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Diffusive Long–time Behavior of Kawasaki Dynamics

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Abstract: If P_t is the semigroup associated with the Kawasaki dynamics on $\mathbb{Z}^d$ and f is a local function on the configuration space, then the variance with respect to the invariant measure μ of $P_t f$ goes to zero as $t \to \infty$ faster than $t^{-d/2+\varepsilon}$, with ε arbitrarily small. The fundamental assumption is a mixing condition on the interaction of Dobrushin and Schlosman type.

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1 Introduction

Consider a Markov process $(\eta_t)_{t\geq 0}$ taking values in an infinite product space $\Omega := S^{\mathbb{Z}^d}$, so that $\eta_t = (\eta_t(x))_{x\in\mathbb{Z}^d}$. S could be, for instance, a subset of $\mathbb{N}$, and the variable $\eta_t(x)$ is sometimes thought of as the number of particles at x at time t. Assume then that this process is reversible with respect to a probability measure μ on Ω which is a Gibbs measure for some interaction J. A very general problem for this class of processes is the study of the relationships between the properties of the interaction J and the behavior of the process. Among the infinite possible ways of constructing Markov processes of this type we single out two special categories: (1) *spin–flip* processes[2] also called *Glauber dynamics*, and (2) (nearest neighbor) *particle–exchange* processes or *Kawasaki dynamics*. In the first case we have that the coordinates of η_t can change only one at a time. More precisely, if $\mathcal{L}^G$ is the generator of the process, then

$$\mathcal{L}^G f(\eta) = \sum_{\eta'} c(\eta,\eta')\,[f(\eta') - f(\eta)]$$

and $c(\eta,\eta') = 0$ unless η and η' differ in exactly one coordinate. Similarly, in a Kawasaki dynamics the transition rate $c(\eta,\eta')$ is zero unless η' can be obtained from η by transferring one particle from x to y where x, y are nearest neighbors in $\mathbb{Z}^d$.

One of the most important result concerning Glauber dynamics is a theorem asserting the *equivalence* between a mixing condition of Dobrushin and Shlosman type [DS87] on the interaction J and the fact that the distribution of η_t converges exponentially fast to the invariant measure μ in a rather strong sense. For a comprehensive account on this subject we refer the reader to the beautiful review paper [Mar99].

For Kawasaki dynamics, which we study in this paper, the situation is more complicated. In fact, even if the interaction J is zero and consequently μ is a product measure, the process is nevertheless an "interacting" (*i.e.* non–product) process. These type of processes are also called "conservative dynamics" because if we run them in a finite volume $\Lambda \subset \mathbb{Z}^d$ then the function $t \to N_\Lambda(\eta_t) := \sum_{x\in\Lambda}\eta_t(x)$ is constant. The specific problem we want to address is: let $(P_t)_{t\geq 0}$ be the semigroup associated with the process, and let f be a real function on Ω. How fast does the quantity $P_t f$ converges to the expectation $\mu(f) := \int_\Omega f d\mu$? Of course there are several ways of interpreting this convergence, however, since μ is supposed to be a reversible measure, one of the most natural quantities to study is the $L^2(\mu)$ distance. Hence we are looking at the long–time behavior of the quantity

$$\|P_t f - \mu f\|^2_{L^2(\mu)} = \mathrm{Var}_\mu(P_t f)\,, \tag{1.1}$$

where Var_μ stands for the variance w.r.t. μ. One of the first things to realize is that the constraint imposed by the conservation law prevents this convergence

[2]the term spin–flip is really appropriate when $S = \{-1, +1\}$

from being exponentially fast even when $J = 0$. It is fairly easy to show (see [Spo91], pag. 175–6) that the quantity (1.1) (with, say $f(\eta) := \eta(0)$) cannot be smaller than $C\, t^{-d/2}$. Actually $t^{-d/2}$ is conjectured to be the correct long–time asymptotics, when (J is such that) μ is somehow close to a product measure, this conjecture being hatched from the idea that these processes are discretized versions of diffusions in $\mathbb{R}^d$. For elliptic diffusions, a standard way of proving the $t^{-d/2}$ decay is [Dav89, Sect 2.4] by means of the so called Nash inequalities stating

$$\|f\|_{L^2}^2 \le C\, \|f\|_{L^1}^{4/(d+2)}\, \mathcal{E}(f)^{d/(d+2)}$$

where $\mathcal{E}$ is the Dirichlet form given by

$$\mathcal{E}(f) := \int_{\mathbb{R}^d} |\nabla f(x)|^2\, dx\,.$$

Unfortunately, in the (morally) infinite dimensional framework of Kawasaki dynamics, this approach has been successful only for a special model called symmetric simple exclusion process [BZ99a, BZ99b] where $S = \{0, 1\}$ and the invariant measure μ is Bernoulli.

It is clear, on the other side, that a piece of information that should be relevant for this problem is the fact that, while the generator of the process has no spectral gap in the infinite volume, if we denote with $\mathcal{L}_\ell$ the generator in $\mathbb{Z}^d \cap [-\ell, \ell]^d$ then we have for large ℓ [LY93, CM00b]

$$\mathrm{gap}(\mathcal{L}_\ell) \sim C\ell^{-2}\,. \tag{1.2}$$

A new approach was then developed in [JLQY99] where thanks to a combination of (1.2) with techniques imported from the hydrodynamic limit theory it was proved that, for the symmetric zero–range process one has

$$\|P_t f - \mu(f)\|_{L^2(\mu)}^2 = \frac{C(f)}{t^{d/2}} + o(t^{-d/2}) \tag{1.3}$$

where $C(f)$ is an explicit quantity. More recently [LY03] the same result (apart from logarithmic corrections) has been extended to the Ginzburg–Landau process with a potential which is a bounded perturbation of a Gaussian potential. Both the zero–range and the Ginzburg–Landau process have an invariant measure which is a product measure. The first results which apply to a process with a non–product invariant measure μ were obtained in [CM00b]. Their main assumption is a mixing condition on μ. In that paper it has been shown in a very simple way that (1.2) supplemented with a soft spectral theoretic argument implies an almost optimal upper bound when $d = 1, 2$. More precisely for all $\varepsilon > 0$ and for all local function f on Ω, there exists $C_{\varepsilon,f} > 0$ such that

$$\|P_t f - \mu(f)\|_{L^2(\mu)}^2 \le \frac{C_{\varepsilon,f}}{t^{d/2-\varepsilon}}\,. \tag{1.4}$$

Their strategy, appealing for its simplicity, seems however unable to yield the correct asymptotics in more than two dimensions.

In the present paper we extend inequality (1.4) to arbitrary values of d, following the original approach of [JLQY99] which the authors predicted would be powerful enough to treat processes with non–trivial invariant measures. We stress, however, that we are unable to prove the sharper equality (1.3). The main reason is that we have been incapable of extending the very precise "hydrodynamical" estimates of [JLQY99, Section 5] to the type of processes we consider in this paper, in which the invariant measure is only assumed to satisfy a certain mixing condition.

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2 Notation and Results

2.1 Lattice and configuration space

The lattice. We consider the d dimensional lattice $\mathbb{Z}^d$ whose elements are called *sites* $x = (x_1, \dots, x_d)$ and where we define the norms

$$|x|_p = \Big[\sum_{i=1}^{d} |x_i|^p\Big]^{1/p} \quad p \geq 1 \quad \text{and} \qquad |x| = |x|_\infty = \max_{i \in \{1,\dots,d\}} |x_i| \, .$$

The associated distance functions are denoted by $d_p(\cdot,\cdot)$ and $d(\cdot,\cdot)$. We define B_L as the *ball* in $\mathbb{Z}^d$ centered at the origin with radius L with respect to the norm $|\cdot|$, *i.e.* $B_L := \{x \in \mathbb{Z}^d : |x| \leq L\}$. Let also, for $y \in \mathbb{Z}^d$, $B_L(y) := B_L + y$, and, more generally, for $A \subset \mathbb{Z}^d$, $B_L(A) := B_L + A = \{x \in \mathbb{Z}^d : d(x, A) \leq L\}$. If Λ is a finite subset of $\mathbb{Z}^d$ we write $\Lambda \Subset \mathbb{Z}^d$. The cardinality of Λ is denoted by $|\Lambda|$. $\mathbb{F}$ is the set of all nonempty finite subsets of $\mathbb{Z}^d$. Two sites x, y are said to be *nearest neighbors* if $|x-y|_1 = 1$. An *edge* of $\mathbb{Z}^d$ is a (unordered) pair of nearest neighbors. We denote by $\mathbb{E}_\Lambda$ the set of all edges with both endpoints are in Λ and by $\overline{\mathbb{E}}_\Lambda$ the set of all edges with at least one endpoint in Λ. Given $\Lambda \subset \mathbb{Z}^d$ we define its interior and exterior n–boundaries as respectively, $\partial_n^- \Lambda = \{x \in \Lambda : \, d(x, \Lambda^c) \leq n\}$, $\partial_n^+ \Lambda = \{x \in \Lambda^c : \, d(x, \Lambda) \leq n\}$. We also let $\delta\Lambda = \overline{\mathbb{E}}_\Lambda \backslash \mathbb{E}_\Lambda$.
For $\ell \in \mathbb{Z}_+$, let $Q_\ell := [0, \ell)^d \cap \mathbb{Z}^d$. A *polycube* is defined as a triple $(\Lambda, \ell, \mathcal{A})$ where $\Lambda \in \mathbb{F}$, $\ell \in \mathbb{Z}_+$, $\mathcal{A} \subset \mathbb{F}$ are such that

(1) for all $V \in \mathcal{A}$ there exists $x \in \ell\mathbb{Z}^d$ such that $V = x + Q_\ell$

(2) $\mathcal{A}$ is a partition of Λ, *i.e.* Λ is the disjoint union of the elements of $\mathcal{A}$.

The configuration space. Our *configuration space* is $\Omega = S^{\mathbb{Z}^d}$, where $S = \{0, 1\}$, or $\Omega_V = S^V$ for some $V \subset \mathbb{Z}^d$. The single spin space S is endowed with the discrete topology and Ω with the corresponding product topology. Given $\eta \in \Omega$ and $\Lambda \subset \mathbb{Z}^d$ we denote by η_Λ the restriction of η to Λ. If U, V are disjoint subsets of $\mathbb{Z}^d$, $\sigma_U\tau_V$ is the configuration on $U \cup V$ which is equal to σ on U and τ on V. We denote by π_x the standard projection from Ω onto S, *i.e.* the map $\eta \mapsto \eta(x)$.

If $\Lambda \in \mathbb{F}$, N_Λ stands for the *number of particles in* Λ, *i.e.* $N_\Lambda = \sum_{x\in\Lambda} \eta(x)$. If $\mathcal{A}$ is a collection of finite subsets of $\mathbb{Z}^d$, we define $N_\mathcal{A}$ as

$$N_\mathcal{A} : \Omega \ni \eta \to (N_\Lambda(\eta))_{\Lambda\in\mathcal{A}} \in \mathbb{N}^\mathcal{A} .$$

We also define the σ–algebras

$$\mathcal{F}_\Lambda = \sigma\{\pi_x : x \in \Lambda\} \qquad \mathcal{G}_{\Lambda,\mathcal{A}} = \sigma\{\pi_x, N_V : x \in \Lambda, V \in \mathcal{A}\} . \tag{2.1}$$

When $\Lambda = \mathbb{Z}^d$ we set $\mathcal{F} = \mathcal{F}_{\mathbb{Z}^d}$ and $\mathcal{F}$ coincides with the Borel $\sigma-$algebra on Ω with respect to the topology introduced above.

If f is a function on Ω, S_f denotes the smallest subset of $\mathbb{Z}^d$ such that $f(\eta)$ depends only on η_{S_f}. f is called *local* if S_f is finite. We introduce 3 operators

(1) the *translations*: $\vartheta_x f(\eta) := f(\eta')$ where $\eta'(y) = \eta(y - x)$

(2) the *spin–flip*: $s_x\eta(y) := \begin{cases} \eta(y) & \text{if } y \neq x \\ 1-\eta(y) & \text{if } y = x \end{cases}$

(3) the *particle exchange*: $t_{xy}\eta(z) = \begin{cases} \eta(x) & \text{if } z = y \\ \eta(y) & \text{if } z = x \\ \eta(z) & \text{otherwise.} \end{cases}$

The capitalized versions of s_x, t_{xy} act on functions in the obvious way

$$S_x f := f \circ s_x \qquad T_{xy} f = f \circ t_{xy} . \tag{2.2}$$

The Glauber and Kawasaki "gradients" are then respectively defined as

$$\nabla_x f := S_x f - f \qquad \nabla_{xy} f := T_{xy} f - f .$$

We denote with $\|f\|_u$ the supremum norm of f, *i.e.* $\|f\|_u := \sup_{\eta\in\Omega} |f(\eta)|$ and with $\operatorname{osc}(f)$ the oscillation of f, *i.e.* $\operatorname{osc}(f) := \sup f - \inf f$.

2.2 The interaction and the Gibbs measures

In the following we consider a translation invariant, summable *interaction* J, of finite range r, *i.e.* a collection of functions $J = (J_A)_{A\in\mathbb{F}}$, such that $J_A : \Omega \mapsto \mathbb{R}$ is measurable w.r.t. $\mathcal{F}_A$, and

(H1) $J_{A+x} \circ \vartheta_x = J_A$ for all $A \in \mathbb{F}$, $x \in \mathbb{Z}^d$

(H2) $J_A = 0$ if the diameter of A is greater than r

(H3) $\|J\| := \sum_{A\in\mathbb{F}:\, A\ni 0} \|J_A\|_u < \infty$

Conditions (H1), (H2), (H3) will always be assumed without explicit mention. The Hamiltonian $(H_\Lambda)_{\Lambda\in\mathbb{F}}$ associated with J is defined as

$$H_\Lambda : \Omega \ni \sigma \to \sum_{A\in\mathbb{F}:\, A\cap\Lambda\neq\emptyset} J_A(\sigma) \in \mathbb{R}\,.$$

Clearly $\|H_\Lambda\|_u \le |\Lambda|\|J\|$. For $\sigma,\tau \in \Omega$ we also let $H_\Lambda^\tau(\sigma) := H_\Lambda(\sigma_V \tau_{V^c})$ and τ is called the *boundary condition*. For each $\Lambda \in \mathbb{F}$, $\tau \in \Omega$ the (finite volume) Gibbs measure on $(\Omega,\mathcal{F})$, are given by

$$\mu_\Lambda^\tau(\sigma) := \left(Z_\Lambda^\tau\right)^{-1} \exp[-H_\Lambda^\tau(\sigma)]\, 1\!\!1_{\{\tau_{\Lambda^c}\}}(\sigma_{\Lambda^c})\,, \tag{2.3}$$

where Z_Λ^τ is the proper normalization factor called partition function, and $1\!\!1$ is the indicator function. In the future we are going to consider an interaction J with an explicit additional *chemical potential* λ. In particular we will consider a chemical potential on a polycube $(\Lambda,\ell,\mathcal{A})$ such that λ is constant in each cube $x+Q_\ell \in \mathcal{A}$. For this reason, given such a polycube, and given $\lambda \in \mathbb{R}^{\mathcal{A}}$ we define

$$H_{\mathcal{A},\lambda} := H_\Lambda - \sum_{V\in\mathcal{A}} \lambda_V N_V \qquad \lambda \in \mathbb{R}^{\mathcal{A}}\,. \tag{2.4}$$

The associated finite volume Gibbs measures are denoted by $\mu_{\mathcal{A},\lambda}^\tau$.
Given a bounded measurable function f on Ω, $\mu_\Lambda^\tau f$ denotes expectation of f w.r.t. μ_Λ^τ, while, when the superscript is omitted, $\mu_\Lambda f$ stands for the function $\sigma \mapsto \mu_\Lambda^\sigma(f)$ which is measurable w.r.t. $\mathcal{F}_{\Lambda^c}$. Analogously, if $X\in\mathcal{F}$, $\mu_V(X) := \mu_V(1\!\!1_X)$. $\mu(f,g)$ stands for the covariance (with respect to μ) of f and g. The variance of f is (accordingly) denoted by $\mu(f,f)$ or, alternatively, by $\mathrm{Var}_\mu(f)$.
The set of measures (2.3) satisfies the DLR compatibility conditions

$$\mu_\Lambda(\mu_V(X)) = \mu_\Lambda(X) \qquad \forall\, X\in\mathcal{F} \qquad \forall\, V\subset\Lambda\Subset\mathbb{Z}^d\,. \tag{2.5}$$

A probability measure μ on $(\Omega,\mathcal{F})$ is called a *Gibbs measure* if

$$\mu(\mu_V(X)) = \mu(X) \qquad \forall\, X\in\mathcal{F} \qquad \forall\, V\in\mathbb{F}\,. \tag{2.6}$$

Our main assumption on the interaction J is an exponential *mixing property* for the finite volume Gibbs measures $\mu_{\mathcal{A},\lambda}^\tau$, uniform in the chemical potential λ. More precisely we assume that:

(USM) There exist $\Gamma_0, m, \ell_0 \in (0,\infty)$, and for every local function f on Ω there is $A_f > 0$ which depends only on $|S_f|$ and $\|f\|_u$, such that for all polycubes $(\Lambda,\ell,\mathcal{A})$ with $\ell\ge\ell_0$ for all pairs of local functions f,g we have

$$|\mu_{\mathcal{A},\lambda}^\tau(f,g)| \le \Gamma_0\, A_f\, A_g\, e^{-md(S_f,S_g)} \qquad \forall\lambda\in\mathbb{R}^{\mathcal{A}},\ \forall\tau\in\Omega\,. \tag{2.7}$$

Condition (USM) is easily implied, except for the uniformity in λ, by the Dobrushin and Shlosman's complete analyticity condition (IIIc) in [DS87]. As for the necessity of assuming this uniformity in λ we refer the reader to the remark after the "Definition of property (USMT)" in [CM00b].

By standard arguments it is not hard to check that (USM) implies that there exists $\Gamma = \Gamma(d, r, \|J\|, \Gamma_0)$ such that if $d(S_f, S_g) > r$ then for all $\lambda \in \mathbb{R}^{\mathcal{A}}$

$$|\mu^\tau_{\mathcal{A},\lambda}(f,g)| \le \\ \le \mu^\tau_{\mathcal{A},\lambda}(|f|)\, \mu^\tau_{\mathcal{A},\lambda}(|g|) \Big\{\exp\Big[\Gamma \sum_{x\in\partial_r^- S_f} \sum_{y\in\partial_r^- S_g} e^{-m|x-y|}\Big] - 1\Big\} \quad \forall \tau \in \Omega\,. \tag{2.8}$$

This inequality becomes effective when S_f and S_g are "far apart" enough, in which case it can be written in a simpler form. More precisely there exists $\Gamma_1 = \Gamma_1(d, r, \|J\|, \Gamma_0, m)$ such that if

$$\big(|\partial_r^- S_f \cap \Lambda| \wedge |\partial_r^- S_g \cap \Lambda|\big)\, e^{-md(S_f,S_g)/3} \le \Gamma_1^{-1} \tag{2.9}$$

then

$$|\mu^\tau_{\mathcal{A},\lambda}(f,g)| \le \mu^\tau_{\mathcal{A},\lambda}(|f|)\, \mu^\tau_{\mathcal{A},\lambda}(|g|)\, e^{-md(S_f,S_g)/2} \quad \forall \lambda \in \mathbb{R}^{\mathcal{A}},\ \forall \tau \in \Omega\,. \tag{2.10}$$

From (2.6) the following well known fact easily follows

Proposition 2.1. *Under hypothesis (USM) there is exactly one Gibbs meassure for J which we denote with μ.*

We introduce the *(multi–)canonical Gibbs measures* on $(\Omega, \mathcal{F})$: let $(\Lambda, \ell, \mathcal{A})$ be a polycube[3] and let $M = (M_V)_{V\in\mathcal{A}}$ be a possible choice for the number of particles in each cube $V \in \mathcal{A}$, *i.e.*

$$M \in \mathbb{M}_\ell^{\mathcal{A}} \quad \text{where} \quad \mathbb{M}_\ell := \{0, 1, \ldots, \ell^d\}\,.$$

Then we define (remember (2.1))

$$\nu^\tau_{\mathcal{A},M} := \mu^\tau_\Lambda(\,\cdot \mid N_{\mathcal{A}} = M) \tag{2.11}$$

$$G_{\mathcal{A}} := \mu(\cdot \mid \mathcal{G}_{\Lambda^c,\mathcal{A}})\,. \tag{2.12}$$

We have, for $f \in L^1(\mu)$

$$\nu^\sigma_{\mathcal{A},N_{\mathcal{A}}(\sigma)}(f) = G_{\mathcal{A}}(f)(\sigma) \qquad \mu\text{–a.e.}$$

in this way we can write the "multicanonical DLR equations" as

$$\mu_W(f) = \mu_W(G_{\mathcal{A}}(f)) \qquad \text{if } \Lambda \subset W\,.$$

In the special case where $\mathcal{A} = \{\Lambda\}$ consists of a single element we (slightly) improperly write

$$\nu^\tau_{\Lambda,N} := \nu^\tau_{\{\Lambda\},N} \qquad G_\Lambda := G_{\{\Lambda\}}\,.$$

[3]multi–canonical measures can obviously be defined on an arbitrary partition of Λ

2.3 The dynamics

We consider the so–called Kawasaki dynamics, a Markov process with generator $\mathcal{L}_V$, where $V \Subset \mathbb{Z}^d$ and

$$(\mathcal{L}_V f)(\sigma) = \sum_{e \in \mathbb{E}_V} c_e(\sigma)\,(\nabla_e f)(\sigma) \qquad \sigma \in \Omega\,, \quad f : \Omega \mapsto \mathbb{R}\,. \tag{2.13}$$

The nonnegative real quantities $c_e(\sigma)$ are the *transition rates* for the process. The general assumptions on the transition rates are

(K1) *Finite range.* c_e is measurable w.r.t. $\mathcal{F}_{B_r(e)}$.

(K2) *Detailed balance.* For all $e \in \mathbb{E}_{\mathbb{Z}^d}$ we have $\nabla_e \left[c_e\, e^{-H_e}\right] = 0$.

(K3) *Positivity and boundedness.* There exist positive real numbers c_m, c_M such that $c_m \le c_e(\sigma) \le c_M$ for all $e \in \mathbb{E}_{\mathbb{Z}^d}$ and $\sigma \in \Omega$.

We denote by $\mathcal{L}^\tau_{V,N}$ the operator $\mathcal{L}_V$ acting on $L^2(\Omega, \nu^\tau_{V,N})$. Assumptions (1), (2) and (3) guarantee that there exists a unique Markov process whose generator is $\mathcal{L}^\tau_{V,N}$, and whose semigroup we denote by $(P_t^{V,N,\tau})_{t\ge 0}$. $\mathcal{L}^\tau_{V,N}$ is a bounded operator on $L^2(\Omega, \nu^\tau_{V,N})$ and $\nu^\tau_{V,N}$ is its unique invariant measure. Moreover $\nu^\tau_{V,N}$ is *reversible* with respect to the process, *i.e.* $\mathcal{L}^\tau_{V,N}$ is self–adjoint on $L^2(\Omega, \nu^\tau_{V,N})$. With $(P_t)_{t\ge 0}$ we denote the *infinite volume semigroup* which is reversible w.r.t. μ, while $\mathcal{L}$ stands for the generator of $(P_t)_{t\ge 0}$.

A fundamental quantity associated with the dynamics of a reversible system is the spectral gap of the generator, *i.e.*

$$\mathrm{gap}(\mathcal{L}^\tau_{V,N}) = \inf \mathrm{spec}\,(-\mathcal{L}^\tau_{V,N} \restriction 1^\perp)$$

where $1^\perp$ is the subspace of $L^2(\Omega, \nu^\tau_{V,N})$ orthogonal to the constant functions.

If Q is a probability measure on $(\Omega, \mathcal{F})$, $V \subset \mathbb{Z}^d$, and $X \subset \mathbb{E}_{\mathbb{Z}^d}$ we let[4]

$$\mathcal{E}_{Q,V}(f) := \frac{1}{2} \sum_{e \in \mathbb{E}_V} Q\left[c_e\,(\nabla_e f)^2\right] \qquad \mathcal{E}_{Q,X}(f) := \frac{1}{2} \sum_{e \in X} Q\left[c_e\,(\nabla_e f)^2\right]\,. \tag{2.14}$$

When Q equals the unique infinite volume Gibbs measure μ, we (may) omit it as a subscript. Analogously we omit the subscript V when $V = \mathbb{Z}^d$, so we let for simplicity

$$\mathcal{E}_V := \mathcal{E}_{\mu,V} \qquad \mathcal{E}_X := \mathcal{E}_{\mu,X} \qquad \mathcal{E} := \mathcal{E}_{\mu,\mathbb{Z}^d} \tag{2.15}$$

The *Dirichlet form* associated with the generator $\mathcal{L}^\tau_{V,N}$ is then given by $\mathcal{E}_{\nu^\tau_{V,N},V}(f)$. The gap can also be characterized as

$$\mathrm{gap}(\mathcal{L}^\tau_{V,N}) = \inf_{f \in L^2(\nu^\tau_{V,N})\,:\, f \perp 1} \frac{\mathcal{E}_{\nu^\tau_{V,N},V}(f)}{\nu^\tau_{V,N}(f,f)}\,. \tag{2.16}$$

[4] again with some abuse of notation

2.4 Main result

Constants. Throughout this paper we tacitly assume to have chosen once and for all a value of the dimension d of the lattice $\mathbb{Z}^d$, an interaction J of finite range r satisfying (H1), (H2), (H3), a set of transition rates $(c_e)_{e\in\mathbb{E}_{\mathbb{Z}^d}}$ satisfying (K1), (K2), (K3). Our main result and most of the results contained in this work hold when the interaction J is such that the mixing hypothesis (USM) is also satisfied. With the word "constant" we denote any quantity which depends solely on the paramenters which have been fixed by means of these hypotheses, namely $d, r, \|J\|, c_m, c_M, \Gamma_0, m, \ell_0$. Analogously "for x large enough" means *for x larger than some constant*. For simplicity we write things like "Assume (USM). Then for all $\varepsilon > 0$ there is $C > 0$ such that …" without reiterating that C depends not only on ε, but in principle, on all the paramenters mentioned above.

Theorem 2.2. *Assume (USM). Then for all $\varepsilon > 0$ and for all local functions f on Ω there is $A(\varepsilon, f) \in (0,\infty)$ such that*

$$\mu\big[\big(P_t f - \mu f\big)^2\big] \le \frac{A(\varepsilon, f)}{t^{d/2-\varepsilon}} \qquad \forall t > 0$$

Remarks 2.3.

(a) This result has been proved for $d = 1, 2$ in [CM00b], so we are going to consider only the case $d \ge 3$.

(b) One might want to be more ambitious and study, instead of the quadratic fluctuations of $P_t f$, the convergence to the invariant measure in some stronger sense, say $L^\infty(\mu)$. We refer the reader to the introduction of [JLQY99] where it is explained how, for these kind of models, the long time behavior of the quantity $|P_t f(\eta) - \mu(f)|$ has a nontrivial dependence on the starting point η, which makes pointwise estimates a much harder problem.

3 Outline of the proof of Theorem 2.2

Let $d \ge 3$, let, as usual, μ be the unique infinite volume Gibbs measure for the interaction J, and define $\langle f, g\rangle := \mu(fg)$, $\|f\| := \mu(f^2)^{1/2}$. Let f be a local function such that $\mu f = 0$, let $f_t := P_t f$ and let $K_t := \lfloor\sqrt{t}\rfloor$. In the following it will be convenient to average over spatial translations, hence we define

$$R_j f := |B_j|^{-1} \sum_{x\in B_j} \vartheta_x f\,.$$

Then we write

$$\mu\big[\big(P_t f - \mu f\big)^2\big] = \|f_t\|^2 \le 2\|f_t - R_{K_t} f_t\|^2 + 2\|R_{K_t} f_t\|^2\,. \tag{3.1}$$

The second term in (3.1) is by far the easier. In fact, since P_s is a contraction in $L^2(\mu)$, we have, for all $s, t > 0$

$$\begin{aligned}\|R_{K_t} f_s\|^2 = \|P_s R_{K_t} f\|^2 \le \|R_{K_t} f\|^2 &= \frac{1}{|B_{K_t}|^2} \sum_{x,y \in B_{K_t}} \mu(\vartheta_x f\, \vartheta_y f) \\ &= \frac{1}{|B_{K_t}|^2} \sum_{x,y \in B_{K_t}} \mu((\vartheta_{x-y} f) f) \le \frac{1}{|B_{K_t}|} \sum_{z \in B_{2K_t}} \mu((\vartheta_z f) f)\end{aligned}$$

so, using our mixing assumption (2.10), we obtain that there is $A_1 = A_1(f) > 0$ such that

$$\|R_{K_t} f_s\|^2 \le A_1\, t^{-d/2} \qquad \forall s, t > 0\,. \tag{3.2}$$

Thus, letting $\varphi(t) := \|f_t - R_{K_t} f_t\|^2$, what we need to do is to show that

$$\varphi(t) \le A_2\, t^{-d/2+\varepsilon}\,. \tag{3.3}$$

Inequality (3.3) is implied, by iteration, by the following statement

$$\exists \delta < 4^{-d/2} \text{ such that } \forall t \ge 0 \quad \varphi(t) \le \delta \varphi(t/4) + A_3\, t^{-d/2+\varepsilon}\,. \tag{3.4}$$

In order to prove (3.4) we write, using (3.2)

$$\begin{aligned}\varphi(t) &\le 2\|f_t - R_{K_{t/4}} f_t\|^2 + 2\|R_{K_t} f_t - R_{K_{t/4}} f_t\|^2 \\ &\le 2\|f_t - R_{K_{t/4}} f_t\|^2 + 4\|R_{K_{t/4}} f_t\|^2 + 4\|R_{K_t} f_t\|^2 \\ &\le 2\|f_t - R_{K_{t/4}} f_t\|^2 + A_1'\, t^{-d/2}\,.\end{aligned} \tag{3.5}$$

Let then

$$\psi(t, K) := \|f_t - R_K f_t\|^2 \qquad t \ge 0,\ K \in \mathbb{Z}_+\,.$$

We claim that in order to prove (3.4) it is sufficient to show that for some $A_4 = A_4(\varepsilon, f)$ we have

$$\exists \delta < 4^{-d/2}\ s.t.\ \forall K \le K_t \quad \int_t^{2t} \psi(s, K)\, ds \le \frac{\delta}{2} \int_t^{2t} \psi(s/2, K)\, ds + \frac{A_4}{t^{d/2-1-\varepsilon}}\,. \tag{3.6}$$

In fact, since $\psi(\cdot, K)$ is nonincreasing (3.6) implies

$$\psi(2t, K) \le \frac{\delta}{2}\, \psi(t/2, K) + \frac{A_4}{t^{d/2-\varepsilon}}$$

and, using (3.5), we find

$$\varphi(t) \le 2\psi(t, K_{t/4}) + \frac{A_1'}{t^{d/2}} \le \delta\psi(t/4, K_{t/4}) + \frac{A_1'}{t^{d/2}} + \frac{A_4'}{t^{d/2-\varepsilon}} \le \delta\varphi(t/4) + \frac{A_3}{t^{d/2-\varepsilon}}\,.$$

Hence the theorem follows from (3.6).

3.1 Proof of statement (3.6)

Let $K \le K_t$, let $(B_{L_2}, \ell, \mathcal{A})$ be a polycube, and choose two more integers L, L_1 such that $\ell \le L < L_1 < L_2$. We anticipate[5] that we are going to choose $\ell = L \sim \sqrt{t}$, $L_1 \sim \sqrt{t} \log t$ and $L_2 \sim \sqrt{t}\,(\log t)^2$ (precise definitions in (3.23)). Let $\Lambda_1 := B_{L_1}$, $\Lambda_2 := B_{L_2}$, and define

$$g_t := P_t(f - R_K f) \qquad g_{x,t} := \vartheta_x g_t \,. \tag{3.7}$$

Thanks to translation invariance, we have, since $\mu\, g_{x,t} = \mu f = 0$,

$$\psi(t, K) = \frac{1}{|B_L|} \sum_{x \in B_L} \mu(g_{x,t}^2)\,. \tag{3.8}$$

For simplicity we define the following orthogonal projections in $L^2(\mu)$

$$Q_1 = \mu(\,\cdot\,|\,\mathcal{F}_{\Lambda_1}) \quad Q_2 = \mu(\,\cdot\,|\,\mathcal{F}_{\Lambda_2}) \quad Q_{\mathcal{A}} = \mu(\,\cdot\,|\,N_{\mathcal{A}})\,.$$

Then, since $G_{\mathcal{A}} Q_{\mathcal{A}} = Q_{\mathcal{A}} G_{\mathcal{A}} = Q_{\mathcal{A}}$, we have

$$\begin{aligned}\mu(g_{x,t}^2) &= \|g_{x,t}\|^2 = \|(I - Q_1) g_{x,t}\|^2 + \|Q_1 g_{x,t}\|^2 \\ &= \|(I - Q_1) g_{x,t}\|^2 + \|G_{\mathcal{A}} Q_1 g_{x,t}\|^2 + \|(1 - G_{\mathcal{A}}) Q_1 g_{x,t}\|^2 \\ &= \|(I - Q_1) g_{x,t}\|^2 + \|Q_{\mathcal{A}} Q_1 g_{x,t}\|^2 \\ &\quad + \|(I - Q_{\mathcal{A}}) G_{\mathcal{A}} Q_1 g_{x,t}\|^2 + \|(I - G_{\mathcal{A}}) Q_1 g_{x,t}\|^2\,.\end{aligned} \tag{3.9}$$

On the other side, since $Q_{\mathcal{A}} Q_2 = Q_{\mathcal{A}}$ and $Q_2 Q_1 = Q_1$

$$\begin{aligned}\|Q_{\mathcal{A}} Q_1 g_{x,t}\| &\le \|Q_{\mathcal{A}} Q_2 g_{x,t}\| + \|Q_{\mathcal{A}}(Q_1 - Q_2) g_{x,t}\| \\ &\le \|Q_{\mathcal{A}} g_{x,t}\| + \|(Q_2 - Q_1) g_{x,t}\| = \|Q_{\mathcal{A}} g_{x,t}\| + \|Q_2 (I - Q_1) g_{x,t}\| \\ &\le \|Q_{\mathcal{A}} g_{x,t}\| + \|(I - Q_1) g_{x,t}\|\,.\end{aligned} \tag{3.10}$$

From (3.9), (3.10) we get

$$\begin{aligned}\mu(g_{x,t}^2) &\le 3\,\mu\,[\mathrm{Var}(g_{x,t}\,|\,\mathcal{F}_{\Lambda_1})] + 2\,\mu\,\big[\mu(g_{x,t}\,|\,N_{\mathcal{A}})^2\big] \\ &\quad + \mu\big[\mathrm{Var}(G_{\mathcal{A}} Q_1 g_{x,t}\,|\,N_{\mathcal{A}})\big] + \mu\,[\,G_{\mathcal{A}}(Q_1 g_{x,t}, Q_1 g_{x,t})\,]\end{aligned} \tag{3.11}$$

where $\mathrm{Var}(f\,|\,\cdot)$ stands for the conditional variance of f (w.r.t. μ). We now proceed to estimate each of the four terms in (3.11) and we are going to prove that (3.6) holds.

First term in (3.11). In Section 4 we generalize the so–called "cutoff estimate" (Proposition 3.1 of [JLQY99]) to the case where the measure μ is no longer a product measure, but it satisfies our mixing condition (USM). The result is (more or less) the same as in [JLQY99].

[5] for those readers who do not like proceeding on a "need-to-know" basis

Proposition 3.1. *Assume (USM). Then there exists $C > 0$ such that, for all local functions g on Ω, for all $t \geq 1$ such that $S_g \subset B_{3\lfloor\sqrt{t}\rfloor}$, and for all $L \in \mathbb{Z}_+$, we have*

$$\mu\,[\mathrm{Var}(P_t g \,|\, \mathcal{F}_{B_L})] \leq C\, e^{-L/\sqrt{t}}\, \mu(g^2)\,. \tag{3.12}$$

If we apply this result to the first term of (3.11) we find, for all $x \in B_L$,

$$\mu\,[\mathrm{Var}(g_{x,t} \,|\, \mathcal{F}_{\Lambda_1})] \leq C\, e^{-L_1/\sqrt{t}}\, \|g_x\|^2 \qquad \text{if } S_g \subset B_{3\lfloor\sqrt{t}\rfloor - L}\,. \tag{3.13}$$

Second term in (3.11). This term keeps track of the fluctuation of the number of particles in the various blocks which make up the polycube $(\Lambda_2, \ell, \mathcal{A})$. We use the following result whose proof appears in section 7. The integral of the second term in (3.11) can be estimated as follows:

Proposition 3.2. *Assume (USM). Then, for all $\varepsilon > 0$, for all local function f on Ω, there exists $A = A(f, \varepsilon)$ such that: for all polycubes $(\Lambda, \ell, \mathcal{A})$ for all positive integers K, L, taking into account definitions (3.7), and for all $t > 0$ we have*

$$\int_0^t \frac{1}{|B_L|} \sum_{x \in B_L} \mu\left[\mu(g_{x,s} \,|\, N_{\mathcal{A}})^2\right] ds \leq \frac{A\, K^2}{L^d} \left[L^{\varepsilon}\, |\mathcal{A}|\, \log \ell + \frac{t}{L^2}\right]. \tag{3.14}$$

Third term in (3.11). Since $\mathrm{Var}(f) \leq \mathrm{osc}(f)^2/2$, we get

$$\mu\big[\mathrm{Var}(G_{\mathcal{A}} Q_1 g_{x,t} \,|\, N_{\mathcal{A}})\big] \leq \frac{1}{2} \sup_{M \in \mathbb{M}_\ell^{\mathcal{A}}} \sup_{\sigma,\tau \in \Omega} \left[\nu^{\sigma}_{\mathcal{A},M}(Q_1 g_{x,t}) - \nu^{\tau}_{\mathcal{A},M}(Q_1 g_{x,t})\right]^2 \cdot \tag{3.15}$$

In order to estimate the difference appearing in the RHS of (3.15) we use the following result which will be proved in Section 5 (see Corollary 5.7):

Proposition 3.3. *Assume (USM). Then there exists $C > 0$ such that for all polycubes $(B_L, \ell, \mathcal{A})$, for all functions f on Ω such that $S_f \subset B_L$, and for all $M \in \mathbb{M}_\ell^{\mathcal{A}}$, we have*

$$\sup_{\sigma,\tau \in \Omega} |\nu^{\sigma}_{\mathcal{A},M}(f) - \nu^{\tau}_{\mathcal{A},M}(f)| \leq \|f\|_u \left[C\, L^{d-1}\, \frac{(\log \ell)^{3/2}}{\ell^d}\right]^{\lfloor d(S_f, B_L^c)/[(3d+4)\ell]\rfloor - 2} \tag{3.16}$$

From (3.15) and (3.16) (applied to the polycube $(\Lambda_2, \ell, \mathcal{A})$) and thanks to the fact that $Q_1 g_{x,t}$ is measurable w.r.t. $\mathcal{F}_{B_{L_1}}$, we get

$$\mu\big[\mathrm{Var}(G_{\mathcal{A}} Q_1 g_{x,t} \,|\, N_{\mathcal{A}})\big] \leq \|f\|_u^2 \left[C\, L_2^{d-1}\, \frac{(\log \ell)^{3/2}}{\ell^d}\right]^{2\lfloor (L_2 - L_1)/[(3d+4)\ell]\rfloor - 4}. \tag{3.17}$$

Fourth term in (3.11). In Section 6 we prove a Poincaré inequality for the multi–canonical measure, more precisely

Proposition 3.4. *Assume (USM). Then for all $\gamma \in (0,(d-1)^{-1})$ there exists C_γ such that for all polycubes $(B_L,\ell,\mathcal{A})$ with $L \le \ell^{1+\gamma}$ we have, for all local functions f,*

$$\mu\,[\,G_{\mathcal{A}}(f,f)\,] \le C_\gamma\,\ell^2\,\mathcal{E}_{B_L}(f)\,. \tag{3.18}$$

Choose $\gamma := \gamma_0 := [2(d-1)]^{-1}$. If $L_2 \le \ell^{1+\gamma_0}$ we can apply Proposition 3.4 to our polycube $(\Lambda_2,\ell,\mathcal{A})$. In this way we can estimate the fourth term in (3.11) as

$$\mu\,[\,G_{\mathcal{A}}(Q_1 g_{x,t}\,,\,Q_1 g_{x,t})\,] \le C_{\gamma_0}\,\ell^2\,\mathcal{E}_{\Lambda_2}(Q_1 g_{x,t})\,. \tag{3.19}$$

In order to find a suitable upper bound to the Dirichlet form appearing in the RHS of (3.19) we proceed as follows: given an edge e of $\mathbb{Z}^d$ we have, for all $f \in L^2(\mu)$

$$\begin{aligned}\|\nabla_e Q_1 f\| &\le \|\nabla_e f\| + \|\nabla_e(I-Q_1)f\| \le \|\nabla_e f\| + \|(I-Q_1)f\| + \|T_e(I-Q_1)f\|\\ &\le \|\nabla_e f\| + \|(I-Q_1)f\|\left(1+\|e^{-\nabla_e H_e}\|_u^{1/2}\right)\\ &\le \|\nabla_e f\| + \|(I-Q_1)f\|\left(1+e^{\|J\|}\right).\end{aligned}$$

Thanks to Proposition 3.1 (applied to the sigma–algebra $\mathcal{F}_{B_{L_1}}$), and using the fact that $S_{g_x} \subset B_L(S_g)$, we obtain that for some constant C_1

$$\|\nabla_e Q_1 g_{x,t}\|^2 \le 2\|\nabla_e g_{x,t}\|^2 + C_1\,e^{-L_1/\sqrt{t}}\,\|g_x\|^2 \quad \text{if } S_g \subset B_{3\lfloor\sqrt{t}\rfloor - L}\,. \tag{3.20}$$

From (2.14), (3.19), (3.20) we get that there is $C_2 > 0$ such that

$$\mu\,[\,G_{\mathcal{A}}(Q_1 g_{x,t}, Q_1 g_{x,t})\,] \le C_2\,\ell^2\Big[\mathcal{E}(g_{x,t}) + e^{-L_1/\sqrt{t}}\|g_x\|^2\Big] \quad \text{if } S_g \subset B_{3\lfloor\sqrt{t}\rfloor - L}\,. \tag{3.21}$$

For any zero mean function f in the domain of $\mathcal{E}$ we have

$$\mu(f^2) \ge -\int_0^t \frac{d}{ds}\mu(f_s^2)ds = 2\int_0^t \mathcal{E}(f_s)ds \ge 2t\mathcal{E}(f_t)\,,$$

hence

$$\mathcal{E}(g_{x,t}) = \mathcal{E}(P_{3t/4}\,g_{x,t/4}) \le \frac{2\mu(g_{x,t/4}^2)}{3t}\,.$$

From (3.21) it follows that if $S_g \subset B_{3\lfloor\sqrt{t}\rfloor - L}$, then

$$\frac{1}{|B_L|}\sum_{x\in B_L}\mu\,[\,G_{\mathcal{A}}(Q_1 g_{x,t}, Q_1 g_{x,t})\,] \le C_3\left[\frac{\ell^2}{t}\,\psi(t/4,K) + e^{-L_1/\sqrt{t}}\,\|g\|^2\right]. \tag{3.22}$$

End of proof of Theorem 2.2. To conclude the proof we choose appropriate values for ℓ, L, L_1, L_2 and collect the various pieces together. Choose then a real number α such that $5\,C_3\,\alpha^2 < 4^{-d/2}$, and let[6]

$$\ell = L := 2\lfloor\alpha\sqrt{t}\rfloor + 1 \quad L_1 := \lfloor(d/2)\sqrt{t}\log t\rfloor \quad 2L_2 + 1 := \ell\,(2\lfloor(\log t)^2\rfloor + 1)\,. \tag{3.23}$$

Inequality (3.6) then follows from (3.8), (3.11), (3.13) (3.14), (3.15), (3.17), (3.22), and this proves the theorem. ☐

[6] the following (apparently?) paranoic definitions are due to the fact that ℓ must be an *odd* integer which divides $2L_2 + 1$.

4 Cutoff estimate and proof of Proposition 3.1

In this section we prove Proposition 3.1. We observe that the factor 3 appearing in the assumption $S_g \subset B_{3\lfloor\sqrt{t}\rfloor}$ is completely arbitrary. By redefining the constant C one can replace this 3 with any number. We follow the strategy of Proposition 3.1 in [JLQY99], with suitable modifications required by the fact that, in our case, μ is not a product measure.

Lemma 4.1. *Assume (USM) and let, for $j \in \mathbb{N}$,*

$$A_j := \mu(\cdot \,|\, \mathcal{F}_{B_j}) \qquad D_j := \mathbb{E}_{B_j} \backslash \mathbb{E}_{B_{j-r}} \qquad \overline{D}_j := D_j \cup \delta B_j \,.$$

Then, there exists a constant $C > 0$ such that for all $\vartheta > 0$, and for all local functions g on Ω, we have (remember (2.15))

$$|\,\mu(A_j g\, \mathcal{L}g)\,| \leq \mathcal{E}_{B_{j-r}}(g) + \vartheta\, C\, \mathcal{E}_{\overline{D}_j}(g) + \frac{C}{\vartheta}\, \mu[\,(A_{j+r}g - A_j g)^2\,]\,.$$

Proof. We let $\langle f, g\rangle := \mu(fg)$, $\|f\| := \mu(f^2)^{1/2}$, and we define, for $x \in \mathbb{Z}^d$, $e \in \mathbb{E}_{\mathbb{Z}^d}$

$$h_e^j := \frac{e^{-\nabla_e H_e}}{A_j(e^{-\nabla_e H_e})} \qquad h_x^j := \frac{e^{-\nabla_x H_{\{x\}}}}{A_j(e^{-\nabla_x H_{\{x\}}})} \qquad U_e^j := 1 - h_e^j \,.$$

A straightforward computation shows that if $e = \{x, y\} \subset B_j$ then we have (remember (2.2))

$$\nabla_e A_j f = A_j(\nabla_e f) + T_e\, A_j[f U_e^j]\,. \tag{4.1}$$

In the special case in which $e \subset B_{j-r}$ we have $h_e^j = 1$, thus, (4.1) reduces to

$$\nabla_e A_j f = A_j(\nabla_e f)\,. \tag{4.2}$$

If instead $e = \{x, y\} \in \delta B_j$ then the formula is slightly more complicated. Assume $x \in B_j$, $y \in B_j^c$, and let $q_e(\sigma) = 1\!\!1_{\{\sigma(x) \neq \sigma(y)\}}$. Then

$$\nabla_e A_j f = q_e \left\{ A_j[\nabla_e f (1 + h_y^j)] + A_j[f V_{xy}^j] + S_x\, A_j[f W_{xy}^j] \right\} \tag{4.3}$$

where

$$\begin{aligned} V_{xy}^j &:= h_y^j\, q_{xy} - (1 - q_{xy}) \\ W_{xy}^j &:= 1 - h_x^j\, q_{xy} - q_{xy}\, S_y\, (h_x^j / h_y^j)\,. \end{aligned}$$

It is easy to verify that

$$A_j V_{xy}^j = A_j W_{xy}^j = 0\,.$$

By definition we have

$$\mu(A_j g\, (-\mathcal{L}g)) = \mathcal{E}(A_j g, g) = \frac{1}{2} \sum_{e:\, e \cap B_j \neq \emptyset} \mu\big(c_e \nabla_e(A_j g) \nabla_e g\big)\,,$$

so, letting, $Y_e := \mu\big(c_e \nabla_e(A_j g)\nabla_e g\big)$, we can write

$$|\mu(A_j g\, (-\mathcal{L}g))| \leq X_1 + X_2 + X_3$$

where

$$X_1 := \frac{1}{2}\Big|\sum_{e\subset B_{j-r}} Y_e\Big| \qquad X_2 := \frac{1}{2}\Big|\sum_{e\in D_j} Y_e\Big| \qquad X_3 := \frac{1}{2}\Big|\sum_{e\in \delta B_j} Y_e\Big| .$$

For what concerns those edges $e \subset B_{j-r}$ which contribute to X_1 we observe that $c_e A_j(f) = A_j(c_e f)$. From this equality, from the fact that A_j is an orthogonal projection in $L^2(\mu)$, and from (4.2), it follows that, for each $e \subset B_{j-r}$

$$Y_e = \mu\big(c_e A_j(\nabla_e g)\nabla_e g\big) = \|A_j(\sqrt{c_e}\,\nabla_e g)\|^2 \le \|\sqrt{c_e}\,\nabla_e g\|^2 = \mu[c_e\,(\nabla_e g)^2]$$

hence

$$X_1 \le \mathcal{E}_{B_{j-r}}(g)\,. \tag{4.4}$$

In order to estimate X_2 we use (4.1) and we get (c_m, c_M are the minimum and maximum transition rates)

$$X_2 \le \frac{c_M}{2}\sum_{e\in D_j} \mu[(A_j|\nabla_e g|)^2] + \frac{c_M}{2}\sum_{e\in D_j} \mu\big[|\nabla_e g|\,|T_e A_j(gU_e^j)|\big]\,.$$

Using $xy \le (\vartheta x^2 + \vartheta^{-1}y^2)/2$ in the second term, we get

$$X_2 \le \frac{c_M}{c_m}\Big(1+\frac{\vartheta}{2}\Big)\,\mathcal{E}_{D_j}(g) + \frac{c_M}{4\vartheta}\sum_{e\in D_j}\mu\big[T_e\big(\,A_j(g\,U_e^j)\,\big)^2\big]\,.$$

Since $\|J\| < \infty$, there exists $C_0 > 0$ such that for all edged e and all sites x

$$\mu(T_e f) \le C_0\,\mu(f) \qquad \mu(S_x f) \le C_0\,\mu(f) \qquad\quad \forall f > 0\,. \tag{4.5}$$

In this way we obtain

$$X_2 \le \frac{c_M}{c_m}\Big(1+\frac{\vartheta}{2}\Big)\,\mathcal{E}_{D_j}(g) + \frac{c_M C_0}{4\vartheta}\sum_{e\in D_j}\|A_j(g\,U_e^j)\|^2\,. \tag{4.6}$$

The term X_3 can be estimated using (4.3) and (4.5) as

$$X_3 \le \frac{c_M}{c_m}\,C_1\,\vartheta\,\mathcal{E}_{\delta B_j}(g) + \frac{c_M C_1}{\vartheta}\sum_{e\in\delta B_j}\big[\|A_j(gV_e^j)\|^2 + \|A_j(gW_e^j)\|^2\big] \tag{4.7}$$

where C_1 is some positive constant. Collecting the terms in (4.4), (4.6), (4.7), we find that there exists a constant $C_2 > 0$ such that

$$\begin{aligned} |\,\mu(A_j g\,(-Lg))| &\le \mathcal{E}_{B_{j-r}}(g) + C_2\,\vartheta\mathcal{E}_{\overline{D}_j}(g) \\ &+ \frac{C_2}{\vartheta}\Big[\sum_{e\in D_j}\|A_j(gU_e^j)\|^2 + \sum_{e\in\delta B_j}\|A_j(gV_e^j)\|^2 + \sum_{e\in\delta B_j}\|A_j(gW_e^j)\|^2\Big]\,. \end{aligned} \tag{4.8}$$

In order to estimate the three sums which appear in (4.8) we use the following elementary Hilbert space inequality.

Proposition 4.2. *Let $(V, \langle\cdot,\cdot\rangle)$ be a Hilbert space, and let $(u_i)_{i=1}^n$ be a finite sequence of elements of V. Define*

$$M := \max_{i=1,\dots,n} \sum_{j=1}^{n} |\langle u_i, u_j\rangle| .$$

Then, for all $v \in V$, we have

$$\sum_{i=1}^{n} \langle v, u_i\rangle^2 \le M\, \|v\|^2 . \tag{4.9}$$

Proof. Since $\|v - \sum_{i=1}^n \lambda_i u_i\|^2 \ge 0$ for all $\lambda \in \mathbb{R}^n$, we find, letting $\lambda_i = \vartheta\langle v, u_i\rangle$,

$$\vartheta^2 \sum_{i,j=1}^{n} \langle v, u_i\rangle\langle v, u_j\rangle\langle u_i, u_j\rangle - 2\vartheta \sum_{i=1}^{n} \langle v, u_i\rangle^2 + \|v\|^2 \ge 0 \qquad \forall \vartheta \in \mathbb{R}$$

which, since $\langle v, u_i\rangle\langle v, u_j\rangle \le (\langle v, u_i\rangle^2 + \langle v, u_j\rangle^2)/2$, implies

$$\vartheta^2 M \sum_{i=1}^{n} \langle v, u_i\rangle^2 - 2\vartheta \sum_{i=1}^{n} \langle v, u_i\rangle^2 + \|v\|^2 \ge 0 \qquad \forall \vartheta \in \mathbb{R}$$

and the result follows. □

Consider now the first sum in the RHS of (4.8)

$$\sum_{e\in D_j} \|A_j(gU_e^j)\|^2 = \mu\Big[\sum_{e\in D_j} [A_j(gU_e^j)]^2\Big] .$$

The idea is to use Proposition 4.2 with $\langle f, g\rangle$ replaced by $A_j(fg)$. Thanks to the hypothesis (USM) on the interaction J, there exists a constant $C_3 > 0$ such that

$$\max_{e'\in D_j} \sum_{e\in D_j} |A_j(U_e^j U_{e'}^j)| \le C_3 \qquad \forall j \in \mathbb{Z}_+ . \tag{4.10}$$

By consequence, using (4.9), (4.10), the fact that U_e^j is measurable w.r.t. $\mathcal{F}_{B_{j+r}}$ and that $A_j(U_e^j) = 0$, we get

$$\begin{aligned} \mu\Big[\sum_{e\in D_j} [A_j(gU_e^j)]^2\Big] &= \mu\Big[\sum_{e\in D_j} [A_j(A_{j+r}g)U_e^j)]^2\Big] \\ &= \mu\Big[\sum_{e\in D_j} [A_j(A_{j+r}g - A_j g)U_e^j)]^2\Big] \le C_3\, \mu\big[(A_{j+r}g - A_j g)^2\big] . \end{aligned} \tag{4.11}$$

From (4.8), (4.11) and the analogous inequalities for the terms

$$\sum_{e\in\delta B_j} \|A_j(gV_e^j)\|^2 \qquad \sum_{e\in\delta B_j} \|A_j(gW_e^j)\|^2 .$$

Lemma 4.1 follows. □

4.1 End of proof of Proposition 3.1

Once we have estabilished Lemma 4.1, Proposition 3.1 follows more or less in the same way as in [JLQY99]. We include the argument for completeness.

Let ℓ, L be two positive integers, let $\vartheta > 0$, and let $\alpha_i := e^{i/(\vartheta C)}$ for $i \in \mathbb{N}$, where C is the constant which appears in Lemma 4.1. We assume $C \geq 1$ otherwise we redefine C as $C \vee 1$. Given $g \in L^2(\mu)$ we also let $g_t := P_t g$. Define then the function

$$F(t) := \alpha_{\ell+1}\|A_{2\ell r} g_t\|^2 + \sum_{j=\ell}^{L-1} \alpha_{j+1}\|A_{2(j+1)r} g_t - A_{2jr} g_t\|^2 + \alpha_{L+1}\|g_t - A_{2Lr} g_t\|^2$$

and notice that it can be also written as

$$F(t) = \alpha_{L+1}\|g_t\|^2 + \sum_{j=\ell+1}^{L} (\alpha_{j+1} - \alpha_j)\|A_{2jr} g_t\|^2 .$$

Differentiating and using to Lemma 4.1 we obtain

$$\begin{aligned} F'(t) &= -2\alpha_{L+1}\mathcal{E}(g_t) - 2\sum_{j=\ell+1}^{L} (\alpha_{j+1} - \alpha_j)\mu(A_{2jr} g_t L g_t) \\ &\leq -2\alpha_{L+1}\mathcal{E}(g_t) + 2\sum_{j=\ell+1}^{L} (\alpha_{j+1} - \alpha_j)\Big[\mathcal{E}_{B_{(2j-1)r}}(g_t) + \vartheta\, C\, \mathcal{E}_{\overline{D}_{2jr}}(g_t) \\ &\qquad + \frac{C}{\vartheta}\|A_{(2j+1)r} g_t - A_{2jr} g_t\|^2\Big] . \end{aligned}$$

Using the summation by parts formula we can rewrite $F'(t)$ as

$$\begin{aligned} F'(t) &= -2\alpha_{L+1}\big[\mathcal{E}(g_t) - \mathcal{E}_{B_{(2L+1)r}}(g_t)\big] - 2\alpha_{\ell+1}\mathcal{E}_{B_{(2\ell+1)r}}(g_t) \\ &\quad + 2\sum_{j=\ell+1}^{L} \alpha_{j+1}\big[\mathcal{E}_{B_{(2j-1)r}}(g_t) - \mathcal{E}_{B_{(2j+1)r}}(g_t)\big] \\ &\quad + 2C\sum_{j=\ell+1}^{L} (\alpha_{j+1} - \alpha_j)\Big[\vartheta\mathcal{E}_{\overline{D}_{2jr}}(g_t) + \frac{1}{\vartheta}\|A_{(2j+1)r} g_t - A_{2jr} g_t\|^2\Big] \\ &\leq 2\sum_{j=\ell+1}^{L} \alpha_{j+1}\big[\mathcal{E}_{B_{(2j-1)r}}(g_t) - \mathcal{E}_{B_{(2j+1)r}}(g_t)\big] \\ &\quad + 2C\sum_{j=\ell+1}^{L} (\alpha_{j+1} - \alpha_j)\Big[\vartheta\mathcal{E}_{\overline{D}_{2jr}}(g_t) + \frac{1}{\vartheta}\|A_{(2j+1)r} g_t - A_{2jr} g_t\|^2\Big] . \end{aligned}$$

With our choice for α_i, we have that $\vartheta C(\alpha_{i+1} - \alpha_i) \leq \alpha_{i+1}$ if $\vartheta C \leq 1$. Furthermore

$$\mathcal{E}_{B_{(2j-1)r}}(g_t) + \mathcal{E}_{\overline{D}_{2jr}}(g_t) - \mathcal{E}_{B_{(2j+1)r}}(g_t) \leq 0$$

hence

$$F'(t) \le \frac{2}{\vartheta^2} \sum_{j=\ell+1}^{L} \alpha_{j+1} \, \|A_{(2j+1)r} g_t - A_{2jr} g_t\|^2 \le \frac{2}{\vartheta^2} F(t) \qquad \forall \vartheta \ge C^{-1} .$$

By consequence $F(t) \le F(0) e^{2t/\vartheta^2}$, so, if $S_g \subset B_{2\ell r}$ we have

$$\|g_t - A_{2Lr} g_t\|^2 \le \exp\Big[\frac{2t}{\vartheta^2} - \frac{L-\ell}{\vartheta C}\Big] \|g\|^2$$

which, since $n \to \|A_n g_t\|^2$ is nondecreasing, implies

$$\|g_t - A_L g_t\|^2 \le \exp\Big[\frac{2t}{\vartheta^2} - \frac{\lfloor L/2r \rfloor - \ell}{\vartheta C}\Big] \|g\|^2 \qquad \forall L \in \mathbb{Z}_+ .$$

Choosing now $\ell = 3(\lfloor \sqrt{t}/r \rfloor + 1)$ and $\vartheta = \sqrt{t}/(2rC)$, we obtain Proposition 3.1. □

5 Influence of the boundary condition on multicanonical expectations

In this section we study how the multicanonical expectation $\nu^\tau_{\mathcal{A},M}(f)$ of a function f on Ω is affected by a variation of the boundary condition τ. More precisely we want to find an upper bound to the quantity

$$|\nu^\tau_{\mathcal{A},M}(f) - \nu^\sigma_{\mathcal{A},M}(f)| . \tag{5.1}$$

This problem has been studied, in a particular geometrical setting, in [CM00a]. Following a similar approach we are going to show how to deal with a more general geometry.

Let then $(\Lambda, \ell, \mathcal{A})$ be a polycube and let $M \in \mathbb{M}^{\mathcal{A}}_\ell$ a possible choice for the number of particles in each element of $\mathcal{A}$. In order to study how the quantity $\nu^\tau_{\mathcal{A},M}(f)$ depends on τ, we first approximate this multicanonical expectation with a grand-canonical expectation $\mu^\tau_{\mathcal{A},\lambda}(f)$ in which λ is a suitable chemical potential (remember (2.4)) which we assume constant in each cube of $\mathcal{A}$. The value of λ is determined by the requirement that the expectation of the number of particles in each cube is equal to the number of particles fixed by the multicanonical measure. In other words we want $\mu^\tau_{\mathcal{A},\lambda}(N_V) = M_V$ for all $V \in \mathcal{A}$. The existence of this *tilting field* λ is proved in the appendix of [CM00a]. Thus there is a map $\hat\lambda : (\mathcal{A}, M, \tau) \to \lambda$ such that

$$\mu^\tau_{\mathcal{A},\hat\lambda(\mathcal{A},M,\tau)}(N_V) = M_V \qquad \forall\, V \in \mathcal{A} . \tag{5.2}$$

For brevity we define

$$\tilde\mu^\tau_{\mathcal{A},M} := \mu^\tau_{\mathcal{A},\hat\lambda(\mathcal{A},M,\tau)} .$$

5.1 The basic estimate

The idea for estimating (5.1) is to write

$$
\begin{aligned}
&|\nu^{\tau}_{\mathcal{A},M}(f) - \nu^{\sigma}_{\mathcal{A},M}(f)| \\
&\le |\nu^{\tau}_{\mathcal{A},M}(f) - \tilde{\mu}^{\tau}_{\mathcal{A},M}(f)| + |\tilde{\mu}^{\tau}_{\mathcal{A},M}(f) - \tilde{\mu}^{\sigma}_{\mathcal{A},M}(f)| + |\tilde{\mu}^{\sigma}_{\mathcal{A},M}(f) - \nu^{\sigma}_{\mathcal{A},M}(f)| \,.
\end{aligned}
\tag{5.3}
$$

The first and third term can be estimated using Proposition 5.1 below, a result concerning the "equivalence of the ensembles", while the second term will be taken care of in Proposition 5.2.

Proposition 5.1. *Assume (USM). There exists $C > 0$ such that for all polycubes $(\Lambda, \ell, \mathcal{A})$, for all $M \in \mathbb{M}^{\mathcal{A}}_{\ell}$, for all functions f on Ω such that $|S_f| \le \ell^{d/2}$, we have*

$$
\sup_{\tau\in\Omega} |\tilde{\mu}^{\tau}_{\mathcal{A},M}(f) - \nu^{\tau}_{\mathcal{A},M}(f)| \le C\, \|f\|_u \, |S_f| \, |I_f| \, \ell^{-d} \, (\log \ell)^{\frac{3}{2}} \tag{5.4}
$$

where $I_f := \{V \in \mathcal{A} \,:\, S_f \cap V \neq \emptyset\}$.

Proof. It is a straightforward consequence of Theorem 5.1 in [CM00a] (see aso Theorem 4.4 in [BCO99]). We just observe that the "bad block" estimate in that theorem is good enough for our purposes. □

Proposition 5.2. *Assume (USM). There exist $\zeta, C > 0$ such that for all polycubes $(\Lambda, \ell, \mathcal{A})$, for all $M \in \mathbb{M}^{\mathcal{A}}_{\ell}$, for all functions f on Ω such that $S_f \subset \Lambda$ we have*

$$
\sup_{\tau,\sigma\in\Omega} |\tilde{\mu}^{\tau}_{\mathcal{A},M}(f) - \tilde{\mu}^{\sigma}_{\mathcal{A},M}(f)| \le C\, \|f\|_u \, |S_f| \, (\zeta\ell)^{2+d-d(S_f,W)/\ell} \tag{5.5}
$$

where $W := \{x \in \partial^+_r \Lambda : \tau(x) \neq \sigma(x)\}$.

Proof. The proof of this statement requires some modifications of the proof of Proposition 7.1 in [CM00a], where a different geometry is considered. We first observe that we can assume

$$
\ell \ge \zeta^{-1}, \quad d(S_f, W) \ge (2+d)\ell, \quad |S_f| \le (\zeta\ell)^{d(S_f,W)/\ell - d - 2} \tag{5.6}
$$

otherwise there is nothing to prove. For simplicity we enumerate (in an arbitrary way) the set $\mathcal{A}$

$$
\mathcal{A} = \{\Lambda_1, \Lambda_2, \ldots, \Lambda_n\} \qquad \Lambda_i = y_i + Q_\ell, \quad y_i \in \ell\mathbb{Z}^d \,. \tag{5.7}
$$

and we let $M_i := M_{\Lambda_i}$. Let $\lambda_0, \lambda_1 \in \mathbb{R}^n$ be defined by

$$
\mu^{\tau}_{\mathcal{A},\lambda_0}(N_{\Lambda_i}) = M_i = \mu^{\sigma}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}) \qquad \forall i \in \{1, \ldots, n\} \,. \tag{5.8}
$$

If we denote by h the Radon–Nikodym density of $\mu^{\sigma}_{\Lambda,\lambda_1}$ with respect to $\mu^{\tau}_{\Lambda,\lambda_1}$, *i.e.*

$$
h := \frac{e^{-(H^{\sigma}_{\mathcal{A},\lambda_1} - H^{\tau}_{\mathcal{A},\lambda_1})}}{\mu^{\tau}_{\Lambda,\lambda_1}\big[e^{-(H^{\sigma}_{\mathcal{A},\lambda_1} - H^{\tau}_{\mathcal{A},\lambda_1})}\big]} \tag{5.9}
$$

we can write

$$
\begin{aligned}
|\tilde{\mu}^{\tau}_{\mathcal{A},M}(f) - \tilde{\mu}^{\sigma}_{\mathcal{A},M}(f)| &\le |\mu^{\tau}_{\mathcal{A},\lambda_0}(f) - \mu^{\tau}_{\mathcal{A},\lambda_1}(f)| + |\mu^{\tau}_{\mathcal{A},\lambda_1}(f) - \mu^{\sigma}_{\mathcal{A},\lambda_1}(f)| \\
&= |\mu^{\tau}_{\mathcal{A},\lambda_0}(f) - \mu^{\tau}_{\mathcal{A},\lambda_1}(f)| + |\mu^{\tau}_{\mathcal{A},\lambda_1}(f,h)|\,.
\end{aligned}
\tag{5.10}
$$

The covariance term in the RHS of (5.10) can be bounded using (2.10). In fact we have

$$
S_h \subset W_0 := \partial^+_r W \cap \Lambda\,,
$$

and, using inequalities (5.6) it is easy to show that if the constant ζ is chosen small enough then condition (2.9) is satisfied. Hence thanks to (2.10) and the fact that $\mu^{\tau}_{\mathcal{A},\lambda_1}(h) = 1$, we find

$$
|\mu^{\tau}_{\mathcal{A},\lambda_1}(f,h)| \le \mu^{\tau}_{\mathcal{A},\lambda_1}(|f|)\, e^{-md(S_f,S_h)/2}\,. \tag{5.11}
$$

We are now going to show that

$$
|\mu^{\tau}_{\mathcal{A},\lambda_0}(f) - \mu^{\tau}_{\mathcal{A},\lambda_1}(f)| \le C\,\|f\|_u\,|S_f|\,(\zeta\ell)^{2+d-d(S_f,W)/\ell} \tag{5.12}
$$

which, together with (5.11), proves the Proposition. We start by introducing a chemical potential λ_s, $s \in (0,1)$, which interpolates between λ_0 and λ_1

$$
\mathbb{R}^n \ni \lambda_s = (1-s)\lambda_0 + s\lambda_1 \qquad s \in [0,1]\,.
$$

Let then, for any local function g, and for $i,j = 1,\ldots,n$,

$$
\varphi_i(g) := \textstyle\int_0^1 \mu^{\tau}_{\mathcal{A},\lambda_s}(N_{\Lambda_i}, g)\, ds \tag{5.13}
$$

$$
\psi_i(g) := \mu^{\tau}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}, g) \tag{5.14}
$$

$$
B_{ij} := \varphi_i(N_{\Lambda_j}) = B_{ji}\,. \tag{5.15}
$$

Then we have, letting $Y = \lambda_1 - \lambda_0$,

$$
\mu^{\tau}_{\mathcal{A},\lambda_1}(f) - \mu^{\tau}_{\mathcal{A},\lambda_0}(f) = \int_0^1 \frac{d}{ds}\mu^{\tau}_{\mathcal{A},\lambda_s}(f)\, ds = \sum_{i=1}^n Y_i\, \varphi_i(f) = \langle Y, \varphi(f)\rangle_{\mathbb{R}^n} \tag{5.16}
$$

and, analogously,

$$
\mu^{\tau}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}) - \mu^{\tau}_{\mathcal{A},\lambda_0}(N_{\Lambda_i}) = (BY)_i\,. \tag{5.17}
$$

On the other side we have, by (5.8) and (5.9)

$$
\mu^{\tau}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}) - \mu^{\tau}_{\mathcal{A},\lambda_0}(N_{\Lambda_i}) = \mu^{\tau}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}) - \mu^{\sigma}_{\mathcal{A},\lambda_1}(N_{\Lambda_i}) = \psi_i(h)\,, \tag{5.18}
$$

by consequence, assuming that B is invertible (we prove it later) we obtain

$$
\mu^{\tau}_{\mathcal{A},\lambda_1}(f) - \mu^{\tau}_{\mathcal{A},\lambda_0}(f) = \langle\, B^{-1}\psi(h)\,, \varphi(f)\,\rangle_{\mathbb{R}^n}\,. \tag{5.19}
$$

For any $n \times n$ matrix A, let $\|A\|$ be the norm of A when A is interpreted as an operator acting on $(\mathbb{R}^n, |\cdot|_\infty)$, *i.e.*

$$\|A\| = \max_{i\in\{1,\dots,n\}} \sum_{j=1}^{n} |A_{ij}|\,. \tag{5.20}$$

Let G be any invertible $n \times n$ matrix. We can then write

$$\begin{aligned} |\,\mu^{\tau}_{\mathcal{A},\lambda_1}(f) - \mu^{\tau}_{\mathcal{A},\lambda_0}(f)\,| &= |\,\langle\, GB^{-1}G^{-1}G\psi(h)\,, G^{-1}\varphi(f)\,\rangle_{\mathbb{R}^n}| \\ &\le |GB^{-1}G^{-1}G\psi(h)|_\infty\,|G^{-1}\varphi(f)|_1\,. \end{aligned} \tag{5.21}$$

Write B as a sum $B = D + E$ of its diagonal part D and its off–diagonal part E. Assume also that G is diagonal with $G_{ii} > 0$. Then we have

$$GBG^{-1} = D\,[I + GD^{-1}EG^{-1}]\,,$$

so, if we could prove that

$$\|GD^{-1}EG^{-1}\| \le 1/2 \tag{5.22}$$

it would follow that B is in fact invertible and, since, in general $\|A_1A_2\| \le \|A_1\|\,\|A_2\|$, we obtain

$$GB^{-1}G^{-1} = [I + GD^{-1}EG^{-1}]^{-1}D^{-1} \tag{5.23}$$

with $\|[I + GD^{-1}EG^{-1}]^{-1}\| \le 2$. In this way we can obtain, from (5.21)

$$|\,\mu^{\tau}_{\mathcal{A},\lambda_1}(f) - \mu^{\tau}_{\mathcal{A},\lambda_0}(f)\,| \le 2\,|D^{-1}G\psi(h)|_\infty\,|G^{-1}\varphi(f)|_1\,. \tag{5.24}$$

What is left is then to show that (5.22) holds and to estimate the two factors in the RHS of (5.24), with a suitable choice of G. Since G and D are diagonal we let, for simplicity,

$$G_i := G_{ii}\,, \quad D_i := D_{ii} \qquad i = 1,\dots,n\,.$$

We collect in the following Lemma a set of basic inequalities we are going to use in the rest of the proof. In order to state the results we need some notation: we introduce a distance κ on the set $\{1,\dots,n\}$ as (remember (5.7))

$$\kappa(i,j) := |y_i - y_j|/\ell = \begin{cases} (d(\Lambda_i,\Lambda_j) - 1)/\ell + 1 & \text{if } i \ne j \\ 0 & \text{if } i = j\,. \end{cases} \tag{5.25}$$

Consider also the function $\rho : \mathbb{R} \to [0,\infty)$ defined as

$$\rho(a) = (1 + e^{-a})^{-1}\,. \tag{5.26}$$

The quantity $\rho(a)$ represents the density of particles in the measure μ with no interaction ($J = 0$) and chemical potential equal to a.

$$\mu^{\tau}_{\mathcal{A},J=0,\lambda}(\eta(x)) = \mu^{\emptyset}_{\{x\},J=0,\lambda}(\eta(x)) = \rho(\lambda(x))\,.$$

Keeping in mind (5.25) and (5.26) we have

Lemma 5.3. *Assume (USM). There exists $A > 0$ such that for all $\lambda \in \mathbb{R}^n$ and for all $i, j = 1,\dots,n$ we have*

(1) $e^{-2\|J\|} \le \dfrac{\mu^{\tau}_{\mathcal{A},\lambda}(N_{\Lambda_i})}{\rho(\lambda_i)\,\ell^d} \le e^{2\|J\|}$ *and* $A^{-1} \le \dfrac{|\mu^{\tau}_{\mathcal{A},\lambda}(N_{\Lambda_i}, N_{\Lambda_i})|}{\rho(\lambda_i)\,\ell^d} \le A$

(2) *If* $i \ne j$ *then* $|\mu^{\tau}_{\mathcal{A},\lambda}(N_{\Lambda_i}, N_{\Lambda_j})| \le A\,\rho(\lambda_i)\,\rho(\lambda_j)\,\ell^{d-1}$

(3) *If* $\kappa(i,j) \ge 2$ *and* $\ell \ge A$ *then* $|\mu^{\tau}_{\mathcal{A},\lambda}(N_{\Lambda_i}, N_{\Lambda_j})| \le \rho(\lambda_i)\,\rho(\lambda_j)\,e^{-md(\Lambda_i,\Lambda_j)/3}$

(4) *For all functions* f *on* Ω *we have* $|\mu^{\tau}_{\mathcal{A},\lambda}(N_{\Lambda_i}, f)| \le A\,\|f\|_u\,\rho(\lambda_i)\,\ell^d$

Proof. All inequalities except (3) are taken from Proposition 3.1 in [CM00a]. As for statement (3) it is a direct consequence of (2.10) and the first inequality in statement (1). □

Proof of (5.22) *and* (5.24). If we let

$$\bar\rho_i := \int_0^1 \rho(\lambda_{s,i})\,ds$$

we obtain, using $\int_0^1 \rho(\lambda_{s,i})\,\rho(\lambda_{s,j})\,ds \le \bar\rho_j$, Lemma 5.3, and the fact that $E_{ii} = 0$,

$$\sum_{j=1}^n \Big|\frac{G_i\,E_{ij}}{G_j\,D_i}\Big| \le \frac{A^2}{\ell} \sum_{j:\,\kappa(j,i)=1} \frac{\bar\rho_j}{\bar\rho_i}\,\frac{G_i}{G_j} + A\ell^d \sum_{j:\,\kappa(j,i)\ge 2} \frac{\bar\rho_j}{\bar\rho_i}\,\frac{G_i}{G_j} e^{-md(\Lambda_i,\Lambda_j)/3} \tag{5.27}$$

Let $\zeta > 0$, let I be a subset of $\{1,\dots,n\}$, and define G as

$$G_i := \bar\rho_i\,(\zeta\ell)^{\kappa(i,I)} \qquad i = 1,\dots,n\,. \tag{5.28}$$

A specific choice for I will be made later, since it is unnecessary at the moment. By the triangular inequality we have

$$\frac{G_i}{G_j} \le \frac{\bar\rho_i}{\bar\rho_j}\,(\zeta\ell)^{\kappa(i,j)} \qquad i,j = 1,\dots,n\,,$$

and (5.27) becomes

$$\sum_{j=1}^n |G_i D_i^{-1} E_{ij} G_j^{-1}| \le \zeta\,A^2\,3^d + A\ell^d \sum_{j:\,\kappa(j,i)\ge 2} (\zeta\ell)^{\kappa(i,j)}\,e^{-md(\Lambda_i,\Lambda_j)/3}\,, \tag{5.29}$$

which, taking $\zeta = 3^{-d}A^{-2}/4$ and ℓ large enough, implies (5.22) and, by consequence, (5.24).

We turn then our attention to the two factors in the RHS of (5.24). In order to obtain proper bounds on them we finally choose the set I and complete our definition of the matrix G in (5.28). We define

$$I := \{i \in \{1,\dots,n\} : d(\Lambda_i, W_0) \le \ell/3\}\,. \tag{5.30}$$

At this point we would like to say that $d(\Lambda_i, W_0)$ is roughly equal to $\kappa(i,I)\ell$. More precisely we have

Lemma 5.4. *For all* $i = 1, \dots, n$ *we have*

$$\frac{1}{3}\kappa(i,I)\ell \le d(\Lambda_i, W_0) \le \left[\kappa(i,I) + \frac{1}{3}\right]\ell\,. \tag{5.31}$$

Proof of the Lemma. Let's start with the lower bound on $d(\Lambda_i, W_0)$. We have

$$d(\Lambda_i, W_0) \ge \inf_{j\in I} d(\Lambda_i, \Lambda_j) \ge (\kappa(i,I) - 1)\ell\,,$$

which, when $i \notin I$ can be improved as

$$d(\Lambda_i, W_0) \ge \max\{(\kappa(i,I) - 1)\ell, \ell/3\} \qquad i \in I^c\,.$$

This implies

$$d(\Lambda_i, W_0) \ge \kappa(i,I)\,\ell/3\,, \tag{5.32}$$

which is trivially true also when $i \in I$. For the upper bound we observe that, if $x \in \Lambda_j$ for some $j \in I$, then

$$d(x, W_0) \le d(\Lambda_j, W_0) + \operatorname{diam}\Lambda_j = d(\Lambda_j, W_0) + \ell - 1 \le \ell/3 + (\ell - 1)\,.$$

Thus, if we let $\Lambda_I := \cup_{j\in I}\Lambda_j$, we have that $\Lambda_I \subset B_{\ell/3+\ell-1}(W_0)$, so

$$d(\Lambda_i, W_0) \le d(\Lambda_i, \Lambda_I) + \ell - 1 + \ell/3 = \kappa(i,I)\ell + \ell/3 \quad \square$$

Estimate of $|D^{-1}G\psi(h)|_\infty$ *in* (5.24). Thanks to Lemma 5.3 we can write

$$|D_i^{-1}G_i\,\psi_i(h)| \le A\,\ell^{-d}\,(\zeta\ell)^{\kappa(i,I)}\,|\mu^\tau_{\mathcal{A},\lambda_1}(N_{\Lambda_i}, h)|\,. \tag{5.33}$$

If $i \in I$ we have, since $\mu^\tau_{\mathcal{A},\lambda_1}(h) = 1$

$$|\mu^\tau_{\mathcal{A},\lambda_1}(N_{\Lambda_i}, h)| \le \mu^\tau_{\mathcal{A},\lambda_1}(N_{\Lambda_i} h) + \mu^\tau_{\mathcal{A},\lambda_1}(N_{\Lambda_i})\mu^\tau_{\mathcal{A},\lambda_1}(h) \le 2\ell^d\,,$$

so, by (5.33),

$$|D_i^{-1}G_i\,\psi_i(h)| \le 2A \qquad \forall i \in I\,. \tag{5.34}$$

If instead $i \notin I$ (and ℓ is large enough) we can use (2.10) and we get

$$|\mu^\tau_{\mathcal{A},\lambda_1}(N_{\Lambda_i}, h)| \le \ell^d\,e^{-md(\Lambda_i,W_0)/2}\,,$$

which, together with (5.31) yields, for ℓ large enough,

$$|D_i^{-1}G_i\,\psi_i(h)| \le A\,(\zeta\ell)^{\kappa(i,I)}\,e^{-m\kappa(i,I)\ell/6} \le A \qquad \forall i \in I^c\,. \tag{5.35}$$

From (5.34), (5.35), we finally get

$$|D^{-1}G\,\psi(h)|_\infty \le 2A\,. \tag{5.36}$$

Estimate of $|G^{-1}\varphi(f)|_1$ *in* (5.24) *and end of the proof.* In order to prove (5.12) we have to bound the last factor in (5.24), namely $|G^{-1}\varphi(f)|_1$. We have

$$|G^{-1}\varphi(f)|_1 = \sum_{i=1}^n \frac{|\varphi_i(f)|}{G_i} \le \sum_{i=1}^n (\bar\rho_i)^{-1}\,(\zeta\ell)^{-\kappa(i,I)}\,\int_0^1 |\mu^\tau_{\mathcal{A},\lambda_s}(N_{\Lambda_i}, f)|\,ds\,. \tag{5.37}$$

Observe first that using Lemma 5.4,

$$d(S_f, W_0) \le d(S_f, \Lambda_i) + d(\Lambda_i, W_0) + \operatorname{diam}\Lambda_i \le d(S_f, \Lambda_i) + \ell\kappa(i, I) + \frac{4\ell}{3}. \quad (5.38)$$

If i is such that $d(\Lambda_i, S_f) \le \ell/3$ we use inequality (4) of Lemma 5.3 and we find

$$\begin{aligned}\frac{|\varphi_i(f)|}{G_i} &\le A\,\|f\|_u\,\ell^d\,(\zeta\ell)^{4/3-d(S_f,W_0)/\ell+d(S_f,\Lambda_i)/\ell} \\ &\le A_1\,\|f\|_u\,(\zeta\ell)^{2+d-d(S_f,W_0)/\ell}\end{aligned}$$

where we have set $A_1 := A\zeta^{-d}$. Moreover the number of $i's$ such that $d(\Lambda_i, S_f) \le \ell/3$ is bounded by $(8/3)^d\,|S_f|$, so we have

$$\sum_{i:\,d(\Lambda_i,S_f)\le\ell/3} \frac{|\varphi_i(f)|}{G_i} \le A_2\,\|f\|_u\,|S_f|\,(\zeta\ell)^{2+d-d(S_f,W_0)/\ell} \quad (5.39)$$

where $A_2 := A_1(8/3)^d$. In order to estimate the contribution of those terms with $d(\Lambda_i, S_f) > \ell/3$ we use (2.10) and, again, (5.38) and we obtain

$$\frac{|\varphi_i(f)|}{G_i} \le A_1\,\|f\|_u\,(\zeta\ell)^{4/3+d-d(S_f,W_0)/\ell+d(S_f,\Lambda_i)/\ell}\,e^{-md(S_f,\Lambda_i)/2}. \quad (5.40)$$

Furthermore it is easy to see that, if ℓ is large enough, then

$$\sum_{i:\,d(\Lambda_i,S_f)>\ell/3} (\zeta\ell)^{d(S_f,\Lambda_i)/\ell}\,e^{-md(S_f,\Lambda_i)/2} \le |S_f|\,. \quad (5.41)$$

From (5.40), (5.41) it follows that

$$\sum_{i:\,d(\Lambda_i,S_f)>\ell/3} \frac{|\varphi_i(f)|}{G_i} \le A_1\,\|f\|_u\,|S_f|\,(\zeta\ell)^{4/3+d-d(S_f,W_0)/\ell}\,, \quad (5.42)$$

which, together (5.39) implies

$$|G^{-1}\varphi(f)|_1 \le A_3\,\|f\|_u\,|S_f|\,(\zeta\ell)^{2+d-d(S_f,W_0)/\ell} \quad (5.43)$$

with $A_3 := A_1 + A_2$. Finally from (5.24), (5.36) and (5.43), inequality (5.12) follows, and the proof of Proposition 5.2 is completed. □

Combining inequality (5.3) with Propositions 5.1 and 5.2 we obtain

Corollary 5.5. *Assume (USM). There exists $C > 0$ such that the following holds: let $(\Lambda, \ell, \mathcal{A})$ be a polycube, and consider a pair of boundary conditions $\tau, \sigma \in \Omega$, with $W := \{x \in \partial_r^+\Lambda : \tau(x) \neq \sigma(x)\}$. Then for all functions f on Ω such that $S_f \subset \Lambda$, $d(S_f, W) \ge (3d+2)\ell$ and $|S_f| \le \ell^{d/2}$, for all $M \in \mathbb{M}_\ell^{\mathcal{A}}$, we have*

$$|\nu^\tau_{\mathcal{A},M}(f) - \nu^\sigma_{\mathcal{A},M}(f)| \le C\,\|f\|_u\,|S_f|\,|I_f|\,\ell^{-d}\,(\log\ell)^{3/2} \quad (5.44)$$

where $I_f := \{V \in \mathcal{A} : S_f \cap V \neq \emptyset\}$.

5.2 Improving the basic estimate

Inequality (5.44) can be iterated and consequently improved. What follows is a generalization of the strategy adopted in [CM00a].

Proposition 5.6. *Assume (USM). There exists $C > 0$ such that the following holds: let $(\Lambda, \ell, \mathcal{A})$ be a polycube, and let f be a function on Ω such that $S_f \subset \Lambda$. Given a pair of boundary conditions $\tau, \sigma \in \Omega$, let $W := \{x \in \partial_r^+\Lambda : \tau(x) \neq \sigma(x)\}$. Assume that there exists an increasing sequence of polycubes $(T_k, \ell, \mathcal{A}_k)$, $k = 0, \dots, n$, such that*

(i) $S_f \subset T_0 \subset T_1 \subset \cdots \subset T_n \subset \Lambda$

(ii) $d(T_n, W) > r$

(iii) $d(\Lambda \backslash T_k, T_{k-1}) \geq (3d+4)\ell$.

Then, for all $M \in \mathbb{M}_\ell^{\mathcal{A}}$,

$$|\nu_{\mathcal{A},M}^\tau(f) - \nu_{\mathcal{A},M}^\sigma(f)| \leq \|f\|_u \left[C \, \frac{(\log \ell)^{3/2}}{\ell^d}\right]^n \prod_{k=1}^n |\partial_r^+ T_k \cap \Lambda| \,. \tag{5.45}$$

Proof. Let

$$f_k := \nu_{\mathcal{A},M}^\tau(f \,|\, \mathcal{F}_{\Lambda\backslash T_k}) \qquad k = 0, \dots, n\,.$$

We denote with M_k the restriction of M to $\mathcal{A}_k$. The function f_k is measurable w.r.t. $\mathcal{F}_{\partial_r^+ T_k \cap \Lambda}$. Denoting with $\tilde{\Omega}$ the set of all $\eta \in \Omega$ such that $\eta_{\Lambda^c} = \tau_{\Lambda^c}$, we can write

$$f_k(\eta) = \nu_{\mathcal{A}_k, M_k}^\eta(f) \qquad \forall \eta \in \tilde{\Omega}\,.$$

Since, by hypothesis, $d(T_k, W) \geq d(T_n, W) > r$, we have

$$\nu_{\mathcal{A},M}^\sigma(f \,|\, \mathcal{F}_{\Lambda\backslash T_k})(\eta) = \nu_{\mathcal{A},M}^\tau(f \,|\, \mathcal{F}_{\Lambda\backslash T_k})(\eta) = \nu_{\mathcal{A}_k, M_k}^\eta(f) = f_k(\eta) \qquad \forall \eta \in \tilde{\Omega}\,,$$

By consequence (remember that $\operatorname{osc}(f) := \sup f - \inf f$)

$$|\nu_{\mathcal{A},M}^\tau(f) - \nu_{\mathcal{A},M}^\sigma(f)| = |\nu_{\mathcal{A},M}^\tau(f_n) - \nu_{\mathcal{A},M}^\sigma(f_n)| \leq \operatorname{osc}(f_n)\,. \tag{5.46}$$

Since f_k is measurable w.r.t. $\mathcal{F}_{\partial_r^+ T_k \cap \Lambda}$

$$\operatorname{osc}(f_k) \leq |\partial_r^+ T_k \cap \Lambda| \sup_{x \in \partial_r^+ T_k \cap \Lambda} \sup_{\eta \in \tilde{\Omega}} |\nabla_x (f_k)(\eta)|\,. \tag{5.47}$$

On the other side, if we let

$$h_k^x(\eta) := \frac{e^{-\nabla_x H_\Lambda(\eta)}}{\nu_{\mathcal{A}_k, M_k}^\eta(e^{-\nabla_x H_\Lambda})}\,,$$

we have, for $x \in \partial_r^+ T_k \cap \Lambda$ and $\eta \in \tilde{\Omega}$

$$|\nabla_x (f_k)(\eta)| = |\nu_{\mathcal{A}_k, M_k}^\eta(f_{k-1}) - \nu_{\mathcal{A}_k, M_k}^{s_x \eta}(f_{k-1})| = |\nu_{\mathcal{A}_k, M_k}^\eta(f_{k-1}, h_k^x)|\,. \tag{5.48}$$

Define now a set $\hat{T}_{k-1}$ slightly larger than T_{k-1}, such that f_{k-1} is measurable w.r.t. $\mathcal{F}_{\hat{T}_{k-1}}$. We let $\hat{T}_{k-1} := B_\ell(T_{k-1}) \cap \Lambda$. The reason for taking the ℓ–boundary of T_{k-1} instead of the r–boundary, which would be enough for the measurability requirement, is that, in this way there exists $\hat{\mathcal{A}}_{k-1} \subset \mathcal{A}_k$, such that $(\hat{T}_{k-1}, \ell, \hat{\mathcal{A}}_{k-1})$ is a polycube. The RHS of (5.48) can be estimated as

$$\begin{aligned} |\nu^\eta_{\mathcal{A}_k,M_k}(f_{k-1}, h^x_k)| &= |\nu^\eta_{\mathcal{A}_k,M_k}(f_{k-1}, \nu^\eta_{\mathcal{A}_k,M_k}(h^x_k \,|\, \mathcal{F}_{\hat{T}_{k-1}})| \\ &\le \operatorname{osc}(f_{k-1}) \operatorname{osc}\big[\nu^\eta_{\mathcal{A}_k,M_k}(h^x_k \,|\, \mathcal{F}_{\hat{T}_{k-1}})\big] . \end{aligned} \tag{5.49}$$

The idea, at this point, is to bound the last factor in the RHS of (5.49) using inequality (5.44). Thanks to hypothesis (iii) the distance between $S_{h^x_k}$ and $\hat{T}_{k-1}$ can be bounded from below as

$$d(S_{h^x_k}, \hat{T}_{k-1}) \ge d(\Lambda \backslash T_k, \hat{T}_{k-1}) - r \ge (3d+4)\ell - \ell - r \ge (3d+2)\ell .$$

So we can apply Corollary 5.5, and, since the uniform norm of h^x_k is at most $\exp(4\|J\|)$, we obtain, with a suitable redefinition of the constant C,

$$\operatorname{osc}\big[\nu^\eta_{\mathcal{A}_k,M_k}(h^x_k \,|\, \mathcal{F}_{\hat{T}_{k-1}})\big] \le C(\log \ell)^{3/2} \ell^{-d} . \tag{5.50}$$

From (5.46), (5.47), (5.48), (5.49), (5.50), it follows that

$$|\nu^\tau_{\mathcal{A},M}(f) - \nu^\sigma_{\mathcal{A},M}(f)| \le \operatorname{osc}(f_0) \prod_{k=1}^n \Big[C\,\ell^{-d} (\log \ell)^{3/2}\,|\partial^+_r T_k \cap \Lambda|\Big] .$$

On the other side, since by hypothesis $S_f \subset T_0$, we have $\operatorname{osc}(f_0) \le \operatorname{osc}(f) \le 2\|f\|_u$, and the Proposition is proved. □

In the following Corollary we consider a particular situation where previous result can be applied and we write down a more explicit expression for the RHS of (5.45).

Corollary 5.7. *Assume (USM). Then there exists $C > 0$ such that the following holds: let $(\Lambda, \ell, \mathcal{A})$ be a rectangular polycube, i.e. a polycube such that $\Lambda = I_1 \times \cdots \times I_d$, where $I_i = [a_i, b_i) \cap \mathbb{Z}$, and assume that $|I_i| \le L$ for $i = 1, \ldots, n$. Then, for all functions f on Ω such that $S_f \subset \Lambda$, for all $M \in \mathbb{M}^{\mathcal{A}}_\ell$, for all $\tau, \sigma \in \Omega$ we have*

$$|\nu^\tau_{\mathcal{A},M}(f) - \nu^\sigma_{\mathcal{A},M}(f)| \le \|f\|_u \left[C\,L^{d-1}\,\frac{(\log \ell)^{3/2}}{\ell^d}\right]^{\lfloor d(S_f,W)/[(3d+4)\ell]\rfloor - 2} \tag{5.51}$$

where $W := \{x \in \mathbb{Z}^d : \tau(x) \ne \sigma(x)\}$.

Proof. Let j be the smallest integer such that $S_f \subset (B_{j\ell} + y) \cap \Lambda$ for some $y \in \ell\mathbb{Z}^d$. Inequality (5.51) follows (after a redefinition of C) from Proposition 5.6, if one takes

$$T_k := (B_{[j+k(3d+4)]\ell} + y) \cap \Lambda \qquad k = 0, \ldots, n$$

where $n = \lfloor d(S_f, W)/[(3d+4)\ell]\rfloor - 2$. □

6 Poincaré inequality

In this section we prove Proposition 3.4. Our goal is to obtain a Poincaré–type inequality for the multicanonical measures $\nu^{\tau}_{\mathcal{A},M}$ on the polycube $(B_L, \ell, \mathcal{A})$ when $L \le \ell^{1+\gamma}$ with $\gamma < (d-1)^{-1}$. This restriction on γ is really fictitious and springs from the fact that the quantity appearing in brackets in the RHS of (5.51) must be much smaller than one. In order to overcome this difficulty one could iterate inequality (5.51) again and obtain a result suitable for larger values of L.

We also observe that (3.18) is weaker than the standard Poincarè inequality associated with the measure $\nu^{\tau}_{\mathcal{A},M}$, for two reasons: first of all the inequality (3.18) is averaged with respect to the infinite volume measure μ, and, moreover the Dirichlet form in the RHS of (3.18) contains also those terms $(\nabla_{xy} f)^2$ in which x and y belong to different cubes of $\mathcal{A}$. This weaker inequality is anyway sufficient for our purposes.

Before starting with our proof, we want to remark that an inequality somehow close to the one we are trying to demonstrate requires basically no effort[7]. Let in fact $\mathcal{A}_0$, $\mathcal{A}_1$ be two partitions of B_L such that $\mathcal{A}_1$ is finer than $\mathcal{A}_0$. Then $\mathcal{G}_{B_L^c,\mathcal{A}_1}$ is also finer than $\mathcal{G}_{B_L^c,\mathcal{A}_0}$, hence we have (remember notation (2.12))

$$\mu[\, G_{\mathcal{A}_1}(f,f)\,] \le \mu[\, G_{\mathcal{A}_0}(f,f)\,] \tag{6.1}$$

and, in particular, $\mu[\, G_{\mathcal{A}}(f,f)\,] \le \mu[\, G_{B_L}(f,f)\,]$. On the other side the canonical measure satisfies (see [LY93] and [CM00b]) a Poincaré inequality which says

$$\nu^{\tau}_{B_L,N}(f,f) \le C_0\, L^2\, \mathcal{E}_{\nu^{\tau}_{B_L,N},B_L}(f)\,. \tag{6.2}$$

As an aside, we observe that by taking the expectation of (6.2) we get

$$\mu[\, G_{\mathcal{A}}(f,f)\,] \le \mu[\, G_{B_L}(f,f)\,] \le C_0\, L^2\, \mathcal{E}_{B_L}(f) \le C_0\, \ell^{2(1+\gamma)}\, \mathcal{E}_{B_L}(f)\,. \tag{6.3}$$

Unfortunately this inequality is not sufficient for our purposes, and the rest of this section is devoted to eliminating the factor γ from the RHS of (6.3).

We use the iterative approach which was introduced in [Mar99]. We let

$$\delta = 3(3d+4)\ell$$

and, following [BCC02], we define a sequence of exponentially increasing length scales

$$w_k := 4\delta\, (3/2)^{k/d} \qquad k = 0,1,2,\dots \tag{6.4}$$

Our choice of δ represents the minimum distance which yields an exponent equal to 1 in the RHS of (5.51). Then we define $\mathcal{R}_k$ as the set of all Λ in $\mathbb{Z}^d$ such that

(1) Λ is a rectangle, $\Lambda = \big([a_1,b_1) \times \cdots \times [a_d,b_d)\big) \cap \mathbb{Z}^d$ and $a_i, b_i \in \ell\mathbb{Z}^d$ for $i = 1,\dots,n$

[7] other than parasiting earlier work

(2) $\Lambda \subset \big([0, w_{k+1}) \times \cdots \times [0, w_{k+d}) \big) \cap \mathbb{Z}^d$ modulo translations and permutations of the coordinates

From (1) it follows that there is a unique $\mathcal{B} \subset \mathbb{F}$ such that $(\Lambda, \ell, \mathcal{B})$ is a polycube. We will sometimes (improperly) write $(\Lambda, \ell, \mathcal{B}) \in \mathcal{R}_k$, meaning $\Lambda \in \mathcal{R}_k$. The length scales w_k have been chosen in such a way that if $\Lambda \in \mathcal{R}_k$ then Λ can be written as $\Lambda = \Lambda_1 \cup \Lambda_2$, where Λ_1 and Λ_2 are two elements of $\mathcal{R}_{k-1}$ with an overlap of thickness δ. If we assume this fact for a moment (we will prove it in a stronger form in Lemma 6.2) the idea of the proof becomes clear. Given a polycube $(\Lambda, \ell, \mathcal{B})$ we define $\Phi(\mathcal{B}) \in [0, \infty]$ as the infimum of all postive real numbers c such that

$$\mu[\, G_{\mathcal{B}}(f,f)\,] \le c\, \mathcal{E}_\Lambda(f) \qquad \text{for all local functions } f \text{ on } \Omega \tag{6.5}$$

and we let

$$\Phi_k := \sup_{(\Lambda,\ell,\mathcal{B}) \in \mathcal{R}_k} \Phi(\mathcal{B})\,. \tag{6.6}$$

Let $\Lambda \in \mathcal{R}_k$ and let $\Lambda_1, \Lambda_2 \in \mathcal{R}_{k-1}$ such that $\Lambda = \Lambda_1 \cup \Lambda_2$ and $d(\Lambda \backslash \Lambda_1, \Lambda \backslash \Lambda_2) \ge \delta$. We know that there exist $\mathcal{B}_1$ and $\mathcal{B}_2$, subsets of $\mathcal{B}$, such that $(\Lambda_1, \ell, \mathcal{B}_1)$ and $(\Lambda_2, \ell, \mathcal{B}_2)$ are polycubes. Consider the multicanonical measure $\nu^\tau_{\mathcal{A},M}$, and let M_i be the restriction of M to $\mathcal{B}_i$. Then for each local function g measurable w.r.t. $\mathcal{F}_{\Lambda \backslash \Lambda_2}$ we have

$$\|\nu^\tau_{\mathcal{A},M}(g) - \nu^\tau_{\mathcal{A},M}(g \,|\, \mathcal{F}_{\Lambda \backslash \Lambda_1})\|_u \le \sup_{\substack{\eta,\eta' :\, \eta(x) = \eta'(x) = \tau(x) \\ \text{for all } x \in \Lambda^c}} \|\nu^\eta_{\Lambda_1, M_1}(g) - \nu^{\eta'}_{\Lambda_1, M_1}(g)\|_u\,.$$

Since $d(\Lambda \backslash \Lambda_1, \Lambda \backslash \Lambda_2) \ge \delta$, thanks to (5.51) we obtain for all $\Lambda \subset B_L$

$$\|\nu^\tau_{\mathcal{A},M}(g) - \nu^\tau_{\mathcal{A},M}(g \,|\, \mathcal{F}_{\Lambda \backslash \Lambda_1})\|_u \le \|g\|_u\, C\, \frac{(\log \ell)^{3/2}}{\ell^d}\, L^{d-1} =: \alpha\, \|g\|_u \tag{6.7}$$

where the last equality represents a definition of α. We can apply at this point Lemma 3.1 in [BCC02]. We are going to reformulate this result in a more general way than the original statement, but the proof given in [BCC02] applies word by word.

Lemma 6.1 ([BCC02]). *Let $(\Omega, \mathcal{F}, \mu)$ be a probability space, and let $\mathcal{F}_1$, $\mathcal{F}_2$ be two sub–σ–algebras of $\mathcal{F}$. Assume that for some $\varepsilon \in [0, \sqrt{2} - 1)$, $p \in [1, \infty]$, we have*

$$\begin{aligned} &\|\mu(g \,|\, \mathcal{F}_1) - \mu(g)\|_p \le \varepsilon\, \|g\|_p \qquad \forall g \in L^p(\Omega, \mathcal{F}_2, \mu) \\ &\|\mu(g \,|\, \mathcal{F}_2) - \mu(g)\|_p \le \varepsilon\, \|g\|_p \qquad \forall g \in L^p(\Omega, \mathcal{F}_1, \mu) \end{aligned}$$

Then

$$\mathrm{Var}_\mu(f) \le (1 - 2\varepsilon - \varepsilon^2)^{-1}\, \mu[\mathrm{Var}_\mu(f \,|\, \mathcal{F}_1) + \mathrm{Var}_\mu(f \,|\, \mathcal{F}_2)] \qquad \forall f \in L^2(\mu)\,.$$

Thanks to this result, from inequality (6.7) and the one obtained by exchanging indices 1 and 2, letting

$$1 + \alpha_1 := (1 - 2\alpha - \alpha^2)^{-1}$$

we obtain,

$$\nu^{\tau}_{\mathcal{A},M}(f,f) \le (1+\alpha_1)\, \nu^{\tau}_{\mathcal{A},M}\left[\nu^{\tau}_{\mathcal{A},M}(f,f \mid \mathcal{F}_{\Lambda\setminus\Lambda_1}) + \nu^{\tau}_{\mathcal{A},M}(f,f \mid \mathcal{F}_{\Lambda\setminus\Lambda_2})\right]. \tag{6.8}$$

After taking the expectation of this inequality w.r.t. μ, recalling the definition of Φ_k (6.6), we get

$$\mu[\, G_{\mathcal{B}}(f,f)\,] \le (1+\alpha_1)\, \Phi_{k-1}\left[\mathcal{E}_{\Lambda}(f) + \mathcal{E}_{\Lambda_1\cap\Lambda_2}(f)\right]. \tag{6.9}$$

If, at this point, we estimate the overlap term $\mathcal{E}_{\Lambda_1\cap\Lambda_2}(f)$ simply with $\mathcal{E}_{\Lambda}(f)$ we run into troubles, since we would find the iterative inequality $\Phi_k \le 2\,(1+\alpha_1)\,\Phi_{k-1}$ which does not look very promising. The idea [Mar99] is to write several different "copies" of inequality (6.9), where each copy corresponds to a different choice of the subsets Λ_1, Λ_2. For this purpose we need the following result:

Lemma 6.2. *For all $k \in \mathbb{Z}_+$, for all $\Lambda \in \mathcal{R}_k\setminus\mathcal{R}_{k-1}$ there esists a collection of polycubes $(\Lambda_n^{(i)}, \ell, \mathcal{B}_n^{(i)})$ where $n = 1,2$ and $i = 1,\dots,s_k := \lfloor (3/2)^{k/d} \rfloor$, such that for all $i,j = 1,\dots,s_k$ we have*

(1) $\Lambda = \Lambda_1^{(i)} \cup \Lambda_2^{(i)}$ *and* $\Lambda_n^{(i)} \in \mathcal{R}_{k-1}$ *for all* $n = 1,2$

(2) $d(\Lambda\setminus\Lambda_1^{(i)}, \Lambda\setminus\Lambda_2^{(i)}) \ge \delta$

(3) *If* $i \ne j$ *then* $\Lambda_1^{(i)} \cap \Lambda_2^{(i)} \cap \Lambda_1^{(j)} \cap \Lambda_2^{(j)} = \emptyset$.

Proof. Since $\Lambda \in \mathcal{R}_k$ we can assume that $\Lambda = \big([0,b_1) \times \cdots \times [0,b_d)\big) \cap \mathbb{Z}^d$ with $b_j \le w_{k+j}$ for $j = 1,\dots,d$. Define

$$\Lambda_1^{(i)} := \Big([0,b_1) \times \cdots \times [0,b_{d-1}) \times \Big[0\,,\Big\lfloor \frac{b_d}{2\ell} \Big\rfloor \ell + i\delta\Big)\Big) \cap \Lambda \tag{6.10}$$

$$\Lambda_2^{(i)} := \Big([0,b_1) \times \cdots \times [0,b_{d-1}) \times \Big[\Big\lfloor \frac{b_d}{2\ell} \Big\rfloor \ell + (i-1)\delta,\, b_d\Big)\Big) \cap \Lambda\,. \tag{6.11}$$

It is straightforward to check that $\Lambda_1^{(i)}$ and $\Lambda_1^{(i)}$ satisfy the required properties (for more details see [BCC02]). ☐

From Lemma 6.2 and inequality (6.9) we get

$$\mu[\, G_{\mathcal{B}}(f,f)\,] \le (1+\alpha_1)\, \Phi_{k-1}\left[\mathcal{E}_{\Lambda}(f) + \mathcal{E}_{\Lambda_1^{(i)}\cap\Lambda_2^{(i)}}(f)\right] \qquad i = 1,\dots,s_k\,. \tag{6.12}$$

Thanks to (3) of Lemma 6.2 we have that $\sum_{i=1}^{s_k} \mathcal{E}_{\Lambda_1^{(i)}\cap\Lambda_2^{(i)}}(f) \le \mathcal{E}_{\Lambda}(f)$, thus we can averge (6.12) over i and we find

$$\Phi_k \le \Phi_{k-1}\,(1+\alpha_1)\,(1 + 1/s_k)\,. \tag{6.13}$$

From our assumption on L, it follows that $B_L \subset \mathcal{R}_{k_1}$ with (say) $k_1 := \lfloor 3d \log \ell \rfloor$, since

$$w_{k_1} \ge \delta\,(3/2)^{3\log\ell} \ge \delta\,\ell \ge 2L + 1\,.$$

By consequence we can iterate (6.13) up to $k = k_1$ and obtain an upper bound for the Poincaré constant of the polycube $(B_L, \ell, \mathcal{A})$ as

$$\Phi(\mathcal{A}) \le \Phi_{k_1} \le \Phi_0 \prod_{i=1}^{k_1} (1+\alpha_1)\left(1 + \frac{1}{s_k}\right) \le \Phi_0 \, \exp\Big[k_1\alpha_1 + \sum_{j=1}^{\infty} \frac{1}{s_k}\Big]. \qquad (6.14)$$

Since $\gamma < (d-1)^{-1}$ from the definition of α if follows that there exists $\ell_0(\gamma) > 0$ such that if $\ell \ge \ell_0(\gamma)$ then α is bounded by a negative power of ℓ, hence $k_1\alpha_1 \le 1$. On the other side there exists $K(d)$ such that $\sum_{j=1}^{\infty} s_k^{-1} < K(d)$. Finally, for what concerns Φ_0, we observe that if $(\Lambda, \ell, \mathcal{B}) \in \mathcal{R}_0$ then, since $\mathcal{G}_{\Lambda^c,\mathcal{B}}$ is finer than $\mathcal{G}_{\Lambda^c,\{\Lambda\}}$, by (6.2) we get

$$\mu[\, G_{\mathcal{B}}(f,f)\,] \le \mu[\, G_{\Lambda}(f,f)\,] \le C_0 \, w_d^2 \, \mathcal{E}_\Lambda(f) \le C \, \ell^2 \, \mathcal{E}_\Lambda(f)\,. \qquad (6.15)$$

From (6.14), (6.15) and what we said in between them, it follows that if $\ell \ge \ell_0(\gamma)$ then

$$\Phi(\mathcal{A}) \le C \, e^{1+K(d)} \, \ell^2\,.$$

On the other side if $\ell < \ell_0(\gamma)$ we can simply use (6.2) and obtain

$$\mu[\, G_{\mathcal{B}}(f,f)\,] \le \mu[\, G_{\Lambda}(f,f)\,] \le C_0 \, L^2 \, \mathcal{E}_{B_L}(f) \le C_0 \, \ell_0(\gamma)^{2(1+\gamma)} \, \mathcal{E}_{B_L}(f)$$

hence (3.18) holds if we redefine C_γ suitably. □

7 Fluctuations of the number of particles

We prove here Proposition 3.2. Consider a polycube $(\Lambda, \ell, \mathcal{A})$ and fix $\varepsilon > 0$. For all $M \in \mathbb{M}_\ell^{\mathcal{A}}$, all $x \in B_L$ and all $t \ge 0$, let

$$h^M(\sigma) := \frac{1\!\!1_M(N_{\mathcal{A}}(\sigma))}{\mu\{N_{\mathcal{A}} = M\}} \qquad \text{and} \qquad h^M_{x,t} := \vartheta_x P_t h^M\,.$$

Then, by reversibility and translation invariance, if $s \ge 0$

$$\begin{aligned} \mu(g_{x,s} h^M) &= \mu\left[P_s \vartheta_x (f - R_K f) h^M\right] = \mu\left[(f - R_K f)\vartheta_{-x} P_s h^M\right] \\ &= \frac{1}{|B_K|} \sum_{y \in B_K} \mu\left[(f - \vartheta_y f) h^M_{-x,s}\right]\,. \end{aligned}$$

Thus, using the Cauchy-Schwarz inequality and the invariance of B_L under the mapping $x \to -x$, we can write

$$\begin{aligned} \frac{1}{|B_L|} \sum_{x \in B_L} \mu\left[\mu(g_{x,s} \,|\, N_{\mathcal{A}})^2\right] &= \frac{1}{|B_L|} \sum_{x \in B_L} \sum_{M \in \mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\} \, \mu(g_{x,s} h^M)^2 \\ &= \sum_{M \in \mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\} \, \frac{1}{|B_L|} \sum_{x \in B_L} \mu\Bigg[\frac{1}{|B_K|} \sum_{y \in B_K} (f - \vartheta_y f) \, h^M_{-x,s}\Bigg]^2 \\ &\le \sum_{M \in \mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\} \Bigg[\frac{1}{|B_L|} \sum_{x \in B_L} \frac{1}{|B_K|} \sum_{y \in B_K} \mu[(f - \vartheta_y f) \, h^M_{x,s}]^2\Bigg]\,. \end{aligned} \qquad (7.1)$$

Now we deal with the terms $\mu[(f-\vartheta_y f)\, h^M_{x,s}]^2$. For any $y \in B_K$, there exists a path $(0, y_1, \ldots, y_k = y)$ going from 0 to y which consists of $k = |y|_1$ nearest neighbor steps. Hence we can define $\gamma_y = (e_1, \ldots, e_{|y|_1})$ where each $e_i = (y_{i-1}, y_i)$ is an (oriented) edge in B_K. Finally, for any edge $e = (u, v)$, we define $d_e f := \vartheta_v f - \vartheta_u f$. By the Cauchy-Schwarz inequality we have

$$\mu[(f-\vartheta_y f)\, h^M_{x,s}]^2 = \mu\Big[\sum_{e\in\gamma_y} d_e f\, h^M_{x,s}\Big]^2 \le |\gamma_y| \sum_{e\in\gamma_y} \mu(d_e f\, h^M_{x,s})^2 \,. \tag{7.2}$$

In the next two Lemmas we deals with $\mu(d_e f\, h^M_{x,s})^2$. In the proof it will be clear why, at the very begining, we have subtracted $R_K f$. This leads to having $d_e f$ instead of f in (7.2).

Lemma 7.1. *Assume (USM). For any $\alpha > 0$, there is $C_\alpha > 0$ such that for all local functions f on Ω with $S_f \ni 0$, for all $u \in \mathbb{Z}^d$ with $|u|_1 = 1$, and for all positive integers L, we have*

$$\sup_{\tau,N} |\nu^\tau_{B_L,N}(d_{(0,u)} f)| \le \frac{C_\alpha\, \|f\|_u\, |S_f|}{L^\alpha} \,. \tag{7.3}$$

Proof. Since

$$|\nu^\tau_{B_L,N}(d_{(0,u)} f)| \le\; 2\|f\|_u \sum_{x\in S_f} \nu^\tau_{B_L,N}(|\sigma(x) - \sigma(x+u)|)$$

one can use Lemma 10.1 of [VY97] where estimate (7.3) is proved when f is the particular function $\sigma(0)$ and the result follows. □

Lemma 7.2. *Assume (USM). For all local functions f on Ω, for all $\varepsilon > 0$ there exists $A = A(f, \varepsilon) > 0$ such that if u, v are nearest neighbors in B_K, $e := (u, v)$ and $W_e := u + B_{\lfloor L^\varepsilon \rfloor}$, then for all non negative functions h with $\mu(h) = 1$ we have*

$$\mu(d_e f\, h)^2 \le A\Big[L^{4\varepsilon} \mathcal{E}_{W_e}(\sqrt{h}) + \frac{1}{L^{d+2}}\Big] \,. \tag{7.4}$$

Proof. First we write $\mu(d_e f\, h) = \int \mu(d\tau)\, \nu^\tau_{W_e, N_{W_e}(\tau)}(d_e f\, h)$. For simplicity, we let $\nu^\tau_e := \nu^\tau_{W_e, N_{W_e}(\tau)}$. By the entropy inequality (see for instance Chapter 1 of [ABC$^+$00]), for any $s > 0$,

$$\nu^\tau_e(d_e f\, h) \le \frac{\nu^\tau_e(h)}{s} \log \nu^\tau_e\big(e^{s\, d_e f}\big) + \frac{1}{s} \operatorname{Ent}_{\nu^\tau_e}(h) \;,$$

where, for an arbitrary probability measure ρ on $(\Omega, \mathcal{F})$, and $h \in L^1(\rho)$ with $\rho(h) = 1$, we denote by $\operatorname{Ent}_\rho(h)$ the entropy of $h\rho$ with respect to ρ, *i.e.*

$$\operatorname{Ent}_\rho(h) := \operatorname{Ent}(h\rho \,|\, \rho) = \rho(h \log h) \,. \tag{7.5}$$

The probability measure ν^τ_e is known to satisfy [Yau96, CMR02] a logarithmic Sobolev inequality which states that for all functions g on Ω

$$\operatorname{Ent}_{\nu^\tau_e}(g) \le C L^{2\varepsilon} \mathcal{E}_{W_e}(g) \tag{7.6}$$

for some constant C. Consequently it follows from the Herbst argument [Led99, ABC$^+$00] that

$$\nu_e^\tau\left(e^{s\,d_e f}\right) \le \exp[\,Cs^2\,\|d_e f\|^2_{\mathrm{Lip}}\,L^{2\varepsilon} + s\,\nu_e^\tau(d_e f)\,]$$

with $\|d_e f\|^2_{\mathrm{Lip}} := \sum_{x\in W_e}\|\nabla_x d_e f\|_u^2 \le 4|S_f|\,\|f\|_u =: A_1(f)$. Thus,

$$\nu_e^\tau(d_e f\,h) \le \nu_e^\tau(h)\nu_e^\tau(d_e f) + s\,\nu_e^\tau(h)\,C\,A_1 L^{2\varepsilon} + \frac{1}{s}\,\mathrm{Ent}_{\nu_e^\tau}(h)\;. \tag{7.7}$$

Optimizing over the free parameter s and using (7.6) once again we get

$$\begin{aligned}\nu_e^\tau(d_e f\,h) &\le 2[CA_1L^{2\varepsilon}\nu_e^\tau(h)\ \mathrm{Ent}_{\nu_e^\tau}(h)]^{1/2} + \nu_e^\tau(h)\,\nu_e^\tau(d_e f)\\ &\le [A_2\,L^{4\varepsilon}\nu_e^\tau(h)\,\mathcal{E}_{\nu_e^\tau}(\sqrt{h})]^{1/2} + \nu_e^\tau(h)\,\nu_e^\tau(d_e f)\;.\end{aligned}$$

Now, by Lemma 7.1 (with $\alpha := \frac{d+2}{2\varepsilon}$), there exists $A_3 = A_3(f,\varepsilon)$ such that $\nu_e^\tau(d_e f) \le A_3 L^{-(d+2)/2}$. Thus, since $\mu(h) = 1$, an integration with respect to $\mu(d\tau)$ gives

$$\begin{aligned}\mu(d_e f\,h)^2 &\le 2A_2^2\,L^{4\varepsilon}\!\int\!\mu(d\tau)\,\nu_e^\tau(h)\int\!\mu(d\tau)\,\mathcal{E}_{\nu_e^\tau}(\sqrt{h}) + 2\frac{A_3^2}{L^{d+2}}\Big[\int\!\mu(d\tau)\,\nu_e^\tau(h)\Big]^2\\ &= 2A_2^2\,L^{4\varepsilon}\mathcal{E}_{W_e}(\sqrt{h}) + 2\frac{A_3^2}{L^{d+2}}\;.\end{aligned}$$

And the result of the Lemma follows. □

Back to the inequality (7.1). Using Lemma 7.2 together with (7.2) and the fact that $|\gamma_y| = |y|_1 \le dK$ for any $y \in B_K$, we get that for any $M \in \mathbb{M}_\ell^{\mathcal{A}}$, any $s \ge 0$,

$$\begin{aligned}&\frac{1}{|B_L|}\sum_{x\in B_L}\frac{1}{|B_K|}\sum_{y\in B_K}\mu[(f-\vartheta_y f)\,h^M_{x,s}]^2\\ &\le A\frac{1}{|B_L|}\sum_{x\in B_L}\frac{1}{|B_K|}\sum_{y\in B_K}|\gamma_y|\sum_{e\in\gamma_y}\Big[L^{4\varepsilon}\mathcal{E}_{W_e}\big(\sqrt{h^M_{x,s}}\big) + \frac{1}{L^{d+2}}\Big]\\ &\le A\Big[d^2\frac{K^2}{L^{d+2}} + \frac{L^{4\varepsilon}}{|B_L|\,|B_K|}\sum_{y\in B_K}|\gamma_y|\sum_{e\in\gamma_y}\sum_{x\in B_L}\mathcal{E}_{-x+W_e}\big(\sqrt{h^M_s}\big)\Big]\,.\end{aligned}$$

In the last inequality we used the fact that $\mathcal{E}_{W_e}(\vartheta_x H) = \mathcal{E}_{-x+W_e}(H)$ for any x and any H, due to the translation invariance property. Then, the bound $|\gamma_y| \le dK$ and an explicit computation gives

$$\frac{1}{|B_L|}\sum_{x\in B_L}\frac{1}{|B_K|}\sum_{y\in B_K}\mu[(f-\vartheta_y f)\,h^M_{x,s}]^2 \le \frac{A'}{L^d}\Big[L^{4\varepsilon}K^2\,|W_e|\,\mathcal{E}\big(\sqrt{h^M_s}\big) + \frac{K^2}{L^2}\Big] \tag{7.8}$$

for some other constant A'. It is well known (see [ABC$^+$00, Chapter 2] for instance) that for any f, $\partial_s \operatorname{Ent}(P_s f) \le -4\mathcal{E}(\sqrt{P_s f})$. Thus, as $\operatorname{Ent}(P_s f)$ is non increasing, we have

$$\int_0^t \mathcal{E}\big(\sqrt{h_s^M}\,\big)\, ds \le \frac{1}{4}[\operatorname{Ent}(h^M) - \operatorname{Ent}(h_t^M)] \le \frac{1}{4}\operatorname{Ent}(h^M) = \frac{1}{4}\log\frac{1}{\mu\{N_{\mathcal{A}} = M\}}\,, \tag{7.9}$$

where, in last equality, we have used the definition of entropy. By consequence we have

$$\sum_{M\in\mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\} \int_0^t \mathcal{E}\big(\sqrt{h_s^M}\,\big)\, ds \le \frac{1}{4} \sum_{M\in\mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\}\log\frac{1}{\mu\{N_{\mathcal{A}} = M\}}\,. \tag{7.10}$$

On the other side, since $x \to x\log(1/x)$ is concave, we can use Jensen inequality and obtain

$$\sum_{M\in\mathbb{M}_\ell^{\mathcal{A}}} \mu\{N_{\mathcal{A}} = M\}\log\frac{1}{\mu\{N_{\mathcal{A}} = M\}} \le \log|\mathbb{M}_\ell^{\mathcal{A}}| = d|\mathcal{A}|\log\ell\,. \tag{7.11}$$

Proposition 3.2 then follows, after a redefinition of ε, from (7.1), (7.8), (7.9), (7.10), and from the fact that $|W_e| \le (2L+1)^{d\varepsilon}$. □

Remark 7.3. Let us briefly explain the difference with the product case. In that case, the first term in (7.7) is null. By consequence, on can choose the boxes $|W_e|$ independent of L and so the logarithmic Sobolev constant used in the Herbst argument is also constant.

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