\,\frac{1}{2}\,\frac{\partial}{\partial x_i}\,g^2 e^{-\Phi(x)}\,dx = \frac{1}{2}\,Z^{-1}\int\limits_{\mathbb{R}^\Lambda} A_\Phi^{(1)^{-1}}\boldsymbol{\nabla} A_g^{n-3} g\cdot\boldsymbol{\nabla}(g^2) e^{-\Phi(x)}\,dx \\
&= \frac{1}{2}\,\mathbf{cov}\,(A_g^{n-3}g, g^2) = \frac{1}{2}\Big[\langle g^2 A_g^{n-3} g\rangle_\Lambda - \langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda\Big].
\end{aligned}$$

We obtain
$$\langle g^2 A_g^{n-3} g\rangle_\Lambda = \frac{1}{3}\,\mathbf{cov}\,(A_g^{n-4}g, g^3) = \frac{1}{3}\,\langle g^3 A_g^{n-4}g\rangle_\Lambda - \frac{1}{3}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda.$$

Hence
$$\begin{aligned}
\langle A_g^{n-1} g\rangle_\Lambda &= \frac{1}{2}\cdot\frac{1}{3}\,\langle g^3 A_g^{n-4} g\rangle_\Lambda - \frac{1}{2}\cdot\frac{1}{3}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda - \frac{1}{2}\,\langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda - \langle g\rangle_\Lambda\langle A_g^{n-2}g\rangle_\Lambda \\
&= \frac{1}{2}\cdot\frac{1}{3}\left[\frac{1}{4}\,\langle g^4 A_g^{n-5}g\rangle_\Lambda - \frac{1}{4}\,\langle g^4\rangle_\Lambda\langle A_g^{n-5}g\rangle_\Lambda\right] \\
&\qquad - \frac{1}{2}\cdot\frac{1}{3}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda - \frac{1}{2}\,\langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda - \langle g\rangle_\Lambda\langle A_g^{n-2}g\rangle_\Lambda \\
&= \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{1}{4}\,\langle g^4 A_g^{n-5}g\rangle_\Lambda - \frac{1}{2}\cdot\frac{1}{3}\cdot\frac{1}{4}\,\langle g^4\rangle_\Lambda\langle A_g^{n-5}g\rangle_\Lambda \\
&\qquad - \frac{1}{2}\cdot\frac{1}{3}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda - \frac{1}{2}\,\langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda - \langle g\rangle_\Lambda\langle A_g^{n-2}g\rangle_\Lambda \\
&\ \ \vdots \\
&= \frac{1}{(n-1)!}\,\langle g^{(n-1)}g\rangle_\Lambda - \frac{1}{(n-1)!}\,\langle g^{(n-1)}\rangle_\Lambda\langle g\rangle_\Lambda - \frac{1}{(n-2)!}\,\langle g^{(n-2)}\rangle_\Lambda\langle A_g g\rangle_\Lambda - \cdots \\
&\qquad - \frac{1}{3!}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda - \frac{1}{2!}\,\langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda.
\end{aligned}$$

Thus
$$\begin{aligned}
&\frac{1}{(n-1)!}\,\langle g^{(n-1)}\rangle_\Lambda\langle g\rangle_\Lambda + \frac{1}{(n-2)!}\,\langle g^{(n-2)}\rangle_\Lambda\langle A_g g\rangle_\Lambda + \cdots + \frac{1}{3!}\,\langle g^3\rangle_\Lambda\langle A_g^{n-4}g\rangle_\Lambda \\
&\qquad + \frac{1}{2!}\,\langle g^2\rangle_\Lambda\langle A_g^{n-3}g\rangle_\Lambda + \frac{1}{1!}\,\langle g\rangle_\Lambda\langle A_g^{n-2}g\rangle_\Lambda + \frac{1}{0!}\,\langle g^0\rangle_\Lambda\langle A_g^{n-1}g\rangle_\Lambda = \frac{1}{(n-1)!}\,\langle g^n\rangle_\Lambda,
\end{aligned}$$

i.e.,

$$\sum_{k=0}^{n-1} \frac{\langle g^k \rangle_\Lambda \langle A_g^{n-k-1} g \rangle_\Lambda}{k!} = \frac{1}{(n-1)!} \langle g^n \rangle_\Lambda. \qquad \square$$

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