

Gaussian fluctuations and free energy expansion for Coulomb gases at any temperature

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Abstract. We obtain concentration estimates for the fluctuations of Coulomb gases in any dimension and in a broad temperature regime, including very small and very large temperature regimes which may depend on the number of points. We obtain a full Central Limit Theorem (CLT) for the fluctuations of linear statistics in dimension 2, valid for the first time down to microscales and for temperatures possibly tending to 0 or ∞ as the number of points diverges. We show that a similar CLT can also be obtained in any larger dimension conditional on a “no phase-transition” assumption, as soon as one can obtain a precise enough error rate for the expansion of the free energy – an expansion is obtained in any dimension, but the rate is so far not good enough to conclude. These CLTs can be interpreted as a convergence to the Gaussian Free Field. All the results are valid as soon as the test-function lives on a larger scale than the temperature-dependent minimal scale ρ_β introduced in our previous work (*Ann. Probab.* **49** (2021) 46–121).

Résumé. On obtient des résultats de concentration pour les fluctuations du gaz de Coulomb en toute dimension et dans un large régime de température, incluant des températures très petites et très grandes qui peuvent dépendre du nombre de points. On obtient un Théorème Central Limite (TCL) complet pour les fluctuations des statistiques linéaires en dimension 2, valable pour la première fois jusqu’aux échelles microscopiques et pour des températures pouvant tendre vers 0 ou l’infini quand le nombre de points diverge. On montre qu’un TCL semblable peut aussi être obtenu en toute dimension sous une condition d’absence de transition de phase, dès lors qu’on peut obtenir une erreur suffisamment petite dans le développement de l’énergie libre – un tel développement est prouvé en toute dimension, mais l’erreur n’est pas suffisamment petite pour conclure. Ces TCL sont valables dès que la fonction-test vit à une échelle supérieure à l’échelle minimale ρ_β dépendant de la température, introduite dans le précédent travail (*Ann. Probab.* **49** (2021) 46–121).

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1. Introduction

1.1. Setting of the problem

In this paper we continue our investigation of d -dimensional Coulomb gases (with $d \geq 2$) at the *inverse temperature* β , defined by the Gibbs measure

$$(1.1) \quad d\mathbb{P}_{N,\beta}(X_N) = \frac{1}{Z_{N,\beta}^V} \exp(-\beta N^{\frac{2}{d}-1} \mathcal{H}_N(X_N)) dX_N,$$

where $X_N = (x_1, \dots, x_N)$ is an N -tuple of points in \mathbb{R}^d and $\mathcal{H}_N(X_N)$ is the energy of the system in the state X_N , given by

$$(1.2) \quad \mathcal{H}_N(X_N) := \frac{1}{2} \sum_{1 \leq i \neq j \leq N} g(x_i - x_j) + N \sum_{i=1}^N V(x_i),$$

where

$$(1.3) \quad g(x) := \begin{cases} -\log|x| & \text{if } d = 2, \\ |x|^{2-d} & \text{if } d \geq 3. \end{cases}$$

We will denote in the whole paper by c_d the (explicitly computable) constant such that $-\Delta g = c_d \delta_0$ in dimension d . Thus the energy $\mathcal{H}_N(X_N)$ is the sum of the pairwise repulsive Coulomb interaction between all particles plus the effect on each particle of an external field or confining potential NV whose intensity is proportional to N . The normalizing constant $Z_{N,\beta}^V$ in the definition (1.1), called the *partition function*, is given by

$$(1.4) \quad Z_{N,\beta}^V := \int_{(\mathbb{R}^d)^N} \exp(-\beta N^{\frac{2}{d}-1} \mathcal{H}_N(X_N)) dX_N.$$

We have chosen particular units of measuring the inverse temperature by writing $\beta N^{\frac{2}{d}-1}$ instead of β . As seen in [52] it turns out to be a natural choice by scaling considerations as our β corresponds to the effective inverse temperature governing the microscopic scale behavior, with a balance in the energy and entropy competition at the local level. Of course, this choice does not reduce generality. Indeed, since our estimates are explicit in their dependence on β and N , one may choose β to depend on N if desired.

The Coulomb gas, also called “one-component plasma” in physics, is a standard ensemble of statistical mechanics, which has attracted much attention in the mathematical physics literature, see for instance [2, 24, 27, 39, 40, 45, 59, 62, 76] and references therein. Its study in the two-dimensional case is more developed, thanks in particular to its connection with Random Matrix Theory (see [32, 33, 61]): when $\beta = 2$ and $V(x) = |x|^2$, (1.1) is the law of the (complex) eigenvalues of the Ginibre ensemble of $N \times N$ matrices with normal Gaussian i.i.d entries [36]. Several additional motivations come from quantum mechanics, in particular via the plasma analogy for the fractional quantum Hall effect [37, 49, 82]. For all these aspects one may refer to [33]. The Coulomb case with $d = 3$, which can be seen as a toy model for matter has been for instance studied in [41, 57, 58]. The study of higher-dimensional Coulomb systems is not as much developed. In contrast the one-dimensional log gas analogue has been extensively studied, with many results of CLTs for fluctuations, free energy expansions, and universality [11, 13, 17–20, 38, 42, 81]. The case of the one-dimensional Coulomb gas, for which the interaction is $g(x) = -|x|$ was studied quite thoroughly in [47, 55, 56].

In Coulomb systems, if β is fixed and if V grows fast enough at infinity, then as $N \rightarrow \infty$, the empirical measure

$$\mu_N := \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$$

converges almost surely under the Gibbs measure to a deterministic equilibrium measure μ_∞ with compact support and density equal to $c_d^{-1} \Delta V$ on its support, which can be identified as the unique minimizer among probability measures of the quantity

$$(1.5) \quad \mathcal{E}^V(\mu) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} g(x-y) d\mu(x) d\mu(y) + \int_{\mathbb{R}^d} V(x) d\mu(x),$$

see for instance [77, Chapter 2]. This behavior in fact persists when β tends to 0 as $N \rightarrow \infty$ as long as $\beta \gg N^{-2/d}$, as we will see just below.

The lengthscale of the support of μ_∞ , independent of N , is of order 1, it is called the *macroscopic scale*, while the typical interparticle distance is of order $N^{-1/d}$ and is called the *microscopic scale* or *microscale*. Intermediate lengthscales are called *mesoscales*.

Following [7], instead of μ_∞ we work with a deterministic correction to the equilibrium measure which we call the *thermal equilibrium measure*, which is appropriate for all temperatures and defined as the probability density μ_θ minimizing

$$(1.6) \quad \mathcal{E}_\theta^V(\mu) := \mathcal{E}^V(\mu) + \frac{1}{\theta} \int_{\mathbb{R}^d} \mu \log \mu$$

with

$$(1.7) \quad \theta := \beta N^{\frac{2}{d}}.$$

Here, and in the sequel, we use the same notation for the measure μ and its density. By contrast with μ_∞ , μ_θ is positive and regular in the whole of \mathbb{R}^d with exponentially decaying tails. It is well-known to be the limiting density of the point distribution in the regime in which θ is fixed independently of N and we send $N \rightarrow \infty$, that is, for $\beta \simeq N^{-\frac{2}{d}}$; see for instance [1, 16, 25, 45, 62].

The precise dependence of μ_θ on θ has been studied in [8] where it is shown that when $\theta \rightarrow \infty$, then μ_θ converges to μ_∞ , with quantitative estimates (see below). Using the thermal equilibrium measure allows us to obtain more precise quantitative results valid for the full range of β and N such that $\theta \gg 1$, allowing in particular regimes of small β . Our method would also work for fixed β using the standard equilibrium measure μ_∞ , as in [51], but the thermal equilibrium measure always yields more precise results and a more precise description of the point distribution.

The inverse temperature θ is an important parameter in this problem because $\theta^{-1/2} = \beta^{-1/2} N^{-1/d}$ turns out to be the *characteristic lengthscale* that governs both the *macroscopic and microscopic distributions of the particles*. Concerning the macroscopic distribution we mean that $\theta^{-1/2}$ is the lengthscale of the tails of the noncompactly supported equilibrium measure μ_θ , as was shown in [8]. Concerning the microscopic distribution, we mean that $\theta^{-1/2}$ is very similar to the *minimal lengthscale for rigidity* ρ_β introduced in [7] and described further below. As we are interested for the first time in getting results that are valid for β possibly depending on N , it turns out that *the only parameters that matter are θ and the ratio of the considered lengthscale to the minimal lengthscale*, essentially our results hold whenever both are large.

We are interested in two related things: one is in obtaining free energy expansions with explicit error rates as $N \rightarrow \infty$, and the other is in obtaining Central Limit Theorems for the fluctuations of linear statistics of the form

$$(1.8) \quad \text{Fluct}(\xi) := \sum_{i=1}^N \xi(x_i) - N \int \xi \, d\mu_\theta(x),$$

with ξ regular enough. These two questions are directly related, indeed, as is well-known and first observed in this context by Johansson [42], studying the fluctuations is conveniently done by computing their Laplace transform, which then reduces the problem to computing the ratio of partition functions of two Coulomb gases with different potentials, and so obtaining very precise expansions for these partition functions is key. In this paper we will show that if one has an expansion of $\log Z_{N,\beta}^V$ with a sufficiently good error rate, then one can obtain a CLT for the fluctuations in all dimensions. The needed rate will be obtained and thus the proof completed in dimension 2, with quantitative convergence. The needed rate is so far not available in dimension 3 and larger, however we believe that the rate we obtain here is suboptimal (it is for instance worse than the one obtained in [7] for the case with uniform background) leading to expect that a CLT should hold for larger dimensions as well.

1.2. Comparison with the literature

The study of free energy expansions for Coulomb gases in general dimensions $d \geq 2$ was initiated in [52, 73, 74]. This program of using free energy expansions to derive CLTs for fluctuations of linear statistics was already accomplished in dimension 2 in [51] and [10] with a slightly different proof (one based on transport, the other on loop equations), however only the case of fixed β was treated. Prior CLT results restricted to the determinantal case $\beta = 2$ were obtained in [4, 69]. The results of [4, 51] were the only ones to treat the case where the support of ξ can overlap the boundary of the support of μ_V . Recently, [53] obtained the first “local CLT” in dimension 2 by using the transport method of [51] on the characteristic function.

Here we are particularly interested, like in the companion paper [7], in obtaining such results for a broad range of regimes of β , possibly depending on N and allowing for very large or very small temperatures. Also, while the results in [10, 51] were the first ones to obtain *mesoscopic CLTs* in dimension 2, i.e. to treat the case of ξ supported on small boxes, they were limited to lengthscales $\ell \geq N^\alpha$, $\alpha > -1/2$, i.e. to mesoscales, while here we can treat all scales down to the *temperature-dependent microscale* ρ_β introduced in [7] and defined in (2.11), below which rigidity is expected to be lost. We will not however treat the boundary case as in [4, 51] and will restrict to functions ξ that are both sufficiently regular and supported in the “bulk”, here defined as the set where the density of μ_θ has a good bound from below. In fact it is known in the physics literature that the Coulomb gas density has more fluctuations near the edge, see [3, 29] and references therein, so this limitation is not purely technical, and we do not expect similar results to ours to hold near the boundary when looking at small scales.

Treating the case of nonsmooth ξ , in particular equal to a characteristic function of a ball or cube in (1.8), i.e. evaluating the number of points in a given region, remains a (significantly more) delicate problem. In particular one would like to show whether *hyperuniformity* (see [83]) holds, i.e. whether the variance of the number of points in boxes is smaller than that of a Poisson point process.

The study of fluctuations of linear statistics is much more developed for ensembles in dimension 1, particularly log gases (or β -ensembles), see the works of [17, 18, 21, 42, 48, 81], and also recently Riesz gases [22]. In terms of temperature regimes, the study of fluctuations for large temperature regimes has only recently attracted attention, also mostly for log gases or β -ensembles in dimension 1, see [14, 63, 64] and [38] (itself based on the Stein's method approach of [48]).

In terms of studying fluctuations for dimensions larger than 2, the main progress was made in work of Chatterjee [31], followed by Ganguly–Sarkar [34], who analyzed a *hierarchical Coulomb gas model*. This is a simplified model, introduced by Dyson, in which the interaction is coarse-grained at dyadic scales. They studied it in a temperature regime that corresponds to $\beta = N^{1/3}$ (i.e. very low temperatures) in our setting. They obtained bounds on the variance of number of points in boxes and of linear statistics, but still no CLT. In the physics literature, the papers [41, 54] (see also [35, 59, 60]) contain a well-known prediction of an order $N^{1-1/d}$ for the variance of the number of points in a domain, however there is no prediction for the order of fluctuations of smooth linear statistics. In [31] the order of fluctuations of smooth linear statistics was speculated upon ($N^{1/3}$ vs. $N^{1/6}$) with supporting arguments from the example of orthogonal polynomial ensemble treated in [9] in favor of $N^{1/3}$, and finally it was shown in [34] to be in $N^{1-2/d}$, again still for the hierarchical model instead of the full model and for β of order $N^{1/3}$.

Going from free energy expansion to CLT involves a step which is often treated in dimension 1 or 2 via “loop equations” also called “Dyson–Schwinger equations” (see [10]) or “Ward identities” (see [4, 69]) and techniques related to complex analysis, which are inherently two-dimensional. These equations involve singular terms which are delicate to control. In [51], we introduced a transport approach, based on a change of variables transporting the original equilibrium measure to the perturbed one (perturbed by the effect of changing V into $V + t\xi$), which essentially replaces the loop equations. It was a question whether that approach could be extended to dimensions $d \geq 3$ where the “loop equations” are even more singular. Here we show that it is possible, and that to do so the terms arising in the loop equations have to be understood in a properly “renormalized” way which allows to bound them by the energy. The main result expressing this is Proposition 4.2 which allows to control the first and second derivatives of the energy of a configuration along a transport path by the energy itself, see also Remark 4.5 which explains how to renormalize the loop equation terms. That crucial proposition is in line with a similar result in [51] but it is significantly improved compared to [51]: first it is extended to arbitrary dimension, and second the estimates are refined to give a control not only of the first but also of the second derivative.

In [7], a free energy expansion with a rate was obtained in the case of a uniform background measure (or equilibrium measure). Here, a free energy expansion is obtained for a varying equilibrium measure by transporting it (locally) to a uniform one and using the aforementioned proposition to estimate the difference. The error rate obtained this way is less good than the one in the uniform measure case, and we believe there is room for improving that rate, which would be sufficient to conclude at least in dimension 3 for small enough β .

The proof crucially leverages on the local laws obtained in [7], which is the reason we cannot go below the scale ρ_β at which local laws hold (and do not necessarily expect the same CLT to hold then) and on the use of thermal equilibrium measure introduced there.

2. Main results

In all the paper, we will denote by C a generic positive constant independent of the parameters of the problem, but which may change from line to line. We will use the notation $|f|_{C^\sigma}$ for the Hölder semi-norm of order σ for any $\sigma \geq 0$ (not necessarily integer). For instance $|f|_{C^0} = \|f\|_{L^\infty}$, $|f|_{C^k} = \|D^k f\|_{L^\infty}$ and if $\sigma \in (k, k+1)$ for some k integer, we let

$$|f|_{C^\sigma(\Omega)} = \sup_{x \neq y \in \Omega} \frac{|D^k f(x) - D^k f(y)|}{|x - y|^{\sigma-k}}.$$

We emphasize that with this convention $f \in C^k$ does not mean that f is k times differentiable but rather that $D^{k-1} f$ is Lipschitz.

2.1. Assumptions and further definitions

We assume

$$(2.1) \quad V \in C^{2m+\gamma} \quad \text{for some integer } m \geq 2 \text{ and some } \gamma \in (0, 1],$$

$$(2.2) \quad \begin{cases} V \rightarrow +\infty & \text{as } |x| \rightarrow \infty \quad \text{if } d \geq 3 \\ \liminf_{|x| \rightarrow \infty} V + g = +\infty & \text{if } d = 2, \end{cases}$$

$$(2.3) \quad \begin{cases} \int_{|x| \geq 1} \exp\left(-\frac{\theta}{2} V(x)\right) dx < \infty, & \text{if } d \geq 3, \\ \int_{|x| \geq 1} e^{-\frac{\theta}{2}(V(x) - \log|x|)} dx + \int_{|x| \geq 1} e^{-\theta(V(x) - \log|x|)} |x| \log^2|x| dx < \infty & \text{if } d = 2, \end{cases}$$

These assumptions ensure the existence of the standard equilibrium measure μ_∞ and the thermal equilibrium measure μ_θ (see [8] for the latter). We recall that the equilibrium measure is characterized by the fact that there exists a constant c such that $g * \mu_\infty + V - c$ is 0 in the support of μ_∞ and nonnegative elsewhere. We let $\Sigma := \text{supp } \mu_\infty$ and assume that $\partial \Sigma \in C^1$. We also assume the nondegeneracy conditions that

$$(2.4) \quad \Delta V \geq \alpha > 0 \quad \text{in a neighborhood of } \Sigma$$

and that

$$g * \mu_\infty + V - c \geq \alpha \min(\text{dist}^2(x, \Sigma), 1)$$

which for instance hold if V is strictly convex. Note that (2.1) and (2.2) imply that V is bounded below.

These assumptions allow us to use the results of [8] on the thermal equilibrium measure, which we now recall. They show that μ_∞ well approximates μ_θ except in a boundary layer of size $\theta^{-\frac{1}{2}}$ near $\partial \Sigma$. More precisely there exists $C > 0$ (depending only on V and d) such that

$$(2.5) \quad \mu_\theta \geq \frac{1}{C} \quad \text{in } \Sigma,$$

$$(2.6) \quad \mu_\theta((\Sigma)^c) \leq C\theta^{-\frac{1}{2}}, \quad \left| \int_{\Sigma^c} \mu_\theta \log \mu_\theta \right| \leq C\theta^{-\frac{1}{2}},$$

and letting f_k be defined iteratively by

$$(2.7) \quad f_0 = \frac{1}{c_d} \Delta V \quad f_{k+1} = \frac{1}{c_d} \Delta V + \frac{1}{\theta c_d} \Delta \log f_k$$

we have $|f_k|_{C^{2(m-k-1)+\gamma}(\Sigma)} \leq C$ and for every even integer $n \leq 2m - 4$ and $0 \leq \gamma' \leq \gamma$, if $\theta \geq \theta_0(m)$, we have for all $U \subset \Sigma$

$$(2.8) \quad |\mu_\theta - f_{m-2-n/2}|_{C^{n+\gamma'}(U)} \leq C\theta^{\frac{n+\gamma'}{2}} \exp(-C \log^2(\theta \text{dist}^2(U, \partial \Sigma))) + C\theta^{1+n-m+\frac{\gamma'}{2}}.$$

The functions f_k provide a sequence of improving approximations (which are absent if V happens to be quadratic) to μ_θ defined iteratively. Spelling out the iteration we easily find the following approximation in powers of $1/\theta$

$$(2.9) \quad \mu_\theta \simeq \frac{1}{c_d} \Delta V + \frac{1}{c_d \theta} \Delta \log \frac{\Delta V}{c_d} + \frac{1}{c_d \theta^2} \Delta \left(\frac{\Delta \log \frac{\Delta V}{c_d}}{\Delta V} \right) + \dots \quad \text{well inside } \Sigma$$

up to an order dictated by the regularity of V and the size of θ . In our proof, we will have to stop the approximations at a level which we denote q and which will depend on the regularity of V , i.e. on m .

In all the explicit formula in the results, the quantity μ_θ could thus be replaced by μ_∞ or more precisely by (2.9) if θ is large enough, while making a small error quantified by (2.8).

Throughout the paper, as in [7] we will use the notation

$$(2.10) \quad \chi(\beta) = \begin{cases} 1 & \text{if } d \geq 3 \\ 1 + \max(-\log \beta, 0) & \text{if } d = 2, \end{cases}$$

and emphasize that $\chi(\beta) = 1$ unless $d = 2$ and β is small. The correction factor $\chi(\beta)$ arises in dimension 2 at small β and reflects the fact that the Poisson point process is expected (in dimension 2 only) to have an infinite Coulomb interaction energy (see the discussion in [7]).

In [7] we introduced the minimal scale ρ_β which is defined as

$$(2.11) \quad \rho_\beta = C \max(1, \beta^{-\frac{1}{2}} \chi(\beta)^{\frac{1}{2}}, \beta^{\frac{1}{d-2}-1} \mathbf{1}_{d \geq 5})$$

for some specific $C > 0$, with χ defined above. We believe that ρ_β should really be just $\max(1, \beta^{-\frac{1}{2}}\chi(\beta)^{\frac{1}{2}})$, the third term in (2.11) appearing only for technical reasons. Note this lengthscale is measured in blown-up coordinates, in original coordinates the minimal lengthscale for “rigidity” is thus $N^{-1/d}\rho_\beta$. Neglecting the logarithmic correction in dimension 2, this lengthscale is thus expected to be $N^{-1/d}\max(1, \beta^{-1/2})$ i.e. $\max(N^{-1/d}, \theta^{-1/2})$, hence our claim at the beginning that $\theta^{-1/2}$ is also the characteristic lengthscale for the microscopic distribution of the points (when $\beta \leq 1$).

In [7] we proved that wherever μ_θ is bounded below, for instance in Σ (by (2.5)), local laws controlling the energy in mesoscopic boxes down to the minimal scale ρ_β (see Proposition 3.7 for a precise statement) hold at a distance $\geq d_0$ from the boundary, where d_0 is defined by

$$(2.12) \quad d_0 := C \max\left(\left(\frac{N^{\frac{1}{d}}}{\max(1, \beta^{-\frac{1}{2}}\chi(\beta)^{\frac{1}{2}})}\right)^{-\frac{2}{3}}, N^{\frac{1}{d+2}-\frac{1}{d}}\right)$$

for some appropriate $C > 0$. Again, we do not expect such local laws to necessarily hold up to the boundary, due to the high oscillations of the gas there, see [29].

This leads us to defining a set $\hat{\Sigma}$ as a subset of Σ made of those x ’s such that

$$(2.13) \quad \theta^{m-2+\frac{\gamma}{2}} \exp(-C \log^2(\theta \operatorname{dist}^2(x, \partial\Sigma))) \leq C \quad \text{and} \quad \operatorname{dist}(x, \partial\Sigma) \geq d_0.$$

For any $\varepsilon > 0$, a distance $\geq \theta^{\varepsilon-\frac{1}{2}} + d_0$ from $\partial\Sigma$ suffices to satisfy the first condition. But by definition

$$(2.14) \quad d_0 \geq CN^{-\frac{1}{d}}N^{\frac{1}{3d}}\beta^{-\frac{1}{3}} = C\theta^{-\frac{1}{3}},$$

hence the desired condition is satisfied. Thus we may absorb $\theta^{\varepsilon-\frac{1}{2}}$ into d_0 and simply define

$$(2.15) \quad \hat{\Sigma} := \{x \in \Sigma, \operatorname{dist}(x, \partial\Sigma) \geq d_0\}.$$

With this choice, in view of (2.8), we have that for $\theta \geq \theta_0(m)$

$$(2.16) \quad \forall \sigma \leq 2m + \gamma - 4, \quad |\mu_\theta|_{C^\sigma(\hat{\Sigma})} \leq C.$$

In all the sequel we need to assume that our test function is supported in a cube of sidelength ℓ (possibly depending on N) with

$$(2.17) \quad \rho_\beta N^{-\frac{1}{d}} < \ell \leq C$$

i.e. larger or equal to the minimal lengthscale for rigidity. This natural condition, implies in view of the definition of θ and since $\rho_\beta \geq \beta^{-\frac{1}{2}}$, that

$$(2.18) \quad C \geq \ell \geq \theta^{-\frac{1}{2}}$$

will always be verified. This in turn implies that θ is bounded below independently of N , up to changing C we may say $\theta \geq \theta_0(m)$, hence in particular (2.16) holds. Our results will require some regularity on V and ξ , we have not tried to optimize the regularity assumptions. Most of our results will not really depend on V but will be valid for general background densities μ (generalizing μ_θ) with perturbations taken in a region where μ is bounded below and where the properties (2.16) hold. All the parameters in our results, in particular β , the lengthscale ℓ and the test function ξ may depend on N , but all the constants in our statements will depend only on d and on V (really via the bounds (2.16) and a lower bound on the density μ).

2.2. Concentration results: Bounds on fluctuations

We start with a first bound on the fluctuations (as defined in (1.8)) with minimal assumptions on the regularity of the test function ξ . Let us emphasize that this result requires no heavy lifting, it is a rather quick consequence of our energy splitting with respect to the equilibrium measure and electric formulation.

In the sequel Q_ℓ will denote a hyperrectangle with sidelengths in $[\ell, 2\ell]$, not necessarily centered at 0.

Theorem 1 (First bound on the Laplace transform in any dimension). *Let $d \geq 2$. Assume $V \in C^7$, (2.2)–(2.4) hold, and $\xi \in C^3$, $\text{supp } \xi \subset Q_\ell \subset \hat{\Sigma}$ with ℓ satisfying (2.17). There exists $C > 0$ depending only on d and V such that the following holds. For every t such that*

$$(2.19) \quad C|t| \max(|\xi|_{C^2}, |\xi|_{C^1}) < 1$$

we have

$$(2.20) \quad \begin{aligned} & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\beta t N^{\frac{2}{d}} \text{Fluct}(\xi)))| \\ & \leq C|t|\beta N \ell^d \left(\chi(\beta)\ell |\xi|_{C^3} + \frac{1}{\beta} |\xi|_{C^2} \right) \\ & \quad + Ct^2 \left(N \ell^d |\xi|_{C^2}^2 + |\text{supp } \nabla \xi| \beta N \left(N^{\frac{2}{d}} |\xi|_{C^1}^2 + \frac{1}{\beta} |\xi|_{C^2}^2 \right) \right) + CN \ell^d t^4 |\xi|_{C^2}^4 \end{aligned}$$

where $|\text{supp } \nabla \xi|$ denotes the volume of the support of $\nabla \xi$.

This result is already stronger (in terms of regularity required for ξ and bounds obtained) and more general (in terms of temperature regime and dimension) than the prior results such as [10, 51, 73] obtained for fixed $\beta > 0$. To illustrate, let us consider that $|\xi|_{C^k} \leq C\ell^{-k}$ which happens for instance if ξ is the rescaling at scale ℓ of a fixed function. Applying Theorem 1 in dimension 2 in this situation we get

Corollary 2.1. *Assume the same as above, that $d = 2$ and $|\xi|_{C^k} \leq M\ell^{-k}$ for $k \leq 3$ with ℓ satisfying (2.17). Then for all $|\tau| < C^{-1}M^{-1}(N^{1/d}\ell)^2 \max(\beta, 1)$ ¹ we have*

$$(2.21) \quad |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\tau \min(1, \beta) |\text{Fluct}(\xi)|))| \leq C(1 + \tau^4 M^4)$$

where C depends only on V .

By Tchebychev's inequality, it immediately implies a concentration result: for any $t > 0$, we have

$$(2.22) \quad \mathbb{P}_{N,\beta}(\min(1, \beta) |\text{Fluct}(\xi)| > t) \leq \exp(-t + C(1 + M^4))$$

where C depends only on V , thus this immediately implies that $\text{Fluct}(\xi)$ is typically bounded by $\max(1, \beta^{-1})$ as $N \rightarrow \infty$, a result which is new if $\beta \ll 1$.

An analogous result to Corollary 2.1 in dimension $d \geq 3$ is stated in Corollary 5.5. If ξ is assumed to be more regular, we can obtain a better estimate in dimension $d \geq 2$, for instance we have

Corollary 2.2. *Assume the same as above, $d \geq 2$, $V \in C^\infty$ and $\xi \in C^\infty$ with $|\xi|_{C^k} \leq M\ell^{-k}$ for each k , with ℓ satisfying (2.17). Then if $\beta \geq (\ell N^{\frac{1}{d}})^{2-d}$, for all $|\tau| < C^{-1}M^{-1}\beta N \ell^d$,¹ we have*

$$|\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\tau (N^{\frac{1}{d}} \ell)^{2-d} |\text{Fluct}(\xi)|))| \leq C|\tau|M + C\tau^4 M^4$$

while if $\beta \leq (\ell N^{\frac{1}{d}})^{2-d}$, for all $|\tau| < C^{-1}M^{-1}\beta^{1/2}(N^{1/d}\ell)^{1+d/2}$,¹ we have

$$|\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\tau \beta^{\frac{1}{2}} (N^{\frac{1}{d}} \ell)^{1-\frac{d}{2}} |\text{Fluct}(\xi)|))| \leq C|\tau|M + C\tau^4 M^4,$$

where C depends only on V and d .

A more general estimate is obtained in (5.39). Let us also point out that we expect the quantities that we have bounded to have a divergent mean (unless β tends to 0) and a smaller variance, see Theorem 5, thus once that mean is removed, the bounds we have obtained should not typically be optimal.

These results, or their reformulation as in (2.22), may be compared to prior concentration results of [15, 30] in the regime of fixed β and to the recent result of [65] which is the first one in the framework of the thermal equilibrium measure, thus allowing $\beta \rightarrow 0$. These prior results are in terms of distance from the empirical to equilibrium measure, rather than in terms of direct bounds on fluctuations.

¹In particular $|\tau| < C^{-1}$ suffices in view of (2.17).

2.3. Next order free energy expansion

Our next result concerns free energy expansions with a rate for general equilibrium measures whose density varies. In [7] we obtained a free energy expansion for uniform equilibrium measures in cubes, with an explicit error term proportional to the surface. It is expressed in terms of a function $f_d(\beta)$, the free energy per unit volume, characterized variationally in [52] as the minimum over stationary point processes of β times a Coulomb “renormalized energy” (from [73,74]) plus a (specific) relative entropy. More precisely, there is a constant $C > 0$ depending only on d such that

$$(2.23) \quad -C \leq f_d(\beta) \leq C\chi(\beta)$$

$$(2.24) \quad f_d \text{ is locally Lipschitz in } (0, \infty) \text{ with } |f'_d(\beta)| \leq \frac{C\chi(\beta)}{\beta},$$

and such that if R^d is an integer we have

$$(2.25) \quad \frac{\log K(\square_R, 1)}{\beta R^d} = -f_d(\beta) + O\left(\chi(\beta) \frac{\rho_\beta}{R} + \frac{\beta^{-\frac{1}{d}} \chi(\beta)^{1-\frac{1}{d}}}{R} \log^{\frac{1}{d}} \frac{R}{\rho_\beta}\right)$$

where ρ_β is as in (2.11). Here $K(\square_R, 1)$ is the appropriate partition function for a zoomed Coulomb gas with density 1 in \square_R , the cube of sidelength R when R^d is integer, see (3.35) for a precise definition. The existence of the large volume limit of the free energy per unit volume $f_d(\beta)$ was shown in dimension 2 in [76] and dimension 3 in [58], but here the novelty is in the rate of convergence. The proof in [7] relies on showing almost additivity of the free energy over cubes, via comparison with a subadditive and a superadditive quantity. In effect, this amounts to showing that in the large volume limit, the free energy does not depend on the boundary conditions chosen, up to surface energy errors. This is very much in line with the physics literature, for instance [24,39,47] and accomplished via a screening procedure, originating in the Coulomb gas context in [74].

From this, the idea is to obtain expansions for general equilibrium measures by partitioning the system into small cubes over which μ_θ is close to uniform, using the almost additivity of the free energy of [7], and computing the difference in free energies in each cube by transporting the almost uniform measure μ_θ to the uniform measure of density equal to the average value. The errors will lead to a degraded error estimate compared to (2.25). We believe that such a degradation is unavoidable by this method as the variations of μ_θ introduce a “soft kind” of boundaries between regions of different point densities, and we do not believe our estimates to be optimal.

Theorem 2 (Free energy expansion, general background). *Assume $d \geq 2$. Assume $V \in C^5$ satisfies (2.1)–(2.4). We have*

$$(2.26) \quad \begin{aligned} \log Z_{N,\beta}^V &= -\beta N^{1+\frac{2}{d}} \mathcal{E}_\theta^V(\mu_\theta) + \frac{\beta}{4} (N \log N) \mathbf{1}_{d=2} - N \frac{\beta}{4} \left(\int_{\mathbb{R}^d} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2} \\ &\quad + N \beta \int_{\mathbb{R}^d} \mu_\theta^{2-\frac{2}{d}} f_d(\beta \mu_\theta^{1-\frac{2}{d}}) + N \beta \chi(\beta) O(\mathcal{R}) \end{aligned}$$

where $\mathcal{R} \rightarrow 0$ as a power of $\rho_\beta N^{-1/d}$.

An explicit form of the error term is given in the paper in Theorem 2. To illustrate, if β is of order 1, then the error obtained is $N O(\mathcal{R}) = O(N^{1-\frac{1}{d}+\frac{1}{d+2}} \log N)$. This is a degradation compared to the rate in $(N^{\frac{1}{d}})^{d-1}$ obtained in [7] for uniform densities (and corresponding to a surface error). The largest part of the error is anyway created by a boundary layer imprecision due to the lack of local laws near the boundary. Our results of course agree with previous ones [10,50,52]² and improve them with the explicit rate, and also agree with the predicted formulas for two dimensions in particular in [84], see also [32].

Note also that in dimension 2 and in the case of quadratic V , [28,80] predict an expansion for $\log Z_{N,\beta}^V$ in powers of $N^{\frac{1}{2}}$ hence where the next order term is \sqrt{N} , which corresponds to a boundary term. This \sqrt{N} term was missing in [84]. For general motivation on two-dimensional free energy expansions, in connection to the fractional quantum Hall effect, we also refer to [46].

²The formula appears different because it is expressed in terms of \mathcal{E}_θ^V instead of \mathcal{E}^V as is usually done, so some order N terms are hidden in the entropy part of \mathcal{E}_θ^V .

What will be crucial for us in the sequel is that we can also obtain a localized version for the relative expansion of the free energy, i.e. the difference of $\log Z_{N,\beta}^V$ for two different equilibrium measures which only differ in a cube of size ℓ included in $\hat{\Sigma}$, see Proposition 6.4 for a full statement. Then there is no boundary local law error and the error rate \mathcal{R} can be expressed as a power of $\rho_\beta N^{-1/d}\ell^{-1}$. The power that we can obtain in all generality is $1/2$ yielding an error term $(N\ell^d)^{1-\frac{1}{2d}}$ (modulo a logarithmic correction) for fixed β of order 1, which is still a degradation compared to the rate in $(N^{\frac{1}{d}}\ell)^{d-1}$ obtained in [7] for uniform densities. It is however sufficient to proceed with the proof of the Central Limit Theorems below in dimension $d = 2$ and barely fails to be sufficient in dimension 3.

2.4. Central limit theorems

To state the results, let us define the operator

$$L = \frac{1}{c_d \mu_\theta} \Delta.$$

We phrase the results as the convergence of the Laplace transform of the fluctuations to that of a Gaussian. Compared to known results, explicit corrections to the known variance in $\int |\nabla \xi|^2$ are given as powers of θ^{-1} when ξ is regular enough, indicating the change in the formula for the variance in the cross-over regime when β becomes small (reminiscent for instance of [38]). Moreover the variance $\int |\nabla \xi|^2$ corresponds to a convergence (of $\Delta^{-1}(\sum_{i=1}^N \delta_{x_i} - N\mu_\theta)$) to the Gaussian Free Field (GFF) while the expected variance when θ becomes order 1 no longer corresponds to the GFF but rather to another Gaussian Field.

We should also emphasize that the normalization of the variable is $\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}}$, and not $\frac{1}{\sqrt{N\ell^d}}$ as in the usual CLT for a sum of independent variables. It is in fact a CLT for very nonindependent random variables. However,

$$\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}} \sim \frac{1}{\sqrt{N\ell^d}} \left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)$$

if one believes that $\rho_\beta \sim \beta^{-\frac{1}{2}}$ (see (2.11) and comments below) so in the extreme regime where $N^{\frac{1}{d}}\ell = \rho_\beta$ (which one can also read as $\theta\ell^d = 1$ or the large temperature regime) we recover the standard CLT normalization for iid variables, because $N\ell^d$ is the number of points in the support of ξ . Physically, this means that the system is very rigid, and becomes less and less so as one approaches the minimal scale. When $\beta \ll 1$, there is a gap between the minimal scale $\rho_\beta N^{-1/d}$ and the microscale $N^{-1/d}$ and we expect that the system becomes Poissonian below the minimal scale, based on the loose heuristic that in the Langevin dynamics the diffusion should dominate at small enough scale depending on temperature, and also by analogy with the case of β -ensembles [14,63,64].

2.4.1. The case of dimension 2

The first result is in dimension 2 and extends the result of [10,51] to possibly small or large β and down to the minimal scale.

Theorem 3 (CLT in dimension 2 for possibly small β). *Let $d = 2$. Let $q \geq 0$ be an integer. Assume $V \in C^{2q+7}$, (2.2)–(2.4) hold, and $\xi \in C^{2q+4}$, $\text{supp } \xi \subset Q_\ell \subset \hat{\Sigma}$ with ℓ satisfying (2.17). Assume $N^{\frac{1}{d}}\ell \gg \rho_\beta$ as $N \rightarrow \infty$,³ and*

$$(2.27) \quad \beta^{\frac{1}{2}} \ll (N^{\frac{1}{d}}\ell)^{\frac{1}{4}} \log^{-\frac{3}{4}}(N^{\frac{1}{d}}\ell).$$

Then for any fixed τ ,⁴

$$(2.28) \quad |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(-\tau\beta^{\frac{1}{2}} \text{Fluct}(\xi))) + \tau m(\xi) - \tau^2 v(\xi)| \rightarrow 0 \quad \text{as } \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \rightarrow \infty$$

where

$$(2.29) \quad v(\xi) = -\frac{1}{2c_d} \int_{\mathbb{R}^d} \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2 + \frac{1}{c_d} \int_{\mathbb{R}^d} \sum_{k=0}^q \nabla \xi \cdot \frac{\nabla L^k(\xi)}{\theta^k} - \frac{1}{2\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^2$$

³which implies $\theta \gg 1$, as seen before.

⁴An explicit rate of convergence in inverse powers of $N^{\frac{1}{d}}\ell\rho_\beta^{-1}$, also depending on the rate in (2.27), is provided.

and

$$m(\xi) = -\frac{\beta^{\frac{1}{2}}}{4} \int_{\mathbb{R}^d} \left(\sum_{k=0}^q \frac{\Delta L^k(\xi)}{c_d \theta^k} \right) \log \mu_\theta.$$

When neglecting the corrections in inverse powers of $\frac{1}{\theta}$ in the expressions for $m(\xi)$ and $v(\xi)$ as $\theta \rightarrow \infty$ we obtain

Corollary 2.3. *Under the same assumptions, assume $\xi = \xi_0(\frac{x-x_0}{\ell})$ for ξ_0 a fixed C^4 function. Then $\beta^{1/2}(\text{Fluct}(\xi) + \frac{1}{4c_d} \int_{\mathbb{R}^d} (\Delta \xi) \log \mu_\theta)$ converges⁵ as $N \rightarrow \infty$ to a Gaussian of mean 0 and variance $\frac{1}{c_d} \int_{\mathbb{R}^2} |\nabla \xi_0|^2$.*

By definition of the Gaussian Free Field (GFF) the convergence to a Gaussian with this specific variance can be expressed as a convergence of $\beta^{1/2}$ times the electrostatic potential (see Section 3.1)

$$\Delta^{-1} \left(\sum_{i=1}^N \delta_{x_i} - N \mu_\theta \right),$$

suitably shifted, to the GFF, and the same applies to the result in dimension 3 below. Note here that the mean $m(\xi)$ may be an unbounded deterministic shift to the fluctuation, since β may tend to ∞ as $N \rightarrow \infty$. Also the expression for $m(\xi)$ differs from that appearing in [51] because the fluctuation is computed with respect to μ_θ instead of μ_∞ , and these differ by $\frac{1}{c_d \theta} \Delta \log \frac{\Delta V}{c_d}$ to leading order (see (2.9)). This difference exactly matches the discrepancy in the expression for the mean.

When β is so large that (2.27) fails, we do not expect the same CLT to hold but we can normalize $\text{Fluct}(\xi)$ differently to obtain a convergence result. The fact that $\text{Fluct}(\xi)$ without normalization converges to a limit again reflects a strong rigidity of the system, consistent with the fact that as $\beta \rightarrow \infty$, in this dimension we expect crystallization to a triangular lattice to happen, related to conjectures of Cohn–Kumar and Sandier–Serfaty (see [52,68]).

Theorem 4 (Low temperature and minimizers). *Let $d = 2$. Assume $V \in C^7$, (2.2)–(2.4) hold, and $\xi \in C^4$, $\text{supp } \xi \subset Q_\ell \subset \hat{\Sigma}$ with ℓ satisfying (2.17). Assume $\beta \gg 1$ and $N^{\frac{1}{d}} \ell \gg 1$ as $N \rightarrow \infty$. Then as $N \rightarrow \infty$, we have⁵*

$$\text{Fluct}(\xi) + \frac{1}{4c_d} \int_{\mathbb{R}^d} (\Delta \xi) \log \mu_\theta \rightarrow 0.$$

If X_N minimizes \mathcal{H}_N then the same result holds.

The case of minimizers of \mathcal{H}_N corresponds to $\beta = \infty$ and can be obtained by simply letting $\beta \rightarrow \infty$ in the case with temperature since the constants are independent of β . Note that this generalizes [51] and also complements the results on minimizers or very low temperature states in [5,6,67,72].

2.4.2. The case of higher dimension

We now turn to dimension 3 and higher. As announced above, we will need to assume more regularity on f_d , and even make a quantitative regularity assumption.

While we know that f_d is locally Lipschitz (see (2.24)), its higher regularity is not known and is a delicate question, since points of nondifferentiability of f_d' correspond by definition to phase-transitions. Assuming that f_d'' is bounded can thus be interpreted as assuming that there are no first order phase-transitions at the effective temperatures we are considering: it was noted in [52] that in dimension $d \geq 3$ an effective temperature $\beta \mu_\theta(x)^{1-\frac{2}{d}}$ appears, which depends on both β and the local particle density.

In the physics literature, the existence of phase transitions is discussed in dimensions 2 and 3, and is described as “despite an extensive literature, still a subject of controversy” according to the recent paper [29]. But several papers discuss a phase transition observed numerically in dimension 2 around $\beta = 140$ [26] and in dimension 3 around $\beta = 175$ [23,43], see also the review [44] which proposes explicit expression for $f_d(\beta)$. So in any case, we expect that the condition we place should be true for all but a finite number of β ’s. Note also that our 2D result did not require any condition on β despite the possible existence of a phase-transition, this is due to the lack of $\mu_\theta(x)$ -dependence in the expression involving f_d in (2.26) in contrast with the case $d \geq 3$.

⁵The convergence is in the sense of convergence of the Laplace transforms, which implies convergence in law but is in fact a bit stronger.

When β is very small or very large (i.e. when it tends to 0 or to ∞ as N diverges) and when $d \geq 3$ only, we will need a quantitative assumption on the derivative of f_d : we will assume that

$$(2.30) \quad \|f_d''\|_{\mu_\theta, U} \leq C\beta^{-2}$$

for some C independent of β , where for a generic set U we denote

$$(2.31) \quad \|f_d''\|_{\mu_\theta, U} = \sup_{x \in U} |f_d''(\beta\mu_\theta(x)^{1-\frac{2}{d}})|.$$

Note that we could do with just the assumption that f_d' is bounded in some Hölder space $C^{0,\alpha}$, hence for simplicity we have assumed $\alpha = 1$. When β is fixed (2.30) is just a regularity assumption. When $\beta \rightarrow 0$ it is more quantitative, and it seems reasonable if one extrapolates from (2.24), assuming a regular behavior for the function $f_d(\beta)$, however we do not have a further basis for its reasonableness. One may refer to [24,39] for a treatment of the low β regime by cluster expansions.

The improved rate in $N^{1-\frac{1}{2d}}$ obtained in Proposition 6.4 does not quite suffice to deduce a CLT in dimension $d \geq 3$, but as mentioned above, we do not believe it to be optimal.

The larger the dimension or the smaller the temperature, the more regular we need ξ to be.

Theorem 5 (Conditional CLT in dimension $d \geq 3$ for possibly small β). *Let $d \geq 3$. Let $q > \frac{d}{4} - 1$ be a nonnegative integer. Assume $V \in C^{2q+7}$, (2.2)–(2.4) hold, and $\xi \in C^{2q+4}$, $\text{supp } \xi \subset Q_\ell \subset \hat{\Sigma}$ with ℓ satisfying (2.17). Assume that (2.30) holds relative to Q_ℓ . If $\beta \rightarrow 0$ assume in addition that*

$$(2.32) \quad \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \geq N^\varepsilon \quad \text{for some } \varepsilon > 0$$

and that q is larger than a constant depending on ε .

If a free energy expansion with rate \mathcal{R} as in Proposition 6.3 is found to hold⁶ with

$$(2.33) \quad \mathcal{R} \ll (N^{\frac{1}{d}}\ell)^{\frac{2}{d}-d}\beta^{-1},$$

then for any fixed τ , we have

$$(2.34) \quad |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(-\tau\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}}\text{Fluct}(\xi))) + \tau m(\xi) - \tau^2\ell^{2-d}v(\xi)| \rightarrow 0 \quad \text{as } \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \rightarrow \infty$$

where

$$(2.35) \quad v(\xi) = -\frac{1}{2c_d} \int_{\mathbb{R}^d} \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2 + \frac{1}{c_d} \int_{\mathbb{R}^d} \sum_{k=0}^q \nabla \xi \cdot \frac{\nabla L^k(\xi)}{\theta^k} - \frac{1}{2\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^2$$

and

$$m(\xi) = -N\ell^2\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{-1-\frac{d}{2}} \left(1 - \frac{2}{d}\right) \int_{\mathbb{R}^d} \left(\sum_{k=0}^q \frac{\Delta L^k(\xi)}{c_d \theta^k} \right) (f_d(\beta\mu_\theta^{1-\frac{2}{d}}) + \beta\mu_\theta^{1-\frac{2}{d}} f'_d(\beta\mu_\theta^{1-\frac{2}{d}})).$$

Corollary 2.4. *Under the same assumptions, if $\xi = \xi_0(\frac{x-x_0}{\ell})$ for ξ_0 a C^{2q+4} function with q large enough for $\beta \ll 1$, or $\xi_0 \in C^4$ otherwise, then $\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}}\text{Fluct}(\xi) + m(\xi)$ converges⁵ to a Gaussian of mean 0 and variance $\frac{1}{2c_d} \int |\nabla \xi_0|^2$.*

Just as in dimension 2, this can be interpreted as a convergence of $\beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}}\Delta^{-1}(\sum_{i=1}^N \delta_{x_i} - N\mu_\theta)$ to the GFF. This reveals a strong rigidity down to the minimal scale, but decreasing as β decreases.

Again, when β is large we expect crystallization to a lattice to happen [52] and do not expect the same result to hold. We can instead obtain

⁶when assuming $|\mu|_{C^1} \leq \ell^{-1}$ in that proposition

Theorem 6 (Low temperature and minimizers in dimension $d \geq 3$). *Let $d \geq 3$. Assume $V \in C^7$, (2.2)–(2.4) hold, and $\xi \in C^4$, $\text{supp } \xi \subset Q_\ell \subset \hat{\Sigma}$ with ℓ satisfying (2.17). Assume $\beta \gg 1$ as $N \rightarrow \infty$ and assume in addition that (2.30) holds relative to Q_ℓ . If a free energy expansion with a rate \mathcal{R} as in Proposition 6.3 is found to hold with*

$$(2.36) \quad \mathcal{R} \ll (N^{\frac{1}{d}} \ell)^{\frac{2}{d}-d},$$

we have, as $N \rightarrow \infty$,⁵

$$(2.37) \quad (N^{\frac{1}{d}} \ell)^{1-\frac{d}{2}} \left(\text{Fluct}(\xi) - \frac{N^{\frac{1}{3}}}{3c_d} \int_{\mathbb{R}^d} \Delta \xi \left(f_d(\beta \mu_\theta^{1-\frac{2}{d}}) + \beta \mu_\theta^{1-\frac{2}{d}} f'_d(\beta \mu_\theta^{1-\frac{2}{d}}) \right) \right) \rightarrow 0.$$

In particular if X_N minimizes \mathcal{H}_N then the same result holds.

Note the temperature regime studied in [31,34] corresponds to $\beta = N^{\frac{1}{3}}$ for us and was in fact a low temperature regime. Our result, conditional to (2.30) and an improved rate, would thus be in agreement with (but in principle stronger than) the result of variance in $N^{1/3}$ for $\text{Fluct}(\xi)$ proved in [34] for the hierarchical model. It also complements results in [66].

2.5. Outline of the proof

As in our prior work [7,51,52,73,74], the starting point is to use a next order Coulomb energy, defined for any probability density μ as

$$(2.38) \quad \mathsf{F}_N(X_N, \mu) = \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d \setminus \Delta} g(x-y) d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(x) d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(y),$$

where Δ denotes the diagonal of $\mathbb{R}^d \times \mathbb{R}^d$. This next order energy appears when expanding \mathcal{H}_N around the appropriate measure, which is here μ_θ . Recalling that $\theta = \beta N^{2/d}$ and that the thermal equilibrium measure minimizing (1.6) satisfies

$$(2.39) \quad g * \mu_\theta + V + \frac{1}{\theta} \log \mu_\theta = C_\theta \quad \text{in } \mathbb{R}^d$$

where C_θ is a constant, we obtain through an elementary computation the following “splitting formula”, found in [7]: for all configurations $X_N \in (\mathbb{R}^d)^N$ with pairwise distinct points,⁷ we have

$$(2.40) \quad \mathcal{H}_N(X_N) = N^2 \mathcal{E}_\theta^V(\mu_\theta) - \frac{N}{\theta} \sum_{i=1}^N \log \mu_\theta(x_i) + \mathsf{F}_N(X_N, \mu_\theta)$$

where \mathcal{E}_θ^V is as in (1.6), F_N as in (2.38), and Δ denotes the diagonal in $\mathbb{R}^d \times \mathbb{R}^d$. This separates the leading order $N^2 \mathcal{E}_\theta^V(\mu_\theta)$ from next order terms. We see here $-\frac{1}{\theta} \log \mu_\theta$ playing the role of an effective confinement potential for the system at next order.

We may then define for any probability density μ the next order partition function

$$(2.41) \quad \mathsf{K}_N(\mu) = \int_{(\mathbb{R}^d)^N} \exp(-\beta N^{\frac{2}{d}-1} \mathsf{F}_N(X_N, \mu)) d\mu(x_1) \cdots d\mu(x_N)$$

and $\mathsf{Q}_N(\mu)$ the associated Gibbs measure. Observe here that the integration is with respect to $\mu^{\otimes N}$ instead of the usual Nd -dimensional Lebesgue measure.

The use of the thermal equilibrium measure allows, via the splitting formula, for a remarkably simple rewriting of the partition function as

$$(2.42) \quad Z_{N,\beta}^V = \exp(-\beta N^{1+\frac{2}{d}} \mathcal{E}_\theta^V(\mu_\theta)) \mathsf{K}_N(\mu_\theta)$$

⁷We can proceed as if configurations all had pairwise distinct points, since the complement event has measure zero.

which is directly obtained by inserting (2.40) into (1.4) and using (2.41). In prior works such as [51,73,74] the energy was split with respect to the usual equilibrium measure, and this led to a less simple formula, involving an effective confinement potential.

The study of the free energy expansion now reduces to the analysis of partition functions $K_N(\mu)$ for general positive densities μ .

The control of fluctuations and proof of the CLT is based on the Johansson approach [42] which consists in evaluating the Laplace transform of the fluctuations, then directly reducing to evaluating the ratio of two partition functions, that for the Coulomb gas with potential V and that for the Coulomb gas with potential $V_t := V + t\xi$ for a small t . In the formulation with the thermal equilibrium measure, in view of (2.42) this takes the simple form

$$(2.43) \quad \mathbb{E}_{\mathbb{P}_{N,\beta}}(e^{-\beta t N^{\frac{2}{d}} \sum_{i=1}^N \xi(x_i)}) = \frac{Z_{N,\beta}^{V_t}}{Z_{N,\beta}^V} = \exp(-\beta N^{1+\frac{2}{d}} (\mathcal{E}_\theta^{V_t}(\mu_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta))) \frac{K_N(\mu_\theta^t)}{K_N(\mu_\theta)},$$

where μ_θ^t is the thermal equilibrium measure associated to V_t . In order to prove the CLT, one needs to show that the right-hand side converges as $N \rightarrow \infty$ to the Laplace transform of an appropriate Gaussian law. The precise value of t to be taken here always ends up being small, to be precise it is $t = \tau \ell^2 \beta^{-\frac{1}{2}} (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}}$ for fixed τ and is chosen to obtain a finite variance in the limit (but not necessarily a bounded mean), this is what yields the factor in front of the fluctuation in (2.28) and (2.34).

The evaluation of the fixed term $\exp(-\beta N^{1+\frac{2}{d}} (\mathcal{E}_\theta^{V_t}(\mu_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta)))$ above is not difficult and is done in Lemma 5.3, and the main work is to evaluate the ratio $\frac{K_N(\mu_\theta^t)}{K_N(\mu_\theta)}$. A first difficulty is that, while it is easy to describe the perturbed *usual* equilibrium measure in the interior case (it is just $\mu_\infty + t c_d^{-1} \Delta \xi$, see [79] for the more delicate boundary case), describing the perturbed *thermal* equilibrium measure μ_θ^t exactly is more difficult and has not yet been done in the literature. Instead we replace μ_θ^t by two successive good approximations ν_θ^t and $\tilde{\mu}_\theta^t$ described in Section 5. This induces an error which can be evaluated once one knows good first bounds on $\log K_N(\mu_1) - \log K_N(\mu_0)$ for general probability densities μ_0 and μ_1 , see Lemma 4.9.

Our method here is the transport-based approach of [51], and the approximation μ_θ^t is chosen because it is expressed as a simple transport of μ_θ , in the form $(\text{Id} + t\psi)\#\mu_\theta$ (here $\#$ denotes the push-forward of probability measures) where ψ is an explicit transport map. The map ψ is itself a (truncated) series in inverse powers of θ^{-1} . The number of terms kept in the series, or level of approximation, is the parameter q in our results. It can be chosen at will, the larger the q the more precise the approximation (especially when θ is not tending to ∞ very fast) but the more regularity of ξ and V it requires.

We are then left with evaluating the change of $\log K_N(\mu)$ along a transport. But if μ and $\Phi\#\mu$ are two probability densities, by definition we have

$$(2.44) \quad \begin{aligned} \frac{K_N(\Phi\#\mu)}{K_N(\mu)} &= \frac{1}{K_N(\mu)} \int_{(\mathbb{R}^d)^N} \exp(-\beta N^{\frac{2}{d}-1} \mathsf{F}_N(X_N, \Phi\#\mu)) d(\Phi\#\mu)^{\otimes N}(X_N) \\ &= \frac{1}{K_N(\mu)} \int_{(\mathbb{R}^d)^N} \exp(-\beta N^{\frac{2}{d}-1} \mathsf{F}_N(\Phi(X_N), \Phi\#\mu)) d\mu^{\otimes N}(X_N) \\ &= \mathbb{E}_{Q_N(\mu)}(\exp(-\beta N^{\frac{2}{d}-1} (\mathsf{F}_N(\Phi(X_N), \Phi\#\mu) - \mathsf{F}_N(X_N, \mu)))) \end{aligned}$$

with Q_N the Gibbs measure defined just after (2.41). Thus we just need to evaluate the variation of the energy F_N along a transport. Note that here it is particularly convenient that we have an integral against $\mu^{\otimes N}$ instead of the Lebesgue measure, thanks to the use of the thermal equilibrium measure. This makes the formula (2.44) exact, with no Jacobian term contrarily to [51].

We thus work at evaluating the variation of $\mathsf{F}_N(\Phi_t(X_N), \mu_t)$ along a transport $\Phi_t = \text{Id} + t\psi$, with $\mu_t = \Phi_t\#\mu$ for a generic probability density μ , when t is small enough. This is done in Proposition 4.2. The result is that the first and second derivatives in t of the energy $\mathsf{F}_N(\Phi_t(X_N), \mu_t)$ are both bounded by $C\mathsf{F}_N(X_N, \mu)$, i.e. the energy itself. This extends the result of [51] to higher dimension and is an improvement even in dimension 2 since in [51] only the first derivative was fully controlled, and this turns out crucial later. The proof relies in an essential way on the electric formulation of F_N (see Section 3.1) first introduced in [73,74] and on some new technical energy control estimates, proven in Section 3.2. The first derivative in t of $\mathsf{F}_N(\Phi_t(X_N), \mu_t)$ involves a singular integral term, which we had called “anisotropy” in dimension 2 in [51], but is even more singular thus harder to handle in higher dimension. We show here how to give it a meaning via the electric formulation, effectively describing how to “renormalize the loop equations”.

Thanks to this control we can deduce the bound (of Lemma 4.9) on differences of the form $\log K_N(\mu_1) - \log K_N(\mu_0)$, by interpreting μ_1 as a transport of μ_0 . This bound suffices to obtain the fluctuation bound in Theorem 1 and also to control the errors made when replacing μ_θ^t by its approximations above. It does not however suffice to evaluate the Laplace transform in (2.43) with sufficient precision for the CLT. For that, we use the approach of [51] of comparing two different ways of evaluating $\log \frac{K_N(\mu_1)}{K_N(\mu_0)}$: one via the linearization of F_N just described above, and one by evaluating independently $\log K_N(\mu)$ for a general nonuniform μ . This consists in proving the free energy expansion with a rate, Theorem 2 and more importantly, its localized version Proposition 6.4. To do so, one splits the support of μ into mesoscopic cubes in which μ is almost uniform, and adds up the free energies for uniform measures in cubes obtained in (2.25) via the almost additivity of the free energy proved in [7] (which comes with an additivity error rate). To do so, we use the control of Lemma 4.9 to bound the error made when replacing a varying measure with a uniform one in a small cube. We also need the assumption (2.30) in dimensions $d \geq 3$ to obtain a good enough error rate because in those dimensions and contrarily to dimension 2, the free energy dependence in μ involves a dependence inside the function f_d , see (2.26).

Comparing these two ways of evaluating $\log K_N(\mu_t)$ along a transport and using the good control on the second derivative of this quantity, we are able to obtain an improved estimate on its first derivative, this is the idea borrowed from [51] in dimension 2. Applying to the thermal equilibrium measure, the first derivative in t of $\log K_N((\text{Id} + t\psi)\#\mu_\theta)$ gives the mean of the fluctuation variable (which may be unbounded), while its higher derivatives do not contribute. The variance in the end only comes from the constant exponential term in the right-hand side of (2.43). Assembling these elements provides the convergence of the log Laplace transform of the fluctuation, after subtracting the appropriate mean, to an explicit quadratic function, as desired.

2.6. Plan of the paper

In Section 3 we review the electric formulation of the energy and the associated definitions, we then provide a new multiscale interaction energy control, Proposition 3.5. We conclude the section by reviewing the local laws and almost additivity from [7].

In Section 4 we show how to control the variations of the energy along a transport. The main result there is Proposition 4.2. This is then applied to estimate the difference of free energies when perturbing the background measure.

In Section 5 we choose a specific transport map adapted to the varying thermal equilibrium measure. We then combine the previous elements to provide a first bound on the fluctuations, proving Theorem 1 and Corollary 2.1.

In Section 6 we prove Proposition 6.4 and Theorem 2 by the almost additivity of the free energy.

In Section 7 we prove the main CLT results of Theorems 3, 4, 5 and 6 and their corollaries.

3. Preliminaries

3.1. Electric formulation

We first describe how to reexpress $F_N(X_N, \mu)$ in “electric form”, i.e via the electric (or Coulomb) potential generated by the points. This idea originates in [67, 73, 74] but we use here the precise formulation of [51]. Here, contrarily to [7] we are working at the normal scale, and not at the blown-up scale.

We consider the electrostatic potential h created by the configuration X_N and the background probability μ , defined by

$$(3.1) \quad h(x) = \int_{\mathbb{R}^d} g(x - y) d \left(\sum_{i=1}^N \delta_{x_i} - N\mu \right) (y),$$

which we will sometimes later denote $h^\mu[X_N](x)$ for less ambiguity. Since g is (up to the constant c_d), the fundamental solution to Laplace’s equation in dimension d , we have

$$(3.2) \quad -\Delta h = c_d \left(\sum_{i=1}^N \delta_{x_i} - N\mu \right).$$

We note that h tends to 0 at infinity because $\int \mu = 1$ and the system formed by the positive charges at x_i and the negative background charge $N\mu$ is neutral. We would like to formally rewrite $F_N(X_N, \mu)$ defined in (2.38) as $\int |\nabla h|^2$, however this is not correct due to the singularities of h at the points x_i which make the integral diverge. This is why we use a truncation procedure which allows to give a renormalized meaning to this integral.

We will need to consider configurations with number of points n not necessarily equal to N . Turning to the truncation procedure, by abuse of notation we will extend the definition of $g(\eta)$ to η positive real numbers, by setting $g(\eta) = -\log|\eta|$ if $d = 2$ and $g(\eta) = \eta^{2-d}$ if $d \geq 3$, cf. (1.3). For any number $\eta > 0$, we then let

$$(3.3) \quad f_\eta(x) = (g(x) - g(\eta))_+,$$

where $(\cdot)_+$ denotes the positive part of a number, and point out that f_η is supported in $B(0, \eta)$. We will also use the notation

$$(3.4) \quad g_\eta = g - f_\eta = \min(g, g(\eta)).$$

This is a truncation of the Coulomb kernel. We also denote by $\delta_x^{(\eta)}$ the uniform measure of mass 1 supported on $\partial B(x, \eta)$. This is a smearing of the Dirac mass at x on the sphere of radius η . Since g is harmonic away from the origin, by the mean-value formula, g_η and $g * \delta_0^{(\eta)}$ coincide outside of $B(0, \eta)$, moreover they also have the same Laplacian $-c_d \delta_0^{(\eta)}$ by symmetry and mass considerations, therefore $g * \delta_0^{(\eta)} = g_\eta$ everywhere and

$$(3.5) \quad f_\eta = g * (\delta_0 - \delta_0^{(\eta)})$$

so that

$$(3.6) \quad -\Delta f_\eta = c_d (\delta_0 - \delta_0^{(\eta)}).$$

We also note that

$$(3.7) \quad \int_{\mathbb{R}^d} |f_\eta| \leq C\eta^2, \quad \int_{\mathbb{R}^d} |\nabla f_\eta| \leq C\eta.$$

For any $\vec{\eta} = (\eta_1, \dots, \eta_n) \in \mathbb{R}_+^n$, and any function u satisfying a relation of the form

$$(3.8) \quad -\Delta u = c_d \left(\sum_{i=1}^n \delta_{x_i} - N\mu \right)$$

we then define the truncated potential

$$(3.9) \quad u_{\vec{\eta}} = u - \sum_{i=1}^n f_{\eta_i}(x - x_i).$$

We note that in view of (3.6) the function $u_{\vec{\eta}}$ then satisfies

$$(3.10) \quad -\Delta u_{\vec{\eta}} = c_d \left(\sum_{i=1}^n \delta_{x_i}^{(\eta_i)} - N\mu \right).$$

We then define a particular choice of truncation parameters: if $X_n = (x_1, \dots, x_n)$ is an n -tuple of distinct points in \mathbb{R}^d we denote for all $i = 1, \dots, n$,

$$(3.11) \quad r_i = \frac{1}{4} \min \left(\min_{j \neq i} |x_i - x_j|, N^{-\frac{1}{d}} \right)$$

which we will think of as the *nearest-neighbor distance* for x_i .

The following is proven in [51, Prop. 2.3] and [78, Prop 3.3]. It gives a renormalized meaning to the “electric reformulation” of $F_N(X_n, \mu)$ as $\frac{1}{2c_d} \int |\nabla h|^2$.

Lemma 3.1. *Let X_N be in $(\mathbb{R}^d)^N$ and μ be a probability measure with bounded density. If (η_1, \dots, η_N) is such that $0 < \eta_i \leq r_i$ for each $i = 1, \dots, N$, we have*

$$(3.12) \quad F_N(X_N, \mu) = \frac{1}{2c_d} \left(\int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}|^2 - c_d \sum_{i=1}^N g(\eta_i) \right) - N \sum_{i=1}^N \int_{\mathbb{R}^d} f_{\eta_i}(x - x_i) d\mu(x).$$

This shows in particular that the expression in the right-hand side is independent of the truncation parameter, as soon as the latter is small enough. Choosing for instance $\eta_i = r_i$ this provides an exact electric representation for F .

We next present a Neumann local version of the energy first introduced in [7]: consider U a subset of \mathbb{R}^d with piecewise C^1 boundary, bounded or unbounded (here we will mostly use hyperrectangles and their complements), Ω a subset of U (typically a subcube or ball), and introduce a modified version of the minimal distance

$$(3.13) \quad \tilde{r}_i := \frac{1}{4} \begin{cases} \min\left(\min_{x_j \in \Omega, j \neq i} |x_i - x_j|, \text{dist}(x_i, \partial U \cap \Omega)\right) & \text{if } \text{dist}(x_i, \partial \Omega \setminus \partial U) \geq \frac{1}{2}N^{-\frac{1}{d}}, \\ \min(N^{-\frac{1}{d}}, \text{dist}(x_i, \partial U \cap \Omega)) & \text{otherwise.} \end{cases}$$

This ensures that the balls $B(x_i, \tilde{r}_i)$ remain included in U . If $N\mu(U) = n$ is an integer, for a configuration X_n of points in U , and using the notation \tilde{r} for the vector $(\tilde{r}_1, \dots, \tilde{r}_n)$, we define

$$(3.14) \quad \begin{aligned} F_N^\Omega(X_n, \mu, U) = & \frac{1}{2c_d} \left(\int_{\Omega} |\nabla v_{\tilde{r}}|^2 - c_d \sum_{i, x_i \in \Omega} g(\tilde{r}_i) \right) - N \sum_{i, x_i \in \Omega} \int_U f_{\tilde{r}_i}(x - x_i) d\mu(x) \\ & + \sum_{i, x_i \in \Omega} \left(g\left(\frac{1}{4} \text{dist}(x_i, \partial U)\right) - g\left(\frac{N^{-\frac{1}{d}}}{4}\right) \right)_+, \end{aligned}$$

where

$$(3.15) \quad \begin{cases} -\Delta v = c_d \left(\sum_{i=1}^n \delta_{x_i} - N\mu \right) & \text{in } U \\ \frac{\partial v}{\partial \nu} = 0 & \text{on } \partial U, \end{cases}$$

with $\partial/\partial \nu$ denoting the normal derivative. Note that under the condition $N\mu(U) = n$ the solution of (3.15) exists and is unique up to addition of a constant.

The extra additive term in the second line of (3.14) was needed in [7] to control points getting close to the boundary when proving local laws.

Finally, we write $F_N(X_n, \mu, U)$ for $F_N^U(X_n, \mu, U)$.

3.2. Monotonicity and local energy controls

We need the following result inspired from [51,67] which expresses a monotonicity with respect to the truncation parameter, and allows to deduce a new control of the interaction energy at arbitrary scales α .

Lemma 3.2. *Let U be any open set and u solve*

$$(3.16) \quad -\Delta u = c_d \left(\sum_{i=1}^n \delta_{x_i} - N\mu \right) \quad \text{in } U,$$

and let $u_{\vec{\alpha}}, u_{\vec{\eta}}$ be as in (3.9). Assume $\alpha_i \leq \eta_i$ for each i . Letting I denote $\{i, \alpha_i \neq \eta_i\}$, assume that for each $i \in I$ we have $B(x_i, \eta_i) \subset U$. Then

$$(3.17) \quad \begin{aligned} & \int_U |\nabla u_{\vec{\eta}}|^2 - c_d \sum_{i=1}^n g(\eta_i) - 2Nc_d \sum_{i=1}^n \int_U f_{\eta_i}(x - x_i) d\mu \\ & - \left(\int_U |\nabla u_{\vec{\alpha}}|^2 - c_d \sum_{i=1}^n g(\alpha_i) - 2Nc_d \sum_{i=1}^n \int_U f_{\alpha_i}(x - x_i) d\mu(x) \right) \leq 0, \end{aligned}$$

with equality if $\eta_i \leq r_i$ for each i . Moreover, for $\Omega \subset U$, denoting temporarily

$$(3.18) \quad \mathcal{F}^{\vec{\alpha}} := \frac{1}{2c_d} \left(\int_{\Omega} |\nabla u_{\vec{\alpha}}|^2 - c_d \sum_{i, x_i \in \Omega} g(\alpha_i) - 2Nc_d \sum_{i, x_i \in \Omega} \int_U f_{\alpha_i}(x - x_i) d\mu(x) \right)$$

assuming that

$$(3.19) \quad \alpha_i = \frac{1}{4}N^{-\frac{1}{d}} \quad \text{for } x_i \text{ such that } \text{dist}(x_i, \partial\Omega) \leq \frac{1}{2}N^{-\frac{1}{d}}$$

and $\alpha_i \leq \tilde{r}_i$ if $\text{dist}(x_i, \partial\Omega) \leq \alpha_i$, we have

$$(3.20) \quad \frac{1}{2} \sum_{\substack{i \neq j, x_i, x_j \in \Omega \\ \text{dist}(x_i, \partial\Omega) \geq \alpha_i + \frac{1}{4}N^{-1/d}}} (\mathbf{g}(x_i - x_j) - \mathbf{g}(\alpha_i))_+ \leq \mathbf{F}_N^\Omega(X_n, \mu, U) - \mathcal{F}^{\vec{\alpha}},$$

and

$$(3.21) \quad \begin{cases} \sum_{\substack{i \neq j, x_i, x_j \in \Omega, \text{dist}(x_i, \partial\Omega) \geq 4\alpha, \\ \alpha \leq |x_i - x_j| \leq 2\alpha}} \mathbf{g}(\alpha) \leq C(\mathcal{F}^{\vec{\eta}} - \mathcal{F}^{\vec{\eta}'}) & \text{if } d \geq 3 \\ \sum_{\substack{i \neq j, x_i, x_j \in \Omega, \text{dist}(x_i, \partial\Omega) \geq 4\alpha, \\ \alpha \leq |x_i - x_j| \leq 2\alpha}} 1 \leq C(\mathcal{F}^{\vec{\eta}} - \mathcal{F}^{\vec{\eta}'}) & \text{if } d = 2, \end{cases}$$

where $\vec{\eta}$ is set to be α if $\text{dist}(x_i, \partial\Omega) \geq \alpha$ and \tilde{r}_i otherwise, and $\vec{\eta}'$ is set to be 4α if $\text{dist}(x_i, \partial\Omega) \geq 4\alpha$ and \tilde{r}_i otherwise, and $C > 0$ depends only on d .

Proof. The relation (3.17) is proven for instance in [7, Proof of Lemma B.1]. There it is also shown that if $\alpha_i \leq \eta_i$ for each i , \mathbf{g}_η being as in (3.4), we have

$$(3.22) \quad \frac{1}{2} \sum_{x_i, x_j \in \Omega, i \neq j} (\mathbf{g}_{\alpha_i}(|x_i - x_j| + \alpha_j) - \mathbf{g}(\eta_i))_+ \leq \mathcal{F}^{\vec{\alpha}} - \mathcal{F}^{\vec{\eta}}$$

Letting $\alpha_i \rightarrow 0$ for the points x_i such that $\text{dist}(x_i, \partial\Omega) \geq \eta_i$ while choosing $\alpha_i = \eta_i$ for the others, we find that

$$(3.23) \quad \frac{1}{2} \sum_{x_i, x_j \in \Omega, i \neq j, \text{dist}(x_i, \partial\Omega) \geq \eta_i} (\mathbf{g}(|x_i - x_j|) - \mathbf{g}(\eta_i))_+ \leq \mathbf{F}_N^\Omega(X_n, \mu, U) - \mathcal{F}^{\vec{\eta}},$$

which gives the result (3.20) by substituting η_i by α_i . Here we observed that for $\vec{\alpha}$ such that $\alpha_i \leq \tilde{r}_i$, we have $\mathcal{F}^{\vec{\alpha}} = \mathbf{F}_N^\Omega(X_n, \mu, U)$.

Next, applying (3.22) to $\vec{\eta}$ and $\vec{\eta}'$, we find the results (3.21). \square

The following result shows that despite the cancellations occurring between the two possibly very large terms $\int_{\mathbb{R}^d} |\nabla u_{\vec{\eta}}|^2$ and $c_d \sum_{i=1}^N \mathbf{g}(\eta_i)$, when choosing $\eta_i = \tilde{r}_i$ we may control each of these two terms by the energy i.e. by their difference. It is adapted from [7, Lemma B.2].

Lemma 3.3. *For any configuration X_n in U , and v corresponding via (3.15), letting $\#I_\Omega$ denote $\#(\{X_n\} \cap \Omega)$ where $\{X_n\}$ is the set of points formed by the entries of X_n and $\#$ denotes the cardinality, for any $\Omega \subset U$, and any $\vec{\eta}$ such that $\eta_i \in [\frac{1}{4}\tilde{r}_i, \tilde{r}_i]$, with \tilde{r} computed with respect to Ω as in (3.13), and satisfying condition (3.19), we have*

$$(3.24) \quad \sum_{x_i \in \Omega} \mathbf{g}(\eta_i) \leq 2 \left(\left(\mathbf{F}_N^\Omega(X_n, \mu, U) + \frac{\#I_\Omega}{2} (\log N) \mathbf{1}_{d=2} \right) + C_0 \#I_\Omega N^{1-\frac{2}{d}} \right),$$

$$(3.25) \quad \int_{\Omega} |\nabla v_{\vec{\eta}}|^2 \leq 4c_d \left(\left(\mathbf{F}_N^\Omega(X_n, \mu, U) + \frac{\#I_\Omega}{4} (\log N) \mathbf{1}_{d=2} \right) + C_0 \#I_\Omega N^{1-\frac{2}{d}} \right)$$

with $C_0 > 0$ depending only on an upper bound for μ in Ω . Moreover, for any $\vec{\eta}$ such that $\eta_i \leq \tilde{r}_i$ and satisfying condition (3.19), we have

$$(3.26) \quad \int_{\Omega} |\nabla v_{\vec{\eta}}|^2 \leq 2c_d \mathbf{F}_N^\Omega(X_n, \mu, U) + c_d \sum_{x_i \in \Omega} \mathbf{g}(\eta_i).$$

Proof. We prove the result for $\eta_i = \tilde{r}_i$, the general case is a straightforward adaptation. For every $1 \leq i \leq N$, let us choose $\alpha_i = \alpha = \frac{1}{4}N^{-1/d}$. Applying (3.20), we have

$$(3.27) \quad \begin{aligned} \mathsf{F}_N^\Omega(X_n, \mu) &\geq -\frac{1}{2} \sum_{i, x_i \in \Omega} g(\alpha) - N \|\mu\|_{L^\infty} \|f_\alpha\|_{L^1} \#I_\Omega \\ &\quad + \frac{1}{2} \sum_{\substack{i, j, x_i, x_j \in \Omega \\ \text{dist}(x_i, \partial\Omega) \geq \alpha}} (g(|x_i - x_j|) - g(\alpha))_+. \end{aligned}$$

From the definition of \tilde{r}_i , we see that if $\text{dist}(x_i, \partial\Omega) \geq \frac{1}{4}N^{-1/d}$, there exists $x_j \in \Omega$ such that $4\tilde{r}_i = \min(\min_{j \neq i} |x_i - x_j|, N^{-1/d})$ so that in all cases

$$(3.28) \quad (g(x_i - x_j) - g(\alpha))_+ \geq g(4\tilde{r}_i) - g(\alpha).$$

In view of (3.7), it follows that, if $d \neq 2$,

$$(3.29) \quad \sum_{\substack{i, x_i \in \Omega \\ \text{dist}(x_i, \partial\Omega) \geq \alpha}} g(\tilde{r}_i) \leq C(\mathsf{F}_N^\Omega(X_n, \mu) + \#I_\Omega g(\alpha) + CN \|\mu\|_{L^\infty} \#I_\Omega \alpha^2),$$

with C depending only on d . Now in view of our choice of α and the definition of \tilde{r}_i , if $x_i \in \Omega$ with $\text{dist}(x_i, \partial\Omega) < \alpha$, then $\tilde{r}_i = \alpha$. Hence,

$$\sum_{i, x_i \in \Omega} g(\tilde{r}_i) \leq C(\mathsf{F}_N^\Omega(X_n, \mu) + \#I_\Omega g(\alpha) + CN \|\mu\|_{L^\infty} \#I_\Omega \alpha^2) + \#I_\Omega g(\alpha).$$

Inserting the definition of α into this inequality, we conclude that (3.24) holds if $d \neq 2$. If $d = 2$, we start again from (3.27) and using the same reasoning, we get instead

$$\sum_{i, x_i \in \Omega} g(\tilde{r}_i/\alpha) \leq 2(\mathsf{F}_N^\Omega(X_n, \mu) + \#I_\Omega g(\alpha) + CN \|\mu\|_{L^\infty} \#I_\Omega \alpha^2),$$

and the conclusion follows as well.

We next turn to (3.25). Let us next choose $\alpha_i = \tilde{r}_i$ in (3.20) where we replace the left-hand side by 0. Using that $\tilde{r}_i \leq \frac{1}{4}N^{-1/d}$, we deduce, using again (3.7),

$$\mathsf{F}_N^\Omega(X_n, \mu) \geq \frac{1}{2c_d} \left(\int_\Omega |\nabla v_{\tilde{r}}|^2 - c_d \sum_{i, x_i \in \Omega} g(\tilde{r}_i) \right) - C \#I_\Omega N^{1-\frac{2}{d}},$$

and in view of (3.24), (3.25) follows. In the case $d = 2$ we split $g(\tilde{r}_i)$ into $g(4\tilde{r}_i N^{1/d}) + g(N^{-1/d}/4)$, and then apply (3.24). Finally, (3.26) follows from (3.20) applied to $\alpha_i = \eta_i$. \square

Specializing the relation (3.20) to $\alpha_i = \tilde{r}_i$ if $\text{dist}(x_i, \partial\Omega) < 2N^{-\frac{1}{d}}$ and $\alpha_i = 2N^{-\frac{1}{d}}$ if $\text{dist}(x_i, \partial\Omega) \geq 2N^{-\frac{1}{d}}$, bounding from below \mathcal{F}^α in an obvious way from (3.18) and (3.7), we deduce the following control of short-range interactions

Corollary 3.4. *Under the same assumptions, we have*

$$(3.30) \quad \begin{cases} \sum_{\substack{i \neq j, x_i, x_j \in \Omega, \\ \text{dist}(x_i, \partial\Omega) \geq 3N^{-\frac{1}{d}}, \\ |x_i - x_j| \leq N^{-\frac{1}{d}}}} g(|x_i - x_j|) \leq C(\mathsf{F}_N^\Omega(X_n, \mu, U) + C_0 \#I_\Omega N^{1-\frac{2}{d}}) & \text{if } d \geq 3 \\ \sum_{\substack{i \neq j, x_i, x_j \in \Omega, \\ \text{dist}(x_i, \partial\Omega) \geq 3N^{-\frac{1}{d}}, \\ |x_i - x_j| \leq N^{-\frac{1}{d}}}} g(2|x_i - x_j|N^{\frac{1}{d}}) \leq C \left(\mathsf{F}_N^\Omega(X_n, \mu, U) + \frac{\#I_\Omega}{4} \log N + C_0 \#I_\Omega \right) & \text{if } d = 2. \end{cases}$$

We now present a novel application of the mesoscopic interaction energy control of (3.20) and (3.21) which allows, by combining the estimates obtained over dyadic scales to control general inverse powers of the distances between the points. It is to be combined with Corollary 3.4 to estimate the interaction of microscopically close points.

Proposition 3.5 (Multiscale interaction energy control). *Let $s > 0$ and $N^{-\frac{1}{d}} \leq \ell \leq 1$. We have*

$$\begin{aligned}
 & \sum_{\substack{i \neq j, x_i, x_j \in \Omega \\ N^{-1/d} \leq |x_i - x_j| \leq \ell, \text{dist}(x_i, \partial\Omega) \geq 4\ell}} \frac{1}{|x_i - x_j|^{d-2+s}} \\
 (3.31) \quad & \leq C N^{\frac{s}{d}} \left(\mathsf{F}_N^\Omega(X_n, \mu, U) + \frac{1}{4} (\#I_\Omega \log N) \mathbf{1}_{d=2} \right) + C \#I_\Omega N^{1-\frac{2}{d}+\frac{s}{d}} \\
 & + \begin{cases} C \#I_\Omega N \ell^{2-s} & \text{if } s \neq 2 \\ C \#I_\Omega N \log(\ell N^{\frac{1}{d}}) & \text{if } s = 2, \end{cases}
 \end{aligned}$$

where $C > 0$ depends only on an upper bound for μ and on d .

Proof. Let us for the sake of generality start from any function f such that $f(x)/g(|x|)$ is a positive decreasing function of \mathbb{R} if $d \geq 3$, respectively f a positive decreasing function of \mathbb{R} if $d = 2$. Decomposing over dyadic scales $\leq \ell$, denoting

$$K := \left\lceil \frac{\log(\ell N^{\frac{1}{d}})}{\log 2} \right\rceil,$$

with $[x]$ the smallest integer $\geq x$. We have

$$\begin{aligned}
 & \sum_{\substack{i \neq j, x_i, x_j \in \Omega, \\ N^{-1/d} \leq |x_i - x_j| \leq \ell, \\ \text{dist}(x_i, \partial\Omega) \geq 4\ell}} f(|x_i - x_j|) \leq \sum_{k=0}^{K-1} \sum_{\substack{i \neq j, 2^k N^{-1/d} \leq |x_i - x_j| \leq 2^{k+1} N^{-1/d}, \\ \text{dist}(x_i, \partial\Omega) \geq 4\ell}} f(|x_i - x_j|) \\
 & \leq \sum_{k=0}^{K-1} \sum_{\substack{i \neq j, 2^k N^{-1/d} \leq |x_i - x_j| \leq 2^{k+1} N^{-1/d} \\ \text{dist}(x_i, \partial\Omega) \geq 4 \cdot 2^k N^{-1/d}}} f(2^k N^{-\frac{1}{d}}) \\
 & \leq \sum_{k=0}^{K-1} \frac{f(2^k N^{-\frac{1}{d}})}{g(2^k N^{-\frac{1}{d}})} \sum_{\substack{i \neq j, 2^k N^{-1/d} \leq |x_i - x_j| \leq 2^{k+1} N^{-1/d} \\ \text{dist}(x_i, \partial\Omega) \geq 4 \cdot 2^k N^{-1/d}}} g(2^k N^{-\frac{1}{d}}),
 \end{aligned}$$

where we use that $\text{dist}(x_i, \partial\Omega) \geq 4 \cdot 2^k N^{-1/d}$ and the last line follows from the assumption that f/g is nonincreasing and g nonincreasing. Inserting (3.21), we deduce

$$\sum_{\substack{i \neq j, x_i, x_j \in \Omega, N^{-1/d} \leq |x_i - x_j| \leq \ell, \\ \text{dist}(x_i, \partial\Omega) \geq 4\ell}} f(|x_i - x_j|) \leq C \sum_{k=0}^K \frac{f(2^k N^{-\frac{1}{d}})}{g(2^k N^{-\frac{1}{d}})} (\mathcal{F}^{\vec{\alpha}^k} - \mathcal{F}^{\vec{\alpha}^{k+2}})$$

with for each k , $\alpha_i^k = 2^k N^{-\frac{1}{d}}$ if $\text{dist}(x_i, \partial\Omega) \geq 2^k N^{-\frac{1}{d}}$ and \tilde{r}_i otherwise.

Using Abel's resummation procedure we find

$$\begin{aligned}
 & \sum_{i \neq j, N^{-\frac{1}{d}} \leq |x_i - x_j| \leq \ell, \text{dist}(x_i, \partial\Omega) \geq 4\ell} f(|x_i - x_j|) \\
 & \leq \sum_{k=0}^K \frac{f(2^k N^{-\frac{1}{d}})}{g(2^k N^{-\frac{1}{d}})} \mathcal{F}^{\vec{\alpha}^k} - \sum_{k=2}^{K+2} \frac{f(2^{k-2} N^{-\frac{1}{d}})}{g(2^{k-2} N^{-\frac{1}{d}})} \mathcal{F}^{\vec{\alpha}^k}
 \end{aligned}$$

$$\begin{aligned} &\leq \sum_{k=2}^K \left(\frac{f(2^k N^{-\frac{1}{d}})}{g(2^k N^{-\frac{1}{d}})} - \frac{f(2^{k-2} N^{-\frac{1}{d}})}{g(2^{k-2} N^{-\frac{1}{d}})} \right) \mathcal{F}^{\vec{\alpha}^k} \\ &\quad + \frac{f(2N^{-1/d})}{g(2N^{-1/d})} \mathcal{F}^{\vec{\alpha}^1} + \frac{f(N^{-1/d})}{g(N^{-1/d})} \mathcal{F}^{\vec{\alpha}^0} - \frac{f(2\ell)}{g(2\ell)} \mathcal{F}^{\vec{\alpha}^{K+2}} - \frac{f(\ell)}{g(\ell)} \mathcal{F}^{\vec{\alpha}^{K+1}}. \end{aligned}$$

We next use the decreasing nature of $\mathcal{F}^{\vec{\alpha}}$ with respect to α of (3.17) (applied to $U = \Omega$), hence that of $\mathcal{F}^{\vec{\alpha}^k}$ with respect to k . This monotonicity also allows to bound from above each $\mathcal{F}^{\vec{\alpha}^k}$ by $\mathsf{F}_N^\Omega(X_n, \mu, U)$ and from below (by definition and by (3.7)) as follows

$$\begin{aligned} (3.32) \quad \mathcal{F}^{\vec{\alpha}^k} &\geq -\frac{1}{2} \sum_i g(\alpha_i^k) - CN \sum_i (\alpha_i^k)^2 \geq -\frac{1}{2} \sum_i g(\tilde{r}_i) - CN \sum_i (\alpha_i^k)^2 \\ &\geq -C\mathsf{F}_N^\Omega(X_n, \mu, U) - C\#I_\Omega N^{1-\frac{2}{d}} - CN \sum_{i, x_i \in \Omega} (\alpha_i^k)^2 \\ &\geq -C\mathsf{F}_N^\Omega(X_n, \mu, U) - C\#I_\Omega N^{1-\frac{2}{d}} 2^{2k} \end{aligned}$$

after using (3.24).

Inserting into the above and using the mean-value theorem and the monotonicity of f/g , we obtain if $d \geq 3$,

$$\begin{aligned} (3.33) \quad &\sum_{\substack{i \neq j, N^{-\frac{1}{d}} \leq |x_i - x_j| \leq \ell, \\ \text{dist}(x_i, \partial\Omega) \geq 4\ell}} f(|x_i - x_j|) \\ &\leq C \sum_{k=2}^K -\left(\frac{f}{g}\right)' (2^{k-2} N^{-\frac{1}{d}}) 2^k N^{-\frac{1}{d}} |(\mathcal{F}^{\vec{\alpha}^k})_-| \\ &\quad + 2 \frac{f(N^{-\frac{1}{d}})}{g(N^{-\frac{1}{d}})} \mathsf{F}_N^\Omega(X_n, \mu, U) + (C\mathsf{F}_N^\Omega(X_n, \mu, U) + C\#I_\Omega N \ell^2) \frac{f(\ell)}{g(\ell)}. \end{aligned}$$

If $d \geq 3$, specializing to $f/g = |x|^{-s}$ with $s > 0$, and using (3.32) we find

$$\begin{aligned} (3.34) \quad &\sum_{\substack{i \neq j, N^{-1/d} \leq |x_i - x_j| \leq \ell, \text{dist}(x_i, \partial\Omega) \geq 4\ell}} f(|x_i - x_j|) \\ &\leq C\mathsf{F}_N^\Omega(X_n, \mu, U) N^{\frac{s}{d}} \sum_{k=2}^{[\log(\ell N^{1/d})/\log 2]} 2^{-ks} + C\#I_\Omega N^{1-\frac{2}{d}+\frac{s}{d}} \sum_{k=2}^{[\log(\ell N^{1/d})/\log 2]} 2^{k(2-s)} \\ &\quad + CN^{\frac{s}{d}} (\mathsf{F}_N^\Omega(X_n, \mu, U) + C\#I_\Omega N^{1-\frac{2}{d}}) + C\#I_\Omega N \ell^{2-s} \end{aligned}$$

hence the result (3.31). If $d = 2$, we replace the use of f/g by that of f and the use of $\mathcal{F}^{\vec{\alpha}^k}$ by that of $\mathcal{F}^{\vec{\alpha}^k} + \frac{1}{4}\#I_\Omega \log N$, and obtain the result in a similar way using again (3.21). \square

3.3. Partition functions and local laws

We define the partition functions relative to the set U as

$$(3.35) \quad \mathsf{K}_N(U, \mu) := \int_{U^n} e^{-\beta N^{\frac{2}{d}-1} \mathsf{F}_N(X_n, \mu, U)} d\mu^{\otimes n}(X_n)$$

under the constraint $n = N\mu(U)$. We also let

$$(3.36) \quad \mathsf{Q}_N(U, \mu) = \frac{1}{\mathsf{K}_N(U, \mu)} e^{-\beta N^{\frac{2}{d}-1} \mathsf{F}_N(X_n, \mu, U)} d\mu^{\otimes n}(X_n)$$

be the associated Gibbs measure.

We note that $\mathsf{K}_N(\mathbb{R}^d, \mu)$ coincides with $\mathsf{K}_N(\mu)$ defined in (2.41) and $\mathsf{Q}_N(\mathbb{R}^d, \mu)$ coincides with $\mathbb{P}_{N, \beta}$ in view of (2.40) and (2.41). In all this sequel, if the set U is not specified for the energy or the partition function, then what is meant is $U = \mathbb{R}^d$.

If U is partitioned into p disjoint sets $Q_i, i \in [1, p]$ which are such that $N\mu(Q_i) = n_i$ with n_i integer (in particular the Q_i 's must depend on N) then it is shown in [7] that

$$(3.37) \quad \mathsf{K}_N(U, \mu) \geq \frac{N!}{n_1! \cdots n_p!} \prod_{i=1}^p \mathsf{K}_N(Q_i, \mu),$$

an easy consequence of the subadditivity of the energy F_N . The converse is much harder to prove and was obtained in [7] using the “screening procedure” as a way to control the additivity defect. The result from [7] is

Proposition 3.6 (Almost additivity of the free energy). *Assume that μ is a density bounded above and below by positive constant in Σ . Assume \hat{U} is a subset of Σ at distance larger than d_0 (as in (2.12)) from $\partial\Sigma$ and is a disjoint union of p hyperrectangles Q_i such that $N\mu(Q_i) = n_i$ with n_i integers, of sidelengths in $[R, 2R]$ satisfying*

$$(3.38) \quad RN^{\frac{1}{d}} \geq \rho_\beta + \left(\frac{1}{\beta \chi(\beta)} \log \frac{R^{d-1}}{\rho_\beta^{d-1}} \right)^{\frac{1}{d}}$$

with ρ_β as in (2.11), and in addition, if $d \geq 4$,

$$(3.39) \quad RN^{\frac{1}{d}} \geq \max\left(\beta^{\frac{1}{d-2}-1}, 1\right) N^{\frac{1}{d}} d^{-1}.$$

Then there exists C , depending only on d and the upper and lower bounds for μ in Σ , such that

$$(3.40) \quad \begin{aligned} & \left| \log \mathsf{K}_N(\mathbb{R}^d, \mu) - \left(\log \mathsf{K}_N(\mathbb{R}^d \setminus \hat{U}, \mu) + \sum_{i=1}^p \log \mathsf{K}_N(Q_i, \mu) \right) \right| \\ & \leq CpN^{1-\frac{1}{d}} \left(\beta R^{d-1} \rho_\beta \chi(\beta) + \beta^{1-\frac{1}{d}} \chi(\beta)^{1-\frac{1}{d}} \left(\log \frac{RN^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} R^{d-1} \right). \end{aligned}$$

If U is a subset of Σ equal to a disjoint union of p hyperrectangles Q_i with $N\mu(Q_i) = n_i$ integers, of sidelengths in $[R, 2R]$ with $R \geq \rho_\beta$ satisfying (3.38), then we have, with C as above,

$$(3.41) \quad \begin{aligned} & \left| \log \mathsf{K}_N(U, \mu) - \sum_{i=1}^p \log \mathsf{K}_N(Q_i, \mu) \right| \\ & \leq CpN^{1-\frac{1}{d}} \left(\beta R^{d-1} \chi(\beta) \rho_\beta + \beta^{1-\frac{1}{d}} \chi(\beta)^{1-\frac{1}{d}} \left(\log \frac{RN^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} R^{d-1} \right). \end{aligned}$$

Finally, we will need the following local laws from [7] (here rescaled down to the original scale).

Proposition 3.7 (Local laws). *Assume μ is a density bounded above and below by positive constants in a set Σ whose boundary is a disjoint union of C^1 submanifolds. There exists a constant $C > 0$ depending only on d and the upper and lower bounds for μ in Σ such that the following holds. Assume Q_ℓ is a cube of sidelength $\ell \geq \rho_\beta N^{-1/d}$, with in addition*

$$(3.42) \quad \text{dist}(Q_\ell, \partial\Sigma) \geq d_0$$

in the case $U \setminus \Sigma \neq \emptyset$. We have

(1) (Control of energy)

$$(3.43) \quad \begin{aligned} & \log \mathbb{E}_{\mathsf{Q}_N(U, \mu)} \left(\exp \left(\frac{1}{2} \beta \left(N^{\frac{2}{d}-1} \mathsf{F}_N^{Q_\ell}(\cdot, \mu, U) + \left(\frac{n}{4} \log N \right) \mathbf{1}_{d=2} \right) + C \#(X_n \cap Q_\ell) \right) \right) \\ & \leq C \beta \chi(\beta) N \ell^d \end{aligned}$$

(2) (Control of fluctuations) Letting D denote $\int_{Q_\ell} (\sum_{i=1}^N \delta_{x_i} - N d\mu)$ we have

$$(3.44) \quad \left| \log \mathbb{E}_{Q_N(U, \mu)} \left(\exp \left(\frac{\beta}{C} \frac{D^2}{N^{1-\frac{2}{d}} \ell^d} \min \left(1, \frac{|D|}{N \ell^d} \right) \right) \right) \right| \leq C \beta \chi(\beta) N \ell^d.$$

(3) (Concentration for linear statistics) If φ is a Lipschitz function such that $\|\nabla \varphi\|_{L^\infty} \leq N^{\frac{1}{d}}$ supported in Q_ℓ , we have

$$(3.45) \quad \left| \log \mathbb{E}_{Q_N(U, \mu)} \left(\exp \frac{\beta}{CN \ell^d} \left(\int_{\mathbb{R}^d} \varphi d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) \right)^2 \right) \right| \leq C \beta \chi(\beta) N^{1-\frac{2}{d}} \ell^d \|\nabla \varphi\|_{L^\infty}^2.$$

When choosing $U = \mathbb{R}^d$ we get the results for $\mathbb{P}_{N, \beta}$ since it coincides with $Q_N(\mathbb{R}^d, \mu)$.

We have the following scaling relation about (2.38): if $\lambda > 0$, letting $Y_n = \lambda^{\frac{1}{d}} X_n$ and $\mu'(x) = \frac{\mu(\lambda^{-1/d} x)}{\lambda}$

$$(3.46) \quad F_N(X_n, \mu, U) = \lambda^{1-\frac{2}{d}} F_N(Y_n, \mu', \lambda^{\frac{1}{d}} U) - \left(\frac{n}{4} \log \lambda \right) \mathbf{1}_{d=2}$$

and

$$(3.47) \quad K_N^\beta(U, \mu) = K_N^{\beta \lambda^{1-\frac{2}{d}}}(\lambda^{\frac{1}{d}} U, \mu') e^{\beta(\frac{n}{4} \log \lambda)} \mathbf{1}_{d=2},$$

where we highlighted the β -dependence in a superscript.

4. Comparison of energies through transport

As described in Section 2.5, a major task is to evaluate the difference of energies along a transport, or rather expand it as the transport is close to identity, which is what we describe in this section.

4.1. Variations of energies along a transport

The first statement is a simple computation. For α a multiindex, we denote $|\alpha| = \alpha_1 + \dots + \alpha_d$ and $D^\alpha := \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}$.

Lemma 4.1. *Let μ be a probability density in $L^\infty(\mathbb{R}^d)$ such that $\iint g(x-y) d\mu(x) d\mu(y) < \infty$. Let $\Phi_t = \text{Id} + t\psi$ with ψ supported in a cube Q_ℓ of sidelength ℓ . Assume X_N is a configuration such that $F_N(X_N, \mu) < \infty$. Let*

$$\begin{aligned} A_1(X_N, \mu, \psi) &:= \iint_{\Delta^c} \psi(x) \cdot \nabla g(x-y) d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (x) d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (y) \\ &= \frac{1}{2} \iint_{\Delta^c} (\psi(x) - \psi(y)) \cdot \nabla g(x-y) d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (x) d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (y) \end{aligned}$$

and more generally

$$(4.1) \quad \begin{aligned} A_k(X_N, \mu, \psi) &= \iint_{\Delta^c \cap (Q_\ell \times \mathbb{R}^d)} \sum_{|\alpha|=k} \frac{D^\alpha g(x-y)}{\alpha!} (\psi(x) - \psi(y))^\alpha d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (x) d \left(\sum_{i=1}^N \delta_{x_i} - N \mu \right) (y). \end{aligned}$$

The function $A_k(X_N, \mu, \psi)$ is k -homogeneous in ψ and is the k -th derivative at $t=0$ of $F_N(\Phi_t(X_N), \Phi_t \# \mu)$. Moreover, for $|t| \|\psi\|_{C^1} < 1$, we have

$$(4.2) \quad \frac{d}{dt} F_N(\Phi_t(X_N), \Phi_t \# \mu) = A_1(\Phi_t(X_N), \Phi_t \# \mu, \psi \circ \Phi_t^{-1})$$

and

$$(4.3) \quad \frac{d}{dt} \log K_N(\Phi_t \# \mu) = -\beta N^{\frac{2}{d}-1} \mathbb{E}_{Q_N(\Phi_t \# \mu)} (A_1(\Phi_t(X_N), \Phi_t \# \mu, \psi \circ \Phi_t^{-1})).$$

Proof. We denote $\mu_t = \Phi_t \# \mu$. We return to the definition (2.38) and use it to find that if we set

$$\Xi(t) := \mathsf{F}_N(\Phi_t(X_N), \mu_t)$$

we have by definition of the push-forward

$$\Xi(t) = \frac{1}{2} \iint_{\Delta^c} g(\Phi_t(x) - \Phi_t(y)) d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(x) d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(y)$$

and we may compute its derivatives

$$\begin{aligned} \Xi^{(k)}(t) &= \frac{1}{2} \iint_{\Delta^c} \sum_{|\alpha|=k} \frac{D^\alpha g(\Phi_t(x) - \Phi_t(y))}{\alpha!} (\psi(x) - \psi(y))^\alpha d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(x) d\left(\sum_{i=1}^N \delta_{x_i} - N\mu\right)(y). \end{aligned}$$

The statement about the derivatives at $t = 0$, as well as the relation (4.2) at $t = 0$ then follow immediately. The statement (4.2) can subsequently be extended for any t such that $|t|\psi|_{C^1} < 1$ (this way $\text{Id} + t\psi$ is injective) and (4.3) follows from (2.44). \square

The quantity $\mathsf{A}_1(X_N, \mu, \psi)$ was also estimated in [78], with a functional inequality that contains additive error terms, not sharp enough for our purposes here. Instead we get a better bound in the following proposition, whose proof will occupy the [Appendix](#). It involves using the electric formulation of the energy (see Section 3.1 for the definitions) and computing the difference of energies by transporting the “electric fields”, and giving a renormalized meaning to the term A_1 via the use of truncations. This step is what essentially replaces the loop equations.

Proposition 4.2. *Let μ be a probability measure with a bounded and C^2 density. Let $\ell \geq 2N^{-\frac{1}{d}}$. Let $\psi \in C^2(\mathbb{R}^d, \mathbb{R}^d)$ and assume that there is a set U_ℓ containing an ℓ -neighborhood of the support of $D\psi$. Let finally $\Phi_t = \text{Id} + t\psi$ and $\mu_t = (\text{Id} + t\psi) \# \mu$. Set $\#I_N$ for $\#I_{U_\ell}$ and*

$$(4.4) \quad \Xi(t) := \mathsf{F}_N^{U_\ell}(\Phi_t(X_N), \Phi_t \# \mu) + \left(\frac{\#I_N}{4} \log N \right) \mathbf{1}_{d=2} + C_0 \#I_N N^{1-\frac{2}{d}},$$

where C_0 is the constant in Lemma 3.3 (hence $\Xi \geq 0$). If $t|\psi|_{C^1(U_\ell)}$ is small enough, we have

$$(4.5) \quad \Xi(t) \leq C \Xi(0)$$

$$(4.6) \quad \frac{d}{dt} \mathsf{F}_N(\Phi_t(X_N), \Phi_t \# \mu) = \Xi'(t)$$

$$(4.7) \quad |\Xi'(t)| \leq C |\psi|_{C^1(U_\ell)} \Xi(t),$$

where C depends only on d and $\|\mu\|_{L^\infty(U_\ell)}$ and if moreover $t|\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}})$ is small enough, for any $\alpha' > 0$ and $0 < \sigma \leq 1$, or any $\alpha' > 0$ and $0 < \sigma \leq 1$,

$$\begin{aligned} (4.8) \quad |\Xi''(t)| &\leq C [|\psi|_{C^1}^2 (1 + N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)} + N^{-\frac{2}{d}} |\mu_t|_{C^2(U_\ell)}) + |\psi|_{C^2} \|\psi\|_{L^\infty} (1 + N^{-\frac{\sigma}{d}} |\mu_t|_{C^\sigma(U_\ell)}) \\ &\quad + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) (1 + N^{-\frac{2}{d}} |\mu_t|_{C^2(U_\ell)})] [((N^{\frac{1}{d}} \ell)^{\alpha'(d-2)} \mathbf{1}_{d \geq 3} + \log(\ell N^{\frac{1}{d}}) \mathbf{1}_{d=2}) \Xi(t) \\ &\quad + \ell^{-1} \|\psi\|_{L^\infty} |\psi|_{C^1} [(N^{\frac{1}{d}} \ell)^{-1} (1 + N^{-\frac{1+\sigma}{d}} |\mu_t|_{C^{1+\sigma}(U_\ell)} + N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)}) \Xi(t) \mathbf{1}_{d=2} \\ &\quad + (((N^{\frac{1}{d}} \ell)^{1-2\alpha'} (1 + N^{-\frac{1+\sigma}{d}} |\mu_t|_{C^{1+\sigma}(U_\ell)}) + (N^{\frac{1}{d}} \ell)^{1-\alpha'} N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)}) \Xi(t) \\ &\quad + (N^{\frac{1}{d}} \ell)^{1-2\alpha'} N^{-\frac{1}{d}} \Xi(t)^{\frac{d-1}{d-2}}] \mathbf{1}_{d \geq 3}]] \end{aligned}$$

where C depends only on \mathbf{d} , $\|\mu\|_{L^\infty(U_\ell)}$ and the bounds on $t|\psi|_{C^1}$ and $t|\psi|_{C^2}N^{-\frac{1}{\mathbf{d}}}\log(\ell N^{\frac{1}{\mathbf{d}}})$. Moreover, we have $\Xi'(0) = \mathsf{A}_1(X_N, \mu, \psi)$, $\Xi'(t) = \mathsf{A}_1(\Phi_t(X_N), \Phi_t\#\mu, \psi \circ \Phi_t^{-1})$ and for any $\vec{\eta}$ such that $\eta_i \leq \mathbf{r}_i$ for each i , we have

$$(4.9) \quad \begin{aligned} & \mathsf{A}_1(X_N, \mu, \psi) \\ &= \frac{1}{2c_{\mathbf{d}}} \int_{\mathbb{R}^{\mathbf{d}}} \nabla h_{\vec{\eta}}^\mu [X_N] \cdot ((2D\psi - (\operatorname{div} \psi)\operatorname{Id}) \nabla h_{\vec{\eta}}^\mu) + \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \nabla \tilde{h}_i(x) \cdot (\psi(x) - \psi(x_i)) \\ & \quad + \frac{1}{2} \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \eta_i^{1-\mathbf{d}} ((\psi(x) - \psi(x_i)) \cdot v) - N \sum_{i=1}^N \int_{B(x_i, \eta_i)} \nabla \mathsf{f}_{\eta_i}(x) \cdot (\psi(x) - \psi(x_i)) d\mu(x) \end{aligned}$$

where DT means $(\partial_i T_j)_{ij}$ and $\tilde{h}_i = h^\mu[X_N] - \mathsf{g}(\cdot - x_i)$. Thus the right-hand side in (4.9) is independent of $\vec{\eta}$ as long as $\eta_i \leq \mathbf{r}_i$. We also have

$$(4.10) \quad \begin{aligned} |\mathsf{A}_1(X_N, \mu, \psi)| &\leq C \int_{\mathbb{R}^{\mathbf{d}}} |\nabla h_{\frac{1}{4}\mathbf{r}}^\mu|^2 |D\psi| \\ & \quad + C \sum_{i=1}^N |\psi|_{C^1(B(x_i, \frac{1}{4}\mathbf{r}_i))} \left(\int_{B(x_i, \mathbf{r}_i)} |\nabla h_{\frac{1}{4}\mathbf{r}}^\mu|^2 + \mathbf{r}_i^{2-\mathbf{d}} + N^{1-\frac{2}{\mathbf{d}}} \|\mu\|_{L^\infty} \right), \end{aligned}$$

with C as above.

Remark 4.3. If the density μ is bounded below, the norms $|\mu_t|_{C^1}$ and $|\mu_t|_{C^2}$ can be estimated in terms of the norms of μ and ψ via (5.13) and (5.14) applied to $t\psi$. Disregarding the dependence in the norms of μ , this then yields in place of (4.8)

$$(4.11) \quad \begin{aligned} |\Xi''(t)| &\leq C \left[|\psi|_{C^1}^2 (1 + N^{-\frac{1}{\mathbf{d}}} t |\psi|_{C^2} + N^{-\frac{2}{\mathbf{d}}} (t^2 |\psi|_{C^2}^2 + t |\psi|_{C^3})) + |\psi|_{C^2} \|\psi\|_{L^\infty} (1 + N^{-\frac{1}{\mathbf{d}}} t |\psi|_{C^2}) \right. \\ & \quad \left. + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}}) (1 + N^{-\frac{2}{\mathbf{d}}} (t^2 |\psi|_{C^2}^2 + t |\psi|_{C^3})) \right] ((N^{\frac{1}{\mathbf{d}}}\ell)^{\alpha'(\mathbf{d}-2)} \mathbf{1}_{\mathbf{d}\geq 3} + \log(\ell N^{\frac{1}{\mathbf{d}}}) \mathbf{1}_{\mathbf{d}=2}) \Xi(t) \\ & \quad + \ell^{-1} \|\psi\|_{L^\infty} |\psi|_{C^1} \left[(N^{\frac{1}{\mathbf{d}}}\ell)^{-1} (1 + N^{-\frac{2}{\mathbf{d}}} (t^2 |\psi|_{C^2}^2 + t |\psi|_{C^3}) + t N^{-\frac{1}{\mathbf{d}}} |\psi|_{C^2}) \Xi(t) \mathbf{1}_{\mathbf{d}=2} \right. \\ & \quad \left. + ((N^{\frac{1}{\mathbf{d}}}\ell)^{1-2\alpha'} (1 + N^{-\frac{2}{\mathbf{d}}} (t^2 |\psi|_{C^2}^2 + t |\psi|_{C^3})) + (N^{\frac{1}{\mathbf{d}}}\ell)^{1-\alpha'} N^{-\frac{1}{\mathbf{d}}} (1 + t |\psi|_{C^2})) \Xi(t) \right. \\ & \quad \left. + (N^{\frac{1}{\mathbf{d}}}\ell)^{1-2\alpha'} N^{-\frac{1}{\mathbf{d}}} \Xi(t)^{\frac{\mathbf{d}-1}{\mathbf{d}-2}} \mathbf{1}_{\mathbf{d}\geq 3} \right], \end{aligned}$$

where C depends only on the norms of μ , a lower bound for μ , and on \mathbf{d} .

Since $\Xi'(0) = \mathsf{A}_1(X_N, \mu, \psi)$ and $\Xi''(0) = \mathsf{A}_2(X_N, \mu, \psi)$, in view of (4.7) and (4.5) we have proven

Corollary 4.4. *We have*

$$(4.12) \quad |\mathsf{A}_1(X_N, \mu, \psi)| \leq C |\psi|_{C^1} \left(\mathsf{F}_N^{U_\ell}(X_N, \mu) + \left(\frac{\#I_N}{4} \log N \right) \mathbf{1}_{\mathbf{d}=2} + C_0 \#I_N N^{1-\frac{2}{\mathbf{d}}} \right)$$

where C depends only on \mathbf{d} and $\|\mu\|_{L^\infty}$, and if $\mathbf{d} = 2$,

$$(4.13) \quad \begin{aligned} |\mathsf{A}_2(X_N, \mu, \psi)| &\leq C \left[(|\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty} + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}})) \log(\ell N^{\frac{1}{\mathbf{d}}}) \right. \\ & \quad \left. + \ell^{-1} \|\psi\|_{L^\infty} |\psi|_{C^1} (N^{\frac{1}{\mathbf{d}}}\ell)^{-1} \right] \left(\mathsf{F}_N^{U_\ell}(X_N, \mu) + \left(\frac{\#I_N}{4} \log N \right) \mathbf{1}_{\mathbf{d}=2} + C_0 \#I_N N^{1-\frac{2}{\mathbf{d}}} \right), \end{aligned}$$

where C depends only on \mathbf{d} and the norms of μ .

The relation (4.12) provides an improved (and sharp) functional inequality compared to [78], while (4.13) is new. Let us point out that a shorter proof of (4.12) was provided in [70] and, in dimension $\mathbf{d} = 2$ an estimate similar to (4.13) but with non-optimal right-hand side in [71], both after the first version of this paper was completed.

Remark 4.5. Taylor expanding ψ and using also that for a matrix A , we have

$$\int_{\partial B_1} A v \cdot v \, dS = \text{tr}(A) |B_1|$$

where B_1 is the unit ball of \mathbb{R}^d and v stands for the outer unit normal to ∂B_1 , we find that the sum of the last three terms in the right-hand side of (4.9) is equal to

$$\frac{1}{2d} \sum_{i=1}^N \eta_i^{2-d} (\text{div } \psi)(x_i) + O(\eta_i^{3-d}) + o(1) \quad \text{as } \eta_i \rightarrow 0.$$

This way one obtains how the “loop equation” type term

$$\int_{\mathbb{R}^d} \nabla h_{\eta}^{\mu} \cdot ((2D\psi - (\text{div } \psi)\text{Id}) \nabla h_{\eta}^{\mu})$$

needs to be renormalized as $\eta_i \rightarrow 0$. In dimension 2, one finds as in [51]

$$(4.14) \quad \mathsf{A}_1(X_N, \mu, \psi) = \lim_{\eta_i \rightarrow 0} \frac{1}{2c_d} \int_{\mathbb{R}^d} \nabla h_{\eta}^{\mu} \cdot ((2D\psi - (\text{div } \psi)\text{Id}) \nabla h_{\eta}^{\mu}) + \frac{1}{4} \sum_{i=1}^N \text{div } \psi(x_i).$$

In dimension 3, the renormalization is more complicated, and one needs to assume additional regularity of ψ to compute all the nonvanishing orders. One finds

$$\begin{aligned} \mathsf{A}_1(X_N, \mu, \psi) &= \lim_{\eta_i \rightarrow 0} \frac{1}{2c_d} \int_{\mathbb{R}^d} \nabla h_{\eta}^{\mu} \cdot ((2D\psi - (\text{div } \psi)\text{Id}) \nabla h_{\eta}^{\mu}) + \frac{1}{6} \sum_i \frac{1}{\eta_i} \text{div } \psi(x_i) \\ &\quad + \frac{1}{2} \sum_{j,k,m} \partial_j \partial_k \psi_m(x_i) \int_{\partial B_1} v_k v_j v_m, \end{aligned}$$

with the last term vanishing by symmetry. In higher dimension, more and more derivatives of ψ are needed in order to fully express the expansion.

We also record the following variant for Neumann problems in cubes.

Lemma 4.6. *Assume μ_0 is a positive measure with a bounded and C^2 density in a hyperrectangle Q_ℓ of sidelengths in $[\ell, 2\ell]$, with $\ell \geq N^{-\frac{1}{d}}$ and $N\mu_0(Q_\ell) = n$ an integer. Let $\psi \in C^2(Q_\ell, Q_\ell)$ satisfying $\psi \cdot v = 0$ on ∂Q_ℓ where v denotes the outer unit normal, and let $\Phi_t = \text{Id} + t\psi$ and $\mu_t = \Phi_t \# \mu_0$. Let $\mathsf{Q}_N^{(t)}$ denote the Gibbs measure $\mathsf{Q}_N(Q_\ell, \mu_t)$ as in (3.36), and let $\Xi(t) := \mathsf{F}_N(\Phi_t(X_n), \mu_t, Q_\ell) + (\frac{n}{4} \log N) \mathbf{1}_{d=2} + C_0 n N^{1-\frac{2}{d}}$, with C_0 the constant in Lemma 3.3.*

Then there exists a function $\mathsf{A}_1(X_n, \mu, \psi)$ linear in ψ such that if $t|\psi|_{C^1}$ is small enough

•

$$(4.15) \quad \mathsf{A}_1(-X_n, \mu_0(-\cdot), \psi(-\cdot)) = -\mathsf{A}_1(X_n, \mu_0, \psi)$$

•

$$(4.16) \quad \Xi'(t) = \mathsf{A}_1(\Phi_t(X_n), \mu_t, \psi \circ \Phi_t^{-1})$$

•

$$(4.17) \quad |\Xi'(t)| \leq C |\psi|_{C^1} \Xi(t)$$

•

$$(4.18) \quad \frac{d}{dt} \log \mathsf{K}_N(Q_\ell, \mu_t) = \mathbb{E}_{\mathsf{Q}_N^{(t)}} (-\beta N^{\frac{2}{d}-1} \mathsf{A}_1(\Phi_t(X_n), \mu_t, \psi \circ \Phi_t^{-1}))$$

- if moreover $t|\psi|_{C^2}N^{-\frac{1}{d}}\log(\ell N^{\frac{1}{d}})$ is small enough, for any $\alpha' > 0, 0 < \sigma \leq 1$,

$$\begin{aligned}
(4.19) \quad & |\Xi''(t)| \leq C \left[|\psi|_{C^1}^2 (1 + N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)} + N^{-\frac{2}{d}} |\mu_t|_{C^2(U_\ell)}) + |\psi|_{C^2} \|\psi\|_{L^\infty} (1 + N^{-\frac{\sigma}{d}} |\mu_t|_{C^\sigma(U_\ell)}) \right. \\
& \quad + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) (1 + N^{-\frac{2}{d}} |\mu_t|_{C^2(U_\ell)}) \left. \right] (1 + (N^{\frac{1}{d}} \ell)^{\alpha'(\frac{d}{d}-2)} \mathbf{1}_{d \geq 3} + \log(\ell N^{\frac{1}{d}}) \mathbf{1}_{d=2}) \Xi(t) \\
& \quad + \ell^{-1} \|\psi\|_{L^\infty} |\psi|_{C^1} \left[(N^{\frac{1}{d}} \ell)^{-1} (1 + N^{-\frac{1+\sigma}{d}} |\mu_t|_{C^{1+\sigma}(U_\ell)} + N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)}) \Xi(t) \mathbf{1}_{d=2} \right. \\
& \quad + \left. \left(((N^{\frac{1}{d}} \ell)^{1-2\alpha'} (1 + N^{-\frac{1+\sigma}{d}} |\mu_t|_{C^{1+\sigma}(U_\ell)}) + (N^{\frac{1}{d}} \ell)^{1-\alpha'} N^{-\frac{1}{d}} |\mu_t|_{C^1(U_\ell)}) \Xi(t) \right. \right. \\
& \quad \left. \left. + (N^{\frac{1}{d}} \ell)^{1-2\alpha'} N^{-\frac{1}{d}} \Xi(t)^{\frac{d-1}{d-2}} \right) \mathbf{1}_{d \geq 3} \right],
\end{aligned}$$

where C depends only on d and $\|\mu_0\|_{L^\infty}$.

Proof. If one ignores the part of F_N in the second line of its definition (3.14), then the results (4.17) and (4.16) and (4.19) can be deduced from Proposition 4.2 after periodizing the configuration by doing a reflection with respect to the boundary of Q_ℓ , and extending ψ into a compactly supported map. They can also be deduced by following the same steps as in the proof of Proposition 4.2. Then to include the part

$$(4.20) \quad \sum_{i=1}^n \left(g\left(\frac{1}{4} \text{dist}(x_i, \partial Q_\ell)\right) - g\left(\frac{N^{-\frac{1}{d}}}{4}\right) \right)_+,$$

it suffices to remark that the first derivative of the function $t \mapsto g(\frac{1}{4} \text{dist}(\Phi_t(x_i), \partial Q_\ell))$ is $\frac{1}{4}(\text{dist}(x_i, \partial Q_\ell))^{1-d} \psi(x_i) \cdot v$, where v is the outer unit normal to Q_ℓ , and since ψ is Lipschitz and $\psi \cdot v = 0$ on ∂Q_ℓ , we may bound it by $O(|\psi|_{C^1(Q_\ell)} g(\frac{1}{4} \text{dist}(x_i, \partial Q_\ell)))$. By the same arguments, the second derivative is bounded by $O(|\psi|_{C^1(Q_\ell)}^2 g(\frac{1}{4} \text{dist}(x_i, \partial Q_\ell)))$. Summing this over i gives terms that are straightforwardly bounded in terms of (4.20) hence of F_N itself, so the results (4.17), (4.16) and (4.19) hold.

The statement (4.15) is a simple symmetry argument. The result (4.18) is obtained just as (4.3) from (2.44). \square

4.2. Variation of free energy

We now show estimates that bound the variation of $\log K$ with respect to μ , taking advantage of the transport approach and (4.3), respectively (4.18). We start with the setting of a hyperrectangle.

Lemma 4.7. Assume $\rho_\beta N^{-1/d} \leq \ell \leq C$. Let $\mu_0, \mu_1 \in C^1$ be two densities bounded above and below by positive constants in Q_ℓ , a hyperrectangle of sidelengths in $[\ell, 2\ell]$ with $N\mu_0(Q_\ell) = N\mu_1(Q_\ell) = n$ an integer. Then

$$\begin{aligned}
(4.21) \quad & |\log K_N(Q_\ell, \mu_1) - \log K_N(Q_\ell, \mu_0)| \\
& \leq C\beta\chi(\beta)N\ell^d \left(\ell^2 \left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 |\mu_0|_{C^1} |\mu_1 - \mu_0|_{C^1} + \ell \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\mu_1 - \mu_0|_{C^1} \right),
\end{aligned}$$

where C depends only on d .

Proof. Let us solve

$$(4.22) \quad \begin{cases} -\Delta\xi = \mu_1 - \mu_0 & \text{in } Q_\ell \\ \frac{\partial\xi}{\partial v} = 0 & \text{on } \partial Q_\ell. \end{cases}$$

By elliptic regularity and scaling we have

$$|\xi|_{C^1} \leq C\ell^2 |\mu_1 - \mu_0|_{C^1}, \quad |\xi|_{C^2} \leq C\ell |\mu_1 - \mu_0|_{C^1}.$$

Setting

$$\psi := \frac{\nabla\xi}{\mu_0},$$

we thus have

$$\begin{aligned}
 |\psi|_{C^1} &\leq C \left(\left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 |\mu_0|_{C^1} |\xi|_{C^1} + \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\xi|_{C^2} \right) \\
 (4.23) \quad &\leq C \left(\left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 \ell^2 |\mu_0|_{C^1} |\mu_1 - \mu_0|_{C^1} + \ell \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\mu_1 - \mu_0|_{C^1} \right),
 \end{aligned}$$

where

$$(4.24) \quad -\operatorname{div}(\psi \mu_0) = \mu_1 - \mu_0.$$

Let now $v_s = (\operatorname{Id} + s\psi) \# \mu_0$ and $\mu_s = (1-s)\mu_0 + s\mu_1$. We have

$$\frac{d}{ds} \Big|_{s=0} v_s = -\operatorname{div}(\psi \mu_0) = \mu_1 - \mu_0 = \frac{d}{ds} \Big|_{s=0} \mu_s,$$

thus using (4.18), we have

$$(4.25) \quad \frac{d}{ds} \Big|_{s=0} \log \mathsf{K}_N(Q_\ell, \mu_s) = \frac{d}{ds} \Big|_{s=0} \log \mathsf{K}_N(Q_\ell, v_s) = \mathbb{E}_{Q_N(Q_\ell, \mu_0)}(-\beta N^{\frac{2}{d}-1} \mathsf{A}_1(X_n, \mu_0, \psi)).$$

Inserting (4.17), (4.23) and the local laws (3.43) we deduce that

$$\left| \frac{d}{ds} \Big|_{s=0} \log \mathsf{K}_N(Q_\ell, \mu_s) \right| \leq C \beta \chi(\beta) (N \ell^d + n) \left(\ell^2 \left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 |\mu_0|_{C^1} |\mu_1 - \mu_0|_{C^1} + \ell \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\mu_1 - \mu_0|_{C^1} \right).$$

Since $n \leq N \|\mu_0\|_{L^\infty}$ we find

$$(4.26) \quad \left| \frac{d}{ds} \Big|_{s=0} \log \mathsf{K}_N(Q_\ell, \mu_s) \right| \leq C \beta \chi(\beta) N \ell^d \left(\ell^2 \left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 |\mu_0|_{C^1} |\mu_1 - \mu_0|_{C^1} + \ell \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\mu_1 - \mu_0|_{C^1} \right).$$

The same reasoning can be applied near any $s \in [0, 1]$ yielding

$$(4.27) \quad \left| \frac{d}{ds} \log \mathsf{K}_N(Q_\ell, \mu_s) \right| \leq C \beta \chi(\beta) N \ell^d \left(\ell^2 \left\| \frac{1}{\mu_0} \right\|_{L^\infty}^2 |\mu_0|_{C^1} |\mu_1 - \mu_0|_{C^1} + \ell \left\| \frac{1}{\mu_0} \right\|_{L^\infty} |\mu_1 - \mu_0|_{C^1} \right).$$

Integrating between 0 and 1 gives the result. \square

Next, we want to show the analogous result for $\log \mathsf{K}_N(\mathbb{R}^d, \mu)$ when μ varies only in a hyperrectangle Q_ℓ . The difficulty is to build a transport which also stays compactly supported in Q_ℓ (solving Laplace's equation does not work). For that we use the following.

Lemma 4.8. *Assume f is C^1 and compactly supported in Q_ℓ , a hyperrectangle of sidelengths in $[\ell, 2\ell]$ with $\int_{Q_\ell} f = 0$. Then there exists a vector field $U : Q_\ell \rightarrow \mathbb{R}^d$ compactly supported in Q_ℓ , such that*

$$\operatorname{div} U = f \quad \text{in } Q_\ell$$

and

$$(4.28) \quad \|U\|_{L^\infty(Q_\ell)} \leq C \ell \|f\|_{L^\infty(Q_\ell)}, \quad |U|_{C^1(Q_\ell)} \leq C (\ell |f|_{C^1(Q_\ell)} + \|f\|_{L^\infty(Q_\ell)}),$$

where C depends only on d .

Proof. Without loss of generality we may assume that $Q_\ell = \prod_{i=1}^d [0, \ell_i]$ with $\ell_i \leq 2\ell$. We prove the result by induction on d , as a linearization of Knotte–Rosenblatt rearrangement. The case $d = 1$ is easy, we just let $U(x) = \int_0^x f(s) ds$. Assume then that the result is true up to $d - 1$. Then set

$$g(x_1, \dots, x_{d-1}) = \frac{1}{\ell_d} \int_0^{\ell_d} f(x_1, \dots, x_{d-1}, s) ds.$$

The function g is compactly supported in $\prod_{i=1}^{d-1}[0, \ell_i]$ and of integral 0. Thus by the induction hypothesis we may find a vector field $U'(x_1, \dots, x_{d-1})$ with values in \mathbb{R}^{d-1} , compactly supported in $\prod_{i=1}^{d-1}[0, \ell_i]$ such that $\operatorname{div} U' = g$ in $\prod_{i=1}^{d-1}[0, \ell_i]$ and

$$(4.29) \quad \|U'\|_{L^\infty} \leq C\ell\|g\|_{L^\infty} \leq C\ell\|f\|_{L^\infty}, \quad |U'|_{C^1} \leq C(\ell|g|_{C^1} + \|g\|_{L^\infty}) \leq 2C(\ell|f|_{C^1} + \|f\|_{L^\infty}).$$

Let also

$$u(x_1, \dots, x_d) = \int_0^{x_d} f(x_1, \dots, x_{d-1}, s) ds - \frac{x_d}{\ell_d} \int_0^{\ell_d} f(x_1, \dots, x_{d-1}, s) ds.$$

Again u is compactly supported in Q_ℓ , and

$$\|u\|_{L^\infty} \leq 2\ell_d\|f\|_{L^\infty} \quad |u|_{C^1} \leq C\ell_d|f|_{C^1}.$$

Setting $U(x_1, \dots, x_d) = (U'(x_1, \dots, x_{d-1}), u(x_1, \dots, x_d))$, we have that U is compactly supported in Q_ℓ , that

$$\operatorname{div} U = g + \partial_{x_d} u = f$$

and that (4.28) hold. The result is thus true by induction. \square

Lemma 4.9. *Assume ℓ satisfies (2.17). Let $\mu_0, \mu_1 \in C^1$ be two densities bounded above and below by positive constants in Q_ℓ , a hyperrectangle of sidelengths in $[\ell, 2\ell]$ with $N\mu_0(Q_\ell) = N\mu_1(Q_\ell) = n$ an integer, and coinciding outside Q_ℓ . Then*

$$(4.30) \quad \begin{aligned} & |\log K_N(\mathbb{R}^d, \mu_1) - \log K_N(\mathbb{R}^d, \mu_0)| \\ & \leq C\beta\chi(\beta)N\ell^d(\ell|\mu_0|_{C^1(Q_\ell)}\|\mu_1 - \mu_0\|_{L^\infty(Q_\ell)} + \ell|\mu_1 - \mu_0|_{C^1(Q_\ell)} + \|\mu_1 - \mu_0\|_{L^\infty(Q_\ell)}) \end{aligned}$$

where C depends on d and the upper and lower bounds for μ_0 and μ_1 .

Proof. Let us apply Lemma 4.8 to $f = \mu_1 - \mu_0$, and set $\psi := \frac{-U}{\mu_0}$. We thus have

$$(4.31) \quad -\operatorname{div}(\psi\mu_0) = \mu_1 - \mu_0$$

and

$$(4.32) \quad |\psi|_{C^1} \leq C(\ell|\mu_0|_{C^1}\|\mu_1 - \mu_0\|_{L^\infty} + \ell|\mu_1 - \mu_0|_{C^1} + \|\mu_1 - \mu_0\|_{L^\infty})$$

where C depends on d and the upper and lower bounds for μ_0 and μ_1 .

Let now $v_s = (\operatorname{Id} + s\psi)\#\mu_0$ and $\mu_s = (1-s)\mu_0 + s\mu_1$. We have $\frac{d}{ds}|_{s=0}v_s = -\operatorname{div}(\psi\mu_0) = \mu_1 - \mu_0 = \frac{d}{ds}|_{s=0}\mu_s$, thus using (4.3), we have

$$(4.33) \quad \left. \frac{d}{ds} \right|_{s=0} \log K_N(\mathbb{R}^d, \mu_s) = \left. \frac{d}{ds} \right|_{s=0} \log K_N(\mathbb{R}^d, v_s) = \mathbb{E}_{Q_N(\mathbb{R}^d, \mu_0)}(-\beta N^{\frac{2}{d}-1} \mathbf{A}_1(X_N, \mu_0, \psi)).$$

Inserting (4.7), (4.32) and the local laws (3.43) we deduce that

$$\begin{aligned} & \left| \left. \frac{d}{ds} \right|_{s=0} \log K_N(\mathbb{R}^d, \mu_s) \right| \\ & \leq C\beta\chi(\beta)(N\ell^d + n)(\ell|\mu_0|_{C^1}\|\mu_1 - \mu_0\|_{L^\infty} + \ell|\mu_1 - \mu_0|_{C^1} + \|\mu_1 - \mu_0\|_{L^\infty}). \end{aligned}$$

Since $n \leq N\|\mu_0\|_{L^\infty}$ we find

$$\begin{aligned} & \left| \left. \frac{d}{ds} \right|_{s=0} \log K_N(\mathbb{R}^d, \mu_s) \right| \\ & \leq C\beta\chi(\beta)N\ell^d(\ell|\mu_0|_{C^1}\|\mu_1 - \mu_0\|_{L^\infty} + \ell|\mu_1 - \mu_0|_{C^1} + \|\mu_1 - \mu_0\|_{L^\infty}). \end{aligned}$$

The same reasoning can be applied near any $s \in [0, 1]$ yielding

$$\begin{aligned} & \left| \frac{d}{ds} \log \mathsf{K}_N(\mathbb{R}^d, \mu_s) \right| \\ & \leq C\beta\chi(\beta)N\ell^d(\ell|\mu_0|_{C^1}\|\mu_1 - \mu_0\|_{L^\infty} + \ell|\mu_1 - \mu_0|_{C^1} + \|\mu_1 - \mu_0\|_{L^\infty}). \end{aligned}$$

Integrating between 0 and 1 gives the result. \square

5. Study of fluctuations

We are now in a position to return to (2.43) and estimate its various terms. As explained in Section 2.5, since it is difficult to find and evaluate an exact transport from μ_θ to μ_θ^t , we instead (as in [12,51]) replace μ_θ^t by an approximation $\tilde{\mu}_\theta^t$ of the form $(\text{Id} + t\psi)\#\mu_\theta$, which is the same as μ_θ^t at first order in t .

We recall that

$$(5.1) \quad L := \frac{1}{c_d \mu_\theta} \Delta,$$

and that from (2.16), μ_θ is uniformly bounded in $C^{2m+\gamma-4}$. This way the iterates L^k of L satisfy the estimate

$$(5.2) \quad |L^k(\xi)|_{C^\sigma} \leq C \sum_{m=\min(2k,2)}^{2k+\sigma} |\xi|_{C^m} \quad \text{as long as } 2k + \sigma \leq 2m + \gamma - 4$$

where C depends on V, σ, k . We will use this fact repeatedly.

5.1. Choice of transport

We now choose ψ to define $\tilde{\mu}_\theta^t$. By definition, μ_θ^t being the thermal equilibrium measure associated to $V_t = V + t\xi$, it satisfies

$$(5.3) \quad g * \mu_\theta^t + V + t\xi + \frac{1}{\theta} \log \mu_\theta^t = C_t \quad \text{in } \mathbb{R}^d.$$

Comparing with (2.39) and linearizing in t , we find that we should choose ψ solving

$$(5.4) \quad -g * (\text{div}(\psi \mu_\theta)) + \xi - \frac{1}{\theta \mu_\theta} \text{div}(\psi \mu_\theta) = 0.$$

This can be solved exactly by letting h solve

$$-\frac{\Delta h}{c_d \theta \mu_\theta} + h = \xi$$

then taking

$$\psi = -\frac{\nabla h}{c_d \mu_\theta}.$$

However, this ψ fails to be localized on the support of ξ , and it is delicate to show good bounds for it.

Instead we use two approximations. The first is the transport of μ_θ by the map

$$(5.5) \quad \psi := -\frac{1}{c_d \mu_\theta} \sum_{k=0}^q \frac{\nabla L^k(\xi)}{\theta^k},$$

that is

$$(5.6) \quad \tilde{\mu}_\theta^t := (\text{Id} + t\psi)\#\mu_\theta.$$

The second is

$$(5.7) \quad \nu_\theta^t := \mu_\theta + \frac{t}{c_d} \sum_{k=0}^q \frac{\Delta L^k(\xi)}{\theta^k}.$$

Here q is an integer to be chosen depending on the regularity of V and ξ . The larger q the more precise the approximation. We will show that ν_θ^t is a good approximation of $\tilde{\mu}_\theta^t$. Also ν_θ^t is convenient because it is easy to compute and because it is an approximate solution to (5.3), as we see below.

We note that $\nu_\theta^t - \mu_\theta$ is supported in Q_ℓ which contains the support of ξ . Moreover $\int \nu_\theta^t = \int \mu_\theta = 1$ hence, since $\mu_\theta \geq \frac{\alpha}{2c_d}$ in $\text{supp } \xi \subset \hat{\Sigma}$ by (2.4), for ν_θ^t to be a probability density it suffices that

$$(5.8) \quad \left\| t \sum_{k=0}^q \frac{\Delta L^k(\xi)}{\theta^k} \right\|_{L^\infty} < \frac{\alpha}{4}.$$

We will also need the condition

$$(5.9) \quad \left\| t \frac{1}{\mu_\theta} \sum_{k=0}^q \frac{\nabla L^k(\xi)}{\theta^k} \right\|_{L^\infty} < \frac{\alpha}{2c_d} \quad \text{and} \quad \left| t \frac{1}{\mu_\theta} \sum_{k=0}^q \frac{\nabla L^k(\xi)}{\theta^k} \right|_{C^1} < \frac{\alpha}{2c_d}$$

which ensures in view of (5.5) that

$$(5.10) \quad |t|(\|\psi\|_{L^\infty} + |\psi|_{C^1}) < 1,$$

since without loss of generality we may assume that $\alpha < c_d$.

We start with a general lemma about the error made when replacing an exact transport by a linearized transport. The main point is that the right-hand side is quadratic in ψ . We also insert a general control for transported densities.

Lemma 5.1. *Assume $\mu \in C^3$ is a positive density bounded above and below by positive constants in the support of ψ , where ψ is a C^1 map such that*

$$(5.11) \quad \|\psi\|_{L^\infty} + |\psi|_{C^1} < 1.$$

Then for any $\sigma \in [0, 1]$, we have

$$(5.12) \quad \begin{aligned} & |(\text{Id} + \psi)\#\mu - (\mu - \text{div}(\psi\mu))|_{C^\sigma} \\ & \leq C \left(|\mu|_{C^2} \|\psi\|_{L^\infty}^2 + |\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty} \right)^{1-\sigma} \\ & \quad \times \left(|\mu|_{C^2} |\psi|_{C^1} \|\psi\|_{L^\infty} + |\mu|_{C^3} \|\psi\|_{L^\infty}^2 + |\mu|_{C^1} \|\psi\|_{L^\infty} |\psi|_{C^1} + |\mu|_{C^2} \|\psi\|_{L^\infty}^2 \right. \\ & \quad \left. + |\psi|_{C^1} |\psi|_{C^2} + |\psi|_{C^3} \|\psi\|_{L^\infty} \right)^\sigma \end{aligned}$$

where C depends only on d and the upper and lower bounds for μ . Moreover,

$$(5.13) \quad |(\text{Id} + \psi)\#\mu|_{C^1} \leq C(|\mu|_{C^1} + |\psi|_{C^2})$$

$$(5.14) \quad |(\text{Id} + \psi)\#\mu|_{C^2} \leq C(|\mu|_{C^2} + (|\mu|_{C^1} + |\psi|_{C^2})(1 + |\psi|_{C^2}) + |\psi|_{C^3}),$$

where C depends only on d and the upper and lower bounds for μ .

Proof. Let $\tilde{\mu} := (\text{Id} + \psi)\#\mu$ and $\nu = \mu - \text{div}(\psi\mu)$ and $\Phi = \text{Id} + \psi$. By definition of the push-forward we have

$$(5.15) \quad \tilde{\mu} = \frac{\mu \circ \Phi^{-1}}{\det(\text{Id} + D\psi) \circ \Phi^{-1}}$$

and using a Taylor expansion and (5.11) we may write

$$\|\mu \circ \Phi^{-1} - \mu - \nabla \mu \cdot \psi\|_{L^\infty} \leq C |\mu|_{C^2} \|\psi\|_{L^\infty}^2$$

and also

$$(5.16) \quad \begin{aligned} & |\mu \circ \Phi^{-1} - \mu - \nabla \mu \cdot \psi|_{C^1} \\ & \leq C(|\mu|_{C^2} |\psi|_{C^1} \|\psi\|_{L^\infty} + |\mu|_{C^3} \|\psi\|_{L^\infty}^2 + |\mu|_{C^1} \|\psi\|_{L^\infty} |\psi|_{C^1} + |\mu|_{C^2} \|\psi\|_{L^\infty}^2). \end{aligned}$$

Also by Taylor expansion, we find (again with (5.11)) that

$$(\det(\text{Id} + D\psi) \circ \Phi^{-1})^{-1} = 1 - \text{div } \psi + u$$

with

$$\|u\|_{L^\infty} \leq C(|\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty})$$

and

$$|u|_{C^1} \leq C(|\psi|_{C^1} |\psi|_{C^2} + |\psi|_{C^3} \|\psi\|_{L^\infty}).$$

Combining these relations, it follows that

$$\|\nu - \tilde{\mu}\|_{L^\infty} \leq C(|\mu|_{C^2} \|\psi\|_{L^\infty}^2 + |\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty})$$

and

$$(5.17) \quad \begin{aligned} |\nu - \tilde{\mu}|_{C^1} \leq & C(|\mu|_{C^2} |\psi|_{C^1} \|\psi\|_{L^\infty} + |\mu|_{C^3} \|\psi\|_{L^\infty}^2 + |\mu|_{C^1} \|\psi\|_{L^\infty} |\psi|_{C^1} + |\mu|_{C^2} \|\psi\|_{L^\infty}^2 \\ & + |\psi|_{C^1} |\psi|_{C^2} + |\psi|_{C^3} \|\psi\|_{L^\infty}) \end{aligned}$$

hence (5.12) follows by interpolation.

In the same way, we check that, using again (5.11),

$$\begin{aligned} |\mu \circ \Phi^{-1}|_{C^1} & \leq C|\mu|_{C^1}, \\ |\mu \circ \Phi^{-1}|_{C^2} & \leq C(|\mu|_{C^2} + |\mu|_{C^1}(1 + |\psi|_{C^2})), \end{aligned}$$

as well as

$$|\det(\text{Id} + D\psi) \circ \Phi^{-1}|_{C^1} \leq C|\psi|_{C^2}$$

and

$$|\det(\text{Id} + D\psi) \circ \Phi^{-1}|_{C^2} \leq C(|\psi|_{C^3} + |\psi|_{C^2} + |\psi|_{C^2}^2).$$

The estimates (5.13) and (5.14) follow. \square

Lemma 5.2. *Assume $\theta \geq \theta_0(m)$ so that (2.16) holds, and assume (5.8) and (5.9) hold. The choice (5.5) satisfies*

- *The support of ψ is included in the support of $\nabla \xi$.*
- *We have for every $\sigma \geq 0$ such that $\sigma + 2q + 4 \leq 2m + \gamma$,*

$$(5.18) \quad |\psi|_{C^\sigma} \leq C \sum_{k=0}^q \frac{|\xi|_{C^{\sigma+2k+1}(U)}}{\theta^k}$$

where C depends on V, σ and q .

- *If $2m + \gamma \geq 6$ and (5.10) holds, for $\sigma = 1, 2$, we have*

$$(5.19) \quad |\tilde{\mu}_\theta^t|_{C^\sigma(\hat{\Sigma})} \leq C + Ct \sum_{k=0}^{\sigma+1} |\psi|_{C^k}$$

where C depends on $|\mu_\theta|_{C^1}, |\mu_\theta|_{C^2}$.

- If $2m + \gamma \geq 7$, we have for $0 \leq \sigma \leq 1$,

$$(5.20) \quad \begin{aligned} |\tilde{\mu}_\theta^t - \nu_\theta^t|_{C^\sigma} &\leq Ct^2(|\mu_\theta|_{C^2}\|\psi\|_{L^\infty}^2 + |\psi|_{C^1}^2 + |\psi|_{C^2}\|\psi\|_{L^\infty})^{1-\sigma} \\ &\quad \times (|\mu_\theta|_{C^2}|\psi|_{C^1}\|\psi\|_{L^\infty} + |\mu_\theta|_{C^3}\|\psi\|_{L^\infty}^2 + |\mu_\theta|_{C^1}\|\psi\|_{L^\infty}|\psi|_{C^1} + |\mu_\theta|_{C^2}\|\psi\|_{L^\infty}^2 \\ &\quad + |\psi|_{C^1}|\psi|_{C^2} + |\psi|_{C^3}\|\psi\|_{L^\infty})^\sigma \end{aligned}$$

- Letting

$$(5.21) \quad \varepsilon_t := \mathbf{g} * \nu_\theta^t + V + t\xi + \frac{1}{\theta} \log \nu_\theta^t - C_\theta$$

with C_θ as in (2.39), we have that ε_t is supported in the support of ξ and if $2m + \gamma \geq 2q + 6$,

$$(5.22) \quad \|\varepsilon_t\|_{L^\infty} \leq C \frac{t^2}{\theta} \left(\sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+2}} \right)^2 + C \frac{t}{\theta^{q+1}} \sum_{k=2}^{2q+2} |\xi|_{C^k},$$

and if in addition $2m + \gamma \geq 2q + 7$,

$$(5.23) \quad |\varepsilon_t|_{C^1} \leq Ct^2 \sum_{m=0}^{2q} \frac{1}{\theta^{m+1}} \sum_{p+k=m} |\xi|_{C^{2k+2}} |\xi|_{C^{2p+3}} + C \frac{t}{\theta^{q+1}} \sum_{k=2}^{2q+3} |\xi|_{C^k}.$$

Here all the constants $C > 0$ depend only on \mathbf{d} and V .

Proof. The support of ψ is obviously that of $\nabla \xi$. The relation (5.18) is a direct calculation following from (5.5) and (5.2) (and the discussion above it) with (2.16). The estimate (5.19) is the result of direct computations starting from the explicit form (5.15).

By definition of ψ (5.5) and of L (5.1), we have

$$\operatorname{div}(\psi \mu_\theta) = - \sum_{k=0}^q \frac{\Delta L^k(\xi)}{c_d \theta^k}.$$

Comparing with (5.7) we thus have that

$$(5.24) \quad \tilde{\mu}_\theta^t - \nu_\theta^t = (\operatorname{Id} + t\psi) \# \mu_\theta - (\mu_\theta - t \operatorname{div}(\psi \mu_\theta)).$$

Since we assume $2m + \gamma - 4 \geq 3$, we have that $\mu_\theta \in C^3$ by (2.16). We may then apply Lemma 5.1 to μ_θ and $t\psi$. The condition (5.11) is satisfied because it is implied by (5.9). We then obtain (5.20).

Next, we notice that ε_t is supported in $\operatorname{supp} \xi$ and we observe that

$$(5.25) \quad \mathbf{g} * (\nu_\theta^t - \mu_\theta) = -t \sum_{k=0}^q \frac{1}{\theta^k} L^k(\xi)$$

and is also supported in $\operatorname{supp} \xi$. Since $\mathbf{g} * \mu_\theta + V + \frac{1}{\theta} \log \mu_\theta = C_\theta$ by (2.39) and by definition (5.1) and (5.7), we deduce that

$$(5.26) \quad \begin{aligned} \varepsilon_t &:= \mathbf{g} * \nu_\theta^t + V + t\xi + \frac{1}{\theta} \log \nu_\theta^t - C_\theta = -t \sum_{k=1}^q \frac{1}{\theta^k} L^k(\xi) + \frac{1}{\theta} \log \left(1 + \frac{t}{c_d} \sum_{k=0}^q \frac{1}{\theta^k} \Delta L^k(\xi) \right) \\ &= \frac{1}{\theta} (\log(1 + f) - f) + \frac{t}{\theta^{q+1}} L^{q+1}(\xi) \end{aligned}$$

where

$$f := \frac{t}{c_d} \sum_{k=0}^q \frac{1}{\theta^k} \Delta L^k(\xi) = t \sum_{k=0}^q \frac{1}{\theta^k} L^{k+1}(\xi),$$

hence in view of (5.2), if $2m + \gamma \geq 2q + \sigma + 6$, we have

$$(5.27) \quad |f|_{C^\sigma} \leq Ct \sum_{k=0}^q \frac{1}{\theta^k} \sum_{m=2}^{2k+2+\sigma} |\xi|_{C^m} \leq Ct \sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+2+\sigma}}.$$

We now compute $\nabla(\log(1+f) - f) = \nabla f(\frac{1}{1+f} - 1)$, with (5.27), if $2m + \gamma \geq 2q + \sigma + 6$ we find

$$(5.28) \quad \begin{aligned} |\varepsilon_t|_{C^\sigma} &\leq \frac{C}{\theta} |f|_{C^1}^\sigma \|f\|_{L^\infty}^{2-\sigma} + C \frac{t}{\theta^{q+1}} \sum_{k=2}^{2q+2+\sigma} |\xi|_{C^k} \\ &\leq C \frac{t^2}{\theta} \left(\sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+3}} \right)^\sigma \left(\sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+2}} \right)^{2-\sigma} + C \frac{t}{\theta^{q+1}} \sum_{k=2}^{2q+2+\sigma} |\xi|_{C^k}. \end{aligned}$$

Hence (5.22) and (5.23) hold. \square

5.2. Replacement for (2.43)

Instead of the exact relation (2.43) obtained via the splitting with respect to μ_θ and μ_θ^t , we use a relation with errors obtained by splitting with respect to v_θ^t instead of μ_θ^t . Instead of (2.40), we thus find that if (5.8) and (5.9) is satisfied, using (5.21), we have (with obvious notation)

$$(5.29) \quad \begin{aligned} \mathcal{H}_N^{V_t}(X_N) &= N^2 \mathcal{E}^{V_t}(v_\theta^t) + N \int_{\mathbb{R}^d} (\mathbf{g} * v_\theta^t + V_t) d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right) + \mathsf{F}_N(X_N, v_\theta^t) \\ &= N^2 \mathcal{E}^{V_t}(v_\theta^t) + N \int_{\mathbb{R}^d} \left(-\frac{1}{\theta} \log v_\theta^t + \varepsilon_t \right) d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right) + \mathsf{F}_N(X_N, v_\theta^t) \\ &= N^2 \mathcal{E}_\theta^{V_t}(v_\theta^t) + \mathsf{F}_N(X_N, v_\theta^t) - \frac{N}{\theta} \sum_{i=1}^N \log v_\theta^t(x_i) + N \int_{\mathbb{R}^d} \varepsilon_t d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right) \end{aligned}$$

with \mathcal{E}_θ^V as in (1.6). Inserting into the definition of $Z_{N,\beta}^{V_t}$ and using the definition of θ (1.7), we obtain

$$(5.30) \quad \begin{aligned} Z_{N,\beta}^{V_t} &= \exp(-\beta N^{1+\frac{2}{d}} \mathcal{E}_\theta^{V_t}(v_\theta^t)) \\ &\times \int_{\mathbb{R}^d} \exp\left(-\theta \int_{\mathbb{R}^d} \varepsilon_t d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right) - \beta N^{\frac{2}{d}-1} \mathsf{F}_N(X_N, v_\theta^t)\right) d(v_\theta^t)^{\otimes N}(X_N). \end{aligned}$$

Using the definitions (2.41) and (3.36) we may rewrite this as

$$(5.31) \quad Z_{N,\beta}^{V_t} = \exp(-\beta N^{1+\frac{2}{d}} \mathcal{E}_\theta^{V_t}(v_\theta^t)) \mathsf{K}_N(v_\theta^t) \mathbb{E}_{\mathbf{Q}_N(v_\theta^t)} \left(\exp\left(-\theta \int_{\mathbb{R}^d} \varepsilon_t d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right)\right) \right).$$

Combining with (2.43) and (2.42) we find

$$(5.32) \quad \begin{aligned} \mathbb{E}_{\mathbb{P}_{N,\beta}}(e^{-t\beta N^{\frac{2}{d}} \sum_{i=1}^N \xi(x_i)}) \\ = e^{-\beta N^{1+\frac{2}{d}} (\mathcal{E}_\theta^{V_t}(v_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta))} \frac{\mathsf{K}_N(v_\theta^t)}{\mathsf{K}_N(\mu_\theta)} \mathbb{E}_{\mathbf{Q}_N(v_\theta^t)} \left(\exp\left(-\theta \int_{\mathbb{R}^d} \varepsilon_t d\left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t\right)\right) \right). \end{aligned}$$

We now focus on estimating the terms in the right-hand side. The first constant term will be expanded explicitly in t and bring out the explicit expression of the variance. The last term will be small because ε_t is small thanks to the concentration result (3.45). The ratio of partition functions K_N will for now be estimated by the rough bound of Lemma 4.9. This yields the first bounds of Theorem 1. For the proof of the CLT the ratio of K 's will be further analyzed and precisely expanded in t , this will be done in Section 7.

5.3. Ratio of the reduced partition functions

If (5.8) is satisfied, applying (4.30), in view of (5.7) and (5.2) we have, if $2m + \gamma \geq 2q + 7$,

$$(5.33) \quad |\log \mathsf{K}_N(v_\theta^t) - \log \mathsf{K}_N(\mu_\theta)| \leq C\beta\chi(\beta)N\ell^d|t|\sum_{k=0}^q \left(\ell \frac{|\xi|_{C^{2k+3}}}{\theta^k} + \frac{|\xi|_{C^{2k+2}}}{\theta^k} \right).$$

5.4. Estimating the leading order term

Lemma 5.3. *We have*

$$(5.34) \quad \mathcal{E}_\theta^{V_t}(v_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta) - t \int_{\mathbb{R}^d} \xi \, d\mu_\theta = -t^2 v(\xi) + O\left(\frac{t^3}{\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^3 \right)$$

where

$$(5.35) \quad v(\xi) := -\frac{1}{2c_d} \int_{\mathbb{R}^d} \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2 + \frac{1}{c_d} \int_{\mathbb{R}^d} \sum_{k=0}^q \nabla \xi \cdot \frac{\nabla L^k(\xi)}{\theta^k} - \frac{1}{2\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^2$$

and if $2m + \gamma \geq 2q + 6$,

$$(5.36) \quad \begin{aligned} & \left| \mathcal{E}_\theta^{V_t}(v_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta) - t \int_{\mathbb{R}^d} \xi \, d\mu_\theta \right| \\ & \leq C t^2 |\text{supp } \nabla \xi| \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+1}}^2}{\theta^{2k}} + \frac{|\xi|_{C^1} |\xi|_{C^{2k+1}}}{\theta^k} + \frac{|\xi|_{C^{2k+2}}^2}{\theta^{2k+1}} \right). \end{aligned}$$

Proof. We have

$$\begin{aligned} & \mathcal{E}_\theta^{V_t}(v_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta) \\ &= \left(\frac{1}{2} \iint g(x-y) \, dv_\theta^t(x) \, dv_\theta^t(y) - \frac{1}{2} \iint g(x-y) \, d\mu_\theta(x) \, d\mu_\theta(y) + \int V_t \, dv_\theta^t - \int V \, d\mu_\theta \right) \\ & \quad + \frac{1}{\theta} \left(\int v_\theta^t \log v_\theta^t - \int \mu_\theta \log \mu_\theta \right) \\ &= \frac{1}{2} \iint g(x-y) \, d(v_\theta^t - \mu_\theta)(x) \, d(v_\theta^t - \mu_\theta)(y) + \iint g(x-y) \, d(v_\theta^t - \mu_\theta)(x) \, d\mu_\theta(y) \\ & \quad + \int V \, d(v_\theta^t - \mu_\theta) + t \int \xi \, d\mu_\theta + t \int \xi \, d(v_\theta^t - \mu_\theta) + \frac{1}{\theta} \left(\int v_\theta^t \log v_\theta^t - \int \mu_\theta \log \mu_\theta \right) \\ &= \frac{1}{2} \iint g(x-y) \, d(v_\theta^t - \mu_\theta)(x) \, d(v_\theta^t - \mu_\theta)(y) + \int \left(g * \mu_\theta + V + \frac{1}{\theta} \log \mu_\theta \right) \, d(v_\theta^t - \mu_\theta) \\ & \quad + t \int \xi \, d\mu_\theta + t \int \xi \, d(v_\theta^t - \mu_\theta) + \frac{1}{\theta} \int v_\theta^t (\log v_\theta^t - \log \mu_\theta). \end{aligned}$$

The second term of the right-hand side vanishes by characterization of μ_θ in (5.3), and we are left with

$$\begin{aligned} & \mathcal{E}_\theta^{V_t}(v_\theta^t) - \mathcal{E}_\theta^V(\mu_\theta) - t \int \xi \, d\mu_\theta \\ &= \frac{1}{2c_d} \int |\nabla(g * (v_\theta^t - \mu_\theta))|^2 + t \int \xi \, d(v_\theta^t - \mu_\theta) + \frac{1}{2\theta} \int \mu_\theta \left(\frac{v_\theta^t}{\mu_\theta} - 1 \right)^2 + O\left(\frac{1}{\theta} \int \left(\frac{v_\theta^t}{\mu_\theta} - 1 \right)^3 \mu_\theta \right) \end{aligned}$$

where we Taylor expanded the logarithm. We then use (5.25), (5.7) and the definition of L to see that

$$|\nabla(g * (v_\theta^t - \mu_\theta))|^2 = t^2 \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2$$

and

$$\frac{v_\theta^t}{\mu_\theta} = 1 + t \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k}.$$

We thus find (5.34). Alternatively we can Taylor expand the log only to first order and get instead a bound by

$$Ct^2 \left(\int_{\mathbb{R}^d} \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2 + \left| \int_{\mathbb{R}^d} \sum_{k=0}^q \nabla \xi \cdot \frac{\nabla L^k(\xi)}{\theta^k} \right| + \frac{1}{\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^2 \right)$$

from which we deduce (5.36) from (5.2). \square

5.5. Estimating the last term

We start by estimating the last expectation in the right-hand side. We will use two different controls.

Lemma 5.4. *We have*

$$(5.37) \quad \left| \log \mathbb{E}_{Q_N(v_\theta^t)} \left(\exp \left(-\theta \int_{\mathbb{R}^d} \varepsilon_t d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right) \right) \right| \leq C \sqrt{\chi(\beta)} \beta N^{1+\frac{1}{d}} \ell^d |\varepsilon_t|_{C^1} + C \theta N \ell^d |\varepsilon_t|_{C^1}^2$$

and

$$(5.38) \quad \begin{aligned} & \left| \log \mathbb{E}_{Q_N(v_\theta^t)} \left(\exp \left(-\theta \int \varepsilon_t d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right) \right) \right| \\ & \leq C \|\varepsilon_t\|_{L^\infty} \beta N^{\frac{2}{d}+1} \ell^d + C \|\varepsilon_t\|_{L^\infty}^2 \beta N^{1+\frac{2}{d}} \ell^{d-2} \end{aligned}$$

Proof. By Proposition 3.7, local laws and concentration hold for $Q_N(v_\theta^t)$ in $\hat{\Sigma}$ where v_θ^t is bounded below, (3.45) applies and yields for any φ such that $\|\nabla \varphi\|_{L^\infty} \leq N^{\frac{1}{d}}$,

$$\left| \log \mathbb{E}_{Q_N(v_\theta^t)} \left(\exp \frac{\beta}{CN\ell^d} \left(\int_{\mathbb{R}^d} \varphi d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right)^2 \right) \right| \leq C \beta \chi(\beta) N^{1-\frac{2}{d}} \ell^d \|\nabla \varphi\|_{L^\infty}^2$$

We may then apply this to $\varphi = \sqrt{C} \ell^{\frac{d}{2}} N^{\frac{1}{d}+\frac{1}{2}} \sqrt{\lambda} \varepsilon_t$. Thus, for any λ such that $\sqrt{\lambda C} \ell^{\frac{d}{2}} N^{\frac{1}{2}} |\varepsilon_t|_{C^1} \leq 1$ (which ensures that $\|\nabla \varphi\|_{L^\infty} \leq N^{1/d}$), using also that

$$\theta \int \varepsilon_t d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \leq \theta \lambda \left(\int \varepsilon_t \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right)^2 + \frac{\theta}{4\lambda},$$

we have

$$\log \mathbb{E}_{Q_N(v_\theta^t)} \left(\exp \left(\theta \int \varepsilon_t d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right) \right) \leq C \lambda \beta \chi(\beta) N^2 \ell^{2d} |\varepsilon_t|_{C^1}^2 + \frac{\theta}{4\lambda}$$

and optimizing over $\lambda \leq |\varepsilon_t|_{C^1}^{-2} (N \ell^d)^{-1}$ we find (5.37). We next turn to proving (5.38). This time we bound

$$\left| \int \varepsilon_t d \left(\sum_{i=1}^N \delta_{x_i} - N v_\theta^t \right) \right| \leq \|\varepsilon_t\|_{L^\infty} (\#I_\Omega + N \ell^d)$$

where $\#I_\Omega$ denotes the number of points in each configuration that fall in the set Ω , defined as the support of ξ . We can in turn bound from above

$$\#I_\Omega \leq N \int_{\Omega} dv_\theta^t + D(x, C\ell)$$

where $B(x, C\ell)$ is a ball that contains Q_ℓ and $D(x, \ell) = \int_{B(x, C\ell)} \sum_{i=1}^N \delta_{x_i} - N d\mu$. Arguing as before, we write

$$\theta \|\varepsilon_t\|_{L^\infty} D(x, C\ell) \leq \|\varepsilon_t\|_{L^\infty} \left(D^2(x, C\ell) \beta N^{\frac{2}{d}-1} \ell^{2-d} \lambda + \frac{\theta N \ell^{d-2}}{4\lambda} \right)$$

and thus using (3.44), we find,

$$\log \mathbb{E}_{Q_N(\nu_\theta^t)} (\exp(\theta \|\varepsilon_t\|_{L^\infty} D(x, C\ell))) \leq C \|\varepsilon_t\|_{L^\infty} \lambda \beta \chi(\beta) N \ell^d + \frac{\beta \|\varepsilon_t\|_{L^\infty} N^{1+\frac{2}{d}} \ell^{d-2}}{4\lambda}.$$

Optimizing over $\lambda \leq \|\varepsilon_t\|_{L^\infty}^{-1}$ we find

$$\log \mathbb{E}_{Q_N(\nu_\theta^t)} (\exp(\theta \|\varepsilon_t\|_{L^\infty} D(x, C\ell))) \leq C \|\varepsilon_t\|_{L^\infty} \sqrt{\chi(\beta)} \beta N^{1+\frac{1}{d}} \ell^{d-1} + C \|\varepsilon_t\|_{L^\infty}^2 \beta N^{1+\frac{2}{d}} \ell^{d-2}.$$

After observing that $\sqrt{\chi(\beta)} N^{-\frac{1}{d}} \ell^{-1} \leq 1$ by (2.17) and (2.11), the result follows. \square

5.6. First bounds on the fluctuations – proof of Theorem 1 and corollaries

We are now in a position to estimate the terms in (5.32). Under the conditions (5.8), (5.9), inserting (5.33), (5.36) and (5.38) into (5.32), we obtain that $2m + \gamma \geq 2q + 7$ and $\xi \in C^{2q+3}$,

$$\begin{aligned} (5.39) \quad & \left| \log \mathbb{E}_{\mathbb{P}_{N,\beta}} \left(\exp \left(-\beta t N^{\frac{2}{d}} \left(\sum_{i=1}^N \xi(x_i) - N \int \xi d\mu_\theta \right) \right) \right) \right| \\ & \leq C \beta \chi(\beta) N \ell^d |t| \sum_{k=0}^q \left(\ell \frac{|\xi|_{C^{2k+3}}}{\theta^k} + \frac{|\xi|_{C^{2k+2}}}{\theta^k} \right) + \text{Error}_1 + \text{Error}_2 \end{aligned}$$

with

$$|\text{Error}_1| \leq C t^2 \beta N^{1+\frac{2}{d}} |\text{supp } \nabla \xi| \sum_{k=0}^q \left(\frac{|\xi|_{C^{2k+1}}^2}{\theta^{2k}} + \frac{|\xi|_{C^1} |\xi|_{C^{2k+1}}}{\theta^k} + \frac{|\xi|_{C^{2k+2}}^2}{\theta^{2k+1}} \right)$$

and

$$\begin{aligned} (5.40) \quad & |\text{Error}_2| \leq C \frac{t^2 \beta N^{1+\frac{2}{d}} \ell^d}{\theta} \left(\sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+2}} \right)^2 + C \frac{|t|}{\theta^{q+1}} \beta N^{1+\frac{2}{d}} \ell^d \sum_{k=2}^{2q+2} |\xi|_{C^k} \\ & + C \frac{t^4}{\theta^2} \left(\sum_{k=0}^q \frac{1}{\theta^k} |\xi|_{C^{2k+2}} \right)^4 \beta N^{1+\frac{2}{d}} \ell^{d-2} + C \frac{t^2}{\theta^{2(q+1)}} \left(\sum_{k=2}^{2q+2} |\xi|_{C^k} \right)^2 \beta N^{1+\frac{2}{d}} \ell^{d-2}. \end{aligned}$$

Alternatively, using (5.37) instead of (5.38) we obtain that

$$\begin{aligned} (5.41) \quad & |\text{Error}_2| \leq C \sqrt{\chi(\beta)} \beta N^{1+\frac{1}{d}} \ell^d \left(t^2 \sum_{m=0}^{2q} \frac{1}{\theta^{m+1}} \sum_{p+k=m} |\xi|_{C^{2k+2}} |\xi|_{C^{2p+3}} + \frac{|t|}{\theta^{q+1}} \sum_{k=2}^{2q+3} |\xi|_{C^k} \right) \\ & + C \theta N \ell^d \left(t^4 \left(\sum_{m=0}^{2q} \frac{1}{\theta^{m+1}} \sum_{p+k=m} |\xi|_{C^{2k+2}} |\xi|_{C^{2p+3}} \right)^2 + \frac{t^2}{\theta^{2q+2}} \left(\sum_{k=2}^{2q+3} |\xi|_{C^k} \right)^2 \right). \end{aligned}$$

We first focus on the result requiring the least regularity for V and ξ , which are obtained by choosing $q = 0$ in (5.39). Then the conditions (5.8), (5.9) reduce to (2.19). We get that if $V \in C^{2m+\gamma}$ with $2m + \gamma \geq 7$ and $\xi \in C^3$ (using $\beta N^{\frac{2}{d}} \ell^2 \geq 1$ or

$\theta\ell^2 \geq 1$ to absorb some terms),

$$\begin{aligned}
 (5.42) \quad & \left| \log \mathbb{E}_{\mathbb{P}_{N,\beta}} \left(\exp \left(-\beta t N^{\frac{2}{d}} \left(\sum_{i=1}^N \xi(x_i) - N \int \xi \, d\mu_\theta \right) \right) \right) \right| \\
 & \leq C |t| \beta N \ell^d \left(\chi(\beta) \ell |\xi|_{C^3} + \frac{1}{\beta} |\xi|_{C^2} \right) \\
 & \quad + C t^2 \left(N \ell^d |\xi|_{C^2}^2 + |\text{supp } \nabla \xi| \beta N \left(N^{\frac{2}{d}} |\xi|_{C^1}^2 + \frac{1}{\beta} |\xi|_{C^2}^2 \right) \right) + C N \ell^d t^4 |\xi|_{C^2}^4.
 \end{aligned}$$

This proves Theorem 1.

We now prove Corollary 2.1. The proof will be split into the cases $\beta \leq 1$ and $\beta \geq 1$. For $\beta \leq 1$, applying the result of Theorem 1 with $|\xi|_{C^k} \leq M \ell^{-k}$ with $M \geq 1$, we find

$$\begin{aligned}
 (5.43) \quad & \left| \log \mathbb{E}_{\mathbb{P}_{N,\beta}} \left(\exp \left(-\beta t N^{\frac{2}{d}} \left(\sum_{i=1}^N \xi(x_i) - N \int \xi \, d\mu_\theta \right) \right) \right) \right| \\
 & \leq C |t| M N \ell^{d-2} (1 + \beta \chi(\beta)) + C t^2 M^2 N \ell^d (\beta N^{\frac{2}{d}} \ell^{-2} + \ell^{-4}) + C t^4 M^4 N \ell^{d-8} \\
 & \leq C N \ell^d (M |t| \ell^{-2} (\beta + 1) + M^2 t^2 \beta N^{\frac{2}{d}} \ell^{-2} + M^4 t^4 \ell^{-8})
 \end{aligned}$$

because we can absorb ℓ^{-4} into $\beta N^{\frac{2}{d}} \ell^{-2}$ and $\beta \chi(\beta)$ into 1 since $\beta \leq 1$.

We then choose $t = \tau (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}} \ell^2$ and plug into (5.43). The condition (2.19) is then equivalent to $|t| M \ell^{-2}$ small enough, i.e. $C |\tau| (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}} < 1$. Using that $d = 2$ we then find that

$$\begin{aligned}
 & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}} (\exp(\tau \beta |\text{Fluct}(\xi)|))| \\
 & \leq C (|\tau| M (1 + \beta) + \tau^2 M^2 + M^4 \tau^4 (N^{\frac{1}{d}} \ell)^{-4-d} + C M^2 (N^{\frac{1}{d}} \ell)^{-2} \tau^2).
 \end{aligned}$$

This concludes the proof for $\beta \leq 1$.

For $\beta \geq 1$, we choose instead $t = \tau (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}} \ell^2 \beta^{-1}$. The condition (2.19) is then equivalent to $C |\tau| (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}} \times \beta^{-1} < 1$. With the same reasoning, we then find that

$$\begin{aligned}
 & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}} (\exp(\tau |\text{Fluct}(\xi)|))| \\
 & \leq C (|\tau| M + \tau^2 M^2 \beta^{-1} + M^4 \tau^4 (N^{\frac{1}{d}} \ell)^{-4-d} \beta^{-4} + C (N^{\frac{1}{d}} \ell)^{-2} M^2 \tau^2 \beta^{-1})
 \end{aligned}$$

and obtain the desired result.

Choosing $t = \pm \tau \ell^2 ((1 + \beta) N \ell^d)^{-1}$ we get the following estimate in dimension $d \geq 3$. A stronger one will be obtained below, but assuming more regularity on ξ .

Corollary 5.5. *Let $d \geq 3$. Assume $V \in C^7$, (2.2)–(2.4) hold, and $\xi \in C^3$, $\text{supp } \xi \subset B(x, \ell) \subset \hat{\Sigma}$, for some ℓ satisfying (2.17). Assume $|\xi|_{C^k} \leq M \ell^{-k}$ for all $k \leq 3$. Then for all $|\tau| < C^{-1} M^{-1} (1 + \beta) N \ell^d$ we have*

$$(5.44) \quad \left| \log \mathbb{E}_{\mathbb{P}_{N,\beta}} \left(\exp \left(\tau \frac{\beta}{\beta + 1} (N^{\frac{1}{d}} \ell)^{2-d} |\text{Fluct}(\xi)| \right) \right) \right| \leq C (1 + \tau^4 M^4)$$

where C depends only on V and d .

Again we note that since $N \ell^d \geq \rho_\beta^d \geq 1$ we can apply this to any $|\tau| < C^{-1}$.

Proof. We choose the announced t and plug into (5.43). The condition (2.19) is here equivalent to $C |\tau| ((1 + \beta) N \ell^d)^{-1} < 1$. We find that the left hand side in (5.44) is bounded by

$$|\tau| M + \tau^2 M^2 \frac{\beta (N^{\frac{1}{d}} \ell)^{2-d}}{(1 + \beta)^2} + \frac{\beta}{(1 + \beta)^4} \frac{M^4 \tau^4}{(\ell N^{\frac{1}{d}})^{3d}} \leq C (1 + \tau^4 M^4).$$

Since $(N^{1/d} \ell)^{-4-d} \leq \rho_\beta^{-4-d} \leq \min(1, \beta^{2+d})$ by (2.17), we find the announced result. \square

We now turn to an estimate that can be obtained by assuming more regularity on ξ , starting from (5.41), and prove Corollary 2.2. Such an estimate will be more precise when β is small. Since $V \in C^\infty$, $\xi \in C^\infty$, we can take $q = \infty$. The condition (2.19) then becomes $|t|CM\ell^{-2} < 1$. Using that $\theta\ell^2 > 1$ by (2.17) we can sum the series, which yields

$$\begin{aligned}
 (5.45) \quad & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(-\beta t N^{\frac{2}{d}} \text{Fluct}(\xi))))| \\
 & \leq C|t|M\beta\chi(\beta)N\ell^{d-2} + Ct^2M^2\beta N^{1+\frac{2}{d}}\ell^{d-2} + C\sqrt{\chi(\beta)}\beta N^{1+\frac{1}{d}}\ell^d t^2 M^2 \frac{\ell^{-5}}{\theta} + CN\ell^d t^4 M^4 \frac{\ell^{-10}}{\theta} \\
 & \leq C|t|M\beta\chi(\beta)N\ell^{d-2} + Ct^2M^2\beta N^{1+\frac{2}{d}}\ell^{d-2} + CN\ell^d t^4 M^4 \ell^{-8},
 \end{aligned}$$

where the third term was absorbable by the second.

We now optimize over t . When $\beta \geq (\ell N^{\frac{1}{d}})^{2-d}$, it leads to choosing $t = \tau(\chi(\beta)\beta)^{-1}N^{-1}\ell^{2-d}$. The condition (2.19) then becomes $|\tau|M\beta^{-1}(N\ell^d)^{-1}$ small enough. Using that $\theta\ell^2 \geq 1$, we find

$$\begin{aligned}
 (5.46) \quad & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\tau(N^{\frac{1}{d}}\ell)^{2-d}|\text{Fluct}(\xi)|)))| \\
 & \leq C|\tau|M + CM^2\tau^2\beta^{-1}(N^{\frac{1}{d}}\ell)^{-d+2} + C(\tau^4M^4\beta^{-4}N^{-3}\ell^{-3d}) \\
 & \leq C|\tau|M + C\frac{\tau^2M^2}{\beta(N^{\frac{1}{d}}\ell)^{d-2}} + C\frac{\tau^4M^4}{\beta^4(N^{\frac{1}{d}}\ell)^{3d}} \leq C|\tau|M + C\tau^4M^4,
 \end{aligned}$$

where we have used that $\beta \geq (N^{\frac{1}{d}}\ell)^{2-d}$. (If $d=2$ then this implies that $\beta \geq 1$ which obviously suffices to conclude. If $d \geq 3$ then by (2.17) $(N^{\frac{1}{d}}\ell)^{3d} \geq \rho_\beta^{3d} \geq \beta^{-4}$, which also suffices.)

When $\beta \leq (\ell N^{\frac{1}{d}})^{2-d}$, it leads to choosing $t = \tau\chi(\beta)^{-1}\ell^{1-\frac{d}{2}}N^{-\frac{1}{2}-\frac{1}{d}}\beta^{-\frac{1}{2}}$. The condition (2.19) becomes $CM|\tau| < \beta^{\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{1+\frac{d}{2}}$ (again satisfied as soon as $CM|\tau| < 1$) and we find

$$\begin{aligned}
 (5.47) \quad & |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(\tau\beta^{\frac{1}{2}}(\ell N^{\frac{1}{d}})^{1-\frac{d}{2}} \text{Fluct}(\xi))))| \\
 & \leq C\tau M\beta^{\frac{1}{2}}N^{\frac{1}{2}-\frac{1}{d}}\ell^{\frac{d}{2}-1} + CM^2\tau^2 + C(\tau^4\ell^{-4-d}N^{-1-\frac{4}{d}}\beta^{-2}M^4) \\
 & \leq C\frac{\tau M\beta^{\frac{1}{2}}}{(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}}} + CM^2\tau^2 + \frac{C\tau^4M^4}{\beta^2(N^{\frac{1}{d}}\ell)^{d+4}} \leq C\tau M + C\tau^4M^4
 \end{aligned}$$

where we used that $\beta \leq (N^{\frac{1}{d}}\ell)^{2-d}$, and again by (2.17) $N^{\frac{1}{d}}\ell \geq \beta^{-\frac{1}{2}}$.

6. Free energy expansions for nonuniform densities

We now have all the ingredients at hand to complete the proof of Theorem 2 and Proposition 6.4, the free energy expansion. The reader interested in Theorems 3 and 5 may skip the details of this section, assuming the result of Proposition 6.4.

From [7] we already have the expansion of $\log K_N(\square_R, 1)$, for constant density 1 (see (2.25)), then for all constant densities by a simple rescaling (3.47). The case of a nonuniform density is treated by transporting the nonuniform density to its average value on a small cube of size R and using Lemma 4.6 to estimate the error. Then the almost additivity result over cubes (Proposition 3.6) allows to get an expansion over any domain. The last part is to optimize over R , the size of the cubes over which we partition.

Combining Lemma 4.7 with the known expansion for uniform densities, this leads to the following expansion of the free energy in the varying case.

Lemma 6.1. Assume ℓ satisfies (2.17). Let Q_ℓ be a hyperrectangle of sidelengths in $(\ell, 2\ell)$. Let μ be a C^1 density bounded above and below by positive constants in Q_ℓ , and assume $n = N \int_{Q_\ell} \mu$ is an integer. We have

$$(6.1) \quad \begin{aligned} \log K_N(Q_\ell, \mu) = & -\beta N \int_{Q_\ell} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) + \frac{\beta}{4} N \left(\int_{Q_\ell} \mu \log \mu \right) \mathbf{1}_{d=2} - \left(\frac{\beta}{4} n \log N \right) \mathbf{1}_{d=2} \\ & + O \left(\beta \chi(\beta) \rho_\beta N^{1-\frac{1}{d}} \ell^{d-1} + \beta^{1-\frac{1}{d}} \chi(\beta)^{1-\frac{1}{d}} \ell^{d-1} \left(\log \frac{\ell N^{1/d}}{\rho_\beta} \right)^{\frac{1}{d}} \right) \\ & + O \left(\beta N \ell^d (\chi(\beta) \ell |\mu|_{C^1} + \ell^2 |\mu|_{C^1}^2 \mathbf{1}_{d=2}) \right) \end{aligned}$$

with C depending only on d and the upper and lower bounds for μ .

Proof. Let $\bar{\mu}$ denote the average of μ on Q_ℓ . We know from [7] an expansion for $\log K_N(Q_\ell)$ for constant densities, see (3.47) and (2.25). Scaling these formulae properly and inserting into (4.21) applied with $\mu_0 = \bar{\mu}$ and $\mu_1 = \mu$, we find

$$(6.2) \quad \begin{aligned} \log K_N(Q_\ell, \mu) = & N |Q_\ell| \left(-\beta \bar{\mu}^{2-\frac{2}{d}} f_d(\beta \bar{\mu}^{1-\frac{2}{d}}) - \frac{1}{4} \beta (\bar{\mu} \log \bar{\mu}) \mathbf{1}_{d=2} \right) + \left(\frac{\beta}{4} n \log N \right) \mathbf{1}_{d=2} \\ & + O \left(\beta \chi(\beta) \rho_\beta N^{1-\frac{1}{d}} \ell^{d-1} + \beta^{1-\frac{1}{d}} \chi(\beta)^{1-\frac{1}{d}} \ell^{d-1} \left(\log \frac{\ell N^{1/d}}{\rho_\beta} \right)^{\frac{1}{d}} \right) + O(N \beta \chi(\beta) \ell^{d+1} |\mu|_{C^1}), \end{aligned}$$

where the O depend only on d and the upper and lower bounds for μ .

If $d = 3$ we write using a Taylor expansion that

$$f_d(\beta \mu^{1-\frac{2}{d}}) = f_d(\beta \bar{\mu}^{1-\frac{2}{d}}) + O(\beta \|f'_d\|_{\mu, Q_\ell} \ell^d \|\mu - \bar{\mu}\|_{L^\infty(Q_\ell)}).$$

Integrating against $\mu^{2-\frac{2}{d}}$, using $\int_{Q_\ell} \mu - \bar{\mu} = 0$, we find

$$(6.3) \quad -\beta |Q_\ell| \bar{\mu}^{2-\frac{2}{d}} f_d(\beta \bar{\mu}^{1-\frac{2}{d}}) = -\beta \int_{Q_\ell} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) + O(\beta^2 \|f'_d\|_{\mu, Q_\ell} \ell^d \|\mu - \bar{\mu}\|_{L^\infty(Q_\ell)}).$$

In dimension 2, we may write instead

$$(6.4) \quad \begin{aligned} & -\beta |Q_\ell| \bar{\mu}^{2-\frac{2}{d}} f_d(\beta \bar{\mu}^{1-\frac{2}{d}}) - \frac{\beta}{4} |Q_\ell| (\bar{\mu} \log \bar{\mu}) \mathbf{1}_{d=2} \\ & = -\beta \int_{Q_\ell} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) - \frac{\beta}{4} \left(\int_{Q_\ell} \mu \log \mu \right) \mathbf{1}_{d=2} + O(\beta \ell^d \|\mu - \bar{\mu}\|_{L^\infty(Q_\ell)}^2). \end{aligned}$$

Using that $\|\mu - \bar{\mu}\|_{L^\infty(Q_\ell)} \leq \ell |\mu|_{C^1(Q_\ell)}$, (2.24), and inserting into (6.2), we obtain (6.1). \square

By subdividing a cube and using the almost additivity of the free energy, we may improve the error term in the previous expansion.

Assume that Q_R is split into p hyperrectangles Q_i with $N \int_{Q_i} \mu = n_i$ an integer, and Q_i of sidelengths in $(\ell, 2\ell)$, $\ell \gg N^{-1/d} \rho_\beta$. We may always find such a splitting arguing as in [7, Lemma 3.2], itself relying on [75, Lemma 7.5]. It consists in first splitting Q_R into parallel strips of width close to ℓ . Because μ is bounded below and N is large we may modify the width of the strip slightly until the integral of μ in that strip is in $\frac{1}{N} \mathbb{N}$. We then iterate by splitting each strip into lower dimensional strips in a transverse direction, so that the integral in each piece is in $\frac{1}{N} \mathbb{N}$. Repeating this d times we obtain hyperrectangles with quantized mass.

Using Proposition 3.6, in particular (3.41), we have

$$\begin{aligned} \log K_N(Q_R, \mu) = & \sum_{i=1}^p \log K_N(Q_i, \mu) \\ & + O \left(p \beta \chi(\beta) N \ell^d \left(\rho_\beta \ell^{-1} N^{-\frac{1}{d}} + \beta^{-\frac{1}{d}} \chi(\beta)^{-\frac{1}{d}} \ell^{-1} N^{-\frac{1}{d}} \left(\log \frac{\ell N^{1/d}}{\rho_\beta} \right)^{\frac{1}{d}} \right) \right). \end{aligned}$$

Inserting (6.1) yields,

$$\begin{aligned}
 \log K_N(Q_R, \mu) = & -\beta N \int_{Q_R} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) - \frac{\beta}{4} \left(N \int_{Q_R} \mu \log \mu \right) \mathbf{1}_{d=2} + \left(\frac{\beta}{4} n \log N \right) \mathbf{1}_{d=2} \\
 (6.5) \quad & + O \left(\frac{R^d}{\ell^d} \beta \chi(\beta) N \ell^d \left(\rho_\beta \ell^{-1} N^{-\frac{1}{d}} + \beta^{-\frac{1}{d}} \chi(\beta)^{-\frac{1}{d}} \ell^{-1} N^{-\frac{1}{d}} \left(\log \frac{\ell N^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} \right) \right) \\
 & + O \left(\frac{R^d}{\ell^d} \beta N \ell^d \left(\chi(\beta) \ell |\mu|_{C^1(Q_R)} + \ell^2 |\mu|_{C^1(Q_R)}^2 \mathbf{1}_{d=2} \right) \right).
 \end{aligned}$$

We also choose $\ell < |\mu|_{C^1(Q_R)}^{-1}$, so that the $\ell^2 |\mu|_{C^1}^2$ term can be absorbed into the previous one. We are left with choosing $\ell \leq \min(R, |\mu|_{C^1(Q_R)}^{-1})$ minimizing

$$\rho_\beta (N^{\frac{1}{d}} \ell)^{-1} + \beta^{-\frac{1}{d}} \chi(\beta)^{-\frac{1}{d}} (N^{\frac{1}{d}} \ell)^{-1} \left(\log \frac{\ell N^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} + O(\ell |\mu|_{C^1}).$$

We next show that we can make this $o(1)$ as $N \rightarrow \infty$. We will use the notation $r = \ell N^{\frac{1}{d}}$ and $X = |\mu|_{C^1}$.

We also need to enforce the condition (3.38) so in total the constraints on r are

$$(6.6) \quad \rho_\beta + \left(\frac{1}{\beta \chi(\beta)} \log \frac{r^{d-1}}{\rho_\beta^{d-1}} \right)^{\frac{1}{d}} \leq r \leq N^{\frac{1}{d}} \min(R, |\mu|_{C^1(Q_R)}^{-1}).$$

We next find the optimal value.

Lemma 6.2. *Assume $R \leq C$ and*

$$(6.7) \quad N^{\frac{1}{d}} R \geq \rho_\beta + \left(\frac{1}{\beta \chi(\beta)} \log \frac{R^{d-1}}{\rho_\beta^{d-1}} \right)^{\frac{1}{d}}$$

then

$$\begin{aligned}
 (6.8) \quad & \min_{r \text{ satisfies (6.6)}} \left(\rho_\beta r^{-1} + (\beta \chi(\beta))^{-\frac{1}{d}} r^{-1} \left(\log \frac{r}{\rho_\beta} \right)^{\frac{1}{d}} + r N^{-\frac{1}{d}} X \right) \\
 & \leq C \max \left((\rho_\beta X N^{-\frac{1}{d}})^{\frac{1}{2}} \left(1 + \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta X} \right)^{\frac{1}{d}} \right), \rho_\beta R^{-1} N^{-\frac{1}{d}} \left(1 + \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} \right), \right. \\
 & \quad \left. \rho_\beta N^{-\frac{1}{d}} |\mu|_{C^1} \left(1 + \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta |\mu|_{C^1}} \right)^{\frac{1}{d}} \right) \right)
 \end{aligned}$$

where C depends on the constants above.

Proof. If $\sqrt{\frac{\rho_\beta N^{\frac{1}{d}}}{X}} \geq \min(N^{\frac{1}{d}} R, N^{\frac{1}{d}} |\mu|_{C^1(Q_R)}^{-1})$, we take $r = \min(N^{\frac{1}{d}} R, N^{\frac{1}{d}} |\mu|_{C^1(Q_R)}^{-1})$. We then find the min is less than

$$\begin{aligned}
 & \max \left[\rho_\beta R^{-1} N^{-\frac{1}{d}} + (\beta \chi(\beta))^{-\frac{1}{d}} R^{-1} N^{-\frac{1}{d}} \left(\log \frac{R N^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} + X, \right. \\
 & \quad \left. \rho_\beta N^{-\frac{1}{d}} |\mu|_{C^1} + (\beta \chi(\beta))^{-\frac{1}{d}} N^{-\frac{1}{d}} C (1 + |\mu|_{C^1}) \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta |\mu|_{C^1}} \right)^{\frac{1}{d}} + |\mu|_{C^1}^{-1} X \right] \\
 & \leq C \max \left[\rho_\beta R^{-1} N^{-\frac{1}{d}} + (\beta \chi(\beta))^{-\frac{1}{d}} R^{-1} N^{-\frac{1}{d}} \left(\log \frac{R N^{\frac{1}{d}}}{\rho_\beta} \right)^{\frac{1}{d}} + X, \right.
 \end{aligned}$$

$$\rho_\beta N^{-\frac{1}{d}} |\mu|_{C^1} + (\beta \chi(\beta))^{-\frac{1}{d}} N^{-\frac{1}{d}} |\mu|_{C^1} \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta |\mu|_{C^1}} \right)^{\frac{1}{d}} + |\mu|_{C^1}^{-1} X \Big].$$

We note here that we are able to bound X from above thanks to the condition $\sqrt{\frac{\rho_\beta N^{\frac{1}{d}}}{X}} \geq N^{\frac{1}{d}} R$ respectively $\sqrt{\frac{\rho_\beta N^{\frac{1}{d}}}{X}} \geq N^{\frac{1}{d}} |\mu|_{C^1}^{-1}$. If on the other hand

$$\sqrt{\frac{\rho_\beta N^{\frac{1}{d}}}{X}} \leq \min(N^{\frac{1}{d}} R, N^{\frac{1}{d}} |\mu|_{C^1(Q_R)}^{-1})$$

we take that value for r (we may check it always satisfies (6.6)) and find the min is less than

$$(6.9) \quad CN^{-\frac{1}{2d}} \sqrt{X} \sqrt{\rho_\beta} \left(1 + \frac{(\beta \chi(\beta))^{-\frac{1}{d}}}{\rho_\beta} \left(\log \frac{N^{\frac{1}{d}}}{\rho_\beta X} \right)^{\frac{1}{d}} \right).$$

We also observe that by definition (2.11) we always have $\frac{(\beta \chi(\beta))^{-\frac{1}{d}}}{\rho_\beta} \leq 1$. It follows that (6.8) holds. \square

Choosing this optimal ℓ as a subdivision size, inserting this into (6.5), and rephrasing in terms of the variable ℓ instead of R , we obtain the final result.

Proposition 6.3 (Free energy expansion for general density in a hyperrectangle). *Let ℓ satisfy (6.7). Let Q_ℓ be a hyperrectangle of sidelengths in $(\ell, 2\ell)$. Let μ be a C^1 density bounded above and below by positive constants in Q_ℓ , and assume $N \int_{Q_\ell} \mu = n$ is an integer. Then,*

$$(6.10) \quad \begin{aligned} \log K_N(Q_\ell, \mu) = & -\beta N \int_{Q_\ell} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{Q_\ell} \mu \log \mu \right) \mathbf{1}_{d=2} + \left(\frac{\beta}{4} n \log N \right) \mathbf{1}_{d=2} \\ & + O(\beta \chi(\beta) N \ell^d \mathcal{R}(N, \ell, \mu)), \end{aligned}$$

where

$$(6.11) \quad \mathcal{R}(N, \ell, \mu) := \max(x(1 + |\log x|), (y^{\frac{1}{2}} + y)(1 + |\log y|^{\frac{1}{d}}))$$

after setting

$$(6.12) \quad x := \frac{\rho_\beta}{\ell N^{\frac{1}{d}}}, \quad y := \frac{\rho_\beta |\mu|_{C^1}}{N^{\frac{1}{d}}},$$

and the O depend only on d and the upper and lower bounds for μ .

What is useful here is that we get an explicit error rate. The quantity x is small by (6.7), the estimate is interesting when y is small too.

We now conclude

Proposition 6.4 (Relative expansion, local version). *Let μ and $\tilde{\mu}$ be two densities in C^1 coinciding outside Q_ℓ a hyperrectangle included in $\hat{\Sigma}$ of sidelengths in $(\ell, 2\ell)$ with ℓ satisfying (2.17), and bounded above and below by positive constants in Q_ℓ . Assume $N \int_{Q_\ell} \mu = N \int_{Q_\ell} \tilde{\mu} = n$ is an integer. We have*

$$(6.13) \quad \begin{aligned} \log K_N(\mu) - \log K_N(\tilde{\mu}) = & -\beta N \int_{Q_\ell} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{Q_\ell} \mu \log \mu \right) \mathbf{1}_{d=2} \\ & + \beta N \int_{Q_\ell} \tilde{\mu}^{2-\frac{2}{d}} f_d(\beta \tilde{\mu}^{1-\frac{2}{d}}) + \frac{\beta}{4} N \left(\int_{Q_\ell} \tilde{\mu} \log \tilde{\mu} \right) \mathbf{1}_{d=2} \\ & + O(\beta \chi(\beta) N \ell^d (\mathcal{R}(N, \ell, \mu) + \mathcal{R}(N, \ell, \tilde{\mu}))) \end{aligned}$$

where \mathcal{R} is as in Proposition 6.3, and the O depends only on d and the upper and lower bounds for μ and $\tilde{\mu}$ in Q_ℓ .

Proof. We may apply (3.40) to both μ and $\tilde{\mu}$ and subtract the obtained relations to get that

$$\begin{aligned} \log K_N(\mu) - \log K_N(\tilde{\mu}) &= \log K_N(Q_\ell, \mu) - \log K_N(Q_\ell, \tilde{\mu}) \\ &\quad + O\left(N^{1-\frac{1}{d}}\beta\ell^{d-1}\rho_\beta\chi(\beta) + N^{1-\frac{1}{d}}\beta^{1-\frac{1}{d}}\chi(\beta)^{1-\frac{1}{d}}\left(\log\frac{\ell N^{\frac{1}{d}}}{\rho_\beta}\right)^{\frac{1}{d}}\ell^{d-1}\right). \end{aligned}$$

Inserting the result of (6.10) applied to μ and $\tilde{\mu}$, we deduce

$$\begin{aligned} \log K_N(\mu) - \log K_N(\tilde{\mu}) &= -\beta N \int_Q \mu^{2-\frac{2}{d}} f_d(\beta\mu^{1-\frac{2}{d}}) - \frac{\beta}{4} \left(N \int_Q \mu \log \mu \right) \mathbf{1}_{d=2} \\ &\quad + \beta N \int_Q \tilde{\mu}^{2-\frac{2}{d}} f_d(\beta\tilde{\mu}^{1-\frac{2}{d}}) + \frac{\beta}{4} N \left(\int_Q \tilde{\mu} \log \tilde{\mu} \right) \mathbf{1}_{d=2} \\ &\quad + O\left(\beta\chi(\beta)N\ell^d\left(\mathcal{R}(N, \ell, \mu) + \mathcal{R}(N, \ell, \tilde{\mu}) + N^{-\frac{1}{d}}\ell^{-1}\rho_\beta + \beta^{-\frac{1}{d}}\chi(\beta)^{-\frac{1}{d}}\left(\log\frac{\ell N^{\frac{1}{d}}}{\rho_\beta}\right)^{\frac{1}{d}}\ell^{-1}N^{-\frac{1}{d}}\right)\right). \end{aligned}$$

Using again that $\beta\chi(\beta)^{-\frac{1}{d}} \leq \rho_\beta$ by (2.11), by definition of x we see that we may absorb the last error terms into \mathcal{R} . \square

We now turn to the more precise version of Theorem 2.

Theorem 2 (More precise version). *Assume $d \geq 2$. Assume $V \in C^5$ satisfies (2.1)–(2.4). We have*

$$\begin{aligned} \log Z_{N,\beta}^V &= -\beta N^{1+\frac{2}{d}} \mathcal{E}_\theta^V(\mu_\theta) + \frac{\beta}{4} (N \log N) \mathbf{1}_{d=2} - N \frac{\beta}{4} \left(\int_{\mathbb{R}^d} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2} \\ (6.14) \quad &\quad + N \beta \int_{\mathbb{R}^d} \mu_\theta^{2-\frac{2}{d}} f_d(\beta\mu_\theta^{1-\frac{2}{d}}) + O\left(\beta\chi(\beta)N(d_0(1 + (\log N)\mathbf{1}_{d=2}) + \mathcal{R}(N, d_0(1 + (\log N)\mathbf{1}_{d=2}), \mu_\theta))\right) \end{aligned}$$

where \mathcal{R} is as above for the norms of μ_θ in $\hat{\Sigma}$, and the O depends only on d , an upper bound for μ_θ and a lower bound for μ_θ in $\hat{\Sigma}$.

Proof. We take $m = 2$ and $\gamma = 1$ in the introduction, that is $V \in C^5$. This ensures by (2.16) that μ_θ is uniformly bounded in $C^1(\hat{\Sigma})$.

We partition $\hat{\Sigma}$ into hyperrectangles Q_i of sidelengths in $(N^{-\frac{1}{d}}r, 2N^{-\frac{1}{d}}r)$ where r is the minimizer in the right-hand side of (6.8) for the choice $R = d_0(1 + M(\log N)\mathbf{1}_{d=2})$, such that $N \int_{Q_i} \mu_\theta = n_i$ is an integer. Again, this can be done as in [75, Lemma 7.5]. We keep only the hyperrectangles that are inside $\hat{\Sigma}$. This way the local laws are satisfied in $U := \bigcup_i Q_i$ and (3.40) applies. By (2.6), (2.14), definition of $\hat{\Sigma}$ (2.15) and choice of R , we have

$$(6.15) \quad \mu_\theta(U^c) \leq \frac{C}{\sqrt{\theta}} + Cd_0 + CR \leq CR.$$

We apply (3.40) to μ_θ and combine it with the result of Proposition 6.3 to obtain

$$\begin{aligned} \log K_N(\mathbb{R}^d, \mu_\theta) &= -\beta N \int_{\bigcup_i Q_i} \mu_\theta^{2-\frac{2}{d}} f_d(\beta\mu_\theta^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{\bigcup_i Q_i} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2} \\ (6.16) \quad &\quad - \frac{\beta}{4} N \mu_\theta(U)(\log N) \mathbf{1}_{d=2} + \log K_N(\mathbb{R}^d \setminus U, \mu_\theta) + O\left(\beta\chi(\beta)N|U|\mathcal{R}(N, R, \mu_\theta)\right) \end{aligned}$$

where again we can absorb the errors in (3.40) into the \mathcal{R} . To bound $\log K_N(\mathbb{R}^d \setminus U, \mu_\theta)$ we use (6.15) and a bound proved in [7, Proposition 3.8] combined with [7, Lemma 3.7] (after rescaling the coordinates by a $N^{1/d}$ factor)

$$\begin{aligned} (6.17) \quad &\left| \log K_N(\mathbb{R}^d \setminus U, \mu_\theta) - \frac{\beta}{4} N \mu(U^c)(\log N) \mathbf{1}_{d=2} \right| \\ &\leq C \begin{cases} \beta N \mu_\theta(U^c) + \beta N^{1-\frac{1}{d}} \min(\beta^{\frac{1}{d-2}}, 1) & \text{if } d \geq 3 \\ \beta\chi(\beta)N \mu_\theta(U^c) & \text{if } d = 2 \end{cases} \end{aligned}$$

and if $d = 2$ we need to have

$$\mu_\theta(U^c \cap (\hat{\Sigma})^c) \leq C \frac{\mu_\theta(U^c)}{\log N}.$$

This is ensured by the fact that μ_θ is bounded below in $\hat{\Sigma} \cap U^c$ and the definition (2.15) hence $\mu_\theta(U^c) \geq \frac{R}{C}$ while $\mu_\theta(\hat{\Sigma}^c) \leq Cd_0$ as seen in (2.14), so the desired condition follows by definition of R (if M is chosen large enough).

It remains to bound

$$-\beta N \int_{U^c} \mu_\theta^{2-\frac{2}{d}} f_d(\beta \mu_\theta^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{U^c} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2}.$$

In dimension $d \geq 3$ we use that f_d is bounded in view of (2.23) and μ_θ is bounded to bound all this by $CN\beta \int_{U^c} \mu_\theta \leq CN\beta(R + \theta^{-1/2}) \leq CN\beta R$ by (2.6) and (2.14).

In dimension $d = 2$ we bound $\int_{U^c} \mu_\theta \log \mu_\theta$ by $C(R + \theta^{-\frac{1}{2}}) \leq CR$ in view of (2.6). We conclude that

$$\begin{aligned} & -\beta N \int_{\bigcup_i Q_i} \mu_\theta^{2-\frac{2}{d}} f_d(\beta \mu_\theta^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{\bigcup_i Q_i} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2} \\ &= -\beta N \int_{\mathbb{R}^d} \mu_\theta^{2-\frac{2}{d}} f_d(\beta \mu_\theta^{1-\frac{2}{d}}) - \frac{\beta}{4} N \left(\int_{\mathbb{R}^d} \mu_\theta \log \mu_\theta \right) \mathbf{1}_{d=2} + O(CN\beta \chi(\beta)R). \end{aligned}$$

Inserting this and (6.17) into (6.16) we obtain the result of Theorem 2. \square

7. Proof of the CLT

7.1. Comparing partition functions

Let us denote

$$(7.1) \quad \mathcal{Z}(\beta, \mu) = -\beta \int_{\mathbb{R}^d} \mu^{2-\frac{2}{d}} f_d(\beta \mu^{1-\frac{2}{d}}) - \frac{\beta}{4} \left(\int_{\mathbb{R}^d} \mu \log \mu \right) \mathbf{1}_{d=2}.$$

Lemma 7.1. *Let μ_0 be a probability density. Let $\psi \in C^1$ be supported in a cube Q_ℓ of sidelength ℓ included in a set where μ_0 is bounded above and below by positive constants, and let $\mu_t := (\text{Id} + t\psi) \# \mu_0$. If $d \geq 3$, assume (2.30) relatively to μ_t in Q_ℓ for all t small enough. Let us denote $\mathcal{B}_1(\beta, \mu_0, \psi)$ the derivative at $t = 0$ of the function $\mathcal{Z}(\beta, \mu_t)$. We have*

$$(7.2) \quad \mathcal{Z}(\beta, \mu_t) - \mathcal{Z}(\beta, \mu_0) = \mathcal{B}_1(\beta, \mu_0, \psi) + O(t^2 \beta N \ell^d |\psi|_{C^1}^2)$$

and

$$(7.3) \quad |\mathcal{B}_1(\beta, \mu_0, \psi)| \leq C \beta \ell^d |\psi|_{C^1},$$

for some constant $C > 0$ depending on d and the upper and lower bounds for μ_0 in Q_ℓ .

Proof. Denoting $\Phi_t = \text{Id} + t\psi$, we may write

$$\int_{\mathbb{R}^d} \beta \mu_t^{2-\frac{2}{d}} f_d(\beta \mu_t^{1-\frac{2}{d}}) = \int_{\mathbb{R}^d} \beta \mu_t^{1-\frac{2}{d}} f_d(\beta \mu_t^{1-\frac{2}{d}}) \Phi_t \# \mu_0 = \int_{\mathbb{R}^d} \beta (\mu_t \circ \Phi_t)^{1-\frac{2}{d}} f_d(\beta (\mu_t \circ \Phi_t)^{1-\frac{2}{d}}) d\mu_0.$$

Next we recall that by definition of the push forward we have

$$\mu_t \circ \Phi_t = \frac{\mu_0}{\det(\text{Id} + tD\psi)}$$

hence we may bound

$$(7.4) \quad \left| \frac{d^j}{dt^j} \mu_t \circ \Phi_t \right| \leq C \|\mu_0\|_{L^\infty} |\psi|_{C^1}^j$$

Let us first assume $d \geq 3$. Setting $g(x) = \beta x^{1-\frac{2}{d}} f_d(\beta x^{1-\frac{2}{d}})$, we have

$$\frac{d}{dt} g(\mu_t \circ \Phi_t) = g'(\mu_t \circ \Phi_t) \frac{d}{dt} \mu_t \circ \Phi_t$$

and

$$\frac{d^2}{dt^2} g(\mu_t \circ \Phi_t) = g''(\mu_t \circ \Phi_t) \left(\frac{d}{dt} \mu_t \circ \Phi_t \right)^2 + g'(\mu_t \circ \Phi_t) \frac{d^2}{dt^2} \mu_t \circ \Phi_t.$$

Moreover, by (2.24) and the assumption (2.30) we have $|g^{(k)}(x)| \leq C\beta$ for all k , for x bounded above and below by positive constants. Noting that $\mu_t \circ \Phi_t$ remains bounded above and below by positive constants, we deduce that for $k = 1, 2$,

$$\left| \frac{d^k}{dt^k} g(\mu_t \circ \Phi_t) \right| \leq C\beta |\psi|_{C^1}^k.$$

If $d = 2$, there is no dependence in μ_0 inside f_d . In the same way

$$\int_{\mathbb{R}^d} \mu_t \log \mu_t = \int_{\mathbb{R}^d} \log(\mu_t \circ \Phi_t) d\mu_0$$

and the derivatives of $\log(\mu_t \circ \Phi_t)$ are bounded by $C\beta |\psi|_{C^1}^k$. Integrating against $d\mu_0$ on the support of ψ we deduce that for $k \leq 2$,

$$(7.5) \quad |\phi^{(k)}(t)| \leq C\beta \ell^d |\psi|_{C^1}^k.$$

The result follows by Taylor expansion. \square

As announced in Section 2.5, the proof of the CLT relies on improving the error on the expansion of the free energy by comparing two ways of expanding the relative free energy: one by transport and one by application of Proposition 6.4. The idea is that if one knows a quadratic function on a whole interval up to a given error, then one can estimate it near zero with a much better error.

This is done in the following crucial lemma which contains the “Hölder trick” and the exponential moment control of the “anisotropy”.

Lemma 7.2. *Let $\mu_t = (\text{Id} + t\psi)\#\mu_0$ for some ψ supported in a cube Q_ℓ where μ_0 is bounded below by a positive constant. Assume that*

$$(7.6) \quad |\psi|_{C^k} \leq C\ell^{-k-1} \quad \text{for } k = 0, 1, 2, 3,$$

and that $t\ell^{-2} < 1$ is small enough that the result of Proposition 4.2 holds. For any $\alpha' > 0$, the following holds. Let

$$(7.7) \quad \begin{cases} D_N(\psi)^{-2} := \ell^{-4} \log(N^{\frac{1}{d}} \ell) & \text{if } d = 2 \\ D_N(\psi)^{-2} := \ell^{-4} (\log(\ell N^{\frac{1}{d}}) (N^{\frac{1}{d}} \ell)^{\alpha'(\frac{d}{2}-2)} + (N^{\frac{1}{d}} \ell)^{1-\alpha'} + (N^{\frac{1}{d}} \ell)^{1-2\alpha'+\frac{d}{d-2}}) & \text{if } d \geq 3. \end{cases}$$

Assume we know that for each $s \leq D_N(\psi)$, we have

$$(7.8) \quad \log \frac{\mathcal{K}_N(\mu_s)}{\mathcal{K}_N(\mu_0)} = N(\mathcal{Z}(\beta, \mu_s) - \mathcal{Z}(\beta, \mu_0)) + O(\beta \chi(\beta) N \ell^d \mathcal{R}_s)$$

with

$$(7.9) \quad \max_{s \in [0, D_N(\psi)]} \mathcal{R}_s \leq C.$$

Then for every t satisfying

$$(7.10) \quad |t| < t_0 := C^{-1} \left(\max_{s \in [0, D_N(\psi)]} \mathcal{R}_s \right)^{\frac{1}{2}} D_N(\psi)$$

for some appropriate C depending only on the bound in (7.9), we have

$$(7.11) \quad \log \frac{\mathsf{K}_N(\mu_t)}{\mathsf{K}_N(\mu_0)} = tN\mathcal{B}_1(\beta, \mu_0, \psi) + O\left(t\beta\chi(\beta)N\ell^{\mathsf{d}}\left(\max_{s \in [0, D_N(\psi)]} \mathcal{R}_s\right)^{\frac{1}{2}} D_N(\psi)^{-1}\right) + o(1)\mathbf{1}_{\mathsf{d} \geq 3}.$$

Moreover, if $\mathsf{d} = 2$, we have for all t satisfying (7.10)

$$(7.12) \quad \begin{aligned} & \log \mathbb{E}_{\mathbb{P}_{N,\beta}}[\exp(-t\beta(\mathsf{A}_1(X_N, \mu_0, \psi) + N\mathcal{B}_1(\beta, \mu_0, \psi)))] \\ &= O\left(t\beta\chi(\beta)N\ell^{\mathsf{d}}\left(\max_{s \in [0, D_N(\psi)]} \mathcal{R}_s\right)^{\frac{1}{2}} D_N(\psi)^{-1}\right). \end{aligned}$$

Proof. First we define a good event to be

$$G = \begin{cases} (\mathbb{R}^{\mathsf{d}})^N & \text{if } \mathsf{d} = 2 \\ \{X_N, \mathsf{F}_N^{Q_\ell}(X_N) \leq M(N\ell^{\mathsf{d}})N^{1-\frac{2}{\mathsf{d}}}\} & \text{if } \mathsf{d} \geq 3 \end{cases}$$

where M is some constant. In view of the local laws (3.43) we have that if M is chosen large enough,

$$(7.13) \quad \log \mathbb{P}_{N,\beta}(G^c) \leq -\frac{1}{2}M\beta N\ell^{\mathsf{d}}$$

for N large enough. In view of Proposition 4.2, we have $\mathsf{F}_N^{Q_\ell}(\Phi_t(X_N), \Phi_t\#\mu) \leq C\mathsf{F}_N^{Q_\ell}(X_N, \mu)$ and thus by (2.41) and (3.43) again, we may write

$$(7.14) \quad \begin{aligned} \log \frac{\mathsf{K}_N(\mu_t)}{\mathsf{K}_N(\mu_0)} &= \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}(\exp(-\beta N^{\frac{2}{\mathsf{d}}-1}(\mathsf{F}_N^{Q_\ell}(\Phi_t(X_N), \Phi_t\#\mu) - \mathsf{F}_N^{Q_\ell}(X_N, \mu)))) \\ &= \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}(\mathbf{1}_G \exp(-\beta N^{\frac{2}{\mathsf{d}}-1}(\mathsf{F}_N^{Q_\ell}(\Phi_t(X_N), \Phi_t\#\mu) \leq C\mathsf{F}_N^{Q_\ell}(X_N, \mu)))) + o(1). \end{aligned}$$

Next we wish to insert the expansion of Proposition 4.2 into the exponent. More precisely, we use (4.11) and make use of (7.6), $t\ell^{-2} < 1$ and $N^{\frac{1}{\mathsf{d}}}\ell \geq 1$ to absorb all the terms in factor of t . In dimension $\mathsf{d} = 2$, it yields

$$(7.15) \quad \log \frac{\mathsf{K}_N(\mu_t)}{\mathsf{K}_N(\mu_0)} = \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}[\exp(-\beta t\mathsf{A}_1(X_N, \mu_0, \psi) + t^2 O(D_N(\psi)^{-2}\beta(N\ell^{\mathsf{d}} + \mathsf{F}_N^{Q_\ell}(X_N, \mu_0)))].$$

Equating with the expansion (7.2) and setting

$$(7.16) \quad \gamma = \beta N^{\frac{2}{\mathsf{d}}-1}\mathsf{A}_1(X_N, \mu_0, \psi) + N\mathcal{B}_1(\beta, \mu_0, \psi)$$

we thus find

$$\begin{aligned} & \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}(\exp(-t\gamma + O(\beta t^2 D_N(\psi)^{-2}(N\ell^{\mathsf{d}} + \mathsf{F}_N^{Q_\ell}(X_N, \mu_t))))) \\ &= O(t^2 N\ell^{\mathsf{d}} |\psi|_{C^1}^2 \beta \chi(\beta)) + O(\beta \chi(\beta) N\ell^{\mathsf{d}} (\mathcal{R}_t + \mathcal{R}_0)). \end{aligned}$$

Using Cauchy–Schwarz’s inequality and the local laws (3.43) we then deduce that if $|t|D_N(\psi)^{-1} < C^{-1}$ with $C > 2$ (which follows from (7.10) and (7.9)),

$$(7.17) \quad \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}\left(\mathbf{1}_G \exp\left(-\frac{1}{2}t\gamma\right)\right) = O(\beta \chi(\beta) N\ell^{\mathsf{d}} (t^2 D_N(\psi)^{-2} + \mathcal{R}_t + \mathcal{R}_0)).$$

We next turn to dimension $\mathsf{d} \geq 3$ and apply (4.11), which yields

$$\begin{aligned} \log \frac{\mathsf{K}_N(\mu_t)}{\mathsf{K}_N(\mu_0)} &= \log \mathbb{E}_{\mathbb{Q}_N(\mu_0)}[\mathbf{1}_G \exp(-\beta N^{\frac{2}{\mathsf{d}}-1}t\mathsf{A}_1(X_N, \mu_0, \psi) \\ &\quad + \beta N^{\frac{2}{\mathsf{d}}-1}t^2 O(((\ell^{-4} \log(\ell N^{\frac{1}{\mathsf{d}}})(N^{\frac{1}{\mathsf{d}}}\ell)^{\alpha'(\mathsf{d}-2)} + \ell^{-4}(N^{\frac{1}{\mathsf{d}}}\ell)^{1-\alpha'})(\mathsf{F}_N^{Q_\ell} + N^{1-\frac{2}{\mathsf{d}}}N\ell^{\mathsf{d}}) \\ &\quad + \ell^{-4}(N^{\frac{1}{\mathsf{d}}}\ell)^{1-2\alpha'} N^{-\frac{1}{\mathsf{d}}}(\mathsf{F}_N^{Q_\ell} + N^{2-\frac{2}{\mathsf{d}}}\ell^{\mathsf{d}})^{\frac{\mathsf{d}-1}{\mathsf{d}-2}}))) + o(1). \end{aligned}$$

As above, equating with (7.2) and setting (7.16), we obtain with the local laws (3.43) and the fact that we are in the good event G , that (7.17) also holds in this case $d \geq 3$, up to an added $o(1)$, by choice of (7.7).

We now choose $\alpha < D_N(\psi)$ small enough that

$$\frac{\alpha^2}{D_N(\psi)^2} \leq C(\mathcal{R}_0 + \mathcal{R}_\alpha).$$

For that we choose

$$\alpha = C^{-1} \left(\max_{t \in [0, D_N(\psi)]} \mathcal{R}_t \right)^{\frac{1}{2}} D_N(\psi)$$

which is indeed $< D_N(\psi)$ if $\max_{t \in [0, D_N(\psi)]} \mathcal{R}_t$ is bounded and C is well-chosen.

With this choice we then have

$$(7.18) \quad \log \mathbb{E}_{Q_N(\mu_0)}(\mathbf{1}_G \exp(-\alpha \gamma)) = O\left(\beta \chi(\beta) N \ell^d \max_{t \in [0, D_N(\psi)]} \mathcal{R}_t\right) + o(1) \mathbf{1}_{d \geq 3}$$

and the same applies as well to $-\alpha$.

Using Hölder's inequality we deduce that if t/α is small enough, more precisely if (7.10) holds, we have

$$(7.19) \quad |\log \mathbb{E}_{Q_N(\mu_0)}(\mathbf{1}_G \exp(\gamma t))| \leq C \frac{|t|}{\alpha} \beta \chi(\beta) N \ell^d \max_{s \in [0, D_N(\psi)]} \mathcal{R}_s + o(1) \mathbf{1}_{d \geq 3}.$$

Inserting (7.16) and (7.19) into (7.15), and using the definition of α and (3.43) again, we obtain

$$\begin{aligned} \log \frac{K_N(\mu_t)}{K_N(\mu_0)} &= t N \mathcal{B}_1(\beta, \mu_0, \psi) + O\left(t \beta \chi(\beta) N \ell^d D_N(\psi)^{-1} \left(\max_{t \in [0, D_N(\psi)]} \mathcal{R}_t \right)^{\frac{1}{2}}\right) \\ &\quad + O\left(\beta \chi(\beta) N \ell^d t^2 D_N(\psi)^{-2}\right) + o(1) \mathbf{1}_{d \geq 3}. \end{aligned}$$

Since the second error can be absorbed into the first in view of (7.10), this gives the result. \square

We now specialize to μ_θ with the notation of Section 5.

Corollary 7.3. *Under the same assumptions, if t satisfies (7.10), then if $d = 2$, we have*

$$(7.20) \quad \begin{aligned} \log \frac{K_N(\tilde{\mu}_\theta^t)}{K_N(\mu_\theta)} &= t N \frac{\beta}{4} \int_{\mathbb{R}^d} \operatorname{div}(\psi \mu_\theta) \log \mu_\theta \\ &\quad + O\left(t \beta \chi(\beta) N \ell^d \left(\max_{s \in [0, D_N(\psi)]} \mathcal{R}_s \right)^{\frac{1}{2}} D_N(\psi)^{-1}\right), \end{aligned}$$

and if $d \geq 3$

$$(7.21) \quad \begin{aligned} \log \frac{K_N(\tilde{\mu}_\theta^t)}{K_N(\mu_\theta)} &= t N \left(1 - \frac{2}{d}\right) \int_{\mathbb{R}^d} \operatorname{div}(\psi \mu_\theta) \left(f_d(\beta \mu_\theta^{1-\frac{2}{d}}) + \beta \mu_\theta^{1-\frac{2}{d}} f'_d(\beta \mu_\theta^{1-\frac{2}{d}}) \right) \\ &\quad + O\left(t \beta N \ell^d \left(\max_{s \in [0, D_N(\psi)]} \mathcal{R}_s \right)^{\frac{1}{2}} D_N(\psi)^{-1}\right) + o(1). \end{aligned}$$

Proof. This is just a specialization of Lemma 7.2 to $\mu_0 = \mu_\theta$, ψ of (5.5) and $\mu_t = \tilde{\mu}_\theta^t$. In dimension $d = 2$ we compute directly that

$$\mathcal{B}_1(\beta, \mu_\theta, \psi) = \frac{\beta}{4} \int_{\mathbb{R}^d} \operatorname{div}(\psi \mu_\theta) \log \mu_\theta,$$

In dimension $d \geq 3$, we evaluate that

$$\mathcal{B}_1(\beta, \mu_\theta, \psi) = \left(1 - \frac{2}{d}\right) \beta \int_{\mathbb{R}^d} \operatorname{div}(\psi \mu_\theta) \left(f_d(\beta \mu_\theta^{1-\frac{2}{d}}) + \beta \mu_\theta^{1-\frac{2}{d}} f'_d(\beta \mu_\theta^{1-\frac{2}{d}}) \right).$$

\square

7.2. Conclusion

To prove the CLT, the correct choice of t is

$$(7.22) \quad t = \tau \ell^2 \beta^{-\frac{1}{2}} (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}}$$

and the choice of ψ is (5.5). We note that by definition of ρ_β in (2.11) and the assumption (2.17), τ being fixed, we always have

$$(7.23) \quad |t| \leq C \ell^2 \left(\frac{N^{\frac{1}{d}} \ell}{\rho_\beta} \right)^{-1-\frac{d}{2}} \ll \ell^2.$$

We now wish to evaluate (5.32). We wish to replace v_θ^t by $\tilde{\mu}_\theta^t$ in that formula, for that we use (5.20) and (5.18) and inserting it into (4.30) we obtain that if $V \in C^{5+2q} \cap C^7$

$$(7.24) \quad \begin{aligned} & |\log \mathbf{K}_N(v_\theta^t) - \log \mathbf{K}_N(\tilde{\mu}_\theta^t)| \\ & \leq C \beta \chi(\beta) N \ell^d t^2 \left(\left(\sum_{k=0}^{q+1} \frac{|\xi|_{C^{2k+1}}}{\theta^k} \right)^2 + \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+1}}}{\theta^k} \right) \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+3}}}{\theta^k} \right) \right. \\ & \quad + \ell \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+2}}}{\theta^k} \right) \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+1}}}{\theta^k} \right) + \ell \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+2}}}{\theta^k} \right) \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+3}}}{\theta^k} \right) \\ & \quad \left. + \ell \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+4}}}{\theta^k} \right) \left(\sum_{k=0}^q \frac{|\xi|_{C^{2k+1}}}{\theta^k} \right) \right), \end{aligned}$$

where C depends on the norms of μ_θ in $\text{supp } \xi$ up to C^3 , which are uniformly bounded in terms on V in view of (2.16). We may now evaluate all the terms in (5.32) by combining the results (7.24), (5.37), (5.34) and (7.20)–(7.21) all applied with the choice (7.22) and inserting (5.5). Each of these results generates an error.

We let Error_1 denote the error in the right-hand side of (5.34), Error_2 denote the error in the right-hand side of (5.37), Error_3 the error term in (7.20) or (7.21) and Error_4 the error in (7.24). With this notation, obtain

$$(7.25) \quad |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(-\tau \beta^{\frac{1}{2}} (N^{\frac{1}{d}} \ell)^{1-\frac{d}{2}} \text{Fluct}(\xi))) + \tau m(\xi) - \tau^2 \ell^{2-d} v(\xi)| \leq \sum_{i=1}^4 |\text{Error}_i|$$

with v as in (5.35), that is

$$(7.26) \quad v(\xi) = -\frac{1}{2c_d} \int_{\mathbb{R}^d} \left| \sum_{k=0}^q \frac{1}{\theta^k} \nabla L^k(\xi) \right|^2 + \frac{1}{c_d} \int_{\mathbb{R}^d} \sum_{k=0}^q \nabla \xi \cdot \frac{\nabla L^k(\xi)}{\theta^k} - \frac{1}{2\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^2$$

and with

$$m(\xi) = \begin{cases} -\frac{1}{4} \beta^{\frac{1}{2}} \int_{\mathbb{R}^d} \left(\sum_{k=0}^q \frac{\Delta L^k(\xi)}{c_d \theta^k} \right) \log \mu_\theta & \text{if } d = 2 \\ -N \ell^2 \beta^{\frac{1}{2}} (N^{\frac{1}{d}} \ell)^{-1-\frac{d}{2}} \left(1 - \frac{2}{d} \right) \int_{\mathbb{R}^d} \left(\sum_{k=0}^q \frac{\Delta L^k(\xi)}{c_d \theta^k} \right) (f_d(\beta \mu_\theta^{1-\frac{2}{d}}) + \beta \mu_\theta^{1-\frac{2}{d}} f'_d(\beta \mu_\theta^{1-\frac{2}{d}})) & \text{if } d \geq 3. \end{cases}$$

As soon as we can show that $\sum_{i=1}^4 \text{Error}_i = o(1)$, we obtain that the Laplace transform of a suitable scaling of $\text{Fluct}(\xi)$ converges to that of a Gaussian, proving the Central Limit Theorem. We will now show this when specializing to the setting where $|\xi|_{C^k} \leq C \ell^{-k}$. The interested reader could estimate the error for more general choices of ξ . The more regular ξ and V are, the larger q can be taken, and the better the errors in (7.25), in particular in terms of their dependence in $\theta \gg 1$. Also the variance and the mean contain more correction terms.

In dimension $d = 2$ it suffices to take $q = 0$, hence $\xi \in C^4$ suffices, but better estimates of the variance and mean can be obtained if ξ is more regular. If $d \geq 3$ we will need to take q larger as β gets small.

7.3. Estimating the errors

From now on, we assume

$$(7.27) \quad |\xi|_{C^k} \leq C\ell^{-k} \quad \text{for all } k \leq 2q+4.$$

This way, from (5.5) and $\theta\ell^2 \geq 1$ (see (2.18)), we have that (7.6) holds, where C depends on the norms of μ_θ (bounded by (2.16)). This implies, using also (2.17), that $D_N(\psi)$ defined in (7.7) satisfies

$$(7.28) \quad C^{-1}\ell^2(\log(\ell N^{\frac{1}{d}}))^{-\frac{1}{2}} \leq D_N(\psi) \leq C\ell^2$$

if $d = 2$. In dimension $d \geq 3$, we have instead

$$(7.29) \quad C^{-1}\ell^2(\log(\ell N^{\frac{1}{d}})(N^{\frac{1}{d}}\ell)^{\alpha'(d-2)} + (N^{\frac{1}{d}}\ell)^{1-\alpha'} + (N^{\frac{1}{d}}\ell)^{1-2\alpha'+\frac{d}{d-2}})^{-\frac{1}{2}} \leq D_N(\psi) \leq C\ell^2.$$

We now make a specific choice of α' , so as to minimize the sum appearing above and let

$$(7.30) \quad \alpha' = \frac{2d-2}{d(d-2)}.$$

We find that

$$(7.31) \quad D_N(\psi)^{-1} \leq C\ell^{-2}(N^{\frac{1}{d}}\ell)^{1-\frac{1}{d}}.$$

In view of (7.23) we also deduce that $t|\psi|_{C^1}$ and $t|\psi|_{C^2}N^{-\frac{1}{d}}\log(\ell N^{\frac{1}{d}})$ are small, as needed for Proposition 4.2.

7.3.1. The first error term

By definition it is

$$(7.32) \quad \text{Error}_1 := C\beta N^{1+\frac{2}{d}} \left(\frac{t^3}{\theta} \int_{\mathbb{R}^d} \mu_\theta \left| \sum_{k=0}^q \frac{L^{k+1}(\xi)}{\theta^k} \right|^3 \right)$$

and we have with (5.2), (7.22) and (7.27)

$$(7.33) \quad |\text{Error}_1| \leq C\tau^3\beta^{-\frac{3}{2}}(N^{\frac{1}{d}}\ell)^{-3-\frac{d}{2}} \leq C\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-3-\frac{d}{2}},$$

where we used that $\beta^{-\frac{1}{2}} \leq \rho_\beta$ and $\rho_\beta \geq 1$ by (2.11). This term tends to 0 with an algebraic rate in $N^{1/d}\ell/\rho_\beta$ in all dimensions.

7.3.2. The second error

The next error is Error_2 equal to the right-hand side of (5.37) and already estimated in (5.41), hence with t as in (7.22), it becomes

$$(7.34) \quad \begin{aligned} |\text{Error}_2| &\leq C\sqrt{\chi(\beta)}\beta N^{1+\frac{1}{d}}\ell^d \left(C\tau^2\beta^{-1}\ell^4(N^{\frac{1}{d}}\ell)^{-2-d} \sum_{m=0}^{2q} \frac{1}{\theta^{m+1}} \sum_{p+k=m} |\xi|_{C^{2k+2}}|\xi|_{C^{2p+3}} \right) \\ &\quad + C\sqrt{\chi(\beta)}\beta N^{1+\frac{1}{d}}\ell^d \frac{|\tau|\beta^{-\frac{1}{2}}\ell^2(N^{\frac{1}{d}}\ell)^{-1-\frac{d}{2}}}{\theta^{q+1}} \sum_{k=2}^{2q+3} |\xi|_{C^k} \\ &\quad + C\theta N\ell^d \left(C\tau^2\beta^{-1}\ell^4(N^{\frac{1}{d}}\ell)^{-2-d} \sum_{m=0}^{2q} \frac{1}{\theta^{m+1}} \sum_{p+k=m} |\xi|_{C^{2k+2}}|\xi|_{C^{2p+3}} + C\frac{\beta^{-\frac{1}{2}}\ell^2(N^{\frac{1}{d}}\ell)^{-1-\frac{d}{2}}}{\theta^{q+1}} \sum_{k=2}^{2q+3} |\xi|_{C^k} \right)^2. \end{aligned}$$

When (7.27) holds, we find after inserting the definition of θ and simplifying terms

$$(7.35) \quad \begin{aligned} |\text{Error}_2| &\leq C\sqrt{\chi(\beta)}\beta^{-1}\tau^2(N^{\frac{1}{d}}\ell)^{-3} + C|\tau|\sqrt{\chi(\beta)}\beta^{-\frac{1}{2}-q}(N^{\frac{1}{d}}\ell)^{\frac{d}{2}-2-2q} \\ &\quad + C\tau^4\beta^{-3}(N^{\frac{1}{d}}\ell)^{-6-d} + C\tau^2\beta^{-2q-2}(N^{\frac{1}{d}}\ell)^{-4-4q}. \end{aligned}$$

Next we note that by (2.11) we have $\chi(\beta)\beta^{-1} \leq C\rho_\beta^2$ so using also that $\rho_\beta \geq 1$ we find

$$\begin{aligned}
 |\text{Error}_2| &\leq C\tau^2\rho_\beta^2(N^{\frac{1}{d}}\ell)^{-3} + C|\tau|\rho_\beta^{1+2q}(N^{\frac{1}{d}}\ell)^{\frac{d}{2}-2-2q} \\
 &\quad + C\tau^4\rho_\beta^{\frac{2}{3}}(N^{\frac{1}{d}}\ell)^{-6-d} + C\tau^2\rho_\beta^{4q+4}(N^{\frac{1}{d}}\ell)^{-4-4q} \\
 (7.36) \quad &\leq C\tau^2\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-3} + C\tau^4\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-6-d} + C|\tau|\rho_\beta^{1+2q}(N^{\frac{1}{d}}\ell)^{\frac{d}{2}-2-2q}.
 \end{aligned}$$

The first two terms always tend to 0 by the assumption $N^{\frac{1}{d}}\ell \gg \rho_\beta$. If $d = 2$ we find that the third term is $O(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta})^{-1-2q}$ which tends to 0 for any $q \geq 0$. We then have

$$(7.37) \quad |\text{Error}_2| \leq C(\tau^2 + \tau^4)\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-3} + C|\tau|\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-1-2q} \quad \text{if } d = 2.$$

For $d \geq 3$, if β does not tend to 0, then ρ_β is bounded and the third term tends to 0 since we assumed $q > \frac{d}{4} - 1$. If $\beta \rightarrow 0$ then we use the extra assumption (2.32), from which we may then take q large enough depending on ε (so ξ needs to be regular enough) so that the last term tends to 0. This is the reason for the assumption that q is larger than some constant depending on ε made in Theorem 5.

This concludes the analysis of Error_2 , with again an algebraic convergence to 0 as $N^{1/d}\ell/\rho_\beta \rightarrow \infty$.

7.3.3. The third error

By definition, it is the rate error

$$(7.38) \quad \text{Error}_3 := t\beta\chi(\beta)N\ell^d D_N(\psi)^{-1} \left(\max_{s \in [0, C\ell^2]} \mathcal{R}_s \right)^{\frac{1}{2}}.$$

Inserting (7.22) and (7.28) or (7.31), this is

$$(7.39) \quad |\text{Error}_3| \leq C|\tau|\beta^{\frac{1}{2}}\chi(\beta)(N^{\frac{1}{d}}\ell)^{\frac{d}{2}-1}\beta^{\frac{1}{2}}\chi(\beta) \left(\max_{s \in [0, C\ell^2]} \mathcal{R}_s \right)^{\frac{1}{2}} \times \begin{cases} (\log(\ell N^{\frac{1}{d}}))^{\frac{1}{2}} & \text{if } d = 2 \\ (N^{\frac{1}{d}}\ell)^{1-\frac{1}{d}} & \text{if } d \geq 3. \end{cases}$$

For $d \geq 3$, the convergence of Error_3 is ensured by the assumption (2.33).

We now check that this error term can be made small if $d = 2$.

To evaluate \mathcal{R}_s we need to compare (7.8) and Proposition 6.4. First we note that (5.11) and (5.8), (5.9) are verified by (7.23). Then in view of (5.19) for all $\tilde{\mu}_\theta^t$ with $t < t_0$ we have $|\tilde{\mu}_\theta^t|_{C^1} \leq C + |t|\ell^{-3} \leq \ell^{-1}$ by (7.23), which we input into the definition of \mathcal{R} . In view of (7.8) and Proposition 6.4, we may thus bound

$$\max_{s \in [0, C\ell^2]} \mathcal{R}_s = C \left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{-\frac{1}{2}} \left(\log \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{\frac{1}{d}}.$$

To apply (7.20)–(7.21) we needed (7.10) to be satisfied, that is

$$|\tau|\ell^2\beta^{-\frac{1}{2}}(N^{\frac{1}{d}}\ell)^{-1-\frac{d}{2}} < C\ell^2(\log(\ell N^{\frac{1}{d}}))^{-\frac{1}{2}} \left(\max_{[0, C\ell^2]} \mathcal{R}_t \right)^{\frac{1}{2}},$$

for this it suffices that

$$\left(\log \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{\frac{1}{2}} \left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{-1-\frac{d}{2}} \ll C \left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{-\frac{1}{4}} \left(\log \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{\frac{1}{2d}},$$

which is clearly satisfied as soon as N is large enough, since we assume $N^{1/d}\ell\rho_\beta^{-1} \gg 1$. We may now write

$$|\text{Error}_3| \leq C\beta^{\frac{1}{2}}\chi(\beta) \left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{-\frac{1}{4}} \left(\log \frac{N^{\frac{1}{d}}\ell}{\rho_\beta} \right)^{\frac{1}{2d}} (\log(N^{\frac{1}{d}}\ell))^{\frac{1}{2}}.$$

Thus if $d = 2$, $\text{Error}_3 \rightarrow 0$ algebraically as soon as $\beta \leq 1$, and if $\beta \geq 1$ (then $\rho_\beta = 1$) we use (2.27).

7.3.4. The fourth error term

It is by definition the term in (7.24), and inserting (7.22) and (7.27), we find

$$|\text{Error}_4| \leq C\tau^2\chi(\beta)(N^{\frac{1}{d}}\ell)^{-2} \leq C\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-2}.$$

This term always tends to 0, algebraically.

7.3.5. Conclusion

We may now conclude that all terms are $o(1)$ under our assumptions if $d = 2$, and that they are $o(1)$ in dimension $d \geq 3$ provided (2.30) and (2.33) hold.

Moreover, a rate of convergence as a negative power of $N^{\frac{1}{d}}\ell\rho_\beta^{-1}$ is provided for most of the error terms.

7.4. The case of small temperature – proof of Theorems 4 and 6

Here we may assume $\beta \geq 1$, so $\rho_\beta = 1$ and the convergence rate will be in terms of $N^{\frac{1}{d}}\ell$. In that case, we choose instead $t = s\ell^2\beta^{-1}(N^{\frac{1}{d}}\ell)^{-1-\frac{d}{2}}$ which is equivalent to taking $\tau = s\beta^{-\frac{1}{2}}$, and we retrace the same steps to find instead of (6.8)

$$(7.40) \quad |\log \mathbb{E}_{\mathbb{P}_{N,\beta}}(\exp(-s(N^{\frac{1}{d}}\ell)^{1-\frac{d}{2}} \text{Fluct}(\xi))) + s\beta^{-\frac{1}{2}}m(\xi) - s^2\beta^{-1}v(\xi)| \leq \sum_{i=1}^4 |\text{Error}_i|.$$

The errors appearing here are each smaller than the respective errors produced in the previous proofs because the extra factors in powers of $\beta^{-\frac{1}{2}}$ that appear are all ≤ 1 . Hence we only need to check that Error_3 tends to 0, with

$$|\text{Error}_3| \leq C(N^{\frac{1}{d}}\ell)^{\frac{d}{2}-1} \left(\max_{s \in [0, C\ell^2]} \mathcal{R}_s \right)^{\frac{1}{2}} \times \begin{cases} (\log(\ell N^{\frac{1}{d}}))^{\frac{1}{2}} & \text{if } d = 2 \\ (N^{\frac{1}{d}}\ell)^{1-\frac{1}{d}} & \text{if } d \geq 3. \end{cases}$$

For $d \geq 3$ this is ensured by (2.36). For $d = 2$ we have

$$|\text{Error}_3| \leq C\left(\frac{N^{\frac{1}{d}}\ell}{\rho_\beta}\right)^{-\frac{1}{4}} \log^{\frac{3}{4}} \frac{N^{\frac{1}{d}}\ell}{\rho_\beta}$$

which tends to 0. We may also choose $q = 0$, although the result would be as true with larger q and this concludes the proof.

Appendix: Proof of Proposition 4.2

A.1. A preliminary bound on the potential near the charges

Let μ be a bounded and C^2 probability density on \mathbb{R}^d , and let X_N be in $(\mathbb{R}^d)^N$. We let h be as in (3.1) and sometimes write $h^\mu[X_N]$ to emphasize the X_N and μ dependence. For any $i = 1, \dots, N$ we let

$$(A.1) \quad \tilde{h}_i(x) := h(x) - g(x - x_i).$$

We will use in particular the notation of (3.9). We start by adapting to arbitrary dimensions some results of [51].

Lemma A.1. *Let $\vec{\eta}$ be such that $\eta_i \leq r_i$ for each i . We have for $i = 1, \dots, N$*

$$(A.2) \quad h_{\vec{\eta}} = \begin{cases} h & \text{outside } B(x_i, \eta_i) \\ \tilde{h}_i \text{ (up to a constant)} & \text{in each } B(x_i, \eta_i). \end{cases}$$

In particular, it holds that

$$(A.3) \quad \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}|^2 = \int_{\mathbb{R}^d \setminus \bigcup_{i=1}^N B(x_i, r_i)} |\nabla h|^2 + \sum_{i=1}^N \int_{B(x_i, r_i)} |\nabla \tilde{h}_i|^2.$$

Proof. The first point follows from (3.9) with (3.5) and the fact that the balls $B(x_i, r_i)$ are disjoint by definition hence the $B(x_i, \eta_i)$'s as well. The second point is a straightforward consequence of the first one. \square

We let for $i = 1, \dots, N$

$$(A.4) \quad \lambda_i(X_N, \mu) := \int_{B(x_i, r_i)} |\nabla \tilde{h}_i|^2.$$

We will later often denote it simply by λ_i .

Lemma A.2. *Assume $\mu \in C^{m-2+\sigma}$ for some $\sigma > 0$ and integer $m \geq 1$. For each $i = 1, \dots, N$, we have*

$$(A.5) \quad \|\nabla \tilde{h}_i\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq C(r_i^{-\frac{d}{2}} \lambda_i(X_N, \mu)^{\frac{1}{2}} + N r_i \|\mu\|_{L^\infty})$$

$$(A.6) \quad \|\nabla^m \tilde{h}_i\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq C(r_i^{1-m-\frac{d}{2}} \lambda_i(X_N, \mu)^{\frac{1}{2}} + N r_i^{2-m} \|\mu\|_{L^\infty} + N r_i^\sigma |\mu|_{C^{m-2+\sigma}(B(x_i, r_i))})$$

for some constant C depending only on d .

Proof. We exploit the fact that \tilde{h}_i is regular in each $B(x_i, r_i)$. Recall that $h = g * (\sum_{i=1}^N \delta_{x_i} - N\mu)$ so that

$$(A.7) \quad \tilde{h}_i = g * \left(\sum_{j \neq i} \delta_{x_j} - N\mu \right).$$

We may thus write \tilde{h}_i as $\tilde{h}_i = u + v$ where

$$(A.8) \quad u = g * (-N\mu \chi_i)$$

with χ_i a smooth nonnegative function such that $\chi_i = 1$ in $B(x_i, r_i)$ and $\chi_i = 0$ outside of $B(x_i, 2r_i)$; and v solves

$$(A.9) \quad -\Delta v = 0 \quad \text{in } B(x_i, r_i).$$

Letting $f(x) = v(x_i + r_i x)$, f solves the relation $\Delta f = 0$ in $B(0, 1)$. Elliptic regularity estimates for this equation yield for any integer $m \geq 1$,

$$(A.10) \quad \|\nabla^m f\|_{L^\infty(B(0, \frac{1}{2}))} \leq C \left(\int_{B(0, 1)} |\nabla f|^2 \right)^{\frac{1}{2}},$$

for some C depending on m . Rescaling this relation, and using (A.4) we conclude that

$$(A.11) \quad \|\nabla v\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq \frac{C}{r_i} \left(\frac{1}{r_i^{d-2}} \int_{B(x_i, r_i)} |\nabla v|^2 \right)^{\frac{1}{2}} \leq \frac{C}{r_i^{d/2}} \left(\lambda_i(X_N, \mu) + \int_{B(x_i, r_i)} |\nabla u|^2 \right)^{\frac{1}{2}},$$

and similarly

$$(A.12) \quad \|\nabla^m v\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq \frac{C}{r_i^{m-1+\frac{d}{2}}} \left(\lambda_i(X_N, \mu) + \int_{B(x_i, r_i)} |\nabla u|^2 \right)^{\frac{1}{2}}.$$

The following assertions for u are obtained similarly by elliptic regularity and scaling:

$$(A.13) \quad \|\nabla^m u\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq \begin{cases} CN r_i^{2-m} \|\mu\|_{L^\infty} & \text{for } m \leq 1 \\ CN(r_i^{2-m} \|\mu\|_{L^\infty} + r_i^\sigma |\mu|_{C^{m-2+\sigma}(B(x_i, r_i))}) & \text{for } m \geq 2. \end{cases}$$

Inserting into (A.11)–(A.12) and computing explicitly, we deduce that

$$(A.14) \quad \|\nabla v\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq \frac{C}{r_i^{d/2}} (\lambda_i(X_N, \mu))^{\frac{1}{2}} + N \|\mu\|_{L^\infty} r_i^{1+\frac{d}{2}},$$

and

$$(A.15) \quad \|\nabla^m v\|_{L^\infty(B(x_i, \frac{1}{2}r_i))} \leq \frac{C}{r_i^{m-1+\frac{d}{2}}} (\lambda_i(X_N, \mu))^{\frac{1}{2}} + N r_i^{1+\frac{d}{2}} \|\mu\|_{L^\infty} + C N r_i^\sigma |\mu|_{C^{m-2+\sigma}}.$$

Combining with (A.13), this concludes the proof. \square

A.2. Transporting electric fields

Lemma A.3. *Let X be a vector field on \mathbb{R}^d and Φ a diffeomorphism and define*

$$(A.16) \quad \Phi \# X := (D\Phi \circ \Phi^{-1})^T X \circ \Phi^{-1} |\det D\Phi^{-1}|.$$

Then

$$\operatorname{div}(\Phi \# X) = \Phi \# (\operatorname{div} X)$$

in the sense of distributions, and of push-forward of measures for the right-hand side.

Proof. Let ϕ be a smooth compactly supported test-function, and let $f = \operatorname{div} X$ (in the distributional sense). We have $-\int X \cdot \nabla \phi = \int f \phi$, hence changing variables, we find

$$-\int_{\mathbb{R}^d} X \circ \Phi^{-1} \cdot \nabla \phi \circ \Phi^{-1} |\det D\Phi^{-1}| = \int_{\mathbb{R}^d} (\phi \circ \Phi^{-1})(f \circ \Phi^{-1}) |\det D\Phi^{-1}|,$$

and writing

$$(A.17) \quad \nabla \phi \circ \Phi^{-1} = (D\Phi \circ \Phi^{-1})^T \nabla (\phi \circ \Phi^{-1})$$

we get

$$-\int_{\mathbb{R}^d} X \circ \Phi^{-1} \cdot (D\Phi \circ \Phi^{-1})^T \nabla (\phi \circ \Phi^{-1}) |\det D\Phi^{-1}| = \int_{\mathbb{R}^d} \phi \circ \Phi^{-1} f \circ \Phi^{-1} |\det D\Phi^{-1}|.$$

Since this is true for any $\phi \circ \Phi^{-1}$ with ϕ smooth enough, we deduce that in the sense of distributions, we have

$$\operatorname{div}((D\Phi \circ \Phi^{-1})^T X \circ \Phi^{-1} |\det D\Phi^{-1}|) = f \circ \Phi^{-1} |\det D\Phi^{-1}|$$

which is the desired result. \square

We now turn to the main proof.

A.3. Estimating the first derivative

We will denote $v = \Phi_t \# \mu$, and for any $X_N \in (\mathbb{R}^d)^N$ we let $Y_N := (\Phi_t(x_1), \dots, \Phi_t(x_N)) = (y_1, \dots, y_N)$, hence we let the t -dependence be implicit. We use superscripts μ and v to denote the background measure with respect to which h is computed and sometimes use $[X_N]$ or $[Y_N]$ to emphasize the configuration for which h is computed. Let $\tilde{\eta}$ be such that $\eta_i \leq r_i$. We wish to compute the energy of the transported configuration by using the transported electric field $\Phi_t(\# \nabla h^\mu [X_N])$. The problem is that the transport distorts the truncated measures $\delta_{x_i}^{(\eta_i)}$ and makes them supported in ellipse-like sets instead of spheres. A large part of our work will consist in estimating the error thus made. For this we take a slightly different route than [51] which contained an incorrect passage.

Let us define

$$(A.18) \quad E_{\tilde{\eta}} := \Phi_t \# (\nabla h_{\tilde{\eta}}^\mu [X_N]),$$

$$(A.19) \quad \hat{\delta}_{y_i} := \Phi_t \# \delta_{x_i}^{(\eta_i)},$$

and

$$(A.20) \quad \hat{h} := g * \left(\sum_{i=1}^N \hat{\delta}_{y_i} - N v \right).$$

Note that \hat{h} implicitly depends on $\vec{\eta}$. By Lemma A.3, we have

$$(A.21) \quad -\operatorname{div} E_{\vec{\eta}} = -\Phi_t \# (\Delta h_{\vec{\eta}}^\mu [X_N]) = c_d \left(\sum_{i=1}^N \hat{\delta}_{y_i} - N \nu \right)$$

thus

$$(A.22) \quad \operatorname{div}(E_{\vec{\eta}} - \nabla \hat{h}) = 0.$$

We next use the fact that $\nabla \hat{h}$ is the L^2 projection of $E_{\vec{\eta}}$ onto gradients to deduce it has a smaller L^2 norm. More precisely, we may write

$$\int_{\mathbb{R}^d} |E_{\vec{\eta}}|^2 = \int_{\mathbb{R}^d} |E_{\eta} - \nabla \hat{h}|^2 + |\nabla \hat{h}|^2 + 2 \int_{\mathbb{R}^d} (E_{\eta} - \nabla \hat{h}) \cdot \nabla \hat{h}$$

and use Green's formula and (A.22) to deduce that the last integral vanishes, hence

$$(A.23) \quad \int_{\mathbb{R}^d} |E_{\vec{\eta}}|^2 = \int_{\mathbb{R}^d} |\nabla \hat{h}|^2 + |E_{\vec{\eta}} - \nabla \hat{h}|^2.$$

We also note that $E_{\vec{\eta}} = \nabla h^\mu [X_N]$ in the interior of the set $\{\Phi_t \equiv \operatorname{Id}\}$.

Without loss of generality, we may assume that $t|\psi|_{C^1} < \frac{1}{2}$. We now wish to estimate $\Xi(t) - \Xi(0) = F_N(\Phi_t(X_N), \mu_t) - F_N(X_N, \mu) = F_N(Y_N, \nu) - F_N(X_N, \mu)$.

Step 1 (Splitting the comparison). Applying Lemma 3.1 yields

$$(A.24) \quad F_N(X_N, \mu) = \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^\mu [X_N]|^2 - \frac{1}{2} \sum_{i=1}^N g(\eta_i) - N \sum_{i=1}^N \int_{\mathbb{R}^d} f_{\eta_i}(x - x_i) d\mu(x)$$

and

$$F_N(Y_N, \nu) = \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^\nu [Y_N]|^2 - \frac{1}{2} \sum_{i=1}^N g(\eta_i) - N \sum_{i=1}^N \int_{\mathbb{R}^d} f_{\eta_i}(x - y_i) d\nu(x).$$

Subtracting these relations and using (A.23) we find

$$(A.25) \quad F_N(Y_N, \nu) - F_N(X_N, \mu) = \operatorname{Main} + \operatorname{Rem} + \operatorname{Err} - \frac{1}{2c_d} \int_{\mathbb{R}^d} |E_{\vec{\eta}} - \nabla \hat{h}|^2$$

where

$$(A.26) \quad \operatorname{Main} := \frac{1}{2c_d} \int_{\mathbb{R}^d} |E_{\vec{\eta}}|^2 - \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^\mu [X_N]|^2,$$

$$(A.27) \quad \operatorname{Rem} := \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^\nu [Y_N]|^2 - \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla \hat{h}|^2$$

and

$$(A.28) \quad \operatorname{Err} := -N \sum_{i=1}^N \int_{\mathbb{R}^d} f_{\eta_i}(x - y_i) d\nu(x) + N \sum_{i=1}^N \int_{\mathbb{R}^d} f_{\eta_i}(x - x_i) d\mu(x).$$

Step 2 (The last term). To control the last term, we first show that $E_{\vec{\eta}}$ is close to $\nabla(h_{\vec{\eta}}^\mu [X_N] \circ \Phi_t^{-1})$. Indeed, using (A.16) and (A.17), we find that

$$E_{\vec{\eta}} = ((D\Phi_t \circ \Phi_t^{-1})^T)^2 \nabla(h_{\vec{\eta}}^\mu [X_N] \circ \Phi_t^{-1}) |\det D\Phi_t^{-1}| = \nabla(h_{\vec{\eta}}^\mu [X_N] \circ \Phi_t^{-1}) (I + O(t|\psi|_{C^1(U_\ell)}))$$

after a Taylor expansion in t . It follows that

$$\int_{\mathbb{R}^d} |E_{\vec{\eta}} - \nabla(h_{\vec{\eta}}^\mu [X_N] \circ \Phi_t^{-1})|^2 \leq Ct^2 |\psi|_{C^1(U_\ell)}^2 \int_{\mathbb{R}^d} |\nabla(h_{\vec{\eta}}^\mu [X_N] \circ \Phi_t^{-1})|^2.$$

After another change of variables we find that

$$\int_{\mathbb{R}^d} |E_{\vec{\eta}} - \nabla(h_{\vec{\eta}}^{\mu}[X_N] \circ \Phi_t^{-1})|^2 \leq Ct^2 |\psi|_{C^1(U_{\ell})}^2 \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^{\mu}[X_N]|^2.$$

As seen just above, $\nabla \hat{h}$ is the L^2 projection onto gradients of $E_{\vec{\eta}}$, hence we conclude that

$$(A.29) \quad \int_{\mathbb{R}^d} |E_{\vec{\eta}} - \nabla \hat{h}|^2 \leq \int_{\mathbb{R}^d} |E_{\vec{\eta}} - \nabla(h_{\vec{\eta}}^{\mu}[X_N] \circ \Phi_t^{-1})|^2 \leq Ct^2 |\psi|_{C^1(U_{\ell})}^2 \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^{\mu}[X_N]|^2.$$

Step 3 (The main term). The term Main is evaluated by a simple change of variables using (A.18):

$$(A.30) \quad \text{Main} = \frac{1}{2c_d} \int_{\mathbb{R}^d} (|(D\Phi_t)^T \nabla h_{\vec{\eta}}^{\mu}|^2 |\det D\Phi_t^{-1} \circ \Phi_t| - |\nabla h_{\vec{\eta}}^{\mu}|^2).$$

Writing $\Phi_t = \text{Id} + t\psi$ and $D\Phi_t = \text{Id} + tD\psi$, we have $\Phi_t^{-1} = \text{Id} - t\psi + O(t^2|\psi|^2)$ and

$$|\det D\Phi_t^{-1} \circ \Phi_t| = \det(\text{Id} - tD\psi(x + t\psi(x))) + O(t^2|D\psi|^2) = 1 - t \operatorname{div} \psi + O(t^2(|D\psi|^2 + |\psi|_{C^2} \|\psi\|_{L^\infty})),$$

thus

$$(A.31) \quad \text{Main} = \frac{t}{2c_d} \int_{U_{\ell}} \nabla h_{\vec{\eta}}^{\mu} \cdot \mathcal{A} \nabla h_{\vec{\eta}}^{\mu} + t^2 O\left((|\psi|_{C^1(U_{\ell})}^2 + |\psi|_{C^2(U_{\ell})} \|\psi\|_{L^\infty(U_{\ell})}) \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^{\mu}|^2\right)$$

where

$$(A.32) \quad \mathcal{A} = 2D\psi - (\operatorname{div} \psi)\text{Id}$$

and where the O depends only on d .

Step 4. We now set to evaluate quantities of the form

$$\int_{\mathbb{R}^d} f(\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)})$$

for general functions f . We note that by (A.35) the supports of $\delta_{y_i}^{(\eta_i)}$ and $\hat{\delta}_{y_i}$ are included in an annulus of center y_i , inner radius $\eta_i(1 - |t||\psi|_{C^1(B(y_i, \eta_i))})$ and outer radius $\eta_i(1 + |t||\psi|_{C^1(B(y_i, \eta_i))})$ and assume that

$$(A.33) \quad |t||\psi|_{C^1} < \frac{1}{2}.$$

By definition of $\hat{\delta}_{y_i}$ (A.19) we have

$$(A.34) \quad \int_{\mathbb{R}^d} f(\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)}) = \int_{\partial B(x_i, \eta_i)} f \circ \Phi_t - \int_{\partial B(y_i, \eta_i)} f = \int_{\partial B(y_i, \eta_i)} f(\Phi_t(x + x_i - y_i)) - f.$$

Note that by definition of Φ_t and the definition of y_i as $x_i + t\psi(x_i)$ we have

$$(A.35) \quad \|\Phi_t(x + x_i - y_i) - x\|_{L^\infty(B(y_i, \eta_i))} = \|t\psi(x + x_i - y_i) - t\psi(x_i)\|_{L^\infty(B(y_i, \eta_i))} \leq t\eta_i |\psi|_{C^1(B(x_i, \eta_i))}.$$

It follows that

$$(A.36) \quad \begin{aligned} \left| \int_{\mathbb{R}^d} f(\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)}) \right| &\leq C |f|_{C^1(B(y_i, \frac{3}{2}\eta_i))} \|\Phi_t(x + x_i - y_i) - x\|_{L^\infty(B(y_i, \eta_i))} \\ &\leq C t \eta_i |\psi|_{C^1(B(x_i, \eta_i))} |f|_{C^1(B(x_i, \frac{3}{2}\eta_i))}. \end{aligned}$$

Linearizing (A.34) in t we find that if $f \in C^2(B(y_i, \frac{3}{2}\eta_i))$,

$$\begin{aligned}
 \int_{\mathbb{R}^d} f(\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)}) &= \int_{\partial B(y_i, \eta_i)} \nabla f(x) \cdot (\Phi_t(x + x_i - y_i) - x) + O(t^2 \eta_i^2 |f|_{C^2(B(y_i, \frac{3}{2}\eta_i))} |\psi|_{C^1(B(x_i, \eta_i))}^2) \\
 &= \int_{\partial B(y_i, \eta_i)} \nabla f(x) \cdot (-t\psi(x_i) + t\psi(x + x_i - y_i)) \\
 (A.37) \quad &+ O(t^2 \eta_i^2 |f|_{C^2(B(y_i, \frac{3}{2}\eta_i))} |\psi|_{C^1(B(x_i, \eta_i))}^2) \\
 &= t \int_{\partial B(x_i, \eta_i)} \nabla f(x + y_i - x_i) \cdot (\psi(x) - \psi(x_i)) \\
 &+ O(t^2 \eta_i^2 |f|_{C^2(B(y_i, \frac{3}{2}\eta_i))} |\psi|_{C^1(B(x_i, \eta_i))}^2).
 \end{aligned}$$

Linearizing further ψ and ∇f and using that $\int_{\partial B(x_i, \eta_i)} D\psi(x_i)(x - x_i) = 0$, we may also get

$$\begin{aligned}
 \int_{\mathbb{R}^d} f(\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)}) &= t \int_{\partial B(x_i, \eta_i)} \nabla f(x + y_i - x_i) \cdot D\psi(x_i)(x - x_i) \\
 (A.38) \quad &+ O(t\eta_i^2 |\psi|_{C^2(B(x_i, \eta_i))} |f|_{C^1(B(y_i, \frac{3}{2}\eta_i))} + t^2 \eta_i^2 |f|_{C^2(B(y_i, \frac{3}{2}\eta_i))} |\psi|_{C^1(B(x_i, \eta_i))}^2) \\
 &= O(t\eta_i^2 (|f|_{C^2(B(y_i, \frac{3}{2}\eta_i))} |\psi|_{C^1(B(x_i, \eta_i))} + |\psi|_{C^2(B(x_i, \eta_i))} |f|_{C^1(B(y_i, \frac{3}{2}\eta_i))})).
 \end{aligned}$$

Step 5 (The remainder term). Let us denote

$$(A.39) \quad v_i = \mathbf{g} * (\hat{\delta}_{y_i} - \delta_{y_i}^{(\eta_i)}).$$

By (A.20) we have

$$(A.40) \quad \hat{h} = h_{\bar{\eta}}^v[Y_N] + \sum_{i=1}^N v_i.$$

Thus, integrating by parts we find

$$\begin{aligned}
 2c_d \text{Rem} &= \sum_{i,j} \int \nabla v_i \cdot \nabla v_j - 2 \sum_i \int \nabla v_i \cdot \nabla \hat{h} \\
 &= c_d \sum_{i,j} \int v_i (\hat{\delta}_{y_j} - \delta_{y_j}^{(\eta_j)}) - 2c_d \sum_i \int v_i \left(\hat{\delta}_{y_i} + \sum_{j \neq i} \hat{\delta}_{y_j} - Nv \right) \\
 (A.41) \quad &= -c_d \sum_i \int v_i (\hat{\delta}_{y_i} + \delta_{y_i}^{(\eta_i)}) + c_d \sum_{i \neq j} \int v_i (\hat{\delta}_{y_j} - \delta_{y_j}^{(\eta_j)}) - 2c_d \sum_i \int v_i \left(\sum_{j \neq i} \delta_{y_j}^{(\eta_j)} - Nv \right) \\
 &:= 2c_d (\text{Rem}_1 + \text{Rem}_2 + \text{Rem}_3).
 \end{aligned}$$

Substep 5.1. Let us start by Rem_1 . We observe that

$$\begin{aligned}
 \text{Rem}_1 &= \frac{1}{2} \sum_i \int \mathbf{g} * \delta_{y_i}^{(\eta_i)} \delta_{y_i}^{(\eta_i)} - \int \mathbf{g} * \hat{\delta}_{y_i} \hat{\delta}_{y_i} \\
 &= \frac{1}{2} \sum_i \int_{\partial B(y_i, \eta_i)} \int_{\partial B(y_i, \eta_i)} (\mathbf{g}(\Phi_t(x) - \Phi_t(y)) - \mathbf{g}(x - y)) dx dy.
 \end{aligned}$$

Breaking the double integral into $|x - y| > \delta$ and $|x - y| \leq \delta$ we may write that

$$\begin{aligned} & \frac{1}{2} \int_{\partial B(y_i, \eta_i)} \int_{\partial B(y_i, \eta_i)} (g(\Phi_t(x) - \Phi_t(y)) - g(x - y)) dx dy \\ &= O\left(\int_{(\partial B(y_i, \eta_i))^2, |x-y| \leq C\delta} g(x - y) dx dy\right) + \frac{t}{2} \int_{(\partial B(y_i, \eta_i))^2, |x-y| > \delta} \nabla g(x - y) \cdot (\psi(x) - \psi(y)) \\ &+ O\left(t^2 |\psi|_{C^1(B(y_i, \eta_i))}^2 \int_{(\partial B(y_i, \eta_i))^2, C|x-y| > \delta} |x - y|^{2-d}\right). \end{aligned}$$

Letting $\delta \rightarrow 0$ we find

$$\begin{aligned} & \frac{1}{2} \int_{\partial B(y_i, \eta_i)} \int_{\partial B(y_i, \eta_i)} (g(\Phi_t(x) - \Phi_t(y)) - g(x - y)) dx dy \\ &= \frac{t}{2} \int_{(\partial B(y_i, \eta_i))^2} \nabla g(x - y) \cdot (\psi(x) - \psi(y)) + O\left(t^2 |\psi|_{C^1(B(y_i, \eta_i))}^2 \int_{(\partial B(y_i, \eta_i))^2} |x - y|^{2-d}\right). \end{aligned}$$

With this we claim that

$$(A.42) \quad \text{Rem}_1 = \frac{t}{2} \sum_{i=1}^N \eta_i^{1-d} \int_{\partial B(y_i, \eta_i)} (\psi(x) - \psi(y_i)) \cdot v + O\left(t^2 \sum_{i=1}^N \eta_i^{2-d} |\psi|_{C^1(B(y_i, \eta_i))}^2\right)$$

where v is the outer unit normal. To see this, introduce $g_{\eta_i} = g * \delta_{y_i}^{(\eta_i)}$ and observe that by splitting $\psi(x) - \psi(y)$ into $\psi(x) - \psi(y_i) + \psi(y_i) - \psi(y)$ and symmetrizing the variables

$$\begin{aligned} & \frac{1}{2} \int_{\partial B(y_i, \eta_i)} \int_{\partial B(y_i, \eta_i)} \nabla g(x - y) \cdot (\psi(x) - \psi(y)) \\ &= \int_{\partial B(y_i, \eta_i)} \int_{\partial B(y_i, \eta_i)} \nabla g(x - y) \cdot (\psi(x) - \psi(y_i)) = \int_{\partial B(y_i, \eta_i)} \nabla g_{\eta_i}(x - y_i) \cdot (\psi(x) - \psi(y_i)) dx \end{aligned}$$

and the right-hand side is equal to

$$\frac{1}{2} \int_{\mathbb{R}^d} (\psi(x) - \psi(y_i)) \cdot \text{div } T_{\nabla g_{\eta_i}}$$

where div here is a vector-valued divergence, and for any function h we let $T_{\nabla h}$ denote the stress-energy tensor

$$T_{\nabla h} := 2(\nabla h) \otimes (\nabla h) - |\nabla h|^2 \text{Id},$$

see for instance [78, Lemma 4.2]. We have the identity $\text{div } T_{\nabla h} = 2\nabla h \Delta h$ for smooth functions, and then notice that $\text{div } T_{\nabla g_{\eta_i}} = 0$ away from $\partial B(y_i, \eta_i)$ so that each component of $\text{div } T_{\nabla g_{\eta_i}}$ is the jump of normal component of the corresponding row of $T_{\nabla g_{\eta_i}}$. Since $T_{\nabla g_{\eta_i}}$ jumps from 0 inside $B(y_i, \eta_i)$ to $T_{\nabla g}$ outside $B(y_i, \eta_i)$, the integral transforms into a boundary integral equal to that of (A.42).

Substep 5.2. We next turn to Rem_2 . First we estimate v_i defined in (A.39). Using (A.38) with $f = g(x - \cdot)$ and $f = \nabla g(x - \cdot)$ we obtain

$$(A.43) \quad \forall x \notin B(y_i, 2\eta_i), \quad |v_i|(x) \leq C|t|\eta_i^2 \left(\frac{1}{|x - y_i|^d} |\psi|_{C^1(B(x_i, \eta_i))} + \frac{1}{|x - y_i|^{d-1}} |\psi|_{C^2(B(x_i, \eta_i))} \right)$$

$$(A.44) \quad \forall x \notin B(y_i, 2\eta_i), \quad |\nabla v_i|(x) \leq C|t|\eta_i^2 \left(\frac{1}{|x - y_i|^{d+1}} |\psi|_{C^1(B(x_i, \eta_i))} + \frac{1}{|x - y_i|^d} |\psi|_{C^2(B(x_i, \eta_i))} \right),$$

hence inserting into (A.36), we find

$$(A.45) \quad \left| \sum_i \int_{\mathbb{R}^d} v_i \sum_{j \neq i} (\hat{\delta}_{y_j} - \delta_{y_j}^{(\eta_j)}) \right| \leq C t^2 \sum_{i \neq j} \eta_i^2 \eta_j \left(\frac{|\psi|_{C^1(B(x_i, \eta_i))}^2}{|y_i - y_j|^{d+1}} + \frac{|\psi|_{C^1(B(x_i, \eta_i))} |\psi|_{C^2(B(x_i, \eta_i))}}{|y_i - y_j|^d} \right).$$

We next split the sum into pairs at distance $\leq N^{-1/d}$ which we control by Corollary 3.4 using that

$$\frac{\eta_i^2 \eta_j}{|y_i - y_j|^{d+1}} \leq \frac{1}{|y_i - y_j|^{d-2}}, \quad \frac{\eta_i^2 \eta_j}{|y_i - y_j|^d} \leq \frac{N^{-1/d}}{|y_i - y_j|^{d-2}}$$

since $\eta_i \leq r_i$, and pairs at distance $\geq N^{-1/d}$ for which we use $\eta_i^2 \eta_j \leq N^{-3/d}$ and use Proposition 3.5 applied with $s = 2, 3$. This way, absorbing some terms and using that $\ell \geq N^{-1/d}$, we conclude that

$$\begin{aligned} |\text{Rem}_2| &\leq Ct^2(|\psi|_{C^1(U_\ell)}^2 + N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) |\psi|_{C^1(U_\ell)} |\psi|_{C^2(U_\ell)}) \\ (A.46) \quad &\times \left(\mathsf{F}^{U_\ell}(Y_N, \nu) + \left(\frac{\#I_{U_\ell}}{4} \log N \right) \mathbf{1}_{d=2} + C_0 \#I_{U_\ell} N^{1-\frac{2}{d}} \right). \end{aligned}$$

Substep 5.3. We finish by analyzing the term Rem_3 . By integration by parts, we may write

$$\text{Rem}_3 = \int_{\mathbb{R}^d} \sum_{i=1}^N (\delta_{y_i}^{(\eta_i)} - \hat{\delta}_{y_i}) \tilde{h}_{i,\tilde{\eta}}[Y_N]$$

where $\tilde{h}_{i,\tilde{\eta}}[Y_N] = h_{\tilde{\eta}}^v[Y_N] - g(\cdot - y_i)$. We also let $\tilde{h}_i[Y_N] = h^v[Y_N] - g(\cdot - y_i)$ and observe that $\tilde{h}_i[Y_N]$ and $\tilde{h}_{i,\tilde{\eta}}[Y_N]$ coincide in $B(y_i, \eta_i)$. Using (A.37), (A.6), $\eta_i \leq r_i$ and Young's inequality we deduce

$$\begin{aligned} &\sum_{i=1}^N \int_{\mathbb{R}^d} \tilde{h}_{i,\tilde{\eta}}[Y_N] (\delta_{y_i}^{(\eta_i)} - \hat{\delta}_{y_i}) - t \sum_i \int_{\partial B(x_i, \eta_i)} \nabla \tilde{h}_i[Y_N](x + y_i - x_i) \cdot (\psi(x) - \psi(x_i)) \\ &= O\left(t^2 \sum_{i=1}^N |\tilde{h}_i[Y_N]|_{C^2(B(y_i, 2\eta_i))} \eta_i^2 |\psi|_{C^1(B(x_i, \eta_i))}^2\right) \\ &= O\left(t^2 \sum_{i \in I_{U_\ell}} |\psi|_{C^1(B(x_i, \eta_i))}^2 \eta_i^2 (C r_i^{-1-\frac{d}{2}} \lambda_i(Y_N, \nu)^{\frac{1}{2}} + N(\|\mu\|_{L^\infty} + r_i |\mu|_{C^1(B(y_i, r_i))}))\right) \\ &= O(t^2 \sum_{i \in I_{U_\ell}} |\psi|_{C^1(B(x_i, r_i))}^2 \left(r_i^{2-d} + \int_{B(y_i, r_i)} |\nabla h_{\tilde{\eta}}^v[Y_N]|^2 + N^{1-\frac{2}{d}} (\|\mu\|_{L^\infty} + N^{-\frac{1}{d}} |\mu|_{C^1(B(y_i, r_i))}) \right)). \end{aligned}$$

Using (3.24) in the case $d \geq 3$ (and the fact that the r_i 's computed for X_N and for Y_N differ by at most a multiplicative factor of 2) we conclude that

$$\begin{aligned} (A.47) \quad \text{Rem}_3 &= t \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \nabla \tilde{h}_i[Y_N](x + y_i - x_i) \cdot (\psi(x) - \psi(x_i)) \\ &+ t^2 O(|\psi|_{C^1(U_\ell)}^2 (1 + \|\mu\|_{L^\infty} + N^{-\frac{1}{d}} |\mu|_{C^1(U_\ell)})) \\ &\times \left(\mathsf{F}^{U_\ell}(Y_N, \nu) + \left(\frac{\#I_{U_\ell}}{4} \log N \right) \mathbf{1}_{d=2} + C_0 \#I_{U_\ell} N^{1-\frac{2}{d}} + \int_{U_\ell} |\nabla h_{\tilde{\eta}}^v[Y_N]|^2 \right) \end{aligned}$$

where the O depends only on d .

Step 6 (The error term (A.28)). First we write

$$-\int_{\mathbb{R}^d} \mathsf{f}_{\eta_i}(x - y_i) d\nu + \int_{\mathbb{R}^d} \mathsf{f}_{\eta_i}(x - x_i) d\mu = -\int_{\mathbb{R}^d} \mathsf{f}_{\eta_i}(x - x_i) (d\nu(x + x_i - y_i) - d\mu(x)).$$

Then we may write $\nu(x - x_i + y_i) = \hat{\Phi}_t \# \nu = \hat{\Phi}_t(\# \Phi_t \# \mu) = (\hat{\Phi}_t \circ \Phi_t) \# \mu$, where we let $\hat{\Phi}_t = \text{Id} + x_i - y_i = \text{Id} - t\psi(x_i)$. Since $\hat{\Phi}_t \circ \Phi_t = \text{Id} + t(\psi - \psi(x_i))$, we may write in view of Lemma 5.1 that

$$\nu(x + x_i - y_i) = \mu - t \operatorname{div}((\psi - \psi(x_i)) \mu) + u$$

with

$$\|u\|_{L^\infty} \leq Ct^2(\|\mu\|_{C^2}\|\psi - \psi(x_i)\|_{L^\infty}^2 + |\psi|_{C^1}^2 + \|\psi\|_{C^2}\|\psi - \psi(x_i)\|_{L^\infty}).$$

Thus

$$\begin{aligned} -\int_{\mathbb{R}^d} \mathbf{f}_{\eta_i}(x - y_i) dv + \int_{\mathbb{R}^d} \mathbf{f}_{\eta_i}(x - x_i) d\mu &= -t \int_{\mathbb{R}^d} \nabla \mathbf{f}_{\eta_i} \cdot (\psi(x) - \psi(x_i)) d\mu \\ &\quad + t^2 O((1 + \eta_i^2 \|\mu\|_{C^2}) |\psi|_{C^1}^2 + \eta_i \|\psi\|_{C^2} |\psi|_{C^1}) \int_{\mathbb{R}^d} |\mathbf{f}_{\eta_i}|. \end{aligned}$$

Using (3.7), summing over i and using $\eta_i \leq N^{-1/d}$ we find

$$\begin{aligned} \text{Err} &= -tN \sum_{i=1}^N \int_{\mathbb{R}^d} \nabla \mathbf{f}_{\eta_i} \cdot (\psi(x) - \psi(x_i)) d\mu(x) \\ (A.48) \quad &\quad + t^2 O\left(\sum_{i=1}^N (1 + N^{-\frac{2}{d}} \|\mu\|_{C^2(B(x_i, \eta_i))}) (|\psi|_{C^1(B(x_i, \eta_i))}^2 + |\psi|_{C^1(B(x_i, \eta_i))} |\psi|_{C^2(B(x_i, \eta_i))} N^{-\frac{1}{d}}) N^{1-\frac{2}{d}}\right), \end{aligned}$$

where O depends only on d .

Step 7 (Conclusion). We now define

$$\begin{aligned} L_t &:= \frac{1}{2c_d} \int \nabla h_{\tilde{\eta}}^\mu \cdot (2D\psi - (\operatorname{div} \psi) \operatorname{Id}) \nabla h_{\tilde{\eta}}^\mu [X_N] + \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \nabla \tilde{h}_i [Y_N](x + y_i - x_i) \cdot (\psi(x) - \psi(x_i)) \\ (A.49) \quad &\quad + \frac{1}{2} \sum_{i=1}^N \int_{\partial B(y_i, \eta_i)} \eta_i^{1-d} ((\psi(x) - \psi(y_i)) \cdot v) - N \sum_{i=1}^N \int_{\mathbb{R}^d} \nabla \mathbf{f}_{\eta_i} \cdot (\psi(x) - \psi(x_i)) d\mu. \end{aligned}$$

Combining (A.25), (A.29), (A.28), (A.31), (A.46), (A.47) and (A.48), we find

$$\begin{aligned} \mathsf{F}_N(Y_N, v) - \mathsf{F}_N(X_N, \mu) &= tL_t + t^2 O\left((|\psi|_{C^1(U_\ell)}^2 + |\psi|_{C^2(U_\ell)} \|\psi\|_{L^\infty(U_\ell)}) \int_{\mathbb{R}^d} |\nabla h_{\tilde{\eta}}^\mu [X_N]|^2\right) \\ (A.50) \quad &\quad + t^2 (|\psi|_{C^1(U_\ell)}^2 (1 + \|\mu\|_{L^\infty} + N^{-\frac{1}{d}} \|\mu\|_{C^1(U_\ell)} + N^{-\frac{2}{d}} \|\mu\|_{C^2(U_\ell)}) \\ &\quad + |\psi|_{C^1(U_\ell)} |\psi|_{C^2(U_\ell)} (1 + N^{-\frac{2}{d}} \|\mu\|_{C^2(U_\ell)}) N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}})) \\ &\quad \times O\left(\mathsf{F}^{U_\ell}(Y_N, v) + \left(\frac{\#I_{U_\ell}}{4} \log N\right) \mathbf{1}_{d=2} + C_0 \#I_{U_\ell} N^{1-\frac{2}{d}} + \int_{U_\ell} |\nabla h_{\tilde{\eta}}^\mu [Y_N]|^2\right) \end{aligned}$$

where the O depends only on d .

In particular

$$\mathsf{F}_N(Y_N, v) - \mathsf{F}_N(X_N, \mu) = tL_t + o(t).$$

Comparing with Proposition 4.1, we find that letting Ξ be as in (4.4), we have

$$\begin{aligned} \Xi'(0) &= \mathsf{A}_1(X_N, \psi, \mu) = \lim_{t \rightarrow 0} L_t \\ (A.51) \quad &= \frac{1}{2c_d} \int_{\mathbb{R}^d} \nabla h_{\tilde{\eta}}^\mu \cdot (2D\psi - (\operatorname{div} \psi) \operatorname{Id}) \nabla h_{\tilde{\eta}}^\mu + \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \nabla \tilde{h}_i [X_N] \cdot (\psi(x) - \psi(x_i)) \\ &\quad + \frac{1}{2} \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \eta_i^{1-d} ((\psi(x) - \psi(x_i)) \cdot v) - N \sum_{i=1}^N \int_{\mathbb{R}^d} \nabla \mathbf{f}_{\eta_i} \cdot (\psi(x) - \psi(x_i)) d\mu. \end{aligned}$$

In addition, this implies that the quantity in the right-hand side is independent of the choice of $\vec{\eta}$ as long as $\eta_i \leq r_i$. Taking $\eta_i = \frac{1}{4}r_i$ and bounding the terms in (A.51) we obtain

$$(A.52) \quad \begin{aligned} |\mathbf{A}_1(X_N, \mu, \psi)| &\leq C \left(\int_{\mathbb{R}^d} |\nabla h_{\frac{1}{4}r}^\mu|^2 |D\psi| + \sum_{i=1}^N r_i \|\nabla \tilde{h}_i\|_{L^\infty(B(x_i, \frac{1}{4}r_i))} |\psi|_{C^1(B(x_i, \frac{1}{4}r_i))} \right. \\ &\quad \left. + \sum_{i=1}^N r_i^{2-d} |\psi|_{C^1(B(x_i, \frac{1}{4}r_i))} + \sum_{i=1}^N |\psi|_{C^1(B(x_i, \frac{1}{4}r_i))} \|\mu\|_{L^\infty} N^{1-\frac{2}{d}} \right) \end{aligned}$$

Using (A.5) and Young's inequality, we deduce that

$$(A.53) \quad \begin{aligned} |\mathbf{A}_1(X_N, \mu, \psi)| &\leq C \int_{\mathbb{R}^d} |\nabla h_{\frac{1}{4}r}^\mu|^2 |D\psi| \\ &\quad + C \sum_{i=1}^N |\psi|_{C^1(B(x_i, \frac{1}{4}r_i))} \left(r_i^{2-d} + \int_{B(x_i, r_i)} |\nabla h_{\frac{1}{4}r}^\mu[X_N]|^2 + N^{1-\frac{2}{d}} \|\mu\|_{L^\infty} \right) \end{aligned}$$

which in view of Lemma 3.3 proves (4.10), from which it also follows that

$$|\Xi'(0)| \leq C(1 + \|\mu\|_{L^\infty}) |\psi|_{C^1(U_\ell)} \Xi(0),$$

where C depends only on d . By the same reasoning, for every t such that (A.33) holds, and since $|\psi \circ \Phi_t^{-1}|_{C^1(U_\ell)} \leq |\psi|_{C^1(U_\ell)} (1 + C|t| |\psi|_{C^1(U_\ell)})$, we have $|\Xi'(t)| \leq C(1 + \|\mu\|_{L^\infty}) |\psi|_{C^1} \Xi(t)$. Thus applying Gronwall's lemma we deduce that if (A.33) holds we have

$$(A.54) \quad |\Xi(t) - \Xi(0)| \leq Ct \Xi(0)$$

and thus also

$$(A.55) \quad \Xi(t) \leq C \Xi(0)$$

where C depends only on d and $\|\mu\|_{L^\infty}$, proving (4.7).

A.4. Estimating the second derivative

We now wish to bound $|\Xi''(t)|$, which is new compared to [51]. We will repeatedly use (A.55), i.e. that the energy for Y_N is controlled by that of X_N .

Step 1 (Choice of η_i). We are going to make a different, smaller, choice of $\eta_i \leq \frac{1}{4}r_i$, for reasons that will appear later, and set

$$(A.56) \quad \eta_i = \frac{m}{4} \min((r_i N^{\frac{1}{d}})^\alpha, 1) r_i,$$

for

$$(A.57) \quad m = \begin{cases} (N^{\frac{1}{d}} \ell)^{-1} & \text{if } d = 2 \\ (N^{\frac{1}{d}} \ell)^{-\alpha'}, \alpha' > 0 & \text{if } d \geq 3 \end{cases}$$

and

$$(A.58) \quad \alpha = \begin{cases} 1 & \text{if } d = 2 \\ 2 & \text{if } d \geq 3. \end{cases}$$

This change in $\vec{\eta}$ leads us to a modification in the evaluation of terms $\int |\nabla h_{\vec{\eta}}|^2$ and $\sum_i \eta_i^{2-d}$. In particular, using the definition (A.56) and (3.24), we may write if $d \geq 3$

$$(A.59) \quad \sum_{i \in I_N} g(\eta_i) \leq C m^{2-d} \Xi(0)$$

and if $d = 2$, using the additivity property of the log,

$$(A.60) \quad \sum_{i \in I_N} g(N^{\frac{1}{d}} \eta_i) \leq \sum_{i \in I_N} g\left(\frac{m}{4} (r_i N^{\frac{1}{d}})^{1+\alpha}\right) \leq C \sum_{i \in I_N} g(r_i N^{\frac{1}{d}}) + C \# I_N g(m) \leq C \Xi(0) + C \# I_N g(m).$$

On the other hand, in view of (3.26) (and adding resp. subtracting $\sum_{i \in I_N} g(N^{\frac{1}{d}})$ to the terms in the right-hand side in the case $d = 2$) we have

$$\int_{U_\ell} |\nabla h_{\vec{\eta}}|^2 \leq 2c_d \left(F_N^{U_\ell}(X_N, \mu) + \frac{\# I_N}{4} (\log N) \mathbf{1}_{d=2} + C_0 \# I_N N^{1-\frac{2}{d}} \right) + c_d \sum_{i \in I_N} g(N^{\frac{1}{d}} \eta_i) \mathbf{1}_{d=2} + c_d \sum_{i \in I_N} g(\eta_i) \mathbf{1}_{d \geq 3}$$

so that by (3.24) and (A.59), resp. (A.60) and rearranging terms, we find

$$(A.61) \quad \int_{U_\ell} |\nabla h_{\vec{\eta}}|^2 \leq C \Xi(0) (1 + m^{2-d} \mathbf{1}_{d \geq 3}) + C \# I_N g(m) \mathbf{1}_{d=2}$$

Step 2 (Main term). To bound $|\Xi''(t)|$ we first need to estimate $|L_t - L_0|$. First, let us evaluate the Lipschitz norm in t of $\int \nabla h_{\vec{\eta}}^\mu [X_N] \cdot (\mathcal{A} \nabla h_{\vec{\eta}}^\mu [X_N])$ or more precisely bound

$$\int_{\mathbb{R}^d} \nabla h_{\vec{\eta}}^\nu [Y_N] \cdot (\mathcal{A} \nabla h_{\vec{\eta}}^\nu [Y_N]) - \int_{\mathbb{R}^d} \nabla h_{\vec{\eta}}^\mu [X_N] \cdot (\mathcal{A} \nabla h_{\vec{\eta}}^\mu [X_N])$$

where $\mathcal{A} = 2D\psi - (\operatorname{div} \psi) \operatorname{Id}$.

We start by observing that, using Young's inequality and $t|\psi|_{C^1} \leq \frac{1}{2}$,

$$\begin{aligned} \left| \int_{\mathbb{R}^d} \nabla \hat{h} \cdot \mathcal{A} \nabla \hat{h} - \int_{\mathbb{R}^d} E_{\vec{\eta}} \cdot \mathcal{A} E_{\vec{\eta}} \right| &\leq C |\psi|_{C^1} \|\nabla \hat{h} - E_{\vec{\eta}}\|_{L^2(U_\ell)} (\|\nabla \hat{h}\|_{L^2(U_\ell)} + \|\nabla \hat{h} - E_{\vec{\eta}}\|_{L^2(U_\ell)}) \\ &\leq \frac{1}{2c_d |t|} \int_{U_\ell} |\nabla \hat{h} - E_{\vec{\eta}}|^2 + C |t| |\psi|_{C^1}^2 \int_{U_\ell} |\nabla \hat{h}|^2. \end{aligned}$$

To control $\int_{\mathbb{R}^d} |\nabla \hat{h}|^2$ we use (A.27) and the bounds on Rem₁, Rem₂, Rem₃ (A.42), (A.46) and (A.47) obtained previously to get

$$\begin{aligned} \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla \hat{h}|^2 &\leq \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla h_{\vec{\eta}}^\nu [Y_N]|^2 + C |t| |\psi|_{C^1} \sum_{i \in I_N} \eta_i^{2-d} \\ &\quad + C t^2 (|\psi|_{C^1}^2 (1 + \|\mu\|_{L^\infty} + N^{-\frac{1}{d}} |\mu|_{C^1(U_\ell)}) + N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) |\psi|_{C^1} |\psi|_{C^2}) \\ &\quad \times \left(\mathsf{F}^{U_\ell}(Y_N, \nu) + \left(\frac{\# I_{U_\ell}}{4} \log N \right) \mathbf{1}_{d=2} + C_0 \# I_N N^{1-\frac{2}{d}} + \int_{U_\ell} |\nabla h_{\vec{\eta}}^\nu [Y_N]|^2 \right) \\ &\quad + t |\psi|_{C^1} \sum_{i \in I_N} \eta_i \|\nabla \tilde{h}_i\|_{L^\infty(B(y_i, r_i))}. \end{aligned}$$

Inserting (A.5), (A.61) and (A.59), and absorbing terms via $t|\psi|_{C^1} < \frac{1}{2}$, we obtain

$$\begin{aligned} \frac{1}{2c_d} \int_{\mathbb{R}^d} |\nabla \hat{h}|^2 &\leq C \left(\Xi(0) (1 + m^{2-d} \mathbf{1}_{d \geq 3}) + \# I_N g(m) \mathbf{1}_{d=2} \right) \\ &\quad \times \left(1 + C (|t| |\psi|_{C^1} + t^2 |\psi|_{C^1}^2 N^{-\frac{1}{d}} |\mu|_{C^1(U_\ell)} + t^2 |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}})) \right) \end{aligned}$$

with C depending only on d and $\|\mu\|_{L^\infty}$. When $t|\psi|_{C^1}$ and $t|\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}})$ are small enough, in view of (A.29), it follows that

$$(A.62) \quad \left| \int_{\mathbb{R}^d} \nabla \hat{h} \cdot \mathcal{A} \nabla \hat{h} - \int_{\mathbb{R}^d} E_{\vec{\eta}} \cdot \mathcal{A} E_{\vec{\eta}} \right| \leq C |t| |\psi|_{C^1}^2 (\Xi(0) (1 + C m^{2-d} \mathbf{1}_{d \geq 3}) + \# I_N g(m) \mathbf{1}_{d=2}) + O(t^3)$$

where C depends only on d and $\|\mu\|_{L^\infty}$. Next, we show that

$$(A.63) \quad \left| \int_{\mathbb{R}^d} \nabla \hat{h} \cdot \mathcal{A} \nabla \hat{h} - \int_{\mathbb{R}^d} \nabla h_{\vec{\eta}}^v[Y_N] \cdot \mathcal{A} \nabla h_{\vec{\eta}}^v[Y_N] \right| \leq C|t|(|\psi|_{C^1}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}))(\Xi(0)(1 + m^{2-d} \mathbf{1}_{d \geq 3}) + C \# I_N \mathbf{g}(m) \mathbf{1}_{d=2}) + O(t^2),$$

where the $O(t^2)$ depends on X_N , $\vec{\eta}$ and μ . First we claim that

$$(A.64) \quad \int_{\mathbb{R}^d} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 \leq C(|t| |\psi|_{C^1} + t^2 N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) |\psi|_{C^1} |\psi|_{C^2}) \Xi(0) + C|t| |\psi|_{C^1} m^{2-d} \Xi(0) \mathbf{1}_{d \geq 3}.$$

Indeed $h_{\vec{\eta}}^v - \hat{h} = \sum_{i=1}^N v_i$ (see (A.40)) hence

$$(A.65) \quad \int_{\mathbb{R}^d} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 = \sum_{i=1}^N \int_{\mathbb{R}^d} |\nabla v_i|^2 + \sum_{i \neq j} \int_{\mathbb{R}^d} \nabla v_i \cdot \nabla v_j.$$

But the second term on the right-hand side is exactly Rem_2 so from (A.46) we get

$$(A.66) \quad \left| \int_{\mathbb{R}^d} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 - \sum_{i=1}^N \int_{\mathbb{R}^d} |\nabla v_i|^2 \right| \leq C t^2 (|\psi|_{C^1}^2 + N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) |\psi|_{C^1} |\psi|_{C^2}) \Xi(0).$$

On the other hand

$$\begin{aligned} \int_{\mathbb{R}^d} |\nabla v_i|^2 &= \int_{\mathbb{R}^d} \mathbf{g} * (\delta_{y_i}^{(\eta_i)} - \hat{\delta}_{y_i})(\delta_{y_i}^{(\eta_i)} - \hat{\delta}_{y_i}) \\ &= - \int_{\mathbb{R}^d} \mathbf{g} * \delta_{y_i}^{(\eta_i)} \delta_{y_i}^{(\eta_i)} + \int_{\mathbb{R}^d} \mathbf{g} * \hat{\delta}_{y_i} \hat{\delta}_{y_i} + 2 \int_{\mathbb{R}^d} \mathbf{g} * \delta_{y_i}^{(\eta_i)} (\delta_{y_i}^{(\eta_i)} - \hat{\delta}_{y_i}). \end{aligned}$$

But $\mathbf{g} * \delta_{y_i}^{(\eta_i)} = \mathbf{g}_{\eta_i}$ by definition, it satisfies $|D\mathbf{g}_{\eta_i}| \leq \eta_i^{1-d}$ so by (A.36) the last term is bounded by $Ct|\psi|_{C^1} \eta_i^{2-d}$. In addition the calculation of Rem_1 also gives us $O(t|\psi|_{C^1} \eta_i^{2-d})$ for the first two terms. We conclude directly for $d=2$ and in view of (A.59) for $d \geq 3$ that (A.64) holds.

Next, we note that by (A.44), and $\eta_i \leq N^{-\frac{1}{d}}$,

$$(A.67) \quad \begin{aligned} \int_{B(y_i, 2\eta_i)^c} |\nabla v_i|^2 &\leq C t^2 \eta_i^4 \left(|\psi|_{C^1(B(x_i, \eta_i))}^2 \int_{|x| \geq 2\eta_i} \frac{dx}{|x|^{2d+2}} + |\psi|_{C^2(B(x_i, \eta_i))}^2 \int_{|x| \geq 2\eta_i} \frac{dx}{|x|^{2d}} \right) \\ &\leq C t^2 (|\psi|_{C^1(B(x_i, \eta_i))}^2 \eta_i^{2-d} + |\psi|_{C^2(B(x_i, \eta_i))}^2 N^{-\frac{2}{d}} \eta_i^{2-d}). \end{aligned}$$

Thus, using again (A.59) and combining with (A.66) we deduce that

$$(A.68) \quad \begin{aligned} \left| \int_{\mathbb{R}^d} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 - \sum_{i=1}^N \int_{B(y_i, 2\eta_i)} |\nabla v_i|^2 \right| &\leq C t^2 (|\psi|_{C^1}^2 + N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) |\psi|_{C^1} |\psi|_{C^2}) \Xi(0) + C t^2 (|\psi|_{C^1}^2 + |\psi|_{C^2}^2 N^{-\frac{2}{d}}) (\Xi(0)(1 + m^{2-d} \mathbf{1}_{d \geq 3})). \end{aligned}$$

We can now evaluate, using (A.40),

$$(A.69) \quad \begin{aligned} &\int_{B(y_i, 2\eta_i)} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N] - v_i)|^2 \\ &= \int_{B(y_i, 2\eta_i)} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 - \int_{B(y_i, 2\eta_i)} |\nabla v_i|^2 - 2 \int_{B(y_i, 2\eta_i)} \nabla v_i \cdot \left(\sum_{j \neq i} \nabla v_j \right) \\ &\leq \int_{\mathbb{R}^d} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 - \int_{B(y_i, 2\eta_i)} |\nabla v_i|^2 - 2 \int_{B(y_i, 2\eta_i)} \nabla v_i \cdot \left(\sum_{j \neq i} \nabla v_j \right). \end{aligned}$$

But using that v_j is harmonic in $B(y_i, 2\eta_i)$ for $j \neq i$ and (A.43), (A.44), we may write

$$\begin{aligned} \left| \sum_{j \neq i} \int_{B(y_i, 2\eta_i)} \nabla v_i \cdot \nabla v_j \right| &= \left| \sum_{j \neq i} \int_{\partial B(y_i, 2\eta_i)} v_i \frac{\partial v_j}{\partial \nu} \right| \\ &\leq t^2 \eta_j^2 \sum_{j \neq i} (\eta_j |\psi|_{C^1} + \eta_i^2 |\psi|_{C^2}) \left(\frac{|\psi|_{C^1}}{|y_j - y_i|^{\mathbf{d}+1}} + \frac{|\psi|_{C^2}}{|y_i - y_j|^{\mathbf{d}}} \right). \end{aligned}$$

After summing over i we may control this term similarly as we did for (A.46) via Proposition 3.5 combined with Corollary 3.4. Since the left-hand side of (A.69) is nonnegative, we thus deduce

$$\begin{aligned} (A.70) \quad &\left| \sum_{i=1}^N \int_{B(y_i, 2\eta_i)} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 - \int_{B(y_i, 2\eta_i)} |\nabla v_i|^2 \right| \\ &\leq Ct^2 (|\psi|_{C^1(U_\ell)}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}}) + |\psi|_{C^2}^2 N^{-\frac{2}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}})) \Xi(0) \\ &\quad + Ct^2 (|\psi|_{C^1}^2 + |\psi|_{C^2}^2 N^{-\frac{2}{\mathbf{d}}}) m^{2-\mathbf{d}} \Xi(0) \mathbf{1}_{\mathbf{d} \geq 3}, \end{aligned}$$

and combining with (A.68), we deduce that

$$\begin{aligned} (A.71) \quad &\int_{\mathbb{R}^{\mathbf{d}} \setminus \cup_i B(y_i, 2\eta_i)} |\nabla(\hat{h} - h_{\vec{\eta}}^v[Y_N])|^2 \\ &\leq Ct^2 (|\psi|_{C^1}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}}) + |\psi|_{C^2}^2 N^{-\frac{2}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}})) \Xi(0) \\ &\quad + Ct^2 (|\psi|_{C^1}^2 + |\psi|_{C^2}^2 N^{-\frac{2}{\mathbf{d}}}) m^{2-\mathbf{d}} \Xi(0) \mathbf{1}_{\mathbf{d} \geq 3}. \end{aligned}$$

To prove (A.63), in view of (A.64) and $|\mathcal{A}| \leq |\psi|_{C^1}$, it suffices to show that

$$\begin{aligned} (A.72) \quad &\int |\nabla(h_{\vec{\eta}}^v[Y_N] - \hat{h})| |\mathcal{A}| |\nabla h_{\vec{\eta}}^v[Y_N]| \\ &\leq Ct(|\psi|_{C^1}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}})) (\Xi(0)(1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}) + C\#I_N \mathbf{g}(m) \mathbf{1}_{\mathbf{d}=2}) + O(t^2). \end{aligned}$$

We break the integral into $\bigcup_i B(y_i, \eta_i)$ and the complement. In the complement, the bound comes from (A.71) and Cauchy–Schwarz, using that $|\mathcal{A}| \leq |\psi|_{C^1}$ and (A.61), and we obtain

$$\begin{aligned} (A.73) \quad &\int_{\mathbb{R}^{\mathbf{d}} \setminus \cup_i B(y_i, 2\eta_i)} |\nabla(h_{\vec{\eta}}^v[Y_N] - \hat{h})| |\mathcal{A}| |\nabla h_{\vec{\eta}}^v[Y_N]| \\ &\leq Ct |\psi|_{C^1} (|\psi|_{C^1}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}}) + |\psi|_{C^2}^2 N^{-\frac{2}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}}))^{\frac{1}{2}} \\ &\quad \times (\Xi(0)(1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}) + C\#I_N \mathbf{g}(m) \mathbf{1}_{\mathbf{d}=2}) \\ &\leq Ct (|\psi|_{C^1}^2 + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{\mathbf{d}}} \log(\ell N^{\frac{1}{\mathbf{d}}})) (\Xi(0)(1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}) + C\#I_N \mathbf{g}(m) \mathbf{1}_{\mathbf{d}=2}). \end{aligned}$$

There remains to study the contribution in $\bigcup_i B(y_i, 2\eta_i)$. We may bound it by

$$(A.74) \quad \sum_{i \in I_N} \int_{B(y_i, 2\eta_i)} |\nabla v_i| |\mathcal{A}| |\nabla \mathbf{g} * \delta_{y_i}^{(\eta_i)}| + \int_{B(y_i, 2\eta_i)} |\nabla v_i| |\mathcal{A}| |\nabla \tilde{h}_i[Y_N]| + \int_{B(y_i, 2\eta_i)} |\nabla(\hat{h} - h_{\vec{\eta}}^v - v_i)| |\mathcal{A}| |\nabla h_{\vec{\eta}}^v|.$$

Here we noted that $h_{\vec{\eta}}^v[Y_N] - \mathbf{g} * \delta_{y_i}$ coincides with $\tilde{h}_i[Y_N]$ in $B(x_i, 2\eta_i)$ because $2\eta_i \leq r_i$.

We bound the first piece by computing explicitly. We recall that $\nabla \mathbf{g} * \delta_{y_i}^{(\eta_i)} = (\nabla \mathbf{g}(\cdot - y_i)) \mathbf{1}_{|x - y_i| \geq \eta_i}$. We compute that for $x \notin \partial B(y_i, \eta_i)$, using $y_i - x_i = t\psi(x_i)$,

$$\begin{aligned} \nabla v_i(x) &= \int_{\partial B(x_i, \eta_i)} \nabla \mathbf{g}(x - y - t\psi(y)) - \nabla \mathbf{g}(x - y + x_i - y_i) \\ &= t \int_{\partial B(x_i, \eta_i)} D^2 \mathbf{g}(x - y) \cdot (\psi(x_i) - \psi(x) + \psi(x) - \psi(y)) + O_N(t^2). \end{aligned}$$

We break the right-hand side into

$$t D^2 \mathbf{g} * \delta_{y_i}^{(\eta_i)} (\psi(x_i) - \psi(x)) + O\left(t |\psi|_{C^1} \int_{\partial B(x_i, \eta_i)} |x - y|^{1-\mathbf{d}}\right) + O(t^2).$$

The convolution with the singular measure $\delta_{y_i}^{(\eta_i)}$ can be justified by smoothing out $\delta_{y_i}^{(\eta_i)}$. We deduce that

$$\begin{aligned} (A.75) \quad & \int_{B(y_i, 2\eta_i)} |\nabla v_i| \\ & \leq C|t| |\psi|_{C^1} \int_{B(x_i, 2\eta_i)} |D^2 \mathbf{g}_{\eta_i}(x - x_i)| \eta_i + C|t| |\psi|_{C^1} \int_{B(y_i, 2\eta_i)} \int_{\partial B(x_i, \eta_i)} \frac{dx dy}{|x - y|^{\mathbf{d}-1}} + O(t^2) \\ & \leq C|t| |\psi|_{C^1} \eta_i + O(t^2). \end{aligned}$$

For the last relation we have used that $|D^2 \mathbf{g}_{\eta_i}|$ is a measure with a singular part of mass $\leq C$ on $\partial B(y_i, \eta_i)$ and a diffuse part of density $\leq \eta_i^{-\mathbf{d}}$ in $B(y_i, 2\eta_i) \setminus B(y_i, \eta_i)$.

Thus we conclude that

$$\sum_{i=1}^N \int_{B(y_i, 2\eta_i)} |\nabla v_i| |\mathcal{A}| |\nabla \mathbf{g} * \delta_{y_i}^{(\eta_i)}| \leq C|t| |\psi|_{C^1}^2 \sum_i \eta_i^{2-\mathbf{d}} \leq C|t| |\psi|_{C^1}^2 \Xi(0) (1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}).$$

For the second piece in (A.74) we bound $|\nabla \tilde{h}_i[Y_N]|$ via (A.5), noticing that $B(y_i, 2\eta_i) \subset B(x_i, \frac{1}{2}r_i)$. Combining with (A.75), we find

$$\int_{B(y_i, 2\eta_i)} |\nabla v_i| |\mathcal{A}| |\nabla \tilde{h}_i[Y_N]| \leq C|t| |\psi|_{C^1}^2 \eta_i (r_i^{-\frac{\mathbf{d}}{2}} \lambda_i^{\frac{1}{2}} + N r_i \|\mu\|_{L^\infty}) + O(t^2).$$

Summing, using $\eta_i \leq r_i$ and Young's inequality, we obtain

$$\begin{aligned} & \sum_{i=1}^N \int_{B(y_i, 2\eta_i)} |\nabla v_i| |\mathcal{A}| |\nabla \tilde{h}_i[Y_N]| \\ & \leq C|t| |\psi|_{C^1}^2 \left(\sum_{i=1}^N r_i^{2-\mathbf{d}} + \lambda_i + N \sum_{i=1}^N r_i^2 \right) + O(t^2) \leq C|t| |\psi|_{C^1}^2 \Xi(0) + O(t^2), \end{aligned}$$

using again Lemma 3.3. This concludes the evaluation of (A.74) and combining with (A.73) we have finished the proof of (A.72) hence of (A.63).

Finally, since $E_\eta = \Phi_t \# \nabla h_{\tilde{\eta}}^\mu[X_N]$ we check with a change of variables and direct calculations that

$$\begin{aligned} & \left| \int_{\mathbb{R}^d} E_{\tilde{\eta}} \cdot \mathcal{A} E_{\tilde{\eta}} - \int_{\mathbb{R}^d} \nabla h_{\tilde{\eta}}^\mu[X_N] \cdot \mathcal{A} \nabla h_{\tilde{\eta}}^\mu[X_N] \right| \\ & \leq C|t| \int_{\mathbb{R}^d} |\nabla h_{\tilde{\eta}}^\mu[X_N]|^2 |D\psi|^2 + |t| \int_{\mathbb{R}^d} |D^2 \psi| |\psi| |\nabla h_{\tilde{\eta}}^\mu[X_N]|^2 + O(t^2) \\ & \leq C|t| (|\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty}) (\Xi(0) (1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}) + C \# I_N \mathbf{g}(m) \mathbf{1}_{\mathbf{d}=2}) + O(t^2), \end{aligned}$$

when we used (A.61).

Combining with (A.63) and (A.62) we then bound

$$\begin{aligned} (A.76) \quad & \left| \int_{\mathbb{R}^d} \nabla h_{\tilde{\eta}}^\nu[Y_N] \cdot \mathcal{A} \nabla h_{\tilde{\eta}}^\nu[Y_N] - \int_{\mathbb{R}^d} \nabla h_{\tilde{\eta}}^\mu[X_N] \cdot \mathcal{A} \nabla h_{\tilde{\eta}}^\mu[X_N] \right| \\ & \leq |t| (|\psi|_{C^1}^2 + |\psi|_{C^2} \|\psi\|_{L^\infty}) (\Xi(0) (1 + m^{2-\mathbf{d}} \mathbf{1}_{\mathbf{d} \geq 3}) + \# I_N \mathbf{g}(m) \mathbf{1}_{\mathbf{d}=2}) \\ & \quad + C|t| |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) \Xi(0) + O(t^2), \end{aligned}$$

where C depends only on $\|\mu\|_{L^\infty}$ and $O(t^2)$ may depend on $X_N, \vec{\eta}, \mu, \mathbf{d}$. In view of (A.31) and (A.61), we deduce that

$$(A.77) \quad \begin{aligned} |\text{Main}'(t) - \text{Main}'(0)| &\leq C|t|(|\psi|_{C^1}^2 + |\psi|_{C^2}\|\psi\|_{L^\infty})(\Xi(0)(1 + m^{2-\mathbf{d}}\mathbf{1}_{\mathbf{d} \geq 3}) + \#I_N \mathbf{g}(m)\mathbf{1}_{\mathbf{d}=2}) \\ &\quad + C|t|\|\psi\|_{C^1}\|\psi\|_{C^2}N^{-\frac{1}{\mathbf{d}}}\log(\ell N^{\frac{1}{\mathbf{d}}})\Xi(0) + O(t^2). \end{aligned}$$

Step 3. Next, let us evaluate the first derivative in t of the second term in L_t of (A.49). Making this term more explicit as

$$\begin{aligned} T_t &:= \sum_{i=1}^N \int_{\partial B(x_i, \eta_i)} \nabla \mathbf{g}(x + y_i - x_i - y) \Phi_i \# \left(\sum_{j \neq i} \delta_{x_j} - N\mu \right) (y) \cdot (\psi(x) - \psi(x_i)) \\ &= \sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} \int_{\mathbb{R}^d} \nabla \mathbf{g}(x - y + t\psi(x_i) - t\psi(y)) \left(\sum_{j \neq i} \delta_{x_j} - N\mu \right) (y) \cdot (\psi(x) - \psi(x_i)), \end{aligned}$$

we may compute its first derivative at $t = 0$ as

$$(A.78) \quad T'_0 = \sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} \int_{\mathbb{R}^d} D^2 \mathbf{g}(x - y) d \left(\sum_{j \neq i} \delta_{x_j} - N\mu \right) (y) (\psi(x_i) - \psi(y)) \cdot (\psi(x) - \psi(x_i))$$

$$(A.79) \quad = \sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} D^2 \tilde{h}_i(x) \psi(x_i) \cdot (\psi(x) - \psi(x_i))$$

$$(A.80) \quad - \sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} \int_{\mathbb{R}^d} D^2 \mathbf{g}(x - y) d \left(\sum_{j \neq i} \delta_{x_j} - N\mu(y)(1 - \chi_i)(y) \right) \psi(y) \cdot (\psi(x) - \psi(x_i))$$

$$(A.81) \quad + \sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} \int_{\mathbb{R}^d} D^2 \mathbf{g}(x - y) N\mu(y) \chi_i(y) \psi(y) \cdot (\psi(x) - \psi(x_i))$$

where χ_i is a cutoff function equal to 1 in $B(x_i, N^{-1/\mathbf{d}})$, vanishing outside $B(x_i, 2N^{-1/\mathbf{d}})$ and such that $|\nabla \chi_i| \leq N^{1/\mathbf{d}}$. To bound these terms, we want to insert that $\psi(x) - \psi(x_i) = D\psi(x_i)(x - x_i) + O(|\psi|_{C^2}\eta_i^2)$ and use that $D\psi(x_i)(x - x_i)$ integrates to 0 over $\partial B(x_i, \eta_i)$. Inserting that decomposition, the first term in (A.79) is then equal to

$$\sum_{i \in I_{U_\ell}} \int_{\partial B(x_i, \eta_i)} D\psi(x_i)^T D^2 \tilde{h}_i(x) \psi(x_i) \cdot (x - x_i) + O \left(\sum_{i \in I_{U_\ell}} \|D^2 \tilde{h}_i\|_{L^\infty(B(x_i, \eta_i))} \|\psi\|_{L^\infty} \|\psi\|_{C^2} \eta_i^2 \right).$$

After expanding $D^2 \tilde{h}_i(x) = D^2 \tilde{h}_i(x_i) + O(|D^3 \tilde{h}_i||x - x_i|)$ and using the cancellation, we find that the term in (A.79) is bounded by

$$|(A.79)| \leq C \sum_{i \in I_{U_\ell}} \|D^2 \tilde{h}_i\|_{L^\infty(B(x_i, \frac{1}{2}\mathbf{r}_i))} \|\psi\|_{L^\infty} \|\psi\|_{C^2} \eta_i^2 + \|D^3 \tilde{h}_i\|_{L^\infty(B(x_i, \frac{1}{2}\mathbf{r}_i))} \|\psi\|_{L^\infty} \|\psi\|_{C^1} \eta_i^2.$$

Thanks to (A.6), we may then bound this by

$$\begin{aligned} |(A.79)| &\leq C \sum_{i \in I_N} \eta_i^2 (\mathbf{r}_i^{-1-\frac{\mathbf{d}}{2}} \lambda_i(X_N, \mu)^{\frac{1}{2}} + N(\|\mu\|_{L^\infty} + \mathbf{r}_i^\sigma |\mu|_{C^\sigma(B(x_i, \mathbf{r}_i))})) \|\psi\|_{L^\infty} \|\psi\|_{C^2} \\ &\quad + C \sum_{i \in I_N} \eta_i^2 (\mathbf{r}_i^{-2-\frac{\mathbf{d}}{2}} \lambda_i(X_N, \mu)^{\frac{1}{2}} + N(\mathbf{r}_i^{-1} \|\mu\|_{L^\infty} + \mathbf{r}_i^\sigma |\mu|_{C^{1+\sigma}(B(x_i, \mathbf{r}_i))})) \|\psi\|_{L^\infty} \|\psi\|_{C^1}, \end{aligned}$$

for any $\sigma > 0$. Next, we insert the choice (A.56) and find, using $\eta_i \leq m\mathbf{r}_i \leq mN^{-1/\mathbf{d}}$ and Young's inequality

$$\begin{aligned} |(A.79)| &\leq C \left(\sum_{i \in I_N} \mathbf{r}_i^{2-\mathbf{d}} + \sum_{i \in I_N} \lambda_i(X_N, \mu) \right) \|\psi\|_{L^\infty} \|\psi\|_{C^2} \\ &\quad + m^2 \#I_N N^{1-\frac{2}{\mathbf{d}}} (\|\mu\|_{L^\infty} + N^{-\frac{\sigma}{\mathbf{d}}} |\mu|_{C^\sigma(U_\ell)}) \|\psi\|_{L^\infty} \|\psi\|_{C^2} \end{aligned}$$

$$\begin{aligned}
& + Cm^2 N^{\frac{2\alpha}{d}} \left(\sum_{i \in I_N} r_i^{p(2\alpha - \frac{d}{2})} + \lambda_i(X_N, \mu)^{\frac{q}{2}} \right) \|\psi\|_{L^\infty} |\psi|_{C^1} \\
& + (m^2 N \# I_N (N^{-\frac{1}{d}} \|\mu\|_{L^\infty} + N^{-\frac{2}{d} - \frac{\sigma}{d}} |\mu|_{C^{1+\sigma}(U_\ell)})) \|\psi\|_{L^\infty} |\psi|_{C^1},
\end{aligned}$$

for $p \leq 2$ and $q \geq 2$ conjugate Sobolev exponents. In dimension 2, we choose $p = q = 2$ and by choice $\alpha = \frac{1}{2}$ (see (A.58)) the corresponding sums are all bounded by $\Xi(0)$. In dimension $d \geq 3$, we use the elementary inequality $\sum_i u_i^r \leq (\sum_i u_i)^r$ for all $u_i \geq 0$ and $r \geq 1$ to bound $\sum_{i \in I_N} r_i^{-p \frac{d}{2}}$ by $(\sum_{i \in I_N} r_i^{2-d})^{\frac{p \frac{d}{2}}{d-2}}$ and $\sum_{i \in I_N} \lambda_i(X_N, \mu)^{\frac{q}{2}}$ by $(\sum_{i \in I_N} \lambda_i(X_N, \mu))^{\frac{q}{2}} \leq C \Xi(0)^{\frac{q}{2}}$. Optimizing gives the choice $q = 1 + \frac{d}{d-2}$ and so the sum in the third line is then bounded by $C \Xi(0)^{\frac{d-1}{d-2}}$. In view of the definition of Ξ , we finally obtain

$$\begin{aligned}
(A.82) \quad |(A.79)| & \leq C (\|\psi\|_{L^\infty} |\psi|_{C^2} + m^2 N^{\frac{1}{d}} \|\psi\|_{L^\infty} |\psi|_{C^1}) \Xi(0) + Cm^2 \|\psi\|_{L^\infty} |\psi|_{C^1} \Xi(0)^{\frac{d-1}{d-2}} \mathbf{1}_{d \geq 3} \\
& + m^2 \# I_N N^{1-\frac{2}{d}} (N^{-\frac{\sigma}{d}} \|\psi\|_{L^\infty} |\psi|_{C^2} |\mu|_{C^\sigma(U_\ell)} + N^{-\frac{\sigma}{d}} \|\psi\|_{L^\infty} |\psi|_{C^1} |\mu|_{C^{1+\sigma}(U_\ell)}).
\end{aligned}$$

For the term in (A.80), we argue similarly to bound it by

$$\begin{aligned}
|(A.80)| & \leq C \sum_{x_i, x_j \in U_\ell, i \neq j} \frac{\eta_i^2 \|\psi\|_{L^\infty} |\psi|_{C^2}}{|x_i - x_j|^d} + C \sum_{x_i, x_j \in U_\ell, i \neq j} \frac{\eta_i^2 \|\psi\|_{L^\infty} |\psi|_{C^1}}{|x_i - x_j|^{d+1}} \\
& + CN \sum_{i \in I_N} \eta_i^2 \|\psi\|_{L^\infty} |\psi|_{C^2} \int_{y \in U_\ell, |y - x_i| \geq N^{-1/d}} \frac{d\mu(y)}{|x_i - y|^d} \\
& + CN \sum_{i \in I_N} \eta_i^2 \|\psi\|_{L^\infty} |\psi|_{C^1} \int_{y \in U_\ell, |y - x_i| \geq N^{-1/d}} \frac{d\mu(y)}{|x_i - y|^{d+1}}.
\end{aligned}$$

The first sum may be controlled similarly as we did for (A.46) via Proposition 3.5 combined with Corollary 3.4, using that $\eta_i \leq m N^{-1/d}$, and they are bounded by $Cm^2 (\log(\ell N^{1/d}) \|\psi\|_{L^\infty} |\psi|_{C^2} + N^{1/d} \|\psi\|_{L^\infty} |\psi|_{C^1}) \Xi(0)$. Writing that with (A.56)

$$\frac{\eta_i^2}{|x_i - x_j|^{d+1}} \leq m^2 N^{\frac{2\alpha}{d}} \frac{r_i^{2+2\alpha}}{|x_i - x_j|^{d+1}} \leq m^2 N^{\frac{2\alpha}{d}} \frac{1}{|x_i - x_j|^{d-1-2\alpha}}$$

and using that $\sum_{i \neq j} |x_i - x_j|^{-d+1+2\alpha} \leq (\sum_{i \neq j} |x_i - x_j|^{2-d})^{\frac{-d+1+2\alpha}{2-d}}$ to use Corollary 3.4, we may then bound the second sum in the same way. Finally the last two integrals are bounded by similar terms as in (A.79). We next examine (A.81). Integrating once by parts in y we may bound this term by

$$(A.83) \quad |(A.81)| \leq CN^{1-\frac{1}{d}} \sum_{i \in I_N} \eta_i |\psi|_{C^1} (|\mu|_{C^1(U_\ell)} \|\psi\|_{L^\infty} + \|\mu\|_{L^\infty} |\psi|_{C^1} + \|\mu\|_{L^\infty} \|\psi\|_{L^\infty} N^{\frac{1}{d}})$$

Inserting all these results into (A.78), we conclude that

$$\begin{aligned}
(A.84) \quad |T'_0| & \leq C (|\psi|_{C^1}^2 + m^2 \|\psi\|_{L^\infty} |\psi|_{C^2} (\log(\ell N^{\frac{1}{d}}) + N^{-\frac{\sigma}{d}} |\mu|_{C^\sigma}) \\
& + \|\psi\|_{L^\infty} |\psi|_{C^1} (m^2 N^{\frac{1}{d}} + m^2 N^{-\frac{\sigma}{d}} |\mu|_{C^{1+\sigma}} + m |\mu|_{C^1} + m \|\mu\|_{L^\infty} N^{\frac{1}{d}})) \Xi(0) \\
& + Cm^2 \|\psi\|_{L^\infty} |\psi|_{C^1} \Xi(0)^{\frac{d-1}{d-2}} \mathbf{1}_{d \geq 3},
\end{aligned}$$

where C depends only on $\|\mu\|_{L^\infty}$ and d .

Step 4. We examine the first derivative in t of the third term in L_t of (A.49). Rewriting this term as

$$\frac{1}{2} \sum_i \eta_i^{1-d} \int_{\partial B(x_i, \eta_i)} (\psi(x + y_i - x_i) - \psi(y_i)),$$

we find that derivative is

$$\frac{1}{2} \sum_i \int_{\partial B(x_i, \eta_i)} \eta_i^{1-d} (D\psi(x) - D\psi(x_i)) \cdot \psi(x_i) \leq C |\psi|_{C^2} \|\psi\|_{L^\infty} \Xi(0) (1 + Cm^{2-d} \mathbf{1}_{d \geq 3}),$$

where we used (A.59).

Step 5 (Conclusion). The sum of all the controls we have obtained for $|L_t - L_0|$ and in the order t^2 term in (A.50) is

$$\begin{aligned} & (|\psi|_{C^1}^2 (1 + N^{-\frac{1}{d}} |\mu|_{C^1} + N^{-\frac{2}{d}} |\mu|_{C^2}) + |\psi|_{C^2} \|\psi\|_{L^\infty} + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) (1 + N^{-\frac{2}{d}} |\mu|_{C^2})) \\ & \times (\Xi(0) (1 + m^{2-d} \mathbf{1}_{d \geq 3}) + \#I_N g(m) \mathbf{1}_{d=2}) \\ & + (\|\psi\|_{L^\infty} |\psi|_{C^2} m^2 (\log(\ell N^{\frac{1}{d}}) + N^{-\frac{\sigma}{d}} |\mu|_{C^\sigma})) \\ & + \|\psi\|_{L^\infty} |\psi|_{C^1} (m^2 N^{\frac{1}{d}} + m^2 N^{-\frac{\sigma}{d}} |\mu|_{C^{1+\sigma}} + m |\mu|_{C^1} + m \|\mu\|_{L^\infty} N^{\frac{1}{d}})) \Xi(0) \\ & + m^2 \|\psi\|_{L^\infty} |\psi|_{C^1} \Xi(0)^{\frac{d-1}{d-2}} \mathbf{1}_{d \geq 3}. \end{aligned}$$

Inserting the choice (A.57) we may bound it by a constant times

$$\begin{aligned} A_{N,\psi} := & [|\psi|_{C^1}^2 (1 + N^{-\frac{1}{d}} |\mu|_{C^1} + N^{-\frac{2}{d}} |\mu|_{C^2}) + |\psi|_{C^2} \|\psi\|_{L^\infty} (1 + N^{-\frac{\sigma}{d}} |\mu|_{C^\sigma}) \\ & + |\psi|_{C^1} |\psi|_{C^2} N^{-\frac{1}{d}} \log(\ell N^{\frac{1}{d}}) (1 + N^{-\frac{2}{d}} |\mu|_{C^2})] (1 + (N^{\frac{1}{d}} \ell)^{\alpha'(d-2)} \mathbf{1}_{d \geq 3} + \log(\ell N^{\frac{1}{d}}) \mathbf{1}_{d=2}) \Xi(0) \\ & + \ell^{-1} \|\psi\|_{L^\infty} |\psi|_{C^1} [(N^{\frac{1}{d}} \ell)^{-1} (1 + N^{-\frac{1+\sigma}{d}} |\mu|_{C^{1+\sigma}} + N^{-\frac{1}{d}} |\mu|_{C^1}) \Xi(0) \mathbf{1}_{d=2} \\ & + (((N^{\frac{1}{d}} \ell)^{1-2\alpha'} (1 + N^{-\frac{1+\sigma}{d}} |\mu|_{C^{1+\sigma}}) + (N^{\frac{1}{d}} \ell)^{1-\alpha'} N^{-\frac{1}{d}} |\mu|_{C^1}) \Xi(0) + (N^{\frac{1}{d}} \ell)^{1-2\alpha'} N^{-\frac{1}{d}} \Xi(0)^{\frac{d-1}{d-2}}) \mathbf{1}_{d \geq 3}]. \end{aligned}$$

In view of (A.50), (A.77), (A.84), combined with (A.61), we have obtained that

$$|\Xi(t) - \Xi(0) - tL_0| \leq Ct^2 A_{N,\psi} + O(t^3)$$

yielding

$$|\Xi''(0)| \leq CA_{N,\psi}.$$

We thus have proved the desired result at $t = 0$. The same reasoning applied near t together with the fact that with (A.33),

$$|\psi \circ \Phi_t^{-1}|_{C^2} \leq C |\psi|_{C^2}$$

allows to conclude with (A.54) that (4.7) and (4.8) hold.

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