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Complete Equivalence of the Gibbs Ensembles for One-Dimensional Markov Systems

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We show the equivalence of the Gibbs ensembles at the level of measures for one-dimensional Markov-Systems with arbitrary boundary conditions. That is, the limit of the microcanonical Gibbs ensemble is a Gibbs measure with an interaction depending on the microcanonical constraint. In fact the usual microcanonical condition is replaced by the sharper constraint that all type frequencies of neighboring spins (including the boundary spins) are fixed. When conditioning on a set of different frequencies of neighboring spins compatible with physical quantities like energy density we get the usual microcanonical ensemble. We show that the limit is a Gibbs measure for a nearest neighbor potential depending on the pair measure which maximizes the entropy on the given set of pair measures. For this we show the large deviation property of the pair empirical measure for arbitrary boundary conditions. We establish analogous results for finite range potentials.

KEY WORDS: Equivalence of ensembles; microcanonical entropy; k-sample empirical measure; large deviations; Euler trails.

1. INTRODUCTION

The problem of equivalence of ensembles, tracing back to Gibbs (1902), is one of the classical problems of Statistical Mechanics. Here we are concerned with the equivalence of microcanonical and grandcanonical ensembles in one-dimensional systems, and we ask for equivalence in the strongest possible sense. If equivalence is interpreted in the classical weak sense of thermodynamic functions, it is well known that, under suitable conditions on the interaction, the infinite-volume limits of the specific

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microcanonical entropy and of the Gibbs free energy per volume exist and are related to each other by a Legendre–Fenchel transform, see refs. 1 and 2. We refer to this statement as the equivalence of the Gibbs ensembles at the level of thermodynamic functions. Another approach is to be found in the works of Thompson,[3] Aizenman *et al.*,[4] and Georgii,[5] where one works directly with infinite-volume states, defining the microcanonical and the canonical Gibbs measures by local specifications as in the familiar theory of the Gibbs measures for the grandcanonical Gibbs ensemble. These ensembles are called equivalent in the sense of infinite-volume states, if the microcanonical Gibbs measures are convex mixtures of the grandcanonical Gibbs measures with different parameters.

A more natural but deeper question is the complete asymptotic equivalence of finite volume measures in the sense that the microcanonical and the grandcanonical Gibbs ensembles in finite boxes have the same infinite-volume limits. Since Gibbs' time, many proofs have been offered of this general theorem. Deuschel *et al.*[6] and Georgii[7–10] use a large deviation principle for the empirical measures to prove the equivalence at the level of measures. Lewis *et al.*[11] show the equivalence with a quite different large deviation theory approach. However these papers are limited to the case of periodic boundary conditions or to a spatial averaging of the microcanonical Gibbs ensembles with configurational boundary conditions.

An alternative approach is given by Menzel[12] where he showed a conditional limit theorem for Gibbs measures on $\mathbb{Z}_+$ with finite state space E. This method is based on a conditional probability formula from ref. 13. Georgii and Adams[14] could not use this method for the whole $\mathbb{Z}$ because it came out that the starting point 0 of $\mathbb{Z}_+$ is necessary. This is also the case in ref. 15 where Csiszár *et al.* showed a conditional limit theorem for independent identically distributed random variables $X_1, X_2, \ldots$ taking values in a finite set under Markov conditioning. They do not show the limiting behavior for the two boundary terms. As a referee pointed out there is a paper, ref. 16 based on ref. 15 where they handle the same limit theorem but with constrains similar to microcanonical ones. However the boundary effect is not handled there.

In this paper we establish the complete equivalence in the sense above for one-dimensional Markov systems with finite state space E and arbitrary boundary conditions. To calculate the probabilities of cylinder events, we use the BEST Theorem of graph theory to count explicitly the number of configurations compatible with the given type frequencies of neighboring pairs including the two boundary pairs.

In the usual microcanonical Gibbs ensemble one gives equal weight to configurations in finite subsets of the lattice $\mathbb{Z}$ with the same energy and particle densities. If we consider nearest neighbor interaction of particles at the lattice sites of finite subsets of $\mathbb{Z}$ we have two extra energy contributions coming from the left and right boundary interaction. These contributions from the boundary have a global effect on the microcanonical Gibbs ensemble of a finite subset of the lattice. However, our results imply that in the thermodynamic limit the global effect disappears. See also our results in ref. 17 for the one-dimensional Ising model.

The type frequencies are given by a probability measure P_n on the set $E \times E$ of pairs. We write M^{η}_{n, P_n} for the microcanonical Gibbs ensemble with prescribed type frequencies in a finite set Λ_n with boundary condition $\eta \in \Omega \cup \{\text{per, free}\}$. This microcanonical Gibbs ensemble provides more information than the microcanonical Gibbs ensemble for energy and particle density because several frequencies of pairs with the same energy and particle density can occur. In a second step we only require that the type frequencies are compatible with a microcanonical constraint to get the results for the usual microcanonical Gibbs ensemble with energy and particle density.

Here is an outline of our results. Under appropriate conditions on the pair measures $P_n, n \in \mathbb{N}$, and for arbitrary boundary condition $\eta \in \Omega \cup \{\text{per, free}\}$ we will show for $P_n \to P$ for $n \to \infty$ that

$$M^{\eta}_{n, P_n} \to \nu_P \in \mathcal{G}(\phi^P) \qquad \text{for} \quad n \to \infty,$$

where ν_P is the stationary Markov chain ν_P with pair marginal P, which is the unique Gibbs measure ν_P with a nearest-neighbor interaction ϕ^P given by the pair measure P and without self-interaction. In our second main result the microcanonical constraint is given by a convex set Π of pair measures. Typically, Π consists of all pair measures consistent with certain particle densities and energy levels. We write $M^{\eta}_{n, \Pi}$ for the microcanonical Gibbs ensemble which gives equal weight to configurations with type frequencies given by the set Π. If the entropy has a unique maximum P^* in the set Π, we will show that

$$M^{\eta}_{n, \Pi} \to \nu_{P^*} \in \mathcal{G}(\phi^{P^*}) \qquad \text{for} \quad n \to \infty,$$

i.e., the complete equivalence for general microcanonical constraints of the Gibbs ensembles for a nearest-neighbor interaction. Of course, the limit ν_{P^*} is the one predicted by the thermodynamic formalism.

The methods used for nearest-neighbor interaction can easily be extended to finite range potentials. The microcanonical constraint in this case is given by the frequency of k-samples for arbitrary $k \in \mathbb{N}$, if k is the range of the potential. This gives the complete equivalence for finite range potentials.

Our proofs rely on an explicit counting of configurations with prescribed type frequencies. The number of such configurations is related to the number of Euler paths from the left to the right boundary state (particle) in an oriented multigraph, defined by the given frequencies of pairs. In Sections 2.1 and 2.2 we define the pair empirical measure to count neighboring pairs and define the restricted microcanonical Gibbs ensemble. The main results are stated in Section 2.3. In Section 3 we investigate the cardinality of the set of configurations with given type frequencies with methods of graph theory and give the conditions on the pair measures P_n, whereas the final sections are devoted to the proofs of the main results.

2. RESULTS

2.1. The Setting

For the finite state space E and a finite $\Lambda \subset \mathbb{Z}$ the space of configurations is $\Omega_\Lambda := E^\Lambda$, and for a configuration $\omega \in \Omega_\Lambda$ the state or the particle at the lattice site $i \in \Lambda$ is $\omega_i := \omega(i) \in E$. The marginals $\bar{P}$ and $\bar{\bar{P}}$ of a pair measure $P \in \mathscr{P}(E^2)$, where $\mathscr{P}(E^2)$ is the set of probability measures on E^2, are defined by

$$\bar{P}(x) := \sum_{y \in E} P(x, y) \qquad \text{and} \qquad \bar{\bar{P}}(x) := \sum_{y \in E} P(y, x) \qquad \text{for all} \quad x \in E.$$

We let $\tilde{\mathscr{P}}(E^2) := \{P \in \mathscr{P}(E^2) : \bar{P} = \bar{\bar{P}}\}$ be the set of pair measures with identical marginals.

A configuration in the finite box $\Lambda_n := [-n, n] \cap \mathbb{Z}$ including the two boundary pairs has $v_n := |\Lambda_n| + 1$ neighboring pairs. The pair empirical measure gives weight to frequencies of such configurations.

2.1. Definition. The pair empirical measure with boundary condition $\eta \in \Omega \cup \{\text{per, free}\}$ is the mapping $L_n^{2,\eta}: \Omega \to \mathscr{P}(E^2)$ with

(i) $L_n^{2,\eta}(\omega) := \frac{1}{v_n} (\sum_{i=-n}^{n-1} \delta_{(\omega_i, \omega_{i+1})} + \delta_{(\eta_{-n-1}, \omega_{-n})} + \delta_{(\omega_n, \eta_{n+1})})$ for configurational boundary conditions $\eta \in \Omega$, and with

(ii) $L_n^{2,\text{per}}(\omega) := \frac{1}{(v_n - 1)} (\sum_{i=1}^{n-1} \delta_{(\omega_i, \omega_{i+1})} + \delta_{(\omega_n, \omega_{-n})})$ for periodic boundary conditions, and with

(iii) $L_n^{2,\text{free}}(\omega) := \frac{1}{v_{n-1}} (\sum_{i=-n}^{n-1} \delta_{(\omega_i, \omega_{i+1})})$ for free boundary conditions.

The pair empirical measure with periodic boundary has identical marginals, i.e., $L_n^{2,\text{per}}(\Omega) \subset \tilde{\mathscr{P}}(E^2)$. In general there exist boundary conditions $\eta \in \Omega$ such that the pair empirical measure has no identical marginals, i.e., $L_n^{2,\eta}(\Omega) \not\subset \tilde{\mathscr{P}}(E^2)$. With the free boundary condition we get for all $\omega \in \Omega$:

$$L_n^{2,\text{free}}(\omega) = L_{n-1}^{2,\eta(\omega_{-n},\omega_n)}(\omega)$$

with the boundary condition $\eta(u,s) \in \Omega$ defined by $\eta_{-n}(u,s) = u$ and $\eta_n(u,s) = s$ for all $n \in \mathbb{N}$; therefore the properties of the pair empirical measure with the free boundary condition follow from the pair empirical measure with a configurational boundary condition.

Two configurations in Ω_{Λ_n} with equal pair empirical measure have identical frequencies of neighboring pairs. The set $T_n^\eta(P) := \{\omega \in \Omega_{\Lambda_n} : L_n^\eta(\omega) = P\}$ is called the pair type class of a pair measure P. We call a pair measure P (n,η)-admissible if the pair type class is non-empty, i.e., $T_n^\eta(P) \neq \emptyset$. In Lemma 3.20 we will give precise conditions for a pair measure P to be (n,η)-admissible.

2.2. The Gibbs Ensembles

The Gibbs ensembles are probability measures on the configuration space Ω_Λ for all finite subsets Λ of $\mathbb{Z}$, whereas the infinite volume Gibbs measure is a probability measure on the configuration space Ω of the infinite system, both equipped their with Borel-σ-algebra. We define the microcanonical Gibbs ensemble for a given pair measure P_n as follows, writing 1_A for the indicator function of an event A.

2.2. Definition. (i) Let $\eta \in \Omega \cup \{\text{per}, \text{free}\}$, λ the counting measure on E, and P_n, $n \in \mathbb{N}$, a (n,η)-admissible pair measure, i.e., $T_n^\eta(P_n) \neq \emptyset$. The microcanonical Gibbs ensemble for P_n is the probability measure M_{n,P_n}^η on the configuration space Ω_{Λ_n} with

$$M_{n,P_n}^\eta(\omega) := \frac{1}{Z_{n,P_n}(\eta)} 1_{\{L_n^{2,\eta} = P_n\}}(\omega) = \lambda^{\Lambda_n}(\omega \mid L_n^{2,\eta}(\omega) = P_n)$$

for all $\omega \in \Omega_{\Lambda_n}$ and the normalization constant $Z_{n,P_n}(\eta) := \lambda^{\Lambda_n}(L_n^{2,\eta} = P_n)$.

The grandcanonical Gibbs ensemble is defined as follows. For a given nearest neighbor potential $\phi\colon E\times E\to\mathbb{R}$ and self-interaction $\psi\colon E\to\mathbb{R}$ and $\omega\in\Omega$ let

$$H_{\Lambda_n}^{\text{free}}(\omega):=\sum_{i=-n}^{n-1}\phi(\omega_i,\omega_{i+1})+\sum_{i\in\Lambda_n}\psi(\omega_i)$$

be the Hamiltonian with free boundary condition,

$$H_{\Lambda_n}^{\eta}(\omega):=H_{\Lambda_n}^{\text{free}}(\omega)+\phi(\eta_{-n-1},\omega_{-n})+\phi(\omega_n,\eta_{n+1})$$

be the Hamiltonian with configurational boundary condition $\eta\in\Omega$, and

$$H^{\text{per}}(\omega):=H_{\Lambda_n}^{\text{free}}(\omega)+\phi(\omega_n,\omega_{-n})$$

be the Hamiltonian for periodic boundary condition.

2.3. Definition. The grandcanonical Gibbs ensemble for the given Hamiltonians and boundary condition $\eta\in\Omega\cup\{\text{per},\text{free}\}$ is the probability measure G_n^η on Ω_{Λ_n} with

$$G_n^\eta(\omega):=Z_n(\eta)^{-1}\exp\{-H_{\Lambda_n}^\eta(\omega)\}$$

for all $\omega\in\Omega_{\Lambda_n}$ and the normalization constant $Z_n(\eta)=\sum_{\omega\in\Omega_{\Lambda_n}}\exp\{-H_{\Lambda_n}^\eta(\omega)\}$.

The thermodynamic equilibrium state for the infinite system is the Gibbs measure for the given nearest neighbor potential. For a finite $\Lambda\subset\mathbb{Z}$ we write $\mathscr{T}_\Lambda$ for the Borel-σ-algebra of events outside Λ. We write $\omega\eta_{\mathbb{Z}\setminus\Lambda}\in\Omega$ for a configuration which has ω as projection on Ω_Λ and $\eta_{\mathbb{Z}\setminus\Lambda}$ as projection on the complement.

2.4. Definition. A probability measure $P\in\mathscr{P}(\Omega)$ on the configuration space Ω is called a Gibbs measure for the nearest neighbor (resp. finite range) potential ϕ and self-interaction ψ, if for all events A in the Borel-σ-algebra of the configuration space Ω and for all $\eta\in\Omega$ and all finite $\Lambda\subset\mathbb{Z}$ we have

$$P(A\mid\mathscr{T}_\Lambda)(\eta)=\frac{1}{Z_\Lambda(\eta)}\sum_{\omega\in\Omega_{\Lambda_n}}1_A(\omega\eta_{\mathbb{Z}\setminus\Lambda})\exp\{-H_\Lambda^\eta(\omega)\}$$

with the normalization constant

$$Z_\Lambda(\eta):=\sum_{\omega\in\Omega_{\Lambda_n}}\exp\{-H_\Lambda^\eta(\omega)\}.$$

The set of all Gibbs measures for the nearest neighbor potential (resp. finite range) ϕ and self-interaction ψ is $\mathscr{G}(\phi, \psi)$.

The grandcanonical Gibbs ensemble converges in the thermodynamic limit to the Gibbs measure with the given nearest neighbor (resp. finite range) potential (see ref. 7).

2.3. The Results

A basic ingredient of our results is the existence and the independence on the boundary conditions of the thermodynamic limit of the microcanonical mean entropy. The entropy of a probability measure $P \in \mathscr{P}(E^2)$ is defined as

$$\mathscr{H}(P) := -\sum_{x, y \in E} P(x, y) \log P(x, y),$$

where we adopt the usual convention that $0 \log 0 = 0$.

2.5. Theorem. Let $\eta \in \Omega \cup \{\text{per, free}\}$ and P_n, $n \in \mathbb{N}$, (n, η)-admissible pair measures, i.e., $T_n^\eta(P_n) \neq \emptyset$ for all $n \in \mathbb{N}$. Then if $P_n \to P$ for $n \to \infty$ and P strictly positive, the limit

$$S(P) := \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log Z_{n, P_n}(\eta) = \log\left(\prod_{x \in E}\left(\frac{\bar{P}(x)^{\bar{P}(x)}}{\prod_{y \in E} P(x, y)^{P(x, y)}}\right)\right)$$

exists and is equal to the conditional entropy of P given the marginal $\bar{P}$, i.e., $S(P) = \mathscr{H}(P) - \mathscr{H}(\bar{P})$. In particular $S(P)$ is concave.

In the next theorem we get our first main result, which shows that the restricted microcanonical Gibbs ensemble M_{n, P_n}^η converges to a Gibbs measure with nearest neighbor potential ϕ^P defined by

$$\phi^P(\omega_i, \omega_{i+1}) := \begin{cases} -\log \dfrac{P(\omega_i, \omega_{i+1})}{\bar{P}(\omega_i)}; & \bar{P}(\omega_i) > 0 \\ +\infty; & \bar{P}(\omega_i) = 0 \end{cases}$$

for $\omega \in \Omega$, $i \in \mathbb{Z}$, and vanishing self-interaction $\psi \equiv 0$.

2.6. Theorem. Let $\eta \in \Omega \cup \{\text{per, free}\}$ and $(P_n)_{n \in \mathbb{N}}$ a sequence of (n, η)-admissible pair measures, i.e., $T_n^\eta(P_n) \neq \emptyset$ for all $n \in \mathbb{N}$. If $P_n \to P$ for $n \to \infty$ and P strictly positive, the microcanonical Gibbs ensemble M_{n, P_n}^η

converges to the unique Gibbs measure with nearest neighbor interaction ϕ^P and no self-interaction, i.e.,

$$\lim_{n\to\infty} M^{\eta}_{n,P_n} = \nu_P \in \mathcal{G}(\phi^P).$$

We define a set of pair measures with prescribed expectation values.

2.7. Definition. Let $d \geqslant 1$ and $f\colon E^2 \to \mathbb{R}^d$ be an arbitrary mapping. For $\varDelta \subset \mathbb{R}^d$ we let

$$\varPi^{\varDelta}_f := \{Q \in \widetilde{\mathcal{P}}(E^2) : Q(f) \in \varDelta\}$$

be the set of pair measures with identical marginals and expectation vector in $\varDelta$.

The usual microcanonical Gibbs ensemble is of the form $M^{\eta}_{n,f,\varDelta} := \lambda^{\varLambda_n}(\cdot \mid L^{2,\eta}_n \in \varPi^{\varDelta}_f)$ for suitable f.

2.8. Theorem. Let $\varDelta \subset \mathbb{R}^d$ be a closed convex set with $\mathring{\varDelta} \neq \emptyset$, and let $P^* \in \varPi^{\varDelta}_f$ be the unique measure which maximizes the entropy on $\varPi^{\varDelta}_f$. For an arbitrary boundary condition $\eta \in \Omega \cup \{\text{per}, \text{free}\}$ the microcanonical Gibbs ensemble $M^{\eta}_{n,f,\varDelta}$ converges to the unique Gibbs measure with nearest neighbor interaction ϕ^{P^*} and no self-interaction, i.e.,

$$\lim_{n\to\infty} M^{\eta}_{n,f,\varDelta} = \nu_{P^*} \in \mathcal{G}(\phi^{P^*}).$$

Next we indicate how the preceeding results can be extended to the case of finite range interaction. We condition on k-samples to get as a limit a Gibbs measure with an interaction potential of finite range k. When we have frequencies of k-samples we have $(k-1)$-samples at the boundaries and have to use the k-sample empirical measure.

2.9. Definition. Let $\eta \in \Omega$, $k \in \mathbb{N}$ and $v_n := |\varLambda_n| + k - 1$. The k-sample empirical measure with configurational boundary condition $\eta \in \Omega$ is the mapping $L^{k,\eta}_n\colon \Omega \to \mathcal{P}(E^k)$ with

$$L^{k,\eta}_n(\omega) := \frac{1}{v_n}\Bigg(\sum_{i=-n}^{n-(k-1)} \delta_{(\omega_i,\ldots,\omega_{i+k-1})} + \sum_{i=n-k+2}^{n} \delta_{(\omega_i,\ldots,\omega_n,\eta_{n+1},\ldots,\eta_{i+k-1})}$$
$$+ \sum_{i=-n-k+1}^{-n-1} \delta_{(\eta_i,\ldots,\eta_{-n-1},\omega_{-n},\ldots,\omega_{i+k-1})}\Bigg).$$

The pure k-body interaction ϕ^P is defined by

$$\phi^P(\omega_i,\ldots,\omega_{i+k-1}) = \begin{cases} -\log \dfrac{P(\omega_i,\ldots,\omega_{i+k-1})}{\bar{P}(\omega_i,\ldots,\omega_{i+k-2})}; & \bar{P}(\omega_i,\ldots,\omega_{i+k-2}) > 0 \\ +\infty; & \bar{P}(\omega_i,\ldots,\omega_{i+k-2}) = 0 \end{cases}$$

for $i \in \mathbb{Z}$ and $\omega \in \Omega$. The microcanonical Gibbs ensembles $M^{k,\eta}_{n,P_n}$ and $M^{k,\eta}_{n,f,\Delta}$ are defined analogously to the nearest neighbor case and we have the same results.

2.10. Theorem. Let $\eta \in \Omega$ and P_n, $n \in \mathbb{N}$, probability measures on E^k which are (n,η)-admissible.

(i) The microcanonical Gibbs ensemble $M^{k,\eta}_{n,P_n}$ converges for $P_n \to P$ for $n \to \infty$ and P strictly positive to the unique Gibbs measure with pure k-body interaction ϕ^P, i.e., $\lim_{n\to\infty} M^{\eta,k}_{n,P_n} = \nu_P \in \mathscr{G}(\phi^P)$.

(ii) Let $\Delta \subset \mathbb{R}^d$ be a closed convex set with $\mathring{\Delta} \neq \emptyset$, $f: E^k \to \mathbb{R}^d$ a mapping, $\Pi^\Delta_f = \{Q \in \widetilde{\mathscr{P}}(E^k) : Q(f) \in \Delta\}$ and let $P^* \in \Pi^\Delta_f$ be the unique measure which maximizes the entropy on the set Π^Δ_f. Then the microcanonical Gibbs ensemble $M^{k,\eta}_{n,f,\Delta}$ converges to the unique Gibbs measure with pure k-body interaction ϕ^{P^*}, i.e.,

$$\lim_{n\to\infty} M^{k,\eta}_{n,f,\Delta} = \nu_{P^*} \in \mathscr{G}(\phi^{P^*}).$$

Thus we have derived the complete equivalence of the Gibbs ensembles. If we take a grandcanonical Gibbs ensemble with a nearest neighbor potential (finite range potential) we can calculate (see book of Georgii,[18] Chapter 3) the transition matrix for the corresponding Markov chain which describes the Gibbs measure for the given nearest neighbor potential; and with this transition matrix we get a pair (k-sample) measure P and a sequence $(P_n)_{n\in\mathbb{N}}$ with $P_n \to P$ for $n \to \infty$ and we know from our theorems that the corresponding microcanonical Gibbs ensemble M^η_{n,P_n} converges to the same Gibbs measure. For this we give an example, the one-dimensional lattice gas formulation of the Ising model:[17]

2.11. Example. In the lattice gas formulation of the Ising model we have the state space $E = \{0, 1\}$. The Hamiltonian with arbitrary configurational boundary condition $\eta \in \Omega$ is given by $H^\eta_{\Lambda_n}(\omega) = -\sum_{i=-n}^{n-1} \omega_i\omega_{i+1} - (\omega_n\eta_{n+1} + \omega_{-n}\eta_{-n-1})$. We fix an energy density $\varepsilon > 0$ and particle density $\varrho > 0$ such that $\varepsilon > \varrho$ and $1 - 2\varrho + \varepsilon > 0$. For any $n \in \mathbb{N}$ let ε_n and ϱ_n with $\varepsilon_n \to \varepsilon$ and $\varrho_n \to \varrho$ for $n \to \infty$ energy and particle densities such that there exist some $\omega \in \Omega_{\Lambda_n}$ satisfying $v_n^{-1} H^{\eta}_{\Lambda_n}(\omega) = \varepsilon_n$ and $v_n^{-1} N_{\Lambda_n}(\omega) = \varrho_n$. Here $N_{\Lambda_n}(\omega) = \sum_{i \in \Lambda_n} \omega_i$ is the number of particles (spins) in Λ_n. Then

$$\{\omega \in \Omega_{\Lambda_n} : v_n^{-1} H^{\eta}_{\Lambda_n}(\omega) = \varepsilon_n;\, v_n^{-1} N_{\Lambda_n}(\omega) = \varrho_n\} = T^{\eta}_n(P_n)$$

for the pair measures P_n with $P_n(1,1) = \varepsilon_n$, $\bar{P}_n(1) = \varrho_n + \frac{1}{v_n}\delta_{1,\eta_{-n-1}}$, $P_n(1,0) = (\varrho_n - \varepsilon_n) + \frac{1}{v_n}\delta_{1,\eta_{-n-1}}$, $P_n(0,1) = (\varrho_n - \varepsilon_n) + \frac{1}{v_n}\delta_{1,\eta_{n+1}}$ and $P_n(0,0) = 1 - 2\varrho_n + \varepsilon_n - \frac{1}{v_n}(\delta_{1,\eta_{-n-1}} + \delta_{1,\eta_{n+1}})$ and with limit $P \in \mathscr{P}(E^2)$ given by $P(1,1) = \varepsilon$, $P(0,1) = P(1,0) = \varrho - \varepsilon$ and $P(0,0) = 1 - 2\varrho + \varepsilon$. From our results we know that the microcanonical ensemble M^{η}_{n,P_n} converges to the unique Gibbs measure v_P with nearest neighbor interaction ϕ^P and no self-interaction.

We have to compare this result with the expected result of the thermodynamic formalism. We let $Z_{n,\varepsilon_n,\varrho_n}(\eta)$ be the normalization constant for the microcanonical Gibbs ensemble M^{η}_{n,P_n} given by the pair measure P_n. By theorem (2.3) the microcanonical entropy $s(\varepsilon, \varrho) := \lim_{n\to\infty} \frac{1}{v_n} \log Z_{n,\varepsilon_n,\varrho_n}(\eta)$ exists. Its partial derivatives are the inverse temperature $\beta := \frac{\partial s}{\partial \varepsilon}(\varepsilon, \varrho)$ and the chemical potential $\mu := \frac{\partial s}{\partial \varrho}(\varepsilon, \varrho)$. We let ϕ be the nearest neighbor potential defined by $\phi(\omega_i, \omega_{i+1}) = \beta \omega_i \omega_{i+1}$ and ψ the self-interaction $\psi(x) = \beta\mu x$ for all $x \in E$. In view of Chapter 3 in ref. 18 the associated unique Gibbs measure is the stationary Markov chain for a transition matrix V, which can be computed as follows. Let $g\colon E^3 \to (0,\infty)$ with

$$\begin{aligned} g(x,y,z) &= (Z_{\{i\}}(\eta^{x,z}))^{-1} \sum_{\xi = 0,1} 1_{\{\pi_i = y\}}(\xi_i \eta^{x,z}) \exp\{-H^{\eta^{x,z}}_{\{i\}}(\xi_i)\} \\ &= \frac{e^{-y(\mu + \beta x + \beta z)}}{1 + e^{-(\mu + \beta x + \beta z)}} \end{aligned}$$

the determining function for the configuration $\eta^{x,z}$ which has x as projection on $\{i-1\}$ and z as projection on $\{i+1\}$ and the projection $\pi_i\colon \Omega \to E$, $\omega \to \omega_i$ on $\{i\}$. The corresponding transfer matrix is given by $Q(x,y) = g(a,x,y)/g(a,a,y)$ for all $x, y \in E$ and an arbitrary $a \in E$. We have $V(x,y) = Q(x,y)\, r(y)/qr(x)$ where q is the largest positive eigenvalue and r the corresponding right eigenvector. The result is

$$V = \begin{pmatrix} \dfrac{1 - 2\varrho + \varepsilon}{1 - \varrho} & \dfrac{\varrho - \varepsilon}{1 - \varrho} \\[2ex] \dfrac{\varrho - \varepsilon}{\varrho} & \dfrac{\varepsilon}{\varrho} \end{pmatrix}.$$

This is precisely the transition matrix of v_P. So, the measure v_P is precisely the limit predicted by thermodynamics.

3. COUNTING OF PAIR TYPE CLASSES

In this section we count for fixed $n \in \mathbb{N}$ the configurations $\omega \in \Omega_{\Lambda_n}$ with $L_n^{2,\eta}(\omega) = P$ for an (n, η)-admissible pair measure P, that is we calculate the cardinality of the pair type class $T_n^\eta(P)$. For the given pair measure P we have a frequency matrix $(f(x, y))_{x, y \in E}$ with $f(x, y) := v_n P(x, y)$, $x, y \in E$. We let this matrix be the incidence matrix of an oriented multigraph G with vertex set E and $f(x, y)$ edges from vertex x to vertex y. We have a multigraph because loops, edges from x to x itself, and several edges between different vertices are allowed. Each configuration $\omega \in T_n^\eta(P)$ corresponds to an Euler trail, a trail running through all edges of the graph in the right direction and just once, from the vertex $u := \eta_{-n-1}$ to the vertex $s := \eta_{n+1}$. We therefore have to count the Euler trails. The graph is connected if for every pair (x, y) of distinct vertices there is a path from x to y. The in-degree of a vertex x is the number of edges ending at x, and the out-degree is the number of edges starting at x. We call the graph simple if for all vertices the in-degree equals the out-degree. If the graph G is simple we can calculate the number of Euler circuits, which are Euler trails whose end vertices coincide, by the so-called BEST-theorem. The multigraph G is simple if $u = s$. In the case $u \neq s$ our multigraph becomes simple if we augment him with an additional edge from s to u. In the following we ignore all isolated vertices from E. We thus have the following correspondence:

$$v_n P \in \mathbb{Z}_+^{E \times E} \quad \longleftrightarrow \quad \text{multigraph } G \text{ with vertex set } E \text{ and } v_n \text{ edges}$$

$$v_n(\bar{P} - \bar{\bar{P}}) = \delta_u - \delta_s \quad \longleftrightarrow \quad \text{multigraph } G \text{ simple, if } u = s$$

$$\omega \in T_n^\eta(P) \quad \longleftrightarrow \quad \text{Euler trail from } u \text{ to } s$$

$$\longleftrightarrow \quad \text{Euler circuit with fixed endpoints for the augmented multigraph } \tilde{G}$$

Our pair type class $T_n^\eta(P)$ is non-empty if there exists an Euler circuit in the augmented multigraph $\tilde{G}$. The next theorem tells us when this does occur.

3.12. Theorem. A connected multigraph G has an Euler circuit if and only if G is simple.

Proof. Theorem I.12 in ref. 19. ∎

In the following we list conditions on the pair measures P_n, $n \in \mathbb{N}$, such that the sets $\{\omega \in \Omega_{\Lambda_n} : L_n^{2,\eta}(\omega) = P_n\}$ are non-empty. For that we need the absolute frequencies

(3.13) $$v_n P_n(x, y) \in \mathbb{Z}_+ \qquad \text{for all} \quad x, y \in E.$$

Because of the boundary condition η the two marginals $\bar{P}_n$ and $\bar{\bar{P}}_n$ differ in general, i.e., we have

(3.14) $$\bar{P}_n - \bar{\bar{P}}_n = \frac{1}{v_n}(\delta_{\eta_{-n-1}} - \delta_{\eta_{n+1}}).$$

In Lemma 3.20 we will also need a suitable ordering $x_0, \ldots, x_{l_n}$ of the elements of $D(\bar{P}_n) \cup \{\eta_{n+1}\}$, the union of the support $D(\bar{P}_n) := \{x \in E : \bar{P}_n(x) > 0\}$ of the marginal with the right boundary point, such that we have

(3.15) $$x_0 = \eta_{-n-1} \text{ and } x_{l_n} = \eta_{n+1} \text{ and } P_n(x_i, x_{i+1}) > 0 \text{ for } i = 0, \ldots, v_n;$$

it is therefore possible that an element of the support occurs several times in the ordering. For periodic boundary conditions we need

(3.16) $(v_n - 1)\, P_n(x, y) \in \mathbb{Z}_+$, $\bar{P}_n = \bar{\bar{P}}_n$ and

(3.17) an ordering (3.15) for the elements of $D(\bar{P}_n) \cup \{x\}$ for all $x \in D(\bar{P}_n)$.

In the free boundary case we need

(3.18) $v_{n-1} P_n(x, y) \in \mathbb{Z}_+$ for all $x, y \in E$ and a sequence

$$((u_n, s_n))_{n \in \mathbb{N}} \text{ in } E^2 \text{ with } \bar{P}_n - \bar{\bar{P}}_n = \frac{1}{v_{n-1}}(\delta_{s_n} - \delta_{u_n})$$

and an ordering (3.15) for the elements of $D(\bar{P}_n) \cup \{s_n\}$.

3.19. Remark. For free boundary conditions with (3.18) we have in the case $u_n = s_n$ for all $n \in \mathbb{N}$ because of $\bar{P}_n(x) - \bar{\bar{P}}_n(x)$ for all $x \in E$ several different sequences $((\tilde{u}_n, \tilde{s}_n))_{n \in \mathbb{N}}$ with $\tilde{u}_n = \tilde{s}_n$. In the case of $u_n \neq s_n$ because of $\bar{P}_n(x) - \bar{\bar{P}}_n(x) = \frac{1}{v_{n-1}}(\delta_{x,u_n} - \delta_{x,s_n})$ for all $x \in E$ the states ω_{-n} and ω_n are not free. In this case we have therefore no real free boundary condition. In the following we restrict ourself to configurational boundary conditions. The free boundary condition makes sense when we condition later on a set of different frequencies.

In Lemma 3.20 we show that the pair type class $T_n^\eta(P)$ is not empty if and only if the conditions (3.13)–(3.15) for $\eta \in \Omega$ or (3.16)–(3.17) for

$\eta = \text{per}$ hold. The free boundary condition follows from the configuration one.

In complete analogy to the pair empirical measure we have conditions like in (3.13)–(3.15) for the k-sample empirical measures P_n, $n \in \mathbb{N}$, for example integer absolute frequencies and the difference in the marginals

$$v_n P_n(x_1,\ldots, x_k) \in \mathbb{Z}_+, \qquad v_n(\bar{P}_n - \bar{\bar{P}}_n) = \delta_{(\eta_{-n-k+1},\ldots,\, \eta_{-n-1})} - \delta_{(\eta_{n+1},\ldots,\, \eta_{n+k-1})}$$

For periodic and free boundary condition similar properties have to be fulfilled, but we restrict here on configurational boundary conditions.

3.20. Lemma. (i) For $\eta \in \Omega$ the pair type class $T_n^\eta(P)$ is non-empty, i.e., P is (n, η)-admissible, if and only if P satisfies the conditions (3.13)–(3.15).

(ii) The pair type class $T_n^{\text{per}}(P)$ is non-empty if and only if P satisfies the conditions (3.16)–(3.17).

Proof. From the ordering (3.15) we get an Euler path from u to s. The multigraph is therefore connected. Because of our condition (3.15) all vertices which are not the boundary vertices have same in-degree and out-degree. With our extra edge from s to u we have coinciding in- and out-degrees for all $x \in E$ (we have assumed above that E contains no isolated vertices), that is the augmented multigraph is simple and connected. With Theorem 3.12 we get the result.

(ii) follows directly from Theorem 3.12. ∎

Our microcanonical Gibbs ensembles for the pair measures are well defined and in the next theorem we calculate the cardinality of the pair type class which is the normalization constant for the microcanonical Gibbs ensemble $M^\eta_{n,P}$, i.e., $Z_{n,P}(\eta) = |T^\eta_n(P)|$.

3.21. Theorem. Let $\eta \in \Omega$ and P a pair measure with (3.13)–(3.15). Then

$$Z_{n,P}(\eta) = B^*_{s,u}(P) \prod_{x \in E} \left(\frac{\bar{f}(x)!}{\prod_{y \in E} f(x, y)!} \right),$$

where $\bar{f} := v_n \bar{P}$ and $B^*_{s,u}(P)$ is the (s, u)-minor determinant of the matrix $B^*(P) = (B^*(P)(x, y))_{x, y \in E}$. Here

$$B^*(P)(x, y) := \begin{cases} \delta_{x,y} - \dfrac{P(x, y)}{\bar{P}(x)}; & \bar{P}(x) > 0, \\ \delta_{x,y}; & \bar{P}(x) = 0, \end{cases}$$

and the (s, u)-minor determinant is obtained as the determinant of the matrix which is obtained from $B^*(P)$ by deleting the sth row and uth column. An analogous result is obtained for $\eta = \text{per}$.

Proof. For a simple connected multigraph there are proofs in refs. 20 and 21 which don't refer to graph theory. The graph theoretic approach goes back to Tutte.[22] We sketch here a proof for our augmented multigraph with the so-called BEST-theorem, which gives the number of different Euler circuits in an oriented connected simple multigraph, and show how to get the number of Euler trails in the original multigraph.

BEST Theorem. Let $M = (m(x, y))_{x, y \in E}$ be the incidence matrix of a simple connected oriented multigraph G. Then the number $s(G)$ of different Euler circuits is given by

$$s(G) = |M^*| \prod_{x \in E} (\bar{m}(x) - 1)!$$

where $|M^*|$ is an arbitrary minor determinant of the matrix $M^* = (m^*(x, y))_{x, y \in E}$ with $m^*(x, y) = \bar{m}(x)\, \delta_{x, y} - m(x, y)$ for all $x, y \in E$.

Proof. From Theorem I.13 in ref. 19 we get

$$s(G) = t_y \prod_{x \in E} (\bar{m}(x) - 1)!,$$

where t_y is the number of spanning trees oriented to an arbitrary vertex $y \in E$ in the multigraph G. In particular $t_y = t_x$ for all $x, y \in E$. From ref. 23 it follows that the number of spanning trees oriented to an arbitrary vertex is given by an arbitrary minor determinant of the matrix M^*. ∎

If the boundary points are distinct we need an extra edge from s to u and as incidence matrix we choose $M = (m(x, y))_{x, y \in E}$ with

$$m(x, y) = f(x, y) \qquad \text{for all} \quad (x, y) \neq (s, u) \qquad \text{and}$$
$$m(s, u) = f(s, u) + 1,$$

so that $\bar{m}(x) = \bar{\bar{m}}(x)$ for all $x \in E$. We let $N_{u, s}(M)$ be the number of trails from u to s. If the edges are distinguishable, we have:

$$N_{u, s}(G) = s(G)\, m(s, u) = |M^*|\, m(s, u) \prod_{x \in E} (\bar{m}(x) - 1)!$$

with a minor determinant $|M^*|$ of the matrix $M^* = (m^*(x, y))_{x, y \in E}$ with $m^*(x, y) = \bar{m}(x)\, \delta_{x, y} - m(x, y)$ for all $x, y \in E$. If these edges are not distinguishable, then the number of Euler trails that begin in u and end in s is $U_{u,s}(G)$ and equals the number of configurations $\omega \in T_n^\eta(P)$:

$$U_{u,s}(G) = \frac{|M^*|\, m(s,u) \prod_{x\in E} (\bar{m}(x)-1)!}{\prod_{x,y\in E} m(x,y)!} = \frac{|M^*|}{\prod_{\substack{x\in E\\ x\neq s}} \bar{m}(x)} \frac{\prod_{x\in E} \bar{f}(x)!}{\prod_{x,y\in E} f(x,y)!},$$

and we define $f^*(P)(x,y) := \delta_{x,y} - \frac{P(x,y)}{\bar{P}(x)}$ for all $x, y \in E$, and we conclude

$$\frac{|M^*|}{\prod_{\substack{x\in E\\ x\neq s}} \bar{m}(x)} = B^*_{s,r}(P) \qquad \text{for all} \quad r \in E,$$

which means that $B^*_{s,u}(P)$ does not depend on the left boundary conditions. For periodic boundary conditions the result follows directly from the BEST Theorem. ∎

We will need an explicit expression for the boundary dependent factor $B^*_s(P)$:

3.22. Corollary. Let P be a pair measure with (3.13)–(3.15). Then for all $s \in E$ we have

$$B^*_{s,s}(P) = \sum_{v\in \Upsilon} \prod_{x\in E\setminus\{s\}} \frac{P(x, v(x))}{\bar{P}(x)},$$

with $\Upsilon := \{v: E\setminus\{s\} \to E,\, v^k(x) \neq x\ \forall k \in \mathbb{N},\, x\in E\setminus\{s\}\}$.

Proof. This follows immediately from the number of spanning trees oriented towards s (see the proofs in refs. 23 and 24). ∎

Next we observe that the factorial terms in Theorem 2.5 can be estimated in terms of conditional entropy.

3.23. Lemma. Let P be a pair measure such that $T_n^\eta(P) \neq \emptyset$. Then

$$v_n^{-|E|^2-|E|} e^{v_n(\mathscr{H}(P)-\mathscr{H}(\bar{P}))} \leqslant Z_{n,P}(\eta) \leqslant e^{v_n(\mathscr{H}(P)-\mathscr{H}(\bar{P}))}.$$

Proof. It follows immediately from Corollary 3.22 that

$$\frac{1}{v_n^{|E|}} \leqslant B^*_{s,s}(P) \leqslant 1.$$

With Lemma I.2.5 in ref. 25 we get the result. It is the same result as in 3.1.22 of ref. 26 where no boundary conditions are considered. ∎

Theorem 2.5 is an immediate consequence of the preceeding lemma. The concavity of S follows from the concavity of the conditional entropy $\mathscr{H}(P)-\mathscr{H}(\bar{P})$.[25] ▮

4. PROOF OF THEOREM 2.6

We proceed in three steps. First we calculate the probability for an arbitrary cylinder event, where we divide the system into the subsystems left and right of the cylinder event. Then we approximate the sum by an integral. We can calculate the integral with the Laplace method. For that we need uniform convergence of the integrand and of the function in the exponent. In a last step we show that the errors we make are negligible in the limit $n \to \infty$.

4.1. The Calculation of the Cylinder Probability

Let $i \in \mathbb{Z}$ and $k \in \mathbb{N}$ and $x_0,..., x_k \in E$ and $n \in \mathbb{N}$ be so large that $i \in \Lambda_n$ and $i+k \in \Lambda_n$. Let $\pi_i\colon \Omega \to E$; $\omega \mapsto \omega_i$ be the projection on the lattice site i. Then

$$\begin{aligned}(4.24)\qquad & M^{\eta}_{n, P_n}(\pi_i = x_0,..., \pi_{i+k} = x_k)\\ &= \sharp\{\omega \in \Omega_{\Lambda_n} : \omega_i = x_0,..., \omega_{i+k} = x_k;\ L_n^{2,\eta}(\omega) = P_n\}/Z_{n, P_n}(\eta).\end{aligned}$$

To calculate the numerator of (4.24) we take the two subsystems in $\Lambda_n^1 := \{-n,..., i-1\}$ with boundary condition $\eta^1 \in \Omega$ with $\eta^1_{-n-1} = u$ and $\eta^1_i = x_0$ and in $\Lambda_n^2 := \{i+k+1,..., n\}$ with $\eta^2 \in \Omega$ with $\eta^2_{i+k} = x_k$ and $\eta^2_{n+1} = s$. Both systems are connected via the microcanonical constraint: the frequency of the pairs in both systems and in the cylinder event have to sum up to the given frequency. Let

$$k(x, y) := \sum_{j=0}^{k-1} \delta_{(x_j, x_{j+1})}(x, y) \qquad \text{for all} \quad x, y \in E$$

the number of pairs (x, y) of the cylinder event with marginal $\bar{k}(x) := \sum_{y \in E} k(x, y)$ for all $x \in E$. We write (4.24) as a sum over the frequencies in Λ_n^1 over the product of the number of compatible configurations in Λ_n^1 with boundary condition $\eta^1 \in \Omega$ and in Λ_n^2 with boundary condition $\eta^2 \in \Omega$. For a configuration $\omega \in \{\omega \in \Omega_{\Lambda_n} : \omega_i = x_0,..., \omega_{i+k} = x_k;\ L_n^{2,\eta} = P_n\}$ we let for all $x, y \in E$

$$f_n^1(x, y) := \sum_{j=-n}^{i-2} \delta_{(\omega_j, \omega_{j+1})}(x, y) + \delta_{(u_n, \omega_{-n})}(x, y) + \delta_{(\omega_{i-1}, x_0)}(x, y)$$

be the frequency of the pairs (x, y) in $\omega \in \Omega_{\Lambda_n^1}$ with boundary $\eta^1 \in \Omega$ and

$$f_n^2(x, y) := f(x, y) - k(x, y) - f_n^1(x, y)$$

the frequency of the pairs (x, y) in Λ_n^2 with boundary $\eta^2 \in \Omega$. The associated pair measure P_n^1 is defined by $P_n^1(x, y) := f_n^1(x, y)/v_n^1$ for all $x, y \in E$ with $v_n^1 := n + i + 1$ and with properties analogous to (3.13)–(3.15):

(i) $v_n^1 P_n^1(x, y) \in \mathbb{Z}^+$ for all $x, y \in E$; $\bar{P}_n^1 - \bar{\bar{P}}_n^1 = \frac{1}{v_n^1}(\delta_u - \delta_{x_0})$, $n \in \mathbb{N}$

(ii) there exist an ordering (3.15) for the elements of $D(P_n^1) \cup \{x_0\}$.

We get the pair measure

$$P_n^2(x, y) := \frac{f(x, y) - k(x, y) - f_n^1(x, y)}{v_n^2} \quad \text{for all } x, y \in E \text{ and for all } n \in \mathbb{N},$$

depending on P_n^1 with $v_n^2 := n - i - k + 1$. The so defined pair measures have analogous properties to (i) and (ii). We have to sum the products

$$\sharp\{\omega \in \Omega_{\Lambda_n} : L^{2, \eta^1}_{\{n+i+1\}}(\omega) = P_n^1\} \sharp\{\omega \in \Omega_{\Lambda_n} : L^{2, \eta^2}_{\{n-i-k+1\}}(\omega) = P_n^2\}$$

over all possible pair measures P_n^1. Because of $f_n^2(x, y) \geqslant 0$ we need

$$f_n^1(x, y) \leqslant v_n P_n(x, y) - k(x, y) \qquad \text{for all} \quad x, y \in E$$

and define

$$U(n) := \left\{ Q \in \mathscr{P}(E^2) : v_n^1 Q \in \mathbb{Z}_+^{E \times E};\, Q \leqslant \frac{v_n P_n - k}{v_n^1},\, \bar{Q} - \bar{\bar{Q}} = \frac{1}{v_n^1}(\delta_u - \delta_{x_0}) \right\}.$$

The set $U(n)$ is finite and from (4.24) we thus get the sum over $P_n^1 \in U(n)$

$$\begin{aligned} &M^{\eta}_{n, P_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k) \\ &= \sum_{P_n^1 \in U(n)} \frac{|T^{\eta_1^1}_{\Lambda_n^1}(P_n^1)|\, |T^{\eta_2^2}_{\Lambda_n^2}(P_n^2)|}{|T^{\eta}_n(P_n)|} \\ &= \sum_{P_n^1 \in U(n)} \frac{B^*_{x_0, u}(P_n^1) \prod_{x \in E} \left(\frac{\bar{f}_n^1(x)!}{\prod_{y \in E} f_n^1(x, y)!} \right) B^*_{s, x_k}(P_n^2) \prod_{x \in E} \left(\frac{\bar{f}_n^2(x)!}{\prod_{y \in E} f_n^2(x, y)!} \right)}{B^*_{s, u}(P_n) \prod_{x \in E} \left(\frac{\bar{f}(x)!}{\prod_{y \in E} f(x, y)!} \right)} \end{aligned}$$

We want to approximate the last sum by means of Stirling's formula. We first show that the terms outside a neighborhood of P_n vanish.

4.25. Lemma. Let $\mathscr{U}(P_n)$ be a neighborhood of P_n with $\mathscr{U}(P_n) \subset U(n)$. Then in the sum for $M^{\eta}_{n, P_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k)$ the terms outside $\mathscr{U}(P_n)$ vanish in the limit $n \to \infty$.

Proof. From Lemma 3.23 we conclude with the conditional entropy $S(P) = \mathscr{H}(P) - \mathscr{H}(\bar{P})$:

$$(4.26) \quad \frac{|T^{\eta^1}_{\Lambda^1_n}(P^1_n)|\, |T^{\eta^2}_{\Lambda^2_n}(P^2_n)|}{|T^{\eta}_n(P_n)|} \leqslant \frac{\exp\{v^1_n S(P^1_n)\} \exp\{v^2_n S(P^2_n)\}}{\exp\{v_n S(P_n) - (|E|^2 + |E|) \log v_n\}}$$
$$= v_n^{|E|^2+|E|} \exp\{(i+1)\, S(P^1_n) - (i+k-1)\, S(P^2_n)\}$$
$$\times \exp\{n(S(P^1_n) + S(P^2_n) - 2S(P_n)\}.$$

Outside the neighborhood $\mathscr{U}(P_n)$ of P_n we find (see Lemma 4.33) a $\xi > 0$ with:

$$\exp\{n(S(P^1_n) + S(P^2_n) - 2S(P_n)\} \leqslant e^{-n\xi}.$$

Since $S(P^i_n) \leqslant \log |E|$, $i = 1, 2$, we find a constant C with:

$$\sum_{P^1_n \notin \mathscr{U}(P_n)} \frac{|T^{\eta^1}_{\Lambda^1_n}(P^1_n)|\, |T^{\eta^2}_{\Lambda^2_n}(P^2_n)|}{|T^{\eta}_n(P_n)|} \leqslant C \sum_{P^1_n \notin \mathscr{U}(P_n)} v_n^{|E|^2+|E|} e^{-n\xi} \to 0 \qquad \text{for} \quad n \to \infty,$$

because the number of terms is a power of n. ∎

Since $P_n \to P$ for $n \to \infty$ and P is positive we can assume that there exists an $\alpha > 0$ with

$$P_n(x, y) > \alpha > 0 \quad \text{for all } x, y \in E \quad \text{and for all } n \in \mathbb{N}.$$

With

$$r_n(P^1_n) := \frac{B^*_{x_0, u}(P^1_n)\, B^*_{s, x_k}(P^2_n)}{B^*_{s, u}(P_n)}$$

and the Stirling approximation we find by collecting terms

$$M_n = \sum_{P^1_n \in \mathscr{U}(P_n)} r_n(P^1_n) \prod_{x \in E} \left(\frac{\bar{f}^1_n(x)!\, \bar{f}^2_n(x)! \prod_{y \in E} f(x, y)!}{\bar{f}(x)! \prod_{y \in E} f^1_n(x, y)!\, f^2_n(x, y)!} \right)$$
$$= \sum_{P^1_n \in U(n)} (2\pi n)^{-v/2}\, g(P^1_n)\, K_n(P^1_n) \exp\{n \mathscr{S}_n(P^1_n)\},$$

where $v := |E|^2 - |E|$ and M_n is defined by $M^{\eta}_{n,P_n}(\pi_i = x_0,\ldots, \pi_{i+k} = x_k) = M_n + o(1)$. The function $K_n(Q)$ is coming from all errors of the Stirling approximation and satisfies

$$\sup_{Q\in\mathscr{U}(P_n)} |K_n(Q) - 1| \to 0 \qquad \text{for} \quad n \to \infty,$$

the function g is defined by

$$g(Q) := 2^{\frac{v}{2}} \left(\frac{B^*_{x_0,x_0}(Q)\, B^*_{s,s}(2P - Q)}{B^*_{s,s}(P)} \right)$$
$$\times \prod_{x\in E} \left\{ \left(\frac{\bar{Q}(x)(2\bar{P}(x) - \bar{Q}(x)) \prod_{y\in E} P(x,y)}{\bar{P}(x) \prod_{y\in E} Q(x,y)(2P(x,y) - Q(x,y))} \right)^{\frac{1}{2}} \right.$$
$$\left. \times \left(\frac{\bar{Q}(x)^{(i+1)\bar{Q}(x)} (2\bar{P}(x) - \bar{Q}(x))^{2\bar{P}(x) - \bar{k}(x) - (i+1)\bar{Q}(x)} \prod_{y\in E} P(x,y)^{2P(x,y)}}{\bar{P}(x)^{2\bar{P}(x)} \prod_{y\in E} (Q(x,y)^{(i+1)Q(x,y)} (2P(x,y) - Q(x,y))^{2P(x,y) - k(x,y) - (i+1)Q(x,y)}} \right) \right\},$$

and the function $\mathscr{S}_n$ is defined by

$$\mathscr{S}_n(Q) := S(Q) + S(2P_n - Q) - 2S(P_n)$$

for all $Q \in \mathscr{U}(P_n)$, if $\mathscr{U}(P_n)$ is sufficient small such that we have $Q \leqslant 2P_n$ for all $Q \in \mathscr{U}(P_n)$.

4.2. The Laplace Method

We want to calculate the last sum for $M^{\eta}_{n,P_n}(\pi_i = x_0,\ldots, \pi_{i+k} = x_k)$ with the Laplace method. The function $\mathscr{S}_n$ and its limit $\mathscr{S}$ with $\mathscr{S}(Q) := S(Q) + S(2P - Q) - 2S(P)$, which is defined for all $Q \in U := \{Q \in \widetilde{\mathscr{P}}(E^2) : Q \leqslant 2P\}$, are concave. For $\mathscr{S}$ we have

$$\mathscr{S}(Q) \leqslant 0 \quad \text{for all } \; Q\in U \quad \text{ and } \quad \mathscr{S}(Q) = 0 \Leftrightarrow Q = P.$$

The same holds for the functions $\mathscr{S}_n$, $n \in \mathbb{N}$. We want to express the pair measure $Q \in \mathscr{U}(P_n)$ by an v-dimensional vector. This is possible because our pair measures have approximatively identical marginals, i.e., $\bar{\bar{Q}} = \bar{Q} - \frac{1}{v_n^1}(\delta_u - \delta_{x_0})$. Thus every pair measure $Q \in \mathscr{U}(P_n)$ corresponds to the pair measure $\tilde{Q} = \frac{1}{v_n^1}(v_n^1 Q + \delta_{u,x_0})$ with identical marginals. We have the mapping $\varphi\colon \widetilde{\mathscr{P}}(E^2) \to \mathbb{R}^v$ on the v-dimensional coordinates and define the following sets, where we identify the set of probability measures with the corresponding set in $\mathbb{R}^v$:

(a) The lattice $G(n) := \{Q \in \mathbb{R}^\nu : \text{there exist a } Q \in \mathcal{U}(P_n) \cap U(n) \text{ with } Q = \varphi(\tilde{Q})\}$

(b) $G_n := \{Q \in \mathbb{R}^\nu : \text{there exist a } Q \in \mathcal{U}(P_n) \text{ with } Q = \varphi(\tilde{Q})\}$

(c) $G := \{Q \in \mathbb{R}^\nu : \text{there exist a } Q \in U \text{ with } Q = \varphi(\tilde{Q})\}$

In order to use the Laplace method we write

$$\begin{aligned} M_n &= \sum_{Q \in G(n)} (2\pi n)^{-\nu/2} g(Q) K_n(Q) \exp\{n\mathcal{S}_n(Q)\} \\ &= n^{\frac{\nu}{2}} \int_{G_n} dQ (2\pi)^{-\nu/2} g(Q) K_n(Q) \exp\{n\mathcal{S}_n(Q)\} + R_1(n) \end{aligned}$$

with an error term $R_1(n)$ coming from the integral approximation. We identify the measure P_n with their ν-dimensional variable $P_n \in G_n$ (resp. the measure P with $P \in G$). The essential part of the integral is in a neighborhood of $P_n \in G_n$. We can choose a $\delta > 0$ independently of $n \in \mathbb{N}$, such that

$$\mathcal{U}_\delta(P_n) \subset G_n, \quad \mathcal{U}_\delta(P_n) \ni P \quad \text{and} \quad \mathcal{U}_\delta(P_n) \subset \mathcal{U}_{2\delta}(P)$$

for sufficiently large $n \in \mathbb{N}$. We decompose the last integral into the two contributions

$$I(\delta, n) := \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}} \int_{\mathcal{U}_\delta(P_n)} dQ\, g(Q) K_n(Q) \exp\{n\mathcal{S}_n(Q)\}$$

and

$$R_2(n, \delta) := \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}} \int_{G_n \setminus \mathcal{U}_\delta(P_n)} dQ\, g(Q) K_n(Q) \exp\{n\mathcal{S}_n(Q)\}.$$

To control the first term we expand $\mathcal{S}_n$ in a Taylor series around the maximum point up to second order. Let $\mathbf{H}_n$ be the Hessian matrix for $\mathcal{S}_n$ in the maximum point P_n and let

$$r(\delta) := \max_{S \in \bar{\mathcal{U}}_\delta(P)} \{|r(S)|\}$$

be the bound of the error terms in the Taylor expansion, which is bounded independently of $n \in \mathbb{N}$ because of the uniform convergence of the integrand in the compact set $\bar{\mathscr{U}}_\delta(P)$. The Hessian matrix is negative definite and we get the inequality:

$$(S-P_n)^t\,(\mathbf{H}_n - r(\delta)\,\mathbf{id})(S-P_n) \leqslant 2\mathscr{S}_n(S) \leqslant (S-P_n)^t\,(\mathbf{H}_n + r(\delta)\,\mathbf{id})(S-P_n).$$

Using the abbreviations

$$g_n^+ := \max_{S \in \overline{\mathscr{U}_\delta(P)}} \{g(S)\,K_n(S)\}, \qquad g_n^- := \min_{S \in \overline{\mathscr{U}_\delta(P)}} \{g(S)\,K_n(S)\},$$

we conclude further that $I(\delta, n)$ is sandwiched between the integrals

$$I^{\pm}(\delta, n) := g_n^{\pm} \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}} \int_{\mathscr{U}_\delta(P)} dS \exp\left\{\frac{n}{2}\left((S-P_n)^t\,(\mathbf{H}_n \pm r(\delta)\,\mathbf{id})(S-P_n)\right)\right\}.$$

We can calculate the Gaussian integral and find

$$I^+(\delta, n) \leqslant g_n^+ / \sqrt{\det(-\mathbf{H}_n - r(\delta)\,\mathbf{id})} \qquad \text{and}$$

$$I^-(\delta, n) \geqslant g_n^- / \sqrt{\det(-\mathbf{H}_n + r(\delta)\,\mathbf{id})} - \frac{g_n^-}{2\pi^{\frac{\nu}{2}}}\, I_3(\delta, n)$$

with

$$I_3(\delta, n) := n^{\frac{\nu}{2}} \int_{\mathbb{R}^\nu \setminus \mathscr{U}_\delta(P)} dS \exp\left\{\frac{n}{2}\left((S-P_n)^t\,(\mathbf{H}_n - r(\delta)\,\mathbf{id})(S-P_n)\right)\right\}$$

outside the neighborhood $\mathscr{U}_\delta(P)$. We will show in Lemma 4.32 that

$$R_3(n, \delta) := \left(\frac{g_n^-}{(2\pi)^{\frac{\nu}{2}}}\right)\left(\frac{\sqrt{\det(-\mathbf{H})}}{g(P)}\right) I_3(\delta, n)$$

converges to zero, where $\mathbf{H}$ is the Hessian of $\mathscr{S}$ in the maximum point P and where we changed back to the old variables. Using the uniform convergence of $(K_n)_{n \in \mathbb{N}}$ on $\bar{\mathscr{U}}_\delta(P)$ we thus obtain the following result.

4.27. Proposition. For all $\varepsilon > 0$ there exist a $\delta(\varepsilon) > 0$ and a $n(\varepsilon, \delta) \in \mathbb{N}$ with

$$-\varepsilon + 1 < \frac{I(\delta, n)\,\sqrt{\det(-\mathbf{H})}}{g(P)} < 1 + \varepsilon \qquad \text{for all} \quad n \geqslant n(\varepsilon).$$

We are now able to calculate the cylinder probabilities. We conclude from Proposition 4.27 and the preceding results

$$M^{\eta}_{n,P_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k) = R_1(n) + R_2(n, \delta) + I(\delta, n) + o(1).$$

We have two convergence schemes. On the one hand the functions $(\mathcal{S}_n)_{n\in\mathbb{N}}$ and the the Hessian $(\mathbf{H}_n)_{n\in\mathbb{N}}$ converge for $n\to\infty$. On the other hand we can choose $\delta(\varepsilon)>0$ so small that the error in the Taylor expansion of $\mathcal{S}_n$ is kept small enough. Combining this with the uniform convergence of the functions K_n and $\mathcal{S}_n$ we obtain the following result.

4.28. Proposition. For all $\eta \in \Omega \cup \{\text{per}, \text{free}\}$ and $P_n \to P$ for $n\to\infty$ the cylinder probability converges, i.e.,

$$M^{\eta}_{n,P_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k) \to \frac{g(P)}{\sqrt{\det(-\mathbf{H})}} \qquad \text{for} \quad n\to\infty.$$

Theorem 2.6 will be proved once we have shown that the limit is the cylinder probability of the stationary Markov chain with marginal P.

4.29. Proposition. The equality

$$\frac{g(P)}{\sqrt{\det(-\mathbf{H})}} = \nu_P(\pi_i = x_0, \ldots, \pi_{i+k} = x_k)$$

holds.

Proof. The value of g at the maximum point P is

$$\begin{aligned} g(P) &= 2^{\nu/2}\bar{P}(x_0)\prod_{j=0}^{k-1}\left(\frac{P(x_j, x_{j+1})}{\bar{P}(x_j)}\right)\sqrt{\prod_{x\in E}\Big(\bar{P}(x)\prod_{y\in E}P(x,y)\Big)}^{\,-1} \\ &\quad \times \sum_{v\in\Upsilon}\prod_{x\in E\setminus\{x_0\}} P(x, v(x)) \\ &= \nu_P(\pi_i = x_0, \ldots, \pi_{i+k} = x_k)\sqrt{\prod_{x\in E}\Big(\bar{P}(x)\prod_{y\in E}P(x,y)\Big)}^{\,-1} \\ &\quad \times \sum_{v\in\Upsilon}\prod_{x\in E\setminus\{x_0\}} P(x, v(x)). \end{aligned}$$

From Theorem I.13 in ref. 19 we know that the number of spanning trees t_y oriented towards $y\in E$ is independent of y. Therefore the sum

$$\sum_{v \in \Upsilon} \prod_{x \in E \setminus \{x_0\}} P_n(x, v(x)) = \prod_{x \in E \setminus \{x_0\}} \bar{P}_n(x) \frac{t_{x_0}}{\prod_{x \in E \setminus \{x_0\}} \bar{m}(x)}$$
$$= t_{x_0} v_n^{|E|-1}$$

does not depend explicitly on x_0. This holds also in the limit $P_n \to P$ for $n \to \infty$. Thus we have $g(P) = v_p(\pi_i = x_0,..., \pi_{i+k} = x_k)\, G$ with some constant G. Since probabilities are normalized, we must have $G/\sqrt{\det(-\mathbf{H})} = 1$. This gives the result. ▮

4.3. Error Estimates

In the next lemmas we show first the uniform convergence of $(\mathscr{S}_n)_{n \in \mathbb{N}}$ and then estimate our different error terms.

4.30. Lemma. The sequence $(\mathscr{S}_n)_{n \in \mathbb{N}}$ converges uniformly to the function $\mathscr{S}$.

Proof. This follows readily from the uniform continuity of the entropy $\mathscr{H}$, cf. ref. 25, Lemma I.2.5. ▮

In the next lemma we show that the integral outside of a neighborhood of the maximum point vanishes in the limit.

4.31. Lemma. Let $\delta > 0$ and

$$R_2(n, \delta) := \left(\frac{n}{2\pi}\right)^{\frac{v}{2}} \int_{G_n \setminus \mathscr{U}_\delta(P_n)} dQ\, g(Q)\, K_n(Q)\, e^{n\mathscr{S}_n(Q)}.$$

Then for every $\varepsilon > 0$ there exists a $n(\varepsilon) \in \mathbb{N}$ with $|R_2(n, \delta)| < \varepsilon$ for all $n \geqslant n(\varepsilon)$.

Proof. There exist a $n_0 \in \mathbb{N}$ with

$$\mathscr{U}_{\frac{\delta}{2}}(P) \subset \mathscr{U}_\delta(P_n) \qquad \text{for all} \quad n \geqslant n_0,$$

and replacing G by a small neighborhood we can assume that $G_n \subset G$ for sufficiently large $n \in \mathbb{N}$, hence

$$|R_2(n, \delta)| \leqslant \left(\frac{n}{2\pi}\right)^{\frac{v}{2}} \int_{G \setminus \mathscr{U}_{\frac{\delta}{2}}(P)} dQ\, 1_{G_n}(Q)\, g(Q)\, K_n(Q)\, e^{n\mathscr{S}_n(Q)}$$

for all $n \geqslant n_0$. Next, we have

$$\sup_{Q \in G \setminus \mathcal{U}_{\frac{\delta}{2}}(P)} \{\mathcal{S}_n(Q)\} \leqslant \sup_{Q \in G \setminus \mathcal{U}_{\frac{\delta}{2}}(P)} \{|\mathcal{S}_n(Q) - \mathcal{S}(Q)| + \mathcal{S}(Q)\}$$

and $\alpha(\delta) := \max_{Q \in G \setminus \mathcal{U}_{\frac{\delta}{2}}(P)} \{\mathcal{S}(Q)\} < 0$ because of the concavity of $\mathcal{S}$. Hence

$$|R_2(n, \delta)| \leqslant \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}} \int_{G \setminus \mathcal{U}_{\frac{\delta}{2}}(P)} dQ \, 1_{G_n}(Q) \, g(Q) \, K_n(Q) \, e^{-n\xi}$$

with $\xi = \alpha(\delta)/2$ when n is large enough. Finally the inequality (4.26) implies that gK_n is bounded outside the neighborhood of the maximum point. The lemma thus follows from the dominated convergence theorem. ▮

4.32. Lemma. Let

$$R_3(n, \delta) := \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}} \frac{g_n^-}{g(P)} \sqrt{\det(-\mathbf{H})}$$
$$\times \int_{\mathbb{R}^\nu \setminus \mathcal{U}_\delta(P)} dS \exp\left\{-\frac{n}{2} [(S - P_n)^T (\mathbf{H}_n - r(\delta) \, \mathbf{id})(S - P_n)]\right\}.$$

Then there exist for any $\varepsilon > 0$ a $\delta > 0$ and a $n(\varepsilon) \in \mathbb{N}$ with $|R_3(n, \delta)| < \varepsilon$ for all $n \geqslant n(\varepsilon)$.

Proof. The symmetric matrix $(-\mathbf{H}_n + r(\delta) \, \mathbf{id})$ is positive definite. Therefore the smallest eigenvalue $\lambda_{\min}(n) > 0$ is positive and $\lambda(n)_{\min}$ converges to the smallest eigenvalue of $(-\mathbf{H} + r(\delta) \, \mathbf{id})$ as $n \to \infty$. Hence $(S - P_n)^T (\mathbf{H}_n - r(\delta) \, \mathbf{id})(S - P_n) \geqslant \gamma \, |S - P|^2$ for some $\gamma > 0$ and all sufficiently large n. This gives

$$|R_3(n, \delta)| \leqslant \left(\frac{g_n^-}{g(P)}\right) \sqrt{\det(-\mathbf{H})} \left(\frac{n}{2\pi}\right)^{\frac{\nu}{2}}$$
$$\times \int_{\mathbb{R}^\nu \setminus \mathcal{U}_\delta(P)} dS \exp\left\{-\frac{n}{2} \gamma (S - P)^T (S - P)\right\}.$$

By Chebyshev's inequality, the last term vanishes in the limit $n \to \infty$. ▮

Next we treat the error in the integral approximation.

4.33. Lemma. Let

$$R_1(n) := n^{\frac{\nu}{2}} \Bigg(\sum_{Q \in G(n)} \frac{g(Q)\, K_n(Q)}{(n^2)^{\nu/2}} \exp\{n\mathcal{S}_n(Q)\}$$
$$- \int_{G_n} dQ\, g(Q)\, K_n(Q) \exp\{n\mathcal{S}_n(Q)\} \Bigg).$$

Then $R_1(n) \to 0$ as $n \to \infty$.

Proof. We split R_1 into two terms corresponding to the error outside and inside the neighborhood of the maximum point P_n. In the following let $\mathcal{U}_n := \mathcal{U}_\delta(P_n)$ and define $\mathcal{U}(n) := G(n) \cap \mathcal{U}_n$ for the lattice.

The estimation outside $\mathcal{U}_n$ is similar to Lemma 4.31 for the sum and the integral. In the following we take $\mathbf{H}_n^- := -\mathbf{H}_n(P_n) + r(\delta)\, \mathbf{id}$ and $\mathbf{H}_n^+ := -\mathbf{H}_n(P_n) - r(\delta)\, \mathbf{id}$ and $\delta > 0$ small enough for $\mathbf{H}_n^+$ being positive definite. We get

$$g_n^- n^{\nu/2} \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^-(Q-P_n)}$$
$$\leqslant n^{\nu/2} \int_{\mathcal{U}_n} dQ\, g(Q-P_n)\, K_n(Q-P_n)\, e^{n\mathcal{S}_n(Q-P_n)}$$
$$\leqslant g_n^+ n^{\nu/2} \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^+(Q-P_n)}$$

for the integral and similarly for the sum over $Q \in G(n)$. Since $g_n^+/g_n^- \to 1$ for $n \to \infty$ and δ small enough we therefore only need to estimate the differences

$$S_n^\pm := n^{\nu/2} \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^\pm(Q-P_n)} - n^{\nu/2} \sum_{Q \in \mathcal{U}(n)} \frac{1}{n^\nu} e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^\mp(Q-P_n)}.$$

Now

(4.34)
$$R_1(n)|_{\mathcal{U}_n} \leqslant n^{\nu/2} \Bigg(\int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^-(Q-P_n)} - \sum_{Q \in \mathcal{U}(n)} \frac{1}{n^\nu} e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^-(Q-P_n)} \Bigg)$$
$$+ n^{\nu/2} \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^-(Q-P_n)}$$
$$n^{\nu/2} \Bigg(\int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^+(Q-P_n)} - \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n^-(Q-P_n)} \Bigg).$$

We have to estimate every term in (4.34). We sketch here the proof for the first term: In the following we write $\mathbf{H}_n$ instead of $\mathbf{H}_n^-$. Consider the mapping

$$\Psi\colon \mathcal{U}_n \to \Psi(\mathcal{U}_n), \qquad Q \mapsto \sqrt{\left(\frac{n}{2}\right)}\,\mathbf{H}_n^{\frac{1}{2}}(Q-P_n)$$

with inverse

$$\Psi^{-1}\colon \Psi(\mathcal{U}_n) \to \mathcal{U}_n, \qquad T \mapsto \sqrt{\left(\frac{2}{n}\right)}\,\mathbf{H}_n^{-\frac{1}{2}}\,(T+P_n)$$

and Jacobian

$$|\det D\Psi^{-1}| = \left(\frac{2}{n}\right)^{\frac{\nu}{2}} \frac{1}{\sqrt{\det \mathbf{H}_n}}.$$

Transforming the integral we obtain

$$n^{\nu/2} \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n (Q-P_n)} = \int_{\Psi(\mathcal{U}_n)} dT\, \frac{e^{-(T+P_n)^T (T+P_n)}}{\sqrt{\det \mathbf{H}_n}}.$$

The lattice $\mathcal{U}(n) \subset G(n)$ is transformed to the parallelepiped lattice $\Psi(\mathcal{U}(n))$. The volume V_n of an elementary parallelepiped is

$$\begin{aligned} V_n &= \det\left(\Psi\left(\frac{\mathbf{e}_1}{n}\right),\ldots,\Psi\left(\frac{\mathbf{e}_\nu}{n}\right)\right) = \left(\frac{1}{2n}\right)^{\nu/2} \det(\mathbf{H}_n^{1/2}) \\ &= \left(\frac{1}{2n}\right)^{\frac{\nu}{2}} \sqrt{\det \mathbf{H}_n}. \end{aligned}$$

Hence

$$\sum_{Q \in \mathcal{U}(n)} \frac{1}{n^\nu} e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n (Q-P_n)} = \sum_{T^n \in \Psi(\mathcal{U}(n))} \left(\frac{2}{n}\right)^{\frac{\nu}{2}} \frac{V_n}{\sqrt{\det \mathbf{H}_n}}\, e^{-(T^n+P_n)^T (T^n+P_n)}.$$

The vector $T^n \in \Psi(\mathcal{U}(n))$ is a vertex of an elementary parallelepiped $P(T^n)$. Therefore

$$\begin{aligned} & n^{\nu/2} \left| \int_{\mathcal{U}_n} dQ\, e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n (Q-P_n)} - \sum_{Q \in \mathcal{U}(n)} \frac{e^{-\frac{n}{2}(Q-P_n)^T \mathbf{H}_n (Q-P_n)}}{n^\nu} \right| \\ & \leqslant \sum_{T^n \in \Psi(\mathcal{U}(n))} \frac{1}{\sqrt{\det \mathbf{H}_n}} \int_{P(T^n)} dT\, e^{-|T+P_n|^2} \left|1 - e^{|T+P_n|^2 - |T^n+P_n|^2}\right|. \end{aligned}$$

As the modulus in the last term converges to zero uniformly in n, the last expression tends to zero as $n \to \infty$. The other terms in (4.34) are estimated similar to Lemma 4.32. ▮

5. PROOF OF THEOREM 2.8

To prove the theorem we need the following large deviation result.

5.35. Definition. (i) Let λ be an *a priori* measure on E. The relative entropy $H(Q; \bar{Q} \otimes \lambda)$ of a probability measure $Q \in \mathscr{P}(E^2)$ and $\bar{Q} \otimes \lambda$ is

$$H(Q; \bar{Q} \otimes \lambda) := \sum_{x, y \in E} Q(x, y) \log \frac{Q(x, y)}{\bar{Q}(x) \lambda(y)}.$$

(ii) Let $\varnothing \neq \Pi \subset \widetilde{\mathscr{P}}(E^2)$ closed. A pair measure $P^* \in \Pi$ is called minimal measure for the set Π, if

$$H(P^*; \bar{P}^* \otimes \lambda) = \min_{Q \in \Pi} H(Q; \bar{Q} \otimes \lambda),$$

i.e., it maximizes the entropy on Π.

If λ is the counting measure on E the relative entropy is the negative conditional entropy: $H(Q; \bar{Q} \otimes \lambda) = -S(P) = \mathscr{H}(P) - \mathscr{H}(\bar{P})$. The following proposition establishes a large deviation result for the empirical pair measure with arbitrary boundary conditions.

5.36. Proposition. Let $\varnothing \neq \Pi \subset \widetilde{\mathscr{P}}(E^2)$ with $\Pi = \Pi_0 \cap \widetilde{\mathscr{P}}(E^2)$ for $\Pi_0 \subset \mathscr{P}(E^2)$ with $\Pi_0 \subset \mathring{\Pi}_0$ and $\eta \in \Omega \cup \{\text{per, free}\}$. Then the limit

$$\lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log \lambda^{\Lambda_n}(L_n^{2,\eta} \in \Pi) = -\inf_{Q \in \Pi} H(Q; \bar{Q} \otimes \lambda) = -\min_{Q \in \bar{\Pi}} H(Q; \bar{Q} \otimes \lambda)$$

exists.

Proof. The proof for the pair empirical measure with periodic boundary condition is given in ref. 27, Chapter I. Let $\mathscr{P}_n^\eta$ the set of pair measures with non-empty pair type class. Then $|\mathscr{P}_n^\eta| \leqslant v_n^{|E|^2}$, and therefore

$$\begin{aligned}\lambda^{\Lambda_n}(L_n^{2,\eta} \in \Pi) &= \sum_{Q \in \Pi \cap \mathscr{P}_n^\eta} \lambda^{\Lambda_n}(L_n^{2,\eta} = Q) \\ &\leqslant v_n^{|E|^2} \exp\{-v_n \min_{Q \in \Pi \cap \mathscr{P}_n^\eta} H(Q; \bar{Q} \otimes \lambda)\}.\end{aligned}$$

Similarly,

$$\lambda^{\Lambda_n}(L_n^{2,\eta} \in \Pi) \geqslant \max_{Q \in \Pi \cap \mathscr{P}_n^\eta} \lambda^{\Lambda_n}(L_n^{2,\eta} = Q)$$
$$\geqslant v^{-|E|^2-|E|} \exp\{-v_n \min_{Q \in \Pi \cap \mathscr{P}_n^\eta} H(Q; \bar{Q} \otimes \lambda)\}.$$

It is therefore sufficient to show that

$$\lim_{n \to \infty} \min_{Q \in \Pi \cap \mathscr{P}_n^\eta} H(Q; \bar{Q} \otimes \lambda) = \inf_{Q \in \Pi} H(Q; \bar{Q} \otimes \lambda) = \min_{Q \in \bar{\Pi}} H(Q; \bar{Q} \otimes \lambda)$$

holds. This will follow once we have shown that

$$\limsup_{n \to \infty} \min_{Q \in \Pi \cap \mathscr{P}_n^\eta} H(Q; \bar{Q} \otimes \lambda) \leqslant \min_{Q \in \bar{\Pi}} H(Q; \bar{Q} \otimes \lambda)$$

holds. The latter, however, follows from the assumptions on Π and standard continuity arguments. ∎

Now we are able to prove our Theorem 2.8. We take $D := H(P^*; \bar{P}^* \otimes \lambda) = \min_{Q \in \overline{\Pi_f^\Delta}} H(Q; \bar{Q} \otimes \lambda)$ if P^* is the minimal measure and

$$\Pi^\varepsilon := \{Q \in \bar{\Pi}_f^\Delta : \|Q - P^*\| \geqslant \varepsilon\}$$

for an arbitrary $\varepsilon > 0$. Since Π^ε is compact, $D^\varepsilon := \min_{Q \in \Pi^\varepsilon} H(Q; \bar{Q} \otimes \lambda) > D > 0$. Proposition 5.36 thus gives

$$\frac{1}{v_n} \log \lambda^{\Lambda_n}(\max_{x, y \in E} |L_n^{2,\eta}(x, y) - P^*(x, y)| \geqslant \varepsilon \mid L_n^{2,\eta} \in \Pi_f^\Delta) \to -D^\varepsilon + D < 0$$

for $n \to \infty$, and therefore

$$M_{n,f,\Delta}^\eta(\|L_n^\eta - P^*\| \geqslant \varepsilon) \to 0 \qquad \text{for} \quad n \to \infty.$$

On the other hand the uniform convergence of $\lambda^{\Lambda_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k \mid L_n^{2,\eta} = P)$ to $\bar{P}(x_0) \prod_{j=0}^{k-1} \frac{P(x_j, x_{j+1})}{\bar{P}(x_j)}$ implies the following corollary:

5.37. Corollary. For every $\varepsilon > 0$, $i \in \mathbb{Z}$ and $k \in \mathbb{N}$ there exist a $\zeta > 0$ and a $n_0 \in \mathbb{N}$, such that for all $x_0, \ldots, x_k \in E$

$$\left| \lambda^{\Lambda_n}(\pi_i = x_0, \ldots, \pi_{i+k} = x_k \mid L_n^{2,\eta} = P) - \bar{P}^*(x) \prod_{j=0}^{k-1} \frac{P^*(x_j, x_{j+1})}{\bar{P}^*(x_j)} \right| < \varepsilon,$$

if $P \in \mathscr{P}_n^\eta$ and $\|P - P^*\| \leqslant \zeta$ and $n \geqslant n_0$.

The rest is routine. ∎

6. EXTENSION TO FINITE-RANGE POTENTIALS

To get the results for the k-sample case we have to count the configurations $\omega \in \Omega_{\Lambda_n}$ compatible with a given frequency of k-samples. The number of k-samples $(x_1,..., x_k)$ is $f(x_1,..., x_k) := v_n P_n(x_1,..., x_k)$. In this case G is the oriented multigraph with the $(k-1)$-sample as vertices in E^{k-1} and with $f(x_1,..., x_k)$ edges from vertex $(x_1,..., x_{k-1})$ to vertex $(x_2,..., x_k)$. If we take an extra edge from the vertex $(\eta_{n+1},..., \eta_{n+k-1})$ to the vertex $(\eta_{-n-k+1},..., \eta_{-n-1})$ the graph is simple and connected because of our assumption on the measure P_n. This multigraph corresponds to the multigraph for the pair empirical measure if we identify every k-sample $(x_1,..., x_k)$ with the ordered pair

$$(x_1,..., x_{k-1}; x_2,..., x_k) \in E^{k-1} \times E^{k-1}.$$

Thus the proceeding proofs for the pair empirical measure are applicable and we get as limit measure a Markov chain with transition matrix $(\tilde{Q}(\bar{x}, \bar{y}))_{\bar{x}, \bar{y} \in E^{k-1}}$, where $\tilde{Q}(\bar{x}, \bar{y}) = 0$ except when $(x_2,..., x_k) = (y_1,..., y_{k-1})$, and in this case

$$\tilde{Q}(x_1,..., x_{k-1}, x_2,..., x_k) = \frac{P(x_1,..., x_k)}{\bar{P}(x_1,..., x_{k-1})}.$$

This Markov chain on E^{k-1} is of order 1. We get a transition matrix Q on E of order k by setting

$$Q(x_1,..., x_{k-1}; x_k) := \tilde{Q}(x_1,..., x_{k-1}; x_2,..., x_k).$$

This associated stationary k-order Markov chain is the unique Gibbs measure for the pure k-body potential ϕ^{Q_P}. ▮

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