2022

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Oluwadara Ogunkoya
University Of Alabama At Birmingham

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by

OLUWADARA OGUNKOYA

SHANNON STARR, COMMITTEE CHAIR
DAVID HALPERN
RYOICHI KAWAI
NANDOR SIMANYI
DONGSHENG WU

A DISSERTATION

Submitted to the graduate faculty of The University of Alabama at Birmingham,
in partial fulfillment of the requirements of the degree of
Doctor of Philosophy

BIRMINGHAM, ALABAMA

2022

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OLUWADARA OGUNKOYA

APPLIED MATHEMATICS

ABSTRACT

The first part of this thesis covers some of the background materials that are prerequisite to doing research in many body particle problems. The definitions are given from a mathematical point of view and the proofs to most of the results were not included since they can be found in standard texts.

The second part was done with Christoph Fischbacher. Here, we consider the Heisenberg XXZ spin-J chain ($J \in \mathbb{N}/2$) with anisotropy parameter Δ. Assuming that $\Delta > 2J$ (a necessary but not sufficient condition), and introducing threshold energies $E_K := K\left(1 - \frac{2J}{\Delta}\right)$, we show that the bipartite entanglement entropy (EE) of states belonging to any spectral subspace with energy less than E_{K+1} satisfy a logarithmically corrected area law with prefactor $(2\lfloor K/J \rfloor - 2)$.

The third part is based on work done with Shannon Starr. We considered a spin-1/2 XXZ chain on the 1-D lattice of size N (even) and gave a lower bound for the 'Emptiness Formation Probability' when the anisotropy parameter $\Delta < 0$. Also, we gave a slightly modified result for the upper bound of the 'Emptiness Formation Probability' for the case $\Delta < 1$ as seen in [9].

ACKNOWLEDGEMENTS

My sincere gratitude goes to the God, the giver of life, intellect and grace.

I express my profound thanks to my supervisor; Shannon Starr(Ph.d) for his contributions and for the time spent discussing his ideas to make this work a success. Also, I want to thank Christoph Fischbacher for working together with me on half of the work in this thesis and dedicating his time to explain how to picture entanglement entropy ideas.

I would like to acknowledge the rest of my thesis committee: Ryoichi Kawai(Phd), Nandor Simanyi(Phd), David Halpern(Phd) and Dongsheng Wu(Phd) for their judicious comments and suggestions.

My unalloyed gratitude goes to my parents: Mr. S.O. Ogunkoya and Mrs O.A. Ogunkoya who supported emotionally, prayerfully and never relented on their efforts. Moreso, I owe so much to my wonderful brothers; Olayinka Ogunkoya, Tomiwa Ogunkoya, Ayobami Ogunkoya and Adeola Ogunkoya, you all have been supportive. I appreciate Pastor Fenny Enefaa the entire members of Jesus House Birmingham, Alabama, for their prayers and well wishes.

To my colleagues and the faculties at the department of Mathematics, University of Alabama at Birmingham, with whom I have discussed my project experience and the career implication, I am deeply thankful.

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CHAPTER 1

INTRODUCTION

This thesis is comprised of two parts. Each part involves mathematical analysis to answer a question about the XXZ quantum spin system.

In the first part, the problem is to prove logarithmically-corrected area law bounds for the bipartite entanglement entropy in the spin-J XXZ ferromagnetic spin chain at all energies. This is a question that is of interest in quantum information theory. The second part of the thesis provides new general bounds for the emptiness formation probability in the ground state(s) of the spin-1/2 XXZ quantum antiferromagnet, which is a quantity of some interest to theoretical physicists.

1.1 Bipartite Entanglement Entropy of the Spin-J XXZ Quantum Ferromagnet

In the following, we prove upper bounds for the bipartite entanglement entropy of the spin–J XXZ Heisenberg chain, where $J \in \{1/2, 1, 3/2, 2 \ldots\}$. The spin–1/2 Heisenberg XXZ chain under the presence of a random magnetic field has recently attracted significant interest in the rigorous study of many–body–localization (MBL), where MBL phenomena such as exponential clustering of correlations, zero–velocity Lieb–Robinson bounds and area laws for the entanglement entropy (EE) for states from the lowest energy regime ("droplet" regime) have been shown recently in [4, 5, 10, 11], for a recent survey of these results, cf. also [31].

Recall that for one-dimensional models such as the chain, we say that the entanglement entropy satisfies an area law with respect to the bipartition of the chain into a "right" and a "left" subchain if it is uniformly bounded in the size of the subchain. While an area law is generally considered as an indicator of many-body-localization, many delocalized systems seem to exhibit a logarithmic correction, which means that the entanglement entropy scales like the logarithm of the subchain's length. See the results in [5, 14, 22, 23, 25, 26, 15, 35], where such logarithmic corrections to an area for the entanglement entropy have been obtained.

In what follows, we will adapt the ideas of Beaud and Warzel from [5], where a log–corrected area law for droplet states of the spin–1/2 Heisenberg XXZ chain for the generic case and a true area law under the presence of a disordered magnetic field was shown. With the help of technical refinements, the result here was improved to show a log–corrected energy law also for higher–energy states in [1].

While our results can certainly be viewed as a technical improvement of the spin-1/2 case, we nevertheless believe them to be of additional interest, since they demonstrate that given a discrete many–particle Schrödinger-type operator in one dimension, a logarithmically corrected area law for states in a given energy range follows if the following four criteria are met: (i) a suitable relative bound that controls the hopping operator in terms of the potential, (ii) the potential energetically favoring configurations with a lower number of "building blocks", (iii) a sufficiently low dimension of the space of these building blocks and (iv) a generalized Pauli principle that limits the amount of particles that can occupy any site.

In Section 2.1, we will introduce the model and review previous results. We recall that the Spin-J XXZ model on the chain with anisotropy parameter Δ is unitarily equivalent to a direct sum of discrete N–particle Schrödinger operators of the form $-(2\Delta)^{-1}A_N + V_N$, where A_N is a weighted adjacency operator and V_N is an interaction potential (Prop. 2.2.2). Compared to the previously studied spin-1/2 case, V_N is much more complicated and we determine the set of all its minimizing configurations for sufficiently large N (Prop. 2.2.5). Using that the kinetic term A_N is controlled by the potential V_N in the sense that $-4JV_N \leq A_N \leq 4JV_N$ (Prop. 2.2.4), we use a suitable Combes–Thomas estimate (Thm. 2.3.1) previously shown in [1], which allows as to obtain decay estimates on spectral projections (Thm. 2.3.2). This together with some previous results on estimating the entanglement entropy (Lemma 2.4.1) reduces the problem to showing bounds for the sum of all possible N-particle configurations in the subsystem weighted by their distance to the nearest configuration with sufficiently low potential (Cor. 2.5.3).

1.2 Emptiness Formation Probability of the Spin-1/2 XXZ Quantum Antiferromagnet

For the latter part of the thesis, one of the correlation functions in quantum spin chain is examined. The expectation of finding a block of sidelength L with ferromagnetic alignment in the ground state of the antiferromagnet XXZ spin chain is considered. This is known as Emptiness Formation Probability as used in [21].

We use the graphical representation of thermal equilibrium states for the XXZ quantum spin system. It is known that the model unitarily equivalent to a reflection positive model for the anisotropy parameter satisfying $\Delta \leq 0$, meaning the regime including the isotropic XY model and extending to the antiferromagnetic domain. We combine the graphical representation and reflection positivity to prove rough bounds on the emptiness formation probability, by a method which allows us to generalize an earlier result by Crawford, Ng and one of the authors, who were only able to handle the interval $-1 \leq \Delta \leq 0$ at low positive temperatures.

In [9], an interpolation of the Tóth representation (Theorem 3.3.5) and the Aisenmann-Nachtergaele representation (Theorem 3.3.9) was used to proved a lower bound for the emptiness formation probability of the XXZ spin chain in the case

$-1 \leq \Delta \leq 1$. The representation is the Aizenmann-Nachtergaele-Tóth-Uelstchi (ANTU) represenation. This relied on the Lipschitz continuity of the number of loops as a function of any individual dead-end (loop-back) or interchange process. In the case $\Delta < -1$, a Feymann-Kac approach seems evident. This is independent on the Lipschitz continuity as seen in the Aizenmann-Nachtergaele-Tóth-Uelstchi (ANTU) represenation. The lower bound for the emptiness formation is given in section (3.4.1).

For subsequent sections, a similar approach in obtaining the upper bound as in [9] was adopted which yielded a slightly modified result for the upper bound of the emptiness formation probability for the case $\Delta < 1$.

1.3 Definitions

Definition 1.3.1 *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ denote separable complex Hilbert spaces. A pair $(\mathcal{H}, \otimes)$ is called a tensor product of $\mathcal{H}_1$ and $\mathcal{H}_2$ if $\mathcal{H}$ is a Hilbert space and $\otimes$ is a bilinear mapping*

$$\otimes : \mathcal{H}_1 \times \mathcal{H}_2 \longrightarrow \mathcal{H}, \quad (\varphi, \psi) \mapsto \varphi \otimes \psi \tag{1.3.1}$$

such that the following properties hold:

(i) $\langle \varphi_1 \otimes \psi_1, \varphi_2 \otimes \psi_2 \rangle_{\mathcal{H}} = \langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}_1} \langle \psi_1, \psi_2 \rangle_{\mathcal{H}_2}$ *for all* $\varphi_1, \varphi_2 \in \mathcal{H}_1$ *and* $\psi_1, \psi_2 \in \mathcal{H}_2$.

(ii) If $\{ e_j \}_{j=1,\dots,N}$ *is an orthonormal basis of* $\mathcal{H}_1$*, and* $\{ f_k \}_{k=1,\dots,M}$ *is an orthonormal basis of* $\mathcal{H}_2$*, where* $N, M \in \mathbb{N} \cup \{ \infty \}$*, then* $\{ e_j \otimes f_k \}_{j=1,\dots,N,k=1,\dots,M}$ *is an orthonormal of* $\mathcal{H}$.

Elements of the form $\varphi \otimes \psi$ are called **product states**.

Remark 1.3.2 *From definition* (1.3.1)*, it is clear that* $\dim(\mathcal{H}) = \dim(\mathcal{H}_1) \dim(\mathcal{H}_2)$*, amd it is a simple exercise to prove that* $\|\varphi \otimes \psi\|_{\mathcal{H}} = \|\varphi\|_{\mathcal{H}_1} \|\psi\|_{\mathcal{H}_2}$ *for all* $\varphi \in$

$\mathcal{H}_1$, $\psi \in \mathcal{H}_2$. Also, not every element of $\mathcal{H}_1 \otimes \mathcal{H}_2$ is a product state. e.g. linear combination of product states may not be a product state.

Theorem 1.3.3 *Let $S \in B(\mathcal{H}_1)$ and $T \in B(\mathcal{H}_2)$ (bounded linear map on $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively). Then there exists a unique linear operator $S \otimes T \in B(\mathcal{H}_1 \otimes \mathcal{H}_2)$ such that*

$$(S \otimes T)(\varphi \otimes \psi) = (S\varphi) \otimes (T\psi) \quad \forall\, \varphi \in \mathcal{H}_1, \ \forall\, \psi \in \mathcal{H}_2. \tag{1.3.2}$$

and

$$\|S \otimes T\|_{\mathcal{H}} = \|S\|_{\mathcal{H}_1} \|T\|_{\mathcal{H}_2}. \tag{1.3.3}$$

Proposition 1.3.4 *Let $S, S_1, S_2 \in B(\mathcal{H}_1)$ and $T, T_1, T_2 \in \mathcal{H}_2$.*

(a) The map $(S,T) \mapsto S \otimes T$ is a bilinear.

(b) $(S_1S_2) \otimes (T_1T_2) = (S_1 \otimes T_1)(S_2 \otimes T_2)$

(c) $(S \otimes T)^* = S^* \otimes T^*$. In particular, if S and T are self-adjoint, then $S \otimes T$ is self-adjoint. The converse is false.

(d) $S \otimes T$ is self-adjoint and S (or T) is self-adjoint, then T (or S) is self-adjoint.

(e) If $(S \otimes T)$ is self-adjoint, then there exists $c \in \mathbb{C} \setminus \{ 0 \}$ and self-adjoint operators $\tilde{S}$ and $\tilde{T}$ such that $\tilde{S} = cS$ and $\tilde{T} = \frac{1}{c}T$.

(f) If $\mathcal{H}_1$ and $\mathcal{H}_2$ are finite-dimensional, amd S and T are self-adjoint, with eigenvalues $\{ \lambda_i \}_i$ and $\{ \mu_j \}_j$, respectively, then $\{ \lambda_i \mu_j \}_{ij}$ are the eigenvalues of $S \otimes T$.

(g) Let S and T be self-adjoint. The $H := S \otimes I + I \otimes T$ is self-adjoint, and $e^{itH} = e^{itS} \otimes e^{itT}$ for all $t \in \mathbb{R}$.

1.3.1 States/Pure states

Definition 1.3.5 *A normalized vector $\varphi \in \mathcal{H}$ is called a* **pure state** *of a Quantum Mechanical system. Given an observable (i.e. self-adjoint operator)S in $\mathcal{H}$ and $\varphi \in D(S)$, the expectation value of A when measured for a system in a state φ is $\langle \varphi, A\varphi \rangle$.*

Remark 1.3.6 1. *States are determined up to a constant multiple of modulus one.*

2. *States correspond one-to-one to orthogonal projections of rank one (i.e. onto one-dimensional subspaces): If $\|\varphi\| = 1$, then the orthogonal projection $P_\varphi f = \langle \varphi, f \rangle \varphi$ is rank one. On the other hand, if P is an arbitrary rank one orthogonal projection, then any $\varphi \in R(P)$ with $\|\varphi\| = 1$ will satisfy $P = P_\varphi$*

Definition 1.3.7 *S is* **trace class operator***, denoted $S \in \mathcal{B}_1(\mathcal{H})$, if*

$$\|S\|_1 = \sum_j s_j < \infty \tag{1.3.4}$$

where $s_1 \geq s_2 \geq \cdots > 0$ are the singular values of S (i.e. non-zero eigenvalues of $|T| = (T^*T)^{\frac{1}{2}}$)

Note: $(\mathcal{B}_1(\mathcal{H}), \|\cdot\|_1)$ *is a Banach space.*

Definition 1.3.8 *For $S \in \mathcal{B}_1(\mathcal{H})$, the* **trace of** *$S$ is defined as*

$$\mathrm{Tr}(S) = \sum_j \langle \phi_j, S\phi_j \rangle \tag{1.3.5}$$

where $\{ \phi_j \}$ is an orthonormal basis of $\mathcal{H}$

Note: *If $S \in \mathcal{B}_1(\mathcal{H})$ and $S > 0$ (in particular, self-adjoint), then $\mathrm{Tr}(S) = \|S\|_1$.*

Definition 1.3.9 *A* **mixed state or density matrix** *in $\mathcal{H}$ is a non-negative operator $\rho \in \mathbb{B}_1(\mathcal{H})$ such that*

$$\mathrm{Tr}(\rho) = \sum_j \lambda_j = 1 \tag{1.3.6}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots > 0$ are eigenvalues of ρ (upto multiplicities).

By spectral decomposition, we have that

$$\rho f = \sum_j \lambda_j \langle \phi_j, f\phi_j \rangle \phi_j \qquad \text{using physics notation,} \quad \rho = \sum_j \lambda_j |\phi_j\rangle \langle \phi_j| \tag{1.3.7}$$

This is interpreted as: a system in a mixed state ρ is with probability λ_j in the state ϕ_j. It is hence obvious that mixed state is a generalization of state/pure state where a pure state is equivalent to a mixzed state $\rho = \langle \phi| |\phi\rangle$.

Note: The word **'state'** is often used to refer to a mixed state.

Definition 1.3.10 (Quantum Gibbs state) *Let $H \geq 0$ be self-adjoint with purely discrete spectrum i.e. there exists an orthonormal basis $\{ \phi_j \}$ corresponding to eigenvalues $\{ E_j \}$ with $0 \leq E_1 \leq E_2 \leq \cdots$ and $E_n \to 0$ such that $H\phi_n = E_n$ for all n*

If $e^{-\beta H} \in \mathbb{B}_1(\mathcal{H})$ (defined via fuunctional calculus) for some $\beta > 0$, then

$$\rho_\beta := \frac{e - \beta H}{\mathrm{Tr}\, e^{-\beta H}} \tag{1.3.8}$$

is a mixed state called the **thermal state** *of H at temperature $T = (\kappa\beta)^{-1}$ (κ is the Boltzmann constant).*

1.4 Entropy

Definition 1.4.1 *The* **Renyi entropy** *is mostly used here as it generalizes some other entropies. Let ρ be a mixed state on $\mathcal{H}$, the Renyi entropy of order α, $\alpha \in [0, 1)$,* *is defined:*

$$\mathcal{S}_\alpha(\rho) = \frac{1}{1-\alpha}\log[\operatorname{Tr}(\rho^\alpha)] = \frac{1}{1-\alpha}\log\left(\sum_{j=1}^{\dim(\mathcal{H})}\lambda_j^\alpha\right) \tag{1.4.1}$$

(a) $\mathcal{S}_\alpha \geq 0$ *and* $\mathcal{S}_\alpha$ *is non-increasing in* α.

(b) $\mathcal{S}_\alpha(\rho) = 0$ *if and only if* ρ *is a pure state.*

(c) $\forall\ \alpha,\ \max_\rho \mathcal{S}_\alpha(\rho) = \log(\dim(\mathcal{H}))$. *This is attained when we have the 'maximally mixed state'* $\rho = \frac{1}{\dim(\mathcal{H})}I$.

(d) $\lim_{\alpha\to 1}\mathcal{S}_\alpha = -\operatorname{Tr}(\rho\log\rho) = -\sum_{i=1}^{\dim(\mathcal{H})}\lambda_i\log\lambda_i =: \mathcal{S}(\rho)$ *which is the* ***von Neumann entropy***.

Proposition 1.4.2 (Schmidt Decomposition) *For a pure state* $\phi \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, *there exists orthonormal bases* $\{e_j\}$ *and* f_k *of* $\mathcal{H}_1$ *and* $\mathcal{H}_2$ *respectively and a unique sequence* $s_1 \geq s_2 \geq \cdots \geq 0$ *with* $\sum_j s_j^2 = 1$ *such that*

$$\phi = \sum_j s_j(e_j \otimes f_j) \tag{1.4.2}$$

In particular, ϕ *is a product state if and only if* $s_k \neq 0$ *and* $s_j = 0$ *for* $j \neq k$.

1.5 Partial Traces

Definition 1.5.1 *Let* $A \in \mathcal{B}_1(\mathcal{H}_1 \otimes \mathcal{H}_2)$, *then the unique operator* $\operatorname{Tr}_{\mathcal{H}_2} A \in \mathcal{B}_1(\mathcal{H}_1)$ *defined as*

$$\langle\phi, (\operatorname{Tr}_{\mathcal{H}_2} A)\psi\rangle = \sum_k \langle\phi\otimes f_k, A(\psi\otimes f_k)\rangle \tag{1.5.1}$$

is called the partial trace of A *with respect to* $\mathcal{H}_2$ *or the "restriction of* A *to* $\mathcal{H}_2$*".*

Remark 1.5.2 *(a)* $\{f_k\}$ *is an orthonormal in* $\mathcal{H}_2$ *and* $\phi, \psi \in \mathcal{H}_1$

(b) The partial trace of A with respect to $\mathcal{H}_1$, $\operatorname{Tr}_{\mathcal{H}_1} A \in \mathcal{B}_1(\mathcal{H}_2)$ is defined similarly as

$$\langle \tilde{\phi}, (\operatorname{Tr}_{\mathcal{H}_1} A)\tilde{\psi} \rangle = \sum_j \langle e_j \otimes \tilde{\phi}, A(e_j \otimes \tilde{\psi}) \rangle \tag{1.5.2}$$

for all $\tilde{\phi}, \tilde{\psi} \in \mathcal{H}_2$

(c) We sometimes write $A_1 = \operatorname{Tr}_{\mathcal{H}_2} A$ and $A_2 = \operatorname{Tr}_{\mathcal{H}_1} A$.

(d) If $A \in \mathcal{B}_1(\mathcal{H}_1 \otimes \mathcal{H}_2)$, then

$$\operatorname{Tr}(A) = \operatorname{Tr}(\operatorname{Tr}_{\mathcal{H}_1} A) = \operatorname{Tr}(\operatorname{Tr}_{\mathcal{H}_2} A) \tag{1.5.3}$$

(e) If $A \in \mathcal{B}_1(\mathcal{H}_1)$, $B \in \mathcal{B}_1(\mathcal{H}_2)$, then

$$\operatorname{Tr}_{\mathcal{H}_1}(A \otimes B) = (\operatorname{Tr} A)B \tag{1.5.4}$$

$$\operatorname{Tr}_{\mathcal{H}_2}(A \otimes B) = (\operatorname{Tr} B)A \tag{1.5.5}$$

(f) If $\rho \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is a mixed state, then $\operatorname{Tr}_{\mathcal{H}_1}(\rho)$ and $\operatorname{Tr}_{\mathcal{H}_2} \rho$ are mixed states in $\mathcal{H}_2$ and $\mathcal{H}_1$, respectively.

(g) If $\rho \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is a pure state, then $\operatorname{Tr}_{\mathcal{H}_1}(\rho)$ and $\operatorname{Tr}_{\mathcal{H}_2}(\rho)$ are pure states if and only if ρ is a product state.

1.6 Entanglemnent Entropy

Definition 1.6.1 *Let ρ be a pure state in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Then its (bipartite) entanglement entropy is defined as*

$$\mathcal{E}(\rho) = S(\operatorname{Tr}_{\mathcal{H}_1}(\rho)) = S(\operatorname{Tr}_{H_2}(\rho) \tag{1.6.1}$$

where $S(\cdot)$ denotes the von-Newmann entropy in $\mathcal{H}_2$ and $\mathcal{H}_1$ respectively.

Remark 1.6.2 $S(\rho_1) = S(\rho_2) = 0$ *if and only if* ρ_1 *and* ρ_2 *are pure states which occur only if* ρ *is a product state. Thus, entanglement entropy of pure states* ρ *can be used as a measure of the 'distance' of* ρ *from product states.*

Proof for the second equaility in equation((1.6.1)*) using Schmidt decomposition can be found in various texts.*

Having set up these definitions, we may state the first result in words. For any energy range, if we cut off the spectral projection of the XXZ spin-J ferromagnetic quantum spin chain at that energy level, then all states in the range of the spectral projector satisfy a logarithmic bound on the entanglement entropy. More precisely the entanglement entropy is bounded by the logarithm of the size of the spin chain, times a universal constant depending only on the anisotropy parameter, the spin and the energy cutoff level. Since the dimension is 1, the area of the boundary is 0-dimensional. So a logarithmically corrected area law is precisely what we prove.

1.7 Reflection Positivity

Let $\mathcal{U}$ be a real algebra of of observables (bounded, self-adjoint operators) with unit and let $\mathcal{U}_+$ and $\mathcal{U}_-$ be subalgebras of $\mathcal{U}$ such that $\mathcal{U}_+ \cup \mathcal{U}_- = \mathcal{U}$. Define $\theta : \mathcal{U}_\pm \to \mathcal{U}_\mp$ to be a continuous morphism such that θ has an extension $\tilde{\theta} : \mathcal{U} \to \mathcal{U}$ satisfying $\theta^2 = 1$.

Definition 1.7.1 *A linear functional* $\langle\cdot\rangle_0$ *on* $\mathcal{U}$ *is* **reflection positive (RP)** *with respect to* θ *if and only if* $\langle (A \otimes \mathbb{1}_{\mathcal{U}_-})\tilde{\theta}(A \otimes \mathbb{1}_{\mathcal{U}_-})\rangle_0 \geq 0$ *for all* $A \in \mathcal{U}_+$.

Definition 1.7.2 *A linear functional* $\langle\cdot\rangle_0$ *is* **generalized reflection positive (GRP)** *with respect to* θ *if and only if* $\langle (A_1 \otimes \mathbb{1}_{\mathcal{U}_-})\tilde{\theta}(A_1 \otimes \mathbb{1}_{\mathcal{U}_-}) \cdots (A_n \otimes \mathbb{1}_{\mathcal{U}_-})\tilde{\theta}(A_n \otimes \mathbb{1}_{\mathcal{U}_-})\rangle_0 \geq 0$ *for all* $A_1, \ldots, A_n \in \mathcal{U}_+$

Example 1.7.3 *Consider 2n spin 1/2-Ising spins* $\sigma_{-n+1}, \sigma_{-n+2}, \ldots, \sigma_n$*. Let* $\mathcal{U}$ *be the family of polynomials in all the* σ*'s,* $\mathcal{U}_+$ *(repectively* $\mathcal{U}_-$*) be the polynomials in* $\sigma_1, \ldots, \sigma_n$ *(respectively* $\sigma_0, \sigma_{-1}, \ldots \sigma_{-n+1}$*). Define* θ *such that* $\theta(\sigma_i) = \sigma_{-i+1}$*. The functional* $\langle\cdot\rangle_0$ *such that*

$$\langle A(\sigma)\rangle_0 = \frac{1}{4^n}\sum_{\sigma_i=\pm 1} A(\sigma_i) \tag{1.7.1}$$

is reflection positive.

Proof:

$$\langle A\theta(A)(\sigma)\rangle_0 = \frac{1}{4^n}\sum_{\sigma_i=\pm 1} A(\sigma_i)\theta(A\sigma_i)$$

$$= \frac{1}{4^n}\sum_{\sigma_i=\pm 1} A(\sigma_i)A(\theta(\sigma_i)) \tag{1.7.2}$$

$$= \frac{1}{4^n}\sum_{\sigma_i=\pm 1,\ \sigma_{-i+1}=\pm 1} A(\sigma_i)A(\sigma_{-i+1}) = \frac{1}{4^n}[A(1)+A(-1)]^2 \geq 0$$

Hence, $\langle\cdot\rangle_0$ is refelction positive.

Also, $\langle\cdot\rangle_0$ is generalized reflection positive by a similar argument.

CHAPTER 2

ENTANGLEMENT ENTROPY BOUNDS IN THE HIGHER SPIN XXZ CHAIN

2.1 Model description

For any fixed $J \in \mathbb{N}/2$, we consider the chain of length $L \in \mathbb{N}\backslash\{1\}$, which is described by the Hamiltonian

$$H_L = \sum_{j=1}^{L-1} h_{j,j+1} + J(2J - S_1^3 - S_L^3) \tag{2.1.1}$$

acting on the Hilbert space $\mathcal{H}_L = \bigotimes_{j=1}^{L} \mathbb{C}^{2J+1} = \bigotimes_{j=1}^{L} \mathcal{H}_j$, with the interpretation of $\mathcal{H}_j = \mathbb{C}^{2J+1}$ as being the local Hilbert space describing a spin–J particle located at site j. For later convenience, we also introduce the notation $\Lambda_L = \{1, 2, \dots, L\}$. The two–site Hamiltonian $h_{j,j+1}$ is given by

$$h_{j,j+1} = J^2 - S_j^3 S_{j+1}^3 - \frac{1}{\Delta}(S_j^1 S_{j+1}^1 + S_j^2 S_{j+1}^2) = J^2 - S_j^3 S_{j+1}^3 - \frac{1}{2\Delta}(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) \tag{2.1.2}$$

and the additional term $J(2J - S_1^3 - S_L^3)$ describes a boundary field; usually referred to as "droplet boundary condition". Given the canonical basis $\{\, \delta_i \,\}_{i=-J}^{J}$ of a single-site Hilbert space where

$$(\delta_i)_j = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{else} \end{cases}, \tag{2.1.3}$$

The Spin lowering operator S^- and the Spin raising operator S^+ are defined thus:

$$S^-\delta_j := \begin{cases} \sqrt{J(J+1)-j(j-1)}\,\delta_{j-1}, & j\in\{-J+1,\dots,J\} \\ \\ 0, & j=-J \end{cases} \tag{2.1.4}$$

$$S^+\delta_j := \begin{cases} \sqrt{J(J+1)-j(j+1)}\,\delta_{j-1}, & j\in\{-J,\dots,J-1\} \\ \\ 0, & j=J \end{cases} \tag{2.1.5}$$

The spin–J matrices $S^1 = \frac{S^+ + S^-}{2}$, $S^2 = \frac{S^+ - S^-}{2i}$ and S^3 is the diagonal matrix with respect to $\{\,\delta_j\,\}_{j=-J}^{J}$ (i.e. $S^3\delta_j = j\delta_j$).

Labeling an operator $A_j \in \mathbb{C}^{(2J+1)\times(2J+1)}$ means that it acts as A on the j-th factor of the tensor product and as the identity on all the other factors. i.e.

$$A_j \equiv I \otimes \cdots \otimes \underset{\text{j-th site}}{A} \otimes \cdots \otimes I \tag{2.1.6}$$

In what follows, we assume that the anisotropy parameter Δ satisfies $\Delta > 2J$. While we emphasize that $\Delta > 2J$ is not necessary for the operators $h_{j,j+1}$ to be non-negative (see, e.g. [30, p.16]), it is certainly sufficient (see Proposition 2.2.4 below).

2.2 Equivalence to a direct sum of Schrödinger-type operators

In the following, we are going to discuss the equivalence of the spin-J XXZ Hamiltonian to a direct sum of discrete many-particle Schödinger-type operators. To this end, we will firstly review previous work [12], where we described configurations of particles via functions $\mathbf{m} : \Lambda_L \to \{0, 1, \dots, 2J\}$, where for each $i \in \Lambda_L$, the value $\mathbf{m}(i)$ represents the number of particles that are located at site i when in configuration $\mathbf{m}$.

Equivalently, a configuration of N particles distributed over Λ_L can be described using ordered multisets X with elements in Λ_L. Here, the value of the i-th element $x_i \in X$ represents the location of the i-th particle of a configuration of N particles.

For our purposes, it will be advantageous to use both points of view as they have their respective advantages: the first description involving occupation numbers will be more useful when it comes to analyzing the interaction potential of the Schrödinger-type operators. On the other hand, once it has been shown how the entanglement entropy of a state can be estimated using the Combes-Thomas bound for spectral projections, the problem boils down to a combinatorial problem estimating exponentially weighted sums over a large set of many-particle configurations, for which the multiset point of view will be more convenient.

2.2.1 Previous approach using occupation numbers

In [12, Prop. 2.1], it was shown that the Hamiltonian H_L is unitarily equivalent to a direct sum of many–body Schrödinger operators. One firstly observes that H_L preserves the total magnetization/particle number: to this end, we define the **local particle number operator** $\mathcal{N}^{loc} := (J - S^3)$ acting on $\mathbb{C}^{2J+1}$ which has spectrum $\sigma(\mathcal{N}^{loc}) = \{0, 1, \ldots, 2J-1, 2J\}$. For any site $j \in \{1, \ldots, L\}$, we interpret the eigenvalues of $\mathcal{N}_j^{loc}$ as the number of particles located at site j. We then define the **total particle number operator** $\mathcal{N}_L$ as

$$\mathcal{N}_L := \sum_{j=1}^{L} \mathcal{N}_j^{loc} \,, \tag{2.2.1}$$

where the eigenvalues $\sigma(\mathcal{N}_L) = \{0, 1, 2, \ldots, 2JL-1, 2JL\}$ of $\mathcal{N}_L$ are consequently interpreted as the total number of particles spread across the sites in Λ_L. It can be verified that $[H_L, \mathcal{N}_L] = 0$, and thus we decompose $\mathcal{H}_L = \bigoplus_{N=0}^{2JL} \mathcal{H}_L^N$, where $\mathcal{H}_L^N$ denotes the eigenspace of $\mathcal{N}_L$ corresponding to the eigenvalue N – the space of all

N-particle configurations in $\{1,2,\ldots,L\}$ with the restriction that no site can be occupied by more than $2J$ particles. We also define $H_L^N := H_L \restriction_{\mathcal{H}_L^N}$. Now, let

$$\mathbf{M}_L^N := \left\{ \mathbf{m} : \{1,2,\ldots,L\} \to \{0,1,\ldots,2J\} : \sum_{j=1}^{L} \mathbf{m}(j) = N \right\} , \tag{2.2.2}$$

be the set of all functions from $\{1,2,\ldots,L\}$ to $\{0,1,\ldots,2J\}$ whose values add up to N. For convenience, we also define $\mathbf{M}_L := \bigcup_{N=0}^{2JL} \mathbf{M}_L^N$ – the set of *all* functions from $\{1,2,\ldots,L\}$ to $\{0,1,\ldots,2J\}$. Let $\{e_k\}_{k=0}^{2J}$ denote a normalized eigenbasis of $\mathcal{N}^{loc}$, such that for any $k \in \{0,1,\ldots,2J\}$, we have $\mathcal{N}^{loc} e_k = k \cdot e_k$. We then define for any $\mathbf{m} \in \mathbf{M}_L$

$$\psi_{\mathbf{m}} := \bigotimes_{j=1}^{L} e_{\mathbf{m}(j)} \, . \tag{2.2.3}$$

This means in particular that for any $j \in \{1,2,\ldots,L\}$ we get $\mathcal{N}_j^{loc}\psi_{\mathbf{m}} = \mathbf{m}(j)\psi_{\mathbf{m}}$. In other words, $\psi_{\mathbf{m}}$ describes a configuration of particles, where at each site $j \in \{1,2,\ldots,L\}$, there are exactly $\mathbf{m}(j)$ particles. Since

$$\mathcal{N}_L \psi_{\mathbf{m}} = \left(\sum_{j=1}^{L} \mathbf{m}(j) \right) \psi_{\mathbf{m}} \, , \tag{2.2.4}$$

it immediately follows that

$$\mathcal{H}_L^N = \operatorname{span} \left\{ \psi_{\mathbf{m}} : \mathbf{m} \in \mathbf{M}_L^N \right\} \, . \tag{2.2.5}$$

Now, consider the Hilbert space $\ell^2(\mathbf{M}_L^N) = \left\{ f : \mathbf{M}_L^N \to \mathbb{C} \right\}$ equipped with inner product $\langle f, g \rangle = \sum_{\mathbf{m} \in \mathbf{M}_L^N} \overline{f(\mathbf{m})} g(\mathbf{m})$ and let $\{\phi_{\mathbf{m}}\}_{\mathbf{m} \in \mathbf{M}_L^N}$ denote the canonical basis of $\ell^2(\mathbf{M}_L^N)$, i.e.

$$\phi_{\mathbf{m}}(\mathbf{n}) = \begin{cases} 1 & \text{if} \quad \mathbf{m} = \mathbf{n} \\ 0 & \text{else.} \end{cases} \tag{2.2.6}$$

The Hilbert spaces $\mathcal{H}_L^N$ and $\ell^2(\mathbf{M}_L^N)$ are unitarily equivalent via

$$U_L^N : \mathcal{H}_L^N \to \ell^2(\mathbf{M}_L^N), \quad \psi_{\mathbf{m}} \mapsto \phi_{\mathbf{m}} . \tag{2.2.7}$$

For any $f \in \ell^2(\mathbf{M}_L^N)$, let us now define the adjacency operator A_N, given by

$$(A_N f)(\mathbf{m}) = \sum_{\mathbf{n}:\mathbf{n}\sim\mathbf{m}} w(\mathbf{m},\mathbf{n}) f(\mathbf{n}) , \tag{2.2.8}$$

where for two configurations $\mathbf{m}, \mathbf{n} \in \mathbf{M}_L^N$ to be adjacent (denoted by $\mathbf{m} \sim \mathbf{n}$) is defined as follows:

$$\begin{aligned} &\mathbf{m} \sim \mathbf{n} :\Leftrightarrow \\ &\quad \exists\, j_0 \in \{1,2,\ldots,L-1\} : \mathbf{m}(j_0) - \mathbf{n}(j_0) = \pm 1 \text{ and } \mathbf{m}(j_0+1) - \mathbf{n}(j_0+1) = \mp 1 \\ &\qquad \text{and for any } j \in \{1,2,\ldots,L\} \setminus \{j_0, j_0+1\} : \mathbf{m}(j) = \mathbf{n}(j) . \end{aligned} \tag{2.2.9}$$

This definition should be interpreted in the following way: two configurations $\mathbf{m}, \mathbf{n}$ of N particles distributed over L sites (with the requirement that no site be occupied by more than $2J$ particles) are adjacent if one configuration can be obtained by moving a single particle from the other configuration to the right or left (cf. Figure 2.2.1).

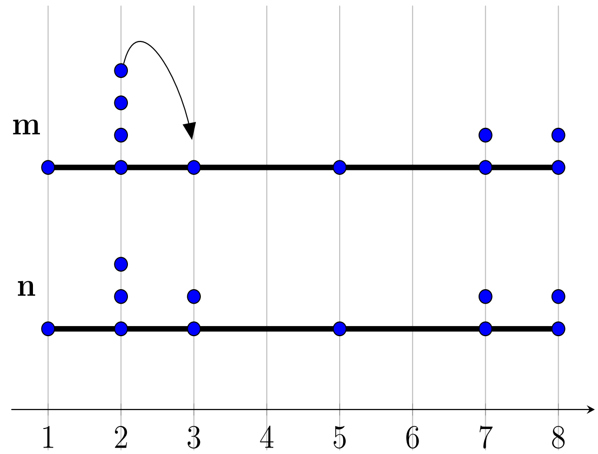

Figure 2.2.1: An example of two adjacent configurations $\mathbf{m}, \mathbf{n} \in \mathbf{M}_8^{11}$ (here: $J = 2$). The values of the functions at a site are represented by blue circles corresponding to particles occupying the respective sites, e.g. $\mathbf{m}(2) = 4$. Since $\mathbf{m}(2) - \mathbf{n}(2) = 4 - 3 = 1$ and $\mathbf{m}(3) - \mathbf{n}(3) = 1 - 2 = -1$, while $\mathbf{m}(j) = \mathbf{n}(j)$ for any other site j, we have $\mathbf{m} \sim \mathbf{n}$. We interpret configuration $\mathbf{n}$ as obtained from configuration $\mathbf{m}$ by a particle hopping to the right from site 2 to site 3. (Represented by an arrow emanating from the hopping particle in configuration $\mathbf{m}$.)

For $\mathbf{m} \sim \mathbf{n}$, the weight function $w(\mathbf{m}, \mathbf{n}) = w(\mathbf{n}, \mathbf{m})$ in (2.2.8) is given by

$$w(\mathbf{m}, \mathbf{n}) = \prod_{j:\mathbf{m}(j) \neq \mathbf{n}(j)} \left(J(\mathbf{m}(j) + \mathbf{n}(j) + 1) - \mathbf{m}(j)\mathbf{n}(j) \right)^{1/2} , \tag{2.2.10}$$

however in what follows, the explicit expression in (2.2.10) will not play a particularly important role. Moreover, for any $\mathbf{m}, \mathbf{n} \in \mathbf{M}_L^N$, we define their distance $d^N(\mathbf{m}, \mathbf{n})$ to be the length of the shortest path connecting $\mathbf{m}$ and $\mathbf{n}$, which we will refer to as graph distance.

Remark 2.2.1 *For more details concerning the construction of the spin-J Heisenberg XXZ model on more general underlying graph (in lieu of just the chain), we refer to [12], where appropriate N-particle graphs were introduced. Similar approaches have been used for the spin-1/2 case in [13, 27]. Consider also [2, 8, 28] and the references therein, where similar constructions have been studied from a graph-theoretic* *point of view.*

Next, we define the full interaction potential V_N, which is a multiplication operator on $\ell^2(\mathbf{M}_L^N)$, to be given by

$$(V_N f)(\mathbf{m}) = V(\mathbf{m})f(\mathbf{m}) = \left(\sum_{j=1}^{L-1} v(\mathbf{m}(j), \mathbf{m}(j+1))\right) f(\mathbf{m}) + J(\mathbf{m}(1) + \mathbf{m}(L))f(\mathbf{m})\,, \tag{2.2.11}$$

where the 'local' two–site potential v is given by

$$v(\mathbf{m}(j), \mathbf{m}(j+1)) = J(\mathbf{m}(j) + \mathbf{m}(j+1)) - \mathbf{m}(j)\mathbf{m}(j+1) \tag{2.2.12}$$

and we refer to the extra term "$J(\mathbf{m}(1) + \mathbf{m}(L))$" as the "**boundary field**".

In what follows, the following two facts will be particularly important: firstly that the operator H_L^N is unitarily equivalent to the Schrödinger-type operator $-(2\Delta)^{-1}A_N + V_N$ (Prop. 2.2.2) and moreover that that kinetic term can be controlled in terms of the potential (Prop. 2.2.4):

Proposition 2.2.2 ([12, Prop. 2.1]) *We have the following unitary equivalence:*

$$U_L^N H_L^N (U_L^N)^* = -\frac{1}{2\Delta} A_N + V_N =: H_N \equiv H_N(L)\,. \tag{2.2.13}$$

Remark on the proof: The only detail which is not discussed in [12] is the unitary equivalence of the boundary field term "$J(\mathbf{m}(1) + \mathbf{m}(L))f(\mathbf{m})$" in (2.2.11) to the boundary field "$J(2J - S_1^3 - S_L^3)$" in (3.3.4), which can be verified by an easy calculation.

Remark 2.2.3 *For the special cases $N = 0$ and $N = 2JL$, note that*

$$\dim(\ell^2(\mathbf{M}_L^0)) = \dim(\ell^2(\mathbf{M}_L^{2JL})) = 1 \ .$$

On these one-dimensional spaces, the operators H_0 and H_{2JL} are just given by $H_0 = 0$ and $H_{2JL} = 4J^2$.

Let us now recall a useful relative bound of A_N in terms of the potential V_N. It is because of this particular feature of the model that we do not have to worry about the explicit form of the weight function w given in (2.2.10).

Proposition 2.2.4 ([12, Lemma 2.9]) *The operators A_N and V_N satisfy the following relative bound:*

$$-4JV_N \leq A_N \leq 4JV_N \ . \tag{2.2.14}$$

Remark on the proof: Strictly speaking, in [12, Lemma 2.9], it was only shown that $A_N \leq 4JV_N$. However, the lower bound $-4JV_N \leq A_N$ follows from a completely analogous argument.

Let us now further analyze the interaction potential V_N and determine all the configurations which minimize its value, the proof can be found in Appendix A.2.1

Proposition 2.2.5 *Let $N \in \{4J, 4J+1, \ldots, 2JL\}$ and define $V_{N,0} := \min\{V(\mathbf{m}) : \mathbf{m} \in \mathbf{M}_L^N\}$. Then*

$$V_{N,0} := 4J^2 \ . \tag{2.2.15}$$

Moreover, – up to overall translations – the minimizers of V_N are given by

$$\mathbf{m}_j^N(x) = \begin{cases} j & \text{if} \quad x = 1 \\ 2J & \text{if} \quad x = 2, \ldots, r \\ 2J - j & \text{if} \quad x = r + 1 \end{cases} \tag{2.2.16}$$

for $N = 2Jr, \ \ 2 \leq r \leq L - 1, \ j = 0, \ldots, 2J - 1$ *and*

$$\mathbf{m}_j^N(x) = \begin{cases} j & \text{if} \quad x = 1 \\ 2J & \text{if} \quad x = 2, \ldots, 1 + \lfloor \frac{N}{2J} \rfloor \\ N(mod\ 2J) - j & \text{if} \quad x = 2 + \lfloor \frac{N}{2J} \rfloor \end{cases} \tag{2.2.17}$$

if N *is not a multiple of* $2J$, $j = 0, \ldots, N(mod\ 2J) - 1$.

Remark 2.2.6 *The following figure provides an example of a minimizer of the form* (2.2.16), *i.e. when* $N \in \{4J, 6J, 8J, \ldots, 2JL\}$*:*

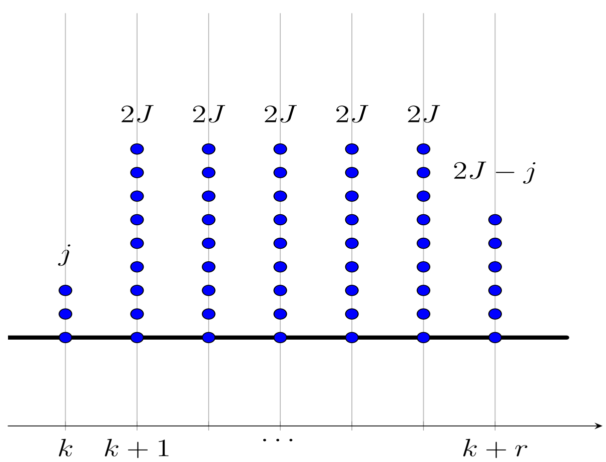

Figure 2.2.2: An example of a minimizer when $N = 2Jr$ as in (2.2.16). Here, $J = 9/2$ and $j = 3$.

Definition 2.2.7 *For any* $K \in \mathbb{N}$, *let* $\mathbf{M}_{L,K}^N = \{\mathbf{m} \in \mathbf{M}_L^N : V(\mathbf{m}) \leq K\}$, *i.e. the set of occupation number functions for which the potential* V_N *is bounded by* K.

2.2.2 An equivalent description using multisets

When it comes to tracking the positions of N individual particles, it will be convenient to introduce ordered N-tuples that satisfy certain conditions. For brevity, in what follows, we will refer to these N-tuples as multisets. Thus, for any $L \in \mathbb{N}$ and any $N \in \{1, \ldots, 2JL\}$, let us define

$$\mathbb{S}_L^N = \left\{ (x_1, x_2, \ldots, x_N) \in \Lambda_L^N : x_1 \leq x_2 \leq \cdots \leq x_N \text{ and } \min_{k \in \{1,2,\ldots,N-2J\}} (x_{k+2J} - x_k) \geq 1 \right\}, \tag{2.2.18}$$

where for any $X = (x_1, x_2, \ldots, x_N) \in \mathbb{S}_L^N$, the value of each individual x_i represents the position of the i-th particle. The condition

$$\min_{k \in \{1,2,\ldots,N-2J\}} (x_{k+2J} - x_k) \geq 1 \tag{2.2.19}$$

reflects the fact that no site can be occupied by more than $2J$ particles and is therefore automatically satisfied if $N \leq 2J$. For later convenience, we also introduce the convention $\mathbb{S}_L^0 := \{\emptyset\}$.

The correspondence between functions of occupation numbers $\mathbf{m} \in \mathbf{M}_L^N$ and N-particle configurations $X \in \mathbb{S}_L^N$ is of course straightforward. For a given $X = (x_1, x_2, \ldots, x_N) \in \mathbb{S}_L^N$, the corresponding function $\mathbf{m}_X \in \mathbf{M}_L^N$ is defined as

$$\mathbf{m}_X(j) := |\{k \in \{1, 2, \ldots, N\} : x_k = j\}| \tag{2.2.20}$$

for any $j \in \Lambda_L$. It is not hard to see that the mapping $X \mapsto \mathbf{m}_X$ is a bijection from $\mathbb{S}_L^N$ to $\mathbf{M}_L^N$. We thus denote by $X_{\mathbf{m}}$ the image of the inverse of that mapping applied to an arbitrary $\mathbf{m} \in \mathbf{M}_L^N$.[1] We will also use $\{\phi_X\}_{X \in \mathbb{S}_L^N}$ to denote the canonical basis of

[1] As an example, consider the multiset corresponding to the occupation function $\mathbf{n}$ in Figure 2.2.1, which would be given by

$$X_{\mathbf{n}} = (1, 2, 2, 2, 3, 3, 5, 7, 7, 8, 8)\,. \tag{2.2.21}$$

$\ell^2(\mathbb{S}_L^N)$, i.e. $\phi_X(Y) = 1$ if $X = Y$ and $\phi_X(Y) = 0$ if $X \neq Y$. Then, the identification of the Hilbert spaces $\ell^2(\mathbf{M}_L^N)$ with $\ell^2(\mathbb{S}_L^N)$ via $\phi_{\mathbf{m}} \mapsto \phi_{X_{\mathbf{m}}}$ is straightforward. So for any $X, Y \in \mathbb{S}_L^N$, we define $X \sim Y :\Leftrightarrow \mathbf{m}_X \sim \mathbf{m}_Y$ as well as $w(X,Y) := w(\mathbf{m}_X, \mathbf{m}_Y)$ and $V(X) := V(\mathbf{m}_X)$. By a slight abuse of notation, we will use the same symbols H_N, A_N and V_N to denote the unitarily equivalent operators on $\ell^2(\mathbb{S}_L^N)$, i.e.

$$(H_N f)(X) = -\frac{1}{2\Delta}(A_N f)(X) + (V_N f)(X) = -\frac{1}{2\Delta}\sum_{Y:X\sim Y} w(X,Y)f(Y) + V(X)f(X) \tag{2.2.22}$$

for any $f \in \ell^2(\mathbb{S}_L^N)$.

For any $X, Y \in \mathbb{S}_L^N$, let $d^N(X,Y) := d^N(\mathbf{m}_X, \mathbf{m}_Y)$. The merit of the multiset-point-of-view will now be made more apparent by the following lemma; its proof can be found in Appendix A.1.

Lemma 2.2.8 *For any two configurations $X, Y \in \mathbb{S}_L^N$, where $X = (x_1, x_2, \ldots, x_N)$ and $Y = (y_1, y_2, \ldots, y_N)$, we have*

$$d^N(X,Y) = \sum_{i=1}^{N} |x_i - y_i| \,. \tag{2.2.23}$$

2.3 Combes–Thomas estimate and bounds on spectral projections

One of the main ingredients of the proof of the bound for the entanglement entropy will be a bound on spectral projections. To be more specific, let $\mathcal{A} \subset \mathbb{S}_L$ be a set of configurations. For any such $\mathcal{A}$, we define $P_{\mathcal{A}}$ to be the orthogonal projection onto the subspace of functions that are supported on $\mathcal{A}$, i.e.

$$(P_{\mathcal{A}}f)(X) = \begin{cases} f(X) & \text{if} \quad X \in \mathcal{A} \\ 0 & \text{if} \quad X \in \mathbb{S}_L \setminus \mathcal{A} \end{cases} . \tag{2.3.1}$$

For later convenience, we also define $\overline{P}_{\mathcal{A}} := \mathbb{1} - P_{\mathcal{A}}$.

Theorem 2.3.1 *For any $N \in \{1, 2, \ldots, 2JL\}$, let Y_N be an arbitrary multiplication operator on $\ell^2(\mathbb{S}_L^N)$ and $z \notin \sigma(H_N + Y_N)$ such that there exists $\kappa_z > 0$ for which*

$$\left\| V_N^{1/2}(H_N + Y_N - z)^{-1} V_N^{1/2} \right\| \leq \frac{1}{\kappa_z} < \infty \, . \tag{2.3.2}$$

Then for all subsets $\mathcal{A}, \mathcal{B} \subseteq \mathbb{S}_L^N$, we have

$$\left\| P_{\mathcal{A}} \left(H_N + Y_N - z\right)^{-1} P_{\mathcal{B}} \right\| \leq \frac{1}{V_{N,0}} \left\| P_{\mathcal{A}} V_N^{1/2} \left(H_N + Y_N - z\right)^{-1} V_N^{1/2} P_{\mathcal{B}} \right\| \leq \frac{2}{V_{N,0}\kappa_z} \, e^{-\eta_z d^N(\mathcal{A},\mathcal{B})}, \tag{2.3.3}$$

where

$$\eta_z = \log\left(1 + \frac{\Delta \kappa_z}{4J}\right). \tag{2.3.4}$$

Proof: An abstract result of this form for Schrödinger-type operators whose kinetic term is controlled by the potential such as in Proposition 2.2.4 was shown in [1, Prop. 3.1]. The theorem now follows.

Now, let $K \in \mathbb{N}$ and for any $\delta \in (0, 1)$, define $E_{K,\delta} := \left(1 - \frac{2J}{\Delta}\right)(K + 1 - \delta)$. Moreover, for any non-negative multiplication operator W_N on $\ell^2(\mathbb{S}_L^N)$, let $Q_{K,\delta}^N \equiv Q_{K,\delta}^N(L, W_N) := \mathbb{1}_{[0,E_{K,\delta}]}(H_N(L) + W_N)$ be the spectral projection of $H_N + W_N$ associated to the energy interval $[0, E_{K,\delta}]$. Lastly, for any $K \in \mathbb{N}$, we introduce the set $\mathbb{S}_{L,K}^N := \{X_{\mathbf{m}} : \mathbf{m} \in \mathbf{M}_{L,K}^N\}$, where the sets $\mathbf{M}_{L,K}^N$ were introduced in Definition 2.2.7.

Theorem 2.3.2 *Let $\mathcal{A} \subset \mathbb{S}_L^N$ be a set of configurations. We then get the following estimate:*

$$\left\|P_{\mathcal{A}} Q_{K,\delta}^N\right\| = \left\|Q_{K,\delta}^N P_{\mathcal{A}}\right\| \leq C_{N,K} e^{-\mu_K d^N(\mathcal{A}, \mathbb{S}_{L,K}^N)}, \tag{2.3.5}$$

where

$$C_{N,K} = C_{N,K}(\Delta, \delta, J) = \max\left\{1, \frac{8K(K+1)}{V_{N,0}\delta^2}\right\} \tag{2.3.6}$$

$$\text{and} \quad \mu_K = \mu_K(\Delta, \delta, J) = \log\left(1 + \frac{\delta(\Delta - 2J)}{16J(K+1)}\right). \tag{2.3.7}$$

Proof: We follow ideas from [10, Proof of Lemma 8.2] and [20]. If $\mathcal{A} \cap \mathbb{S}_{L,K}^N \neq \emptyset$, which implies $d^N(\mathcal{A}, \mathbb{S}_{L,K}^N) = 0$, then (2.3.5) immediately follows from $C_{N,K} \geq 1$. Hence, assume $\mathcal{A} \subset \mathbb{S}_L^N \setminus \mathbb{S}_{L,K}^N$ from now on. Then, let us choose $Y_N = W_N + \gamma P_{\mathbb{S}_{L,K}^N}$ with $\gamma = \left(1 - \frac{2J}{\Delta}\right) K$ and show that the operator $H_N + W_N + \gamma P_{\mathbb{S}_{L,K}^N}$ satisfies the assumptions of Theorem 2.3.1. Observe that for any $E \in [0, E_{K,\delta/2}]$ one has

$$V_N^{-1/2}(H_N + Y_N - E)V_N^{-1/2} \geq -\frac{1}{2\Delta} V_N^{-1/2} A_N V_N^{-1/2} + \mathbb{1} + \gamma P_{\mathbb{S}_{L,K}^N} V_N^{-1} - E V_N^{-1} \tag{2.3.8}$$

$$\geq \left(1 - \frac{2J}{\Delta}\right) + \left(\left(1 - \frac{2J}{\Delta}\right) K - E_{K,\delta/2}\right) V_N^{-1} P_{\mathbb{S}_{L,K}^N} - E_{K,\delta/2} \overline{P}_{\mathbb{S}_{L,K}^N} V_N^{-1} \tag{2.3.9}$$

$$= \left(1 - \frac{2J}{\Delta}\right) \left(\mathbb{1} - (1 - \delta/2) V_N^{-1} P_{\mathbb{S}_{L,K}^N} - (K + 1 - \delta/2) V_N^{-1} \overline{P}_{\mathbb{S}_{L,K}^N}\right). \tag{2.3.10}$$

Now, note that

$$-(1-\delta/2) V_N^{-1} P_{\mathbb{S}_{L,K}^N} \geq -(1-\delta/2) P_{\mathbb{S}_{L,K}^N} \quad \text{as well as} \quad -V_N^{-1} \overline{P}_{\mathbb{S}_{L,K}^N} \geq -\frac{1}{K+1} \overline{P}_{\mathbb{S}_{L,K}^N}, \tag{2.3.11}$$

which we use to further estimate (2.3.10):

$$(2.3.10) \geq \left(1 - \frac{2J}{\Delta}\right)\left(\frac{\delta}{2}P_{\mathbb{S}^N_{L,K}} + \frac{\delta/2}{K+1}\overline{P}_{\mathbb{S}^N_{L,K}}\right) \geq \left(1 - \frac{2J}{\Delta}\right)\frac{\delta}{2(K+1)}\,. \quad (2.3.12)$$

From this, it can be concluded that for any $E \in [0, E_{K,\delta}]$, we have $E \notin \sigma(H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}})$ and moreover that

$$\|V_N^{1/2}(H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - E)^{-1}V_N^{1/2}\| \leq \frac{2(K+1)}{\delta\left(1 - \frac{2J}{\Delta}\right)} \quad (2.3.13)$$

and, by a slight modification (see [10, Lemma 4.3]), one gets for any $\varepsilon \in \mathbb{R}$:

$$\|V_N^{1/2}(H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - E + i\varepsilon)^{-1}V_N^{1/2}\| \leq \frac{4(K+1)}{\delta\left(1 - \frac{2J}{\Delta}\right)}\,. \quad (2.3.14)$$

From Theorem 2.3.1, we therefore get for any $\mathcal{A} \in \mathbb{S}^N_L \setminus \mathbb{S}^N_{L,K}$

$$\|P_{\mathbb{S}^N_{L,K}}(H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - E + i\varepsilon)^{-1}P_{\mathcal{A}}\| \leq \frac{8(K+1)}{V_{N,0}\cdot\delta\left(1 - \frac{2J}{\Delta}\right)}e^{-\mu_K d^N(\mathcal{A},\mathbb{S}^N_{L,K})}, \quad (2.3.15)$$

for any $E \in [0, E_{K,\delta/2}]$ and any $\varepsilon \in \mathbb{R}$. The constant $\mu_K = \mu_K(\Delta, \delta, J)$ is given by

$$\mu_K = \log\left(1 + \frac{\delta(\Delta - 2J)}{16J(K+1)}\right)\,. \quad (2.3.16)$$

Now, let Γ be the circle centered at $\frac{1}{2}E_{K,\delta}$ with radius $R := \frac{1}{2}\left(1 - \frac{2J}{\Delta}\right)(K+1)$. Note that this implies $\operatorname{dist}(\Gamma, [0, E_{K,\delta}]) = \frac{\delta}{2}\left(1 - \frac{2J}{\Delta}\right) =: \delta'$. Moreover, it follows from

Proposition 2.2.4 that

$$H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} \geq -\frac{1}{2\Delta} A_N + V_N + \gamma P_{\mathbb{S}^N_{L,K}} \geq \left(1 - \frac{2J}{\Delta}\right) V_N + \gamma P_{\mathbb{S}^N_{L,K}} \quad (2.3.17)$$

$$\geq \left(1 - \frac{2J}{\Delta}\right) (V_N + K) P_{\mathbb{S}^N_{L,K}} + \left(1 - \frac{2J}{\Delta}\right) V_N \overline{P}_{\mathbb{S}^N_{L,K}} \quad (2.3.18)$$

$$\geq \left(1 - \frac{2J}{\Delta}\right) (K+1)\,, \quad (2.3.19)$$

which means that there is no spectrum of $H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}}$ inside the circle Γ, which implies

$$\oint_\Gamma (H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - z)^{-1} \mathrm{d}z = 0\,. \quad (2.3.20)$$

We therefore get

$$Q^N_{K,\delta} = (Q^N_{K,\delta})^2 = \frac{i}{2\pi} Q^N_{K,\delta} \oint_\Gamma (H_N + W_N - z)^{-1} \mathrm{d}z \quad (2.3.21)$$

$$= \frac{i}{2\pi} Q^N_{K,\delta} \oint_\Gamma [(H_N + W_N - z)^{-1} - (H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - z)^{-1}] \mathrm{d}z \quad (2.3.22)$$

$$= \frac{i\gamma}{2\pi} Q^N_{K,\delta} \oint_\Gamma (H_N + W_N - z)^{-1} P_{\mathbb{S}^N_{L,K}} (H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - z)^{-1} \mathrm{d}z \quad (2.3.23)$$

We then proceed to estimate

$$\|Q^N_{K,\delta} P_{\mathcal{A}}\| \leq \gamma R \max_{z \in \Gamma} \left[\|Q^N_{K,\delta} (H_N + W_N - z)^{-1}\| \|P_{\mathbb{S}^N_{L,K}} (H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - z)^{-1} P_{\mathcal{A}}\| \right] \quad (2.3.24)$$

$$\leq \frac{\gamma R}{\delta'} \max_{z \in \Gamma} \|\|P_{\mathbb{S}^N_{L,K}} (H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} - z)^{-1} P_{\mathcal{A}}\|\,, \quad (2.3.25)$$

where we have used $\|Q^N_{K,\delta}(H_N + W_N - z)^{-1}\| \leq (\delta')^{-1}$. Note that for any $z \in \Gamma$, we have

$$\mathrm{Re}\, z \leq \left(1 - \frac{2J}{\Delta}\right) \left(K + 1 - \frac{\delta}{2}\right) = E_{K,\delta/2}\,, \quad (2.3.26)$$

which means that we can apply (2.3.15) to estimate $\|P_{\mathbb{S}^N_{L,K}}(H_N + W_N + \gamma P_{\mathbb{S}^N_{L,K}} -$

$z)^{-1}P_{\mathcal{A}}\|$ uniformly in $z \in \Gamma$. We then get

$$(2.3.25) \leq \frac{8\gamma R(K+1)}{V_{N,0}\delta'\delta(1-\frac{2J}{\Delta})} e^{-\mu_K d^N(\mathcal{A},\mathbb{S}^N_{L,K})} = \frac{8K(K+1)}{V_{N,0}\delta^2} e^{-\mu_K d^N(\mathcal{A},\mathbb{S}^N_{L,K})} , \qquad (2.3.27)$$

which is the desired result.

Remark 2.3.3 *This result applies in particular to non-negative multiplication operators W_N, that are of the form*

$$W_N(X) = \sum_{i=1}^{N} \nu(x_i) \qquad (2.3.28)$$

for any $X = (x_1, x_2, \ldots, x_N) \in \mathbb{S}^N_L$, where $\nu : \Lambda_L \to \mathbb{R}^+_0$ is an arbitrary non-negative function with domain Λ_L. In this case, W_N corresponds to a background magnetic field in 3-direction, whose value at each site j is given by $\nu(j)$. To be more precise, we have

$$W_N = U^N_L \left(\sum_{j=1}^{L} \mathcal{N}^{loc}_j \nu(j) \restriction_{\mathcal{H}^N_L} \right) (U^N_L)^* , \qquad (2.3.29)$$

where the unitary operator U^N_L was given in (2.2.7)*. See also [12, Remark 2.7].*

2.4 Entanglement Entropy of Higher Energy states

In what follows, we will mainly use ideas and previous results from [1, Sec. 5]. Let $\mathbb{S}_L := \bigcup_{N=0}^{2JL} \mathbb{S}^N_L$, which allows us to identify

$$\ell^2(\mathbb{S}_L) = \bigoplus_{N=0}^{2JL} \ell^2(\mathbb{S}^N_L) . \qquad (2.4.1)$$

Next, let $\psi \in \ell^2(\mathbb{S}_L)$ be normalized. We denote the associated density matrix by $\rho_\psi = |\psi\rangle\langle\psi|$.[2] Analogous to (2.2.18), for any subset $\Gamma \subset \Lambda_L$, and any $N \in \{1, \ldots, 2J|\Gamma|\}$,

[2]Using physicist's notation, for any α, β in a Hilbert space $\mathcal{H}$, the symbol "$|\alpha\rangle\langle\beta|$" denotes the rank-one operator $\psi \mapsto \alpha\langle\beta, \psi\rangle$ for any $\psi \in \mathcal{H}$.

we define

$$\mathbb{S}_\Gamma^N := \left\{(x_1, x_2, \ldots, x_N) \in \Gamma^N : x_1 \le x_2 \le \cdots \le x_N \text{ and } \min_{k\in\{1,2,\ldots,N-2J\}}(x_{k+2J} - x_k) \ge 1\right\} \tag{2.4.2}$$

and – as before – we set $\mathbb{S}_\Gamma^0 := \{\emptyset\}$. Moreover, $\ell^2(\mathbb{S}_\Gamma)$ is defined analogously to (2.4.1). Now, let $\ell \in \mathbb{N}$ such that $1 < \ell < L$. Then, $\Lambda_L = \Lambda_\ell \cup \Lambda_\ell^c$ is a spatial bipartition of Λ_L into two disjoint discrete subintervals, with the corresponding decomposition of the Hilbert space $\ell^2(\mathbb{S}_L) = \ell^2(\mathbb{S}_{\Lambda_\ell}) \otimes \ell^2(\mathbb{S}_{\Lambda_\ell^c})$. Moreover, for any $X \in \mathbb{S}_{\Lambda_\ell}$ and any $Y \in \mathbb{S}_{\Lambda_\ell^c}$, which implies that $X \vee Y \in \mathbb{S}_L$, one naturally identifies $\phi_{X\vee Y} = \phi_X \otimes \phi_Y$.[3]

The reduced state $\rho_1 : \ell^2(\mathbb{S}_{\Lambda_\ell}) \to \ell^2(\mathbb{S}_{\Lambda_\ell})$ is the linear operator given by

$$\rho_1(\psi, \Lambda_\ell) \equiv \rho_1 = \mathrm{Tr}_{\Lambda_\ell^c}(\rho_\psi) = \sum_{X_1, X_2 \in \mathbb{S}_{\Lambda_\ell}} \sum_{Y \in \mathbb{S}_{\Lambda_\ell^c}} \psi(X_1 \vee Y)\overline{\psi(X_2 \vee Y)}|\phi_{X_1}\rangle\langle\phi_{X_2}| \tag{2.4.3}$$

where $\mathrm{Tr}_{\Lambda_\ell^c}(\cdot)$ denotes the partial trace over the subsystem Λ_ℓ^c. Then, the Entanglement Entropy of ρ_ψ, which we denote by $\mathcal{E}(\rho_\psi)$ as in definition (1.6.1) is given by

$$\mathcal{E}(\rho_\psi) = -\mathrm{Tr}(\rho_1 \log \rho_1) =: \mathcal{S}(\rho_1)\,, \tag{2.4.4}$$

where $\mathcal{S}(\rho_1)$ denotes the von Neumann entropy of the reduced state ρ_1.[4] As in [1, 5], we will actually show estimates for the α-Rényi entropies $\mathcal{S}_\alpha$ of ρ_1, which are given by

$$\mathcal{S}_\alpha(\rho_1) := \frac{1}{1-\alpha} \log \mathrm{Tr}[(\rho_1)^\alpha]\,, \tag{2.4.5}$$

where $\alpha \in (0, 1)$. Since for every $\alpha \in (0, 1)$ one has $\mathcal{S}(\rho_1) \le \mathcal{S}_\alpha(\rho_1)$, showing suitable bounds for $\mathcal{S}_\alpha(\rho_1)$ will then readily imply the desired result for the entanglement

[3] For two multisets $X = (x_1, x_2, \ldots, x_j) \in \mathbb{S}_{\Lambda_\ell}$ and $Y = (y_1, y_2, \ldots, y_K) \in \mathbb{S}_{\Lambda_\ell^c}$, the notation "$X \vee Y$" denotes the multiset $(x_1, x_2, \ldots, x_j, y_1, y_2, \ldots, y_k) \in \mathbb{S}_L$. This means in particular that $\mathbf{m}_{X\vee Y} = \mathbf{m}_X + \mathbf{m}_Y$.

[4] We adapt the convention $0 \log 0 = 0$.

entropy $\mathcal{E}(\rho_\psi)$. Let us now further analyze (2.4.3):

$$\rho_1 = \sum_{X_1,X_2\in\mathbb{S}_{\Lambda_\ell}} \psi(X_1)\overline{\psi(X_2)}|\phi_{X_1}\rangle\langle\phi_{X_2}| + \sum_{X_1,X_2\in\mathbb{S}_{\Lambda_\ell}} \sum_{Y\in\mathbb{S}_{\Lambda_\ell^c}\setminus\{\emptyset\}} \psi(X_1\vee Y)\overline{\psi(X_2\vee Y)}|\phi_{X_1}\rangle\langle\phi_{X_2}|, \tag{2.4.6}$$

where the first sum simply corresponds to the contributions in (2.4.3), for which $Y=\emptyset$. Now, let the vector $\Psi\in\ell^2(\mathbb{S}_{\Lambda_\ell})$ be given by $\Psi := \sum_{X_3\in\mathbb{S}_{\Lambda_\ell}} \psi(X_3)\phi_{X_3}$, which clearly satisfies $\|\Psi\|_{\ell^2(\mathbb{S}_{\Lambda_\ell})} \le \|\psi\|_{\ell^2(\mathbb{S}_L)}$ and observe that

$$\sum_{X_1,X_2\in\mathbb{S}_{\Lambda_\ell}} \psi(X_1)\overline{\psi(X_2)}|\phi_{X_1}\rangle\langle\phi_{X_2}| = |\Psi\rangle\langle\Psi| \,. \tag{2.4.7}$$

So, we write $\rho_1 = |\Psi\rangle\langle\Psi| + \hat\rho_1$ with $\hat\rho_1$ being equal to the second sum in (2.4.6). Notice that $\hat\rho_1$ is non-negative since it is the partial trace of a non-negative operator $|\hat\psi\rangle\langle\hat\psi|$ where $|\hat\psi\rangle = \sum_{X\in\mathbb{S}_{\Lambda_\ell}}\sum_{Y\in\mathbb{S}_{\Lambda_\ell^c}\setminus\{\emptyset\}} \psi(X\vee Y)|\phi_{X\vee Y}\rangle$. Let us now focus on $\mathrm{Tr}[(\rho_1)^\alpha]$:

$$\mathrm{Tr}[(\rho_1)^\alpha] = \mathrm{Tr}[(|\Psi\rangle\langle\Psi| + \hat\rho_1)^\alpha] \le 2\mathrm{Tr}[(|\Psi\rangle\langle\Psi|)^\alpha] + 2\mathrm{Tr}[(\hat\rho_1)^\alpha] \le 2 + 2\mathrm{Tr}[(\hat\rho_1)^\alpha] \,, \tag{2.4.8}$$

where we have used the quasi-norm property of $\mathrm{Tr}|\cdot|^\alpha$, cf. [32, Satz 3.21] and the fact that $|\Psi\rangle\langle\Psi|$ is a non-negative rank-one operator with norm less than or equal to one. Let us now further estimate

$$\mathrm{Tr}[(\hat\rho_1)^\alpha] = \sum_{X\in\mathbb{S}_{\Lambda_\ell}} \langle\phi_X, (\hat\rho_1)^\alpha\phi_X\rangle \le \sum_{X\in\mathbb{S}_{\Lambda_\ell}} \langle\phi_X, \hat\rho_1\phi_X\rangle^\alpha = \sum_{j=0}^{2J\ell} \sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} \langle\phi_X, \hat\rho_1\phi_X\rangle^\alpha \tag{2.4.9}$$

$$\le \left| \bigcup_{j=0}^{4J-1} \mathbb{S}^j_{\Lambda_\ell} \right|^{1-\alpha} + \sum_{j=4J}^{2J\ell} \sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} \langle\phi_X, \hat\rho_1\phi_X\rangle^\alpha \tag{2.4.10}$$

where we have used Jensen's inequality for the first estimate in (2.4.9) and the second estimate (2.4.10) just follows from maximizing $\sum\sum\langle\phi_X,\hat{\rho}_1\phi_X\rangle^\alpha$ under the constraint $\sum\sum\langle\phi_X,\hat{\rho}_1\phi_X\rangle \le 1$. We estimate further by noting $|\mathbb{S}^j_{\Lambda_\ell}| \le \ell^j$ and since $\ell \ge 2$,

$$(2.4.10) \le \ell^{4J(1-\alpha)} + \sum_{j=4J}^{2J\ell} \sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} \langle\phi_X,\hat{\rho}_1\phi_X\rangle^\alpha \,. \tag{2.4.11}$$

Now, for each $X \in \mathbb{S}_{\Lambda_\ell}$ with $|X| = j$, we get

$$\langle\phi_X,\hat{\rho}_1\phi_X\rangle = \sum_{Y\in\mathbb{S}_{\Lambda^c_\ell}\setminus\{\emptyset\}} |\psi(X\vee Y)|^2 = \|P_{\mathcal{A}_X}\psi\|^2 \,, \tag{2.4.12}$$

where given any $X \in \mathbb{S}_{\Lambda_\ell}$, we have defined $P_{\mathcal{A}_X} := (P_X \otimes P_{\mathbb{S}_{\Lambda^c_\ell}}) - (P_X \otimes P_{\{\emptyset\}})$. Altogether, these considerations show the following

Lemma 2.4.1 *Let $\psi \in \ell^2(\mathbb{S}_L)$ be normalized. Then, for any $\alpha \in (0,1)$ we get*

$$\mathrm{Tr}[(\rho_1)^\alpha] \le 2 + 2\ell^{4J(1-\alpha)} + 2\sum_{j=4J}^{2J\ell} \sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} \|P_{\mathcal{A}_X}\psi\|^{2\alpha} \,. \tag{2.4.13}$$

2.5 Proof of the logarithmically corrected entanglement bound

In this section, the main result; the logarithmic upper bound for the entanglement entropy is shown.

Theorem 2.5.1 *For any $K \in \{4J^2, 4J^2+1, \dots\}$ and any $\delta > 0$, we get the following estimate*

$$\limsup_{\ell\to\infty}\, \limsup_{L\to\infty} \frac{\sup_W\, \sup_\psi \mathcal{E}(\rho_\psi)}{\log \ell} \le 2\lfloor K/J \rfloor - 2 \,, \tag{2.5.1}$$

where the suprema are taken over all non-negative functions $W : \mathbb{S}_L \to \mathbb{R}^+_0$ and over all normalized elements $\psi \in \mathrm{ran}(Q_{K,\delta}(L,W))$, respectively.

2.5.1 Local distance estimates

The following lemma, whose proof can be found in Appendix A.2.2, provides us with an estimate for the distance of a configuration in $\mathbb{S}_L$ to the nearest configuration in $\mathbb{S}_{L,K}$.

Lemma 2.5.2 *Let $X = (x_1, x_2, \ldots, x_j) \in \mathbb{S}^j_{\Lambda_\ell}$ with $j \geq 4J$ and $Y = (y_1, y_2, \ldots, y_k) \in \mathbb{S}^k_{\Lambda^c_\ell}$, where $k \in \mathbb{N}$. Then, for any $K \geq 4J^2$, we have the following estimate:*

$$d^j(X, \mathbb{S}^j_{\Lambda_\ell,K}) \leq d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K}) \,. \tag{2.5.2}$$

So, the main observation made in Lemma 2.5.2 is that there always exists a configuration in $\mathbb{S}^j_{\Lambda_\ell,K}$ which is at least as close to X as any configuration in $\mathbb{S}^{j+k}_{L,K}$ might be to $X \vee Y$. We now combine Lemmas 2.4.1, 2.5.2 and Theorem 2.3.2. To this end, for any non-negative function $W : \mathbb{S}_L \to \mathbb{R}^+_0$, let us define $Q_{K,\delta} \equiv Q_{K,\delta}(L, W) := \bigoplus_{N=0}^{2JL} Q^N_{K,\delta}(L, W_N)$ – the spectral projection of the full Hamiltonian onto the energy interval $[0, E_{K,\delta}]$ with background potential W. Here, $W_N : \ell^2(\mathbb{S}^N_L) \to \ell^2(\mathbb{S}^N_L)$, denotes the multiplication operator induced by W, i.e. $(W_N f)(X) := W(X)f(X)$, for any $f \in \ell^2(\mathbb{S}^N_L)$ and any $X \in \mathbb{S}^N_L$.

Corollary 2.5.3 *Fix $K \in \mathbb{N}$ and let $\ell \geq 4J$. Let $\psi \in \operatorname{ran}(Q_{K,\delta})$ be normalized. Then, for any $\alpha \in (0, 1)$, we have the following estimate*

$$\operatorname{Tr}[(\rho_1)^\alpha] \leq 2 + 2\ell^{4J(1-\alpha)} + 2C'^{2\alpha}_K \sum_{j=4J}^{2J\ell} \sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-2\alpha\mu_K d^j(X, \mathbb{S}^j_{\Lambda_\ell,K})} \,, \tag{2.5.3}$$

where

$$C'_K = \max\left\{1, \frac{2K(K+1)}{J^2\delta^2}\right\} \,. \tag{2.5.4}$$

Proof: Let $X \in \mathbb{S}^j_{\Lambda_\ell}$, where $j \geq 4J$. Defining $P_{\mathcal{A}_{X,k}} := P_X \otimes P_{\mathbb{S}^k_{\Lambda^c_\ell}}$, and using that

$$P_{\mathcal{A}_X} Q_{K,\delta} = \bigoplus_{k=1}^{2J(L-\ell)} P_{\mathcal{A}_{X,k}} Q^{j+k}_{K,\delta} \tag{2.5.5}$$

we get

$$\|P_{\mathcal{A}_X}\psi\| = \|P_{\mathcal{A}_X} Q_{K,\delta}\psi\| \leq \|P_{\mathcal{A}_X} Q_{K,\delta}\| = \max_{k\in\{1,\ldots,2J(L-\ell)\}} \|P_{\mathcal{A}_{X,k}} Q^{j+k}_{K,\delta}\| \tag{2.5.6}$$

$$\leq \max_{k\in\{1,\ldots,2J(L-\ell)\}} \left(C_{j+k,K} \cdot e^{-\mu_K d^{j+k}(\mathcal{A}_{X,k}, \mathbb{S}^{j+k}_{L,K})}\right) \tag{2.5.7}$$

where we have used Theorem 2.3.2 for the last inequality and the constants $C_{j+k,K}$ and μ_K were given in (2.3.6). Now, since $j + k \geq 4J$ by assumption, it follows from Proposition 2.2.5 that $V_{j+k,0} = 4J^2$ and thus

$$C_{j+k,K} = \max\left\{1, \frac{2K(K+1)}{J^2\delta^2}\right\} = C'_K\ , \tag{2.5.8}$$

independently of j. Now, for any $k \in \{1, \ldots, 2J(L-\ell)\}$, observe that by Lemma 2.5.2, we have

$$d^{j+k}(\mathcal{A}_{X,k}, \mathbb{S}^{j+k}_{L,K}) = \min_{Y\in\mathbb{S}^k_{\Lambda^c_\ell}} d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K}) \geq d^j(X, \mathbb{S}^j_{\Lambda_\ell,K}) \tag{2.5.9}$$

and thus we may proceed to estimate (2.5.7) to get

$$\|P_{\mathcal{A}_X}\psi\| \leq (2.5.7) \leq C'_K \cdot e^{-\mu_K d^j(X, \mathbb{S}^j_{\Lambda_\ell,K})}\ . \tag{2.5.10}$$

Using Lemma 2.4.1, we consequently find

$$\operatorname{Tr}[(\rho_1)^\alpha] \le 2 + 2\ell^{4J(1-\alpha)} + 2C_K'^{2\alpha} \sum_{j=4J}^{2J\ell} \sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-2\alpha\mu_K d^j(X, \mathbb{S}^j_{\Lambda_\ell, K})} \,, \tag{2.5.11}$$

which shows (2.5.3).

2.5.2 Estimates using geometric series

Lemma 2.5.4 *Let $\mathcal{X}^N = \{\, X = (x_1, x_2, \ldots, x_N) \in \mathbb{Z}^N : x_1 < x_2 < \cdots < x_N \,\}$ be the set of spin–1/2 configurations on the infinite chain. Moreover, let $C = (c_1, c_2, \ldots, c_N) = (c, c+1, \ldots, c+(N-1))$ be an arbitrary configuration of N consecutive particles ($c \in \mathbb{Z}$). Then, for any $\gamma > 0$, we get*

$$\sum_{X \in \mathcal{X}^N} e^{-\gamma d^N(X,C)} \le \left(\frac{1}{1-e^{-\gamma}} \right) \left(\prod_{k=1}^{\infty} \frac{1}{1-e^{-k\gamma}} \right)^2 := \mathcal{L}_\gamma < \infty \,. \tag{2.5.12}$$

Proof:

Define

$$\mathcal{X}^{N,0} = \{\, X \in \mathcal{X}^N : x_1 \ge c_1 \,\}, \quad \mathcal{X}^{N,N} = \{\, X \in \mathcal{X}^N : x_N < c_N \,\}$$

and for any $j \in \{\, 1, \ldots, N-1 \,\}$,

$$\mathcal{X}^{N,j} = \{\, X \in \mathcal{X}^N : x_j < c_j,\ x_{j+1} \ge c_{j+1} \,\} \ .$$

Then, $\mathcal{X}^N = \uplus_{j=0}^N \mathcal{X}^{N,j}$, where "$\uplus$" denotes a disjoint union. For any $j \in \{\, 1, \ldots, N-1 \,\}$, *we get by an argument similar to [14, Lemma A.3] that*

$$\sum_{X\in\mathcal{X}^{N,j}} e^{-\gamma d^N(X,C)} = \sum_{x_1<x_2<\cdots<x_j<c_j} e^{-\gamma(|x_1-c_1|+\cdots+|x_j-c_j|)} \sum_{c_{j+1}\le x_{j+1}<x_{j+2}<\cdots<x_N} e^{-\gamma(|x_{j+1}-c_{j+1}|+\cdots+|x_N-c_N|)}$$
$$\le e^{-\gamma j}\left(\prod_{k=1}^{j}\frac{1}{1-e^{-k\gamma}}\right)\left(\prod_{k=1}^{N-j}\frac{1}{1-e^{-k\gamma}}\right) \le e^{-\gamma j}\left(\prod_{k=1}^{\infty}\frac{1}{1-e^{-k\gamma}}\right)^2 . \tag{2.5.13}$$

Analogously, we find

$$\sum_{X\in\mathcal{X}^{N,0}} e^{-\gamma d^N(X,C)} \le \prod_{k=1}^{N}\frac{1}{1-e^{-k\gamma}} \le \left(\prod_{k=1}^{\infty}\frac{1}{1-e^{-k\gamma}}\right)^2 \tag{2.5.14}$$

$$\sum_{X\in\mathcal{X}^{N,N}} e^{-\gamma d^N(X,C)} \le e^{-\gamma N}\prod_{k=1}^{N}\frac{1}{1-e^{-k\gamma}} \le e^{-\gamma N}\left(\prod_{k=1}^{\infty}\frac{1}{1-e^{-k\gamma}}\right)^2 . \tag{2.5.15}$$

Hence,

$$\sum_{X\in\mathcal{X}^{N}} e^{-\gamma d^N(X,C)} = \sum_{j=0}^{N}\sum_{X\in\mathcal{X}^{N,j}} e^{-\gamma d^N(X,C)} \tag{2.5.16}$$
$$\le \sum_{j=0}^{N} e^{-\gamma j}\left(\prod_{k=1}^{\infty}\frac{1}{1-e^{-k\gamma}}\right)^2 \le \left(\frac{1}{1-e^{-\gamma}}\right)\left(\prod_{k=1}^{\infty}\frac{1}{1-e^{-k\gamma}}\right)^2 , \tag{2.5.17}$$

which is the desired result. The infinite product's convergence follows from elementary facts.

Definition 2.5.5 *For any* $\mathbf{m}\in\mathbf{M}_L^N$*, let* $\mathrm{supp}(\mathbf{m}) := \{j\in\{1,2,\ldots,L\} : \mathbf{m}(j)\neq 0\}$ *denote the support of* $\mathbf{m}$*. Then, for any* L*, we define the set* $\mathbf{K}_L$ *of "building bocks"* *in* Λ_L *as follows*

$$\mathbf{K}_L := \{\mathbf{m} \in \mathbf{M}_L : |supp(\mathbf{m})| = 1\} \\ \cup \{\mathbf{m} \in \mathbf{M}_L : \exists\, \alpha, \beta \in \Lambda_L : \mathbf{m}(i) = 2J \ \text{if}\ \alpha \le i \le \beta \ \text{and}\ \mathbf{m}(i) = 0 \ \text{else}\} . \tag{2.5.18}$$

In other words, building blocks are configurations of either a single column of up to $2J$ *particles or of discrete intervals, where each site is occupied by exactly* $2J$ *particles (rectangular blocks).*

Lemma 2.5.6 *Let* $\gamma > 0$. *Then for any* $C \in \mathbf{K}_L$, *we have*

$$\sum_{X \in \mathbb{S}_L^N} e^{-\gamma d^N(X,C)} \le \mathcal{L}_\gamma^{2J} \tag{2.5.19}$$

Proof: *Let* C *be a rectangular block, i.e.* $C = (\overbrace{c, \ldots, c}^{2J\ \ times}, \overbrace{c+1, \ldots, c+1}^{2J\ \ times}, \ldots, \overbrace{c+m, \ldots, c+m}^{2J\ \ times})$ *where* $N = 2J(m+1)$. *For any* N*-particle configuration* $X = (x_1, \ldots, x_N) \in \mathbb{S}_L^N$, *let* $Z_0(X)$ *denote the constraint*

$$Z_0(X) : x_1 \le x_2 \le \cdots \le x_N \,. \tag{2.5.20}$$

Moreover, define the additional constraints

$$Z_i(X) : x_i < x_{i+2J} < x_{i+4J} < \cdots < x_{i+2JR_i} \tag{2.5.21}$$

where $i \in \{\,1, 2, \ldots, 2J\,\}$ *and* $R_i = \max\{\,R \in \{1, 2, \ldots, N\} : i + 2JR \le N\,\}$.

Let

$$\mathbb{M}_L^N := \{\,X \in \Lambda_L^N :\ Z_i(X) \ \ \text{holds}\ \ \forall\, i = 0, \ldots, 2J\,\} \tag{2.5.22}$$

and

$$\Gamma^N := \{ X \in \mathbb{Z}^N : Z_k(X) \text{ holds } \forall k = 1, \dots, 2J \} . \tag{2.5.23}$$

Obviously, $\mathbb{M}_L^N \subseteq \Gamma^N$.

To see that $\mathbb{M}_L^N = \mathbb{S}_L^N$ *(defined in (2.2.18)), note that it is obvious that* $\mathbb{M}_L^N \subseteq \mathbb{S}_L^N$ *since for any* $X \in \mathbb{M}_L^N$*, the constraints* $Z_i(X)$ *imply that* $\min\{ (x_{k+2J} - x_k) : k = 1, \dots, N-2J \} \geq 1$.

Conversely, suppose there exists $X \in \mathbb{S}_L^N \setminus \mathbb{M}_L^N$*, i.e.* X *violates at least one constraint,* $Z_t(X)$ *say, where* $t \neq 0$*. Then there exists* $r \in \mathbb{N}$ *such that* $x_{t+2Jr} \geq x_{t+2J(r+1)}$*. This is a contradiction since* $X \in \mathbb{S}_L^N$*. Hence,* $\mathbb{S}_L^N = \mathbb{M}_L^N$.

Therefore, by Lemma (2.5.4),

$$\begin{aligned} \sum_{X \in \mathbb{S}_L^N} e^{-\gamma d^N(X,C)} &\leq \sum_{X \in \Gamma^N} e^{-\gamma d^N(X,C)} \\ &= \sum_{Z_1(X)} e^{-\gamma(|x_1 - c_1| + \cdots + |x_{1+2JR_1} - c_{1+2JR_1}|)} \times \cdots \\ &\qquad \cdots \times \sum_{Z_{2J}(X)} e^{-\gamma(|x_{2J} - c_{2J}| + \cdots + |x_{2J+2JR_{2J}} - c_{2J+2JR_{2J}}|)} \\ &\leq \mathcal{L}_\gamma^{2J} . \end{aligned} \tag{2.5.24}$$

If $C = (c_1, \dots, c_N)$ *is a column block, i.e.* $c_1 = \cdots = c_N = c$*, where* $c \in \Lambda_L$ *and* $N \leq 2J$*, then*

$$\sum_{X \in \mathbb{S}_L^N} e^{-\gamma d^N(X,C)} \leq \sum_{-\infty < x_1 \leq x_2 \leq \cdots \leq x_N < \infty} e^{-\gamma[|x_1 - c| + \cdots + |x_N - c|]} \tag{2.5.25}$$

$$\leq \sum_{x_1, x_2, \cdots, x_N \in \mathbb{Z}} e^{-\gamma[|x_1 - c| + \cdots + |x_N - c|]} = \left(\frac{1 + e^{-\gamma}}{1 - e^{-\gamma}} \right)^N \leq \mathcal{L}_\gamma^N \leq \mathcal{L}_\gamma^{2J} , \tag{2.5.26}$$

which finishes the proof.

Remark 2.5.7 *Note that for this result, we are making use of the generalized Pauli principle, which requires that no site be occupied by more than* $2J$ *particles.*

2.5.3 Building blocks and potential

Given a value $K \in \mathbb{N}$ and a particle number $N \geq 4J$, it seems rather cumbersome to give a full description of all configurations in $\mathbf{M}_{L,K}^N$. However, it can be shown that any configuration in $\mathbf{M}_{L,K}^N$ can be composed out of no more than K of the "building blocks" as described in Definition 2.5.5 before.

Definition 2.5.8 *Given a configuration* $\mathbf{m} \in \mathbf{M}_L$*, we define the quantity* $B(\mathbf{m})$ *as follows:*

$$B(\mathbf{m}) := |\{i \in \{1, 2, \dots, L-1\} : \mathbf{m}(i) + \mathbf{m}(i+1) \notin \{0, 4J\}\}| + (2 - \delta_{\mathbf{m}(1),0} - \delta_{\mathbf{m}(L),0}). \tag{2.5.27}$$

Moreover, for any $R \in \mathbb{N}$*, we define*

$$\mathbf{B}_{L,R} := \{\mathbf{m} \in \mathbf{M}_L : B(\mathbf{m}) \leq R\} \quad \text{as well as} \quad \mathbf{B}_{L,R}^N := \mathbf{B}_{L,R} \cap \mathbf{M}_L^N \tag{2.5.28}$$

for any $N \in \{0, 1, \dots, 2JL\}$*. Additionally, for multisets, we introduce* $\mathbb{B}_{L,R} = \{X \in \mathbb{S}_L : \mathbf{m}_X \in \mathbf{B}_{L,R}\}$ *and* $\mathbb{B}_{L,R}^N = \mathbb{B}_{L,R} \cap \mathbb{S}_L^N$*.*

Remark 2.5.9 *The purpose of* $B(\mathbf{m})$ *is to count the number of neighboring sites* $\{i, i+1\}$*,* $i = 1, 2, \dots, L-1$*, which are not both occupied by either* 0 *or* $2J$ *particles. Each of the two additional terms in* $(2 - \delta_{\mathbf{m}(1),0} - \delta_{\mathbf{m}(L),0}) = (1 - \delta_{\mathbf{m}(1),0}) + (1 - \delta_{\mathbf{m}(L),0})$ *increases* $B(\mathbf{m})$ *by a value of one if the sites* 1 *or* L *are occupied by any particles (which formally corresponds to including the edges* $\{0, 1\}$ *and* $\{L, L+1\}$ *in the count).*

Remark 2.5.10 *Observe that* $B(\mathbf{m}) \leq J^{-1}V(\mathbf{m})$ *for every* $\mathbf{m} \in \mathbf{M}_L$*. This follows from the fact that* $v(\mathbf{m}(i), \mathbf{m}(i+1)) = 0$ *if and only if* $\mathbf{m}(i) = \mathbf{m}(i+1) = 0$ *or* $\mathbf{m}(i) = \mathbf{m}(i+1) = 2J$ *and* $v(\mathbf{m}(i), \mathbf{m}(i+1)) \geq J$ *else, and comparing the extra term* $(2 - \delta_{\mathbf{m}(1),0} - \delta_{\mathbf{m}(L),0})$ *in* (2.5.27) *with the boundary field term* $J(\mathbf{m}(1) + \mathbf{m}(L))$ *in* (2.2.11)*. For* $K \geq 4J^2$*, define* $\widetilde{K} := \lfloor K/J \rfloor$*, and observe that this implies*

$$\mathbb{S}_{L,K} \subset \mathbb{B}_{L,\widetilde{K}} \quad \textit{and thus in particular} \quad \mathbb{S}^N_{L,K} \subset \mathbb{B}^N_{L,\widetilde{K}} \,. \tag{2.5.29}$$

It is now crucial to observe that any configuration in $\mathbf{B}_{L,\widetilde{K}}$ can always by obtained by composing it out of at most $(\widetilde{K} - 1)$ "building blocks".

Remark 2.5.11 *Observe that for any* $\mathbf{m} \in \mathbf{M}_L$*, there exist* $\{\mathbf{k}^{(i)}\}_{i=1}^{\tau} \subset \mathbf{K}_L$*,* $(\tau \leq L)$*, with pairwise disjoint supports, such that* $\mathbf{m} = \sum_{i=1}^{\tau} \mathbf{k}_i$*. If in addition, we have* $\mathbf{m} \in \mathbf{B}_{L,\widetilde{K}}$*, it follows from* (2.5.27) *that* $\tau \leq (\widetilde{K} - 1)$*, i.e. any configuration in* $\mathbf{B}_{L,\widetilde{K}}$ *can be composed out of no more than* $(\widetilde{K} - 1)$ *building blocks. See Figure 2.5.1 for a pictorial representation of building blocks.*

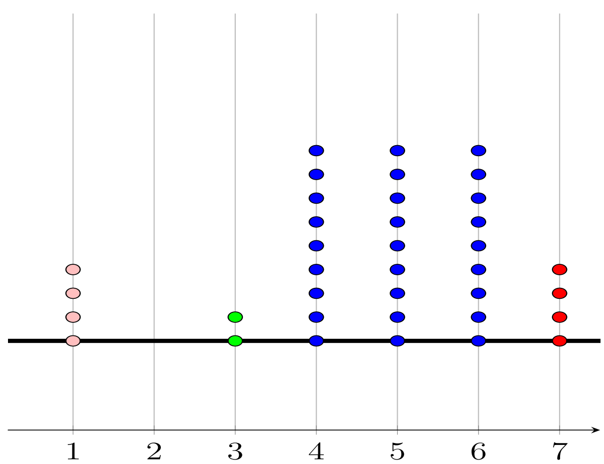

Figure 2.5.1: A configuration $\mathbf{m} \in \mathbf{M}^N_L$ of $N = 37$ particles (here: $J = 9/2$). Moreover, $B(\mathbf{m}) = 6 \leq J^{-1}V(\mathbf{m}) = 26$ and indeed, $\mathbf{m}$ can be written as a composition of $4 \leq (\lfloor J^{-1}V(\mathbf{m}) \rfloor - 1)$ building blocks (represented here by four different colors).

Lemma 2.5.12 *Let* $j \in \{4J, 4J+1, \ldots, 2J\ell\}$*,* $K \in \{4J^2, 4J^2+1, \ldots, 2J\ell\}$ *and* $\widetilde{K} := \lfloor K/J \rfloor$*. Then, for any* $\gamma > 0$*, we get the following estimate*

$$\sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X, \mathbb{S}^j_{\Lambda_\ell, K})} \leq (4Je)^{\widetilde{K}-2} \mathcal{L}^{2J(\widetilde{K}-1)}_{2\alpha\mu_K} \ell^{2\widetilde{K}-3} . \tag{2.5.30}$$

Proof: Analogously to before, we define $\mathbb{B}^j_{\Lambda_\ell, \widetilde{K}} := \mathbb{B}^j_{L, \widetilde{K}} \cap \mathbb{S}_{\Lambda_\ell}$ and observe that due to (2.5.29), we have $\mathbb{S}^j_{\Lambda_\ell, K} \subset \mathbb{B}^j_{\Lambda_\ell, \widetilde{K}}$ and thus, we get

$$\sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X, \mathbb{S}^j_{\Lambda_\ell, K})} \leq \sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} \sum_{Y \in \mathbb{S}^j_{\Lambda_\ell, K}} e^{-\gamma d^j(X,Y)} = \sum_{Y \in \mathbb{S}^j_{\Lambda_\ell, K}} \sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X,Y)} \leq \sum_{Y \in \mathbb{B}^j_{\Lambda_\ell, \widetilde{K}}} \sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X,Y)}. \tag{2.5.31}$$

We now claim that for every $Y \in \mathbb{B}^j_{\Lambda_\ell, \widetilde{K}}$, we get

$$\sum_{X \in \mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X,Y)} \leq \mathcal{L}^{2J(\widetilde{K}-1)}_{\gamma} . \tag{2.5.32}$$

Since $Y \in \mathbb{B}^j_{\Lambda_\ell, \widetilde{K}}$, observe that by Remark 2.5.11, there exist $\mathbf{k}^{(1)}, \mathbf{k}^{(2)}, \ldots, \mathbf{k}^{(\tau)} \in \mathbf{K}_L$ with $\tau \leq (\widetilde{K}-1)$ and pairwise disjoint support such that

$$\mathbf{k}^{(1)} + \mathbf{k}^{(2)} + \cdots + \mathbf{k}^{(\tau)} = \mathbf{m}_Y . \tag{2.5.33}$$

Without loss of generality, we may assume that the building blocks are ordered such that $1 \leq i < s \leq \tau$ implies $\max \operatorname{supp}(\mathbf{k}^{(i)}) < \min \operatorname{supp}(\mathbf{k}^{(s)})$.

For any $i \in \{1, 2 \ldots, \tau\}$, let $K^{(i)} := X_{\mathbf{k}^{(i)}}$ denote the multiset associated with the building block $\mathbf{k}^{(i)}$ and thus $Y = K^{(1)} \vee K^{(2)} \vee \cdots \vee K^{(\tau)}$. Now, decompose any $X \in \mathbb{S}^j_{\Lambda_\ell}$ analogously into $X = X^{(1)} \vee X^{(2)} \vee \cdots \vee X^{(\tau)}$ such that $|X^{(i)}| = |K^{(i)}| =: k_i$ for every $i \in \{1, 2, \ldots, \tau\}$ and $i < s$ implies that $\max(X^{(i)}) < \min(X^{(s)})$.

We then get

$$\sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X,Y)} = \sum_{X^{(1)}\vee\cdots\vee X^{(\tau)}\in\mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma\left(d^{k_1}(X^{(1)},K^{(1)})+\cdots+d^{k_\tau}(X^{(\tau)},K^{(\tau)})\right)} \tag{2.5.34}$$

$$\leq \prod_{i=1}^{\tau}\left(\sum_{X^{(i)}\in\mathbb{S}^{k_i}_{\Lambda_\ell}} e^{-\gamma d^{k_i}(X^{(i)},K^{(i)})}\right) \leq \mathcal{L}_\gamma^{2J\tau} \leq \mathcal{L}_\gamma^{2J(\widetilde{K}-1)}\,, \tag{2.5.35}$$

where we have used Lemma 2.5.6 for estimating the sum in (2.5.35). This shows (2.5.32) which together with (2.5.31) proves that

$$\sum_{X\in\mathbb{S}^j_{\Lambda_\ell}} e^{-\gamma d^j(X,\mathbb{S}^j_{\Lambda_\ell,K})} \leq \sum_{Y\in\mathbb{B}^j_{\Lambda_\ell,\widetilde{K}}} \mathcal{L}_\gamma^{2J(\widetilde{K}-1)} = |\mathbb{B}^j_{\Lambda_\ell,\widetilde{K}}|\cdot\mathcal{L}_\gamma^{2J(\widetilde{K}-1)}\,, \tag{2.5.36}$$

which means that we need to further estimate the number of configurations in Λ_ℓ of $(\widetilde{K}-1)$ or less building blocks of j particles. We do this by a rather rough combinatorial argument: firstly, note that distributing j particles into up to $(\widetilde{K}-1)$ building blocks can be estimated by $\binom{j+\widetilde{K}-2}{\widetilde{K}-2}$. This is clearly an overestimate, since it disregards the constraints in (2.5.18) which building blocks have to satisfy. Next, we have to account for all the possible ways, those $(\widetilde{K}-1)$ or less building blocks can be placed in Λ_ℓ. A trivial upper bound for this is given by $\ell^{\widetilde{K}-1}$, since there are up to ℓ sites one could place each individual building block (disregarding the fact that the supports of the building blocks have to be disjoint and can be larger than one and thus again overestimating). If $\widetilde{K}>2$, we therefore conclude

$$|\mathbb{B}^j_{\Lambda_\ell,\widetilde{K}}| \leq \binom{j+\widetilde{K}-2}{\widetilde{K}-2}\cdot\ell^{\widetilde{K}-1} \leq \left(\frac{(2J\ell+\widetilde{K}-2)e}{\widetilde{K}-2}\right)^{\widetilde{K}-2}\ell^{\widetilde{K}-1} \leq (4Je)^{\widetilde{K}-2}\ell^{2\widetilde{K}-3}\,, \tag{2.5.37}$$

where we have used the estimate $\binom{\alpha}{\beta}\leq\left(\frac{\alpha e}{\beta}\right)^{\beta}$ for the binomial coefficient as well as the fact that $j\leq 2J\ell$ and $4J\leq\widetilde{K}\leq 2\ell$. For the special case $\widetilde{K}=2$, which can only occur of $J = 1/2$, Equation (2.5.37) still follows since $|\mathbb{B}^j_{\Lambda_\ell,\widetilde{K}}| \leq \ell$. This shows the lemma.

2.5.4 Proof of the main result

Proof of Theorem 2.5.1: Let $W : \mathbb{S}_L \to \mathbb{R}_0^+$ be an arbitrary non-negative background potential and let ψ be an arbitrary normalized element of $\mathrm{ran}(Q_{K,\delta}(L,W))$. Combining Corollary 2.5.3 and Lemma 2.5.12 (with the choice $\gamma = 2\alpha\mu_K$) and using that for any $\alpha \in (0,1)$, the α-Rényi entropy is an upper bound for the von Neumann entropy, we obtain

$$\mathcal{E}(\rho_\psi) \leq \frac{1}{1-\alpha} \log \mathrm{Tr}[(\rho_1)^\alpha] \leq \frac{1}{1-\alpha} \log \left(2 + 2\ell^{4J(1-\alpha)} + (4Je)^{\widetilde{K}-1} C_K'^{2\alpha} \mathcal{L}_{2\alpha\mu_K}^{2J(\widetilde{K}-1)} \ell^{2\widetilde{K}-2} \right) , \tag{2.5.38}$$

which does not depend on L. We therefore get

$$\limsup_{\ell\to\infty} \limsup_{L\to\infty} \frac{\sup_W \, \sup_\psi \mathcal{E}(\rho_\psi)}{\log \ell} \leq \frac{2\widetilde{K}-2}{1-\alpha} = \frac{2\lfloor K/J \rfloor - 2}{1-\alpha} . \tag{2.5.39}$$

Since this is true for all $\alpha \in (0,1)$, one can take $\alpha \to 0$, which yields the desired result.

Remark 2.5.13 *Note that for $J = 1/2$, the constant in* (2.5.1)*, is given by* $(4K-2)$*. In [1], where only the case $J = 1/2$ was treated, the better bound* $(2K-1)$ *was established. The main reason for this discrepancy is that in this special case, one can actually show that any configuration* $\mathbf{m}$ *with* $V(\mathbf{m}) \leq K$ *can actually be composed out of no more than K building blocks rather than out of no more than* $\widetilde{K} - 1 = 2K - 1$ *building blocks.*

CHAPTER 3

GENERALIZATION OF EMPTINESS FORMATION BOUNDS USING REFLECTION POSITIVITY

3.1 Classical spin systems on $\mathbb{Z}^d$

Let $d \in \mathbb{N}$ and $G = (\mathcal{V}, \mathcal{E})$ be a finite graph on $\mathbb{Z}^d$, where $\mathcal{E}$ is the collection of pairs $\{ i, j \}$ for $i \neq j$ and $\langle i, j \rangle$ means i and j are nearest neighbors. S_i represents a spin at the site $i \in \mathcal{V}$ i.e. random variable with values in a closed subset C of $\mathbb{R}^n$, $n \geq 1$. We hereby consider some spin systems:

1. **The $O(n)$ model:** Let $C := S^{n-1} = \{ x \in \mathbb{R}^n : |x| = 1 \}$ and let the *a priori* measure m be the surface measure on C. The Hamiltonian is given as

$$H(S) := -J \sum_{\langle i,j \rangle} S_i \cdot S_j \tag{3.1.1}$$

   where $J \geq 0$ and the product is the usual dot product in $\mathbb{R}^n$. H preserves rotation since for any orthogonal $n-$dimensional matrix M, $MS_i \cdot MS_j = S_i \cdot S_j$. Also, m is 'globally' rotation invariant since $m \circ A^{-1} = m$ for all spin sites.

   The case $n = 2$ is the *rotor model* while the case $n = 3$ is the *(classical) Heisenberg ferromagnet.*

2. **Ising model:** This is formally the $O(1)$ model where $C = \{ -1, +1 \}$ with

uniform *a priori* measure and the Hamiltonian given as

$$H(S) := -J \sum_{\langle i,j \rangle} S_i S_j \tag{3.1.2}$$

where the ground state energy is obtained when all the spins align (for $J \geq 0$) or when the spins anti-align (for $J \leq 0$). (This is true also for all the $O(n)$ models).

3. **Potts model:** This is a generalization of the ising model beyond two spin states (i.e $C = \{1, \ldots r\}$, $r < \infty$) with uniform *a priori* measure and Hamiltonian

$$H(S) := -J \sum_{\langle i,j \rangle} \delta_{S_i S_j} \tag{3.1.3}$$

The case $r = 2$ can be can be seen as the Ising model within an additive constant (see [6])

3.2 Definition and statement of main results

3.2.1 Emptiness Formation Probability (EFP)

For spin 1/2, recall that the eigenvalues of the spin matrix S^3 are $\pm(1/2)$. Therefore, define projections unto the eigenvectors corresponding to these eigenvalues as the two operators $(\frac{1}{2}\mathbb{1} \pm S^3)$. As long as $N \geq L$, we may view $\mathbb{B}_L$ as a subset of the graph $\mathcal{G}$ (whose vertex set is $\mathbb{B}_N$). We define the projection operator

$$\mathbf{Q}_L = \prod_{\mathbf{i} \in \mathbb{B}_L} \left[\frac{1}{2}\mathbb{1}_{\mathbf{i}} + S^3_{\mathbf{i}}\right] \tag{3.2.1}$$

The range of $\mathbf{Q}_L$ is the subspace spanned by all spin states having all spins up on the sub-box $\mathbb{B}_L$. The expectation of $\mathbf{Q}_L$ (i.e expectation of having a sequence of up spins on $\mathbb{B}_L$) in the ground state of thee XXZ model is called **Emptines Formation**

probability in physics literatures.

Theorem 3.2.1 *Suppose $d \in \mathbb{N}$ is fixed. For $\Delta < -1$, there are constants $c, C \in (0, \infty)$ such that, whenever $L \leq \frac{N}{2}$,*

$$\langle \mathbf{Q}_L \rangle \geq C e^{-c\beta L^{d+1}} \tag{3.2.2}$$

Theorem 3.2.2 *For each $\Delta < 1$, there exists $L_0 \in \mathbb{N}$, and $\tilde{c}$, $\tilde{C} > 0$ such that for all $L \geq L_0$, we have*

$$\langle \hat{\mathbf{Q}}_{N,L} \rangle_{N,\Delta,\beta} \leq C e^{-cN^d \min(L,\beta)} \tag{3.2.3}$$

3.3 Graphical representations for the XXZ model

3.3.1 Tóth's representation for the Heisenberg ferromagnet

The origin of the Tóth's representation can be found in [3] and [33].

Lemma 3.3.1 (Trotter product formula [18, Prop. 2.11]) . *For all $X, Y \in \mathbb{M}_n(\mathbb{C})$, we have that*

$$e^{A+B} = \lim_{N \to 0} \left(e^{\frac{X}{N}} e^{\frac{Y}{N}} \right)^N \tag{3.3.1}$$

Proposition 3.3.2 (Duhamel's formula [17, Prop. 3.1]) . *Let A and B be $n \times n$ matrices. Then*

$$\begin{aligned} e^{A+B} &= e^A + \int_0^1 e^{tA} B e^{(1-t)(A+B)} dt \\ &= \sum_{k \geq 0} \int_{0 < t_1 < \cdots < t_k < 1} e^{t_1 A} B e^{(t_2 - t_1)A} B \cdots B e^{(1-t_k)A} dt_1 \cdots dt_k. \end{aligned} \tag{3.3.2}$$

Consider the finite graph $G = (\mathcal{V}, \mathcal{E})$ on $\mathbb{Z}^d$ and the Hilbert space

$$\mathcal{H}_{\mathcal{V}} = \bigotimes_{j \in \mathcal{V}} \mathcal{H}_j \tag{3.3.3}$$

where $\mathcal{H}_j$ is a copy of $\mathbb{C}^2$. Define the XXZ Hamiltonian $H_{\mathcal{G},\Delta} : \mathcal{H}_{\mathcal{V}} \longrightarrow \mathcal{H}_{\mathcal{V}}$ as

$$H_{\mathcal{G},\Delta} := \sum_{\{i,j\}\in\mathcal{E}} h_{ij}^{\Delta} = -\sum_{\{i,j\}\in\mathcal{E}} (S_i^x S_j^x + S_i^y S_j^y + \Delta \cdot S_i^z S_j^z) \tag{3.3.4}$$

where S^x, S^y and S^z are the normalized Pauli matrices given by;

$$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.3.5}$$

and consider the notation

$$|\tfrac{1}{2}\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |-\tfrac{1}{2}\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.3.6}$$

The parameter $\Delta \in \mathbb{R}$ is called the anisotropy parameter. $H_{\mathcal{V},\Delta}$ is ferromagnetic for $\Delta > 0$ and it is unitarily equivalent to the antiferromagnetic XXZ when $\Delta < 0$ as seen in (B.1.1). The case $\Delta = 0$ gives the XX Hamiltonian.

We define the Partition function as

$$Z_{\mathcal{G},\Delta}(\beta) := \mathrm{Tr}(e^{-\beta H_{\mathcal{G},\Delta}}) \tag{3.3.7}$$

and the Equilibrium state as

$$\langle X\rangle_{\mathcal{G},\Delta,\beta} := \frac{\mathrm{Tr}(X e^{-\beta H_{\mathcal{G},\Delta}})}{Z_{\mathcal{G},\Delta}(\beta)}, \qquad \beta \geq 0 \tag{3.3.8}$$

For graphs $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ in any dimension d, d finite, we define $\mathcal{V}$ to be the box $\mathbb{B}_N$, $N \in \mathbb{N}$ as

$$\mathbb{B}_N = \big\{\mathbf{i} = (i_1, \ldots, i_d) \in \mathbb{Z}^d : 0 \leq i_1, \ldots, i_d \leq N-1\big\} \tag{3.3.9}$$

and the edge set $\mathcal{E}$ as

$$\mathcal{E} = \mathbb{T}_N = \{\,\{\,\mathbf{i},\mathbf{j}\,\} : \mathbf{i},\mathbf{j} \in \mathbb{B}_N \text{ and } \mathbf{j}-\mathbf{i} \in \{\,e_1,\ldots,e_d,-(N-1)e_1,\ldots,-(N-1)e_d\,\}\,\} \tag{3.3.10}$$

where $e_1,\ldots,e_d$ are the canonical basis vector in $\mathbb{Z}^d$ and the multiples of the canonical basis vectors in (3.3.10) show periodic boundary conditions. Hence the graph is the discrete torus on $\mathbb{Z}^d$.

In what follows, we restrict N to be even for bipartite graphs and by a slight abuse of notation, we write $H_{\mathcal{G},\Delta},\ Z_{\mathcal{G},\Delta}(\beta),\ \langle X\rangle_{\mathcal{G},\Delta,\beta}$ in place of the Hamiltonian , the Partition function and the Equilibrium state with respective to the discrete torus on $\mathbb{Z}^d$ and $|\mathbb{B}_N| = N^d$.

3.3.2 Poisson edge process on the graph

Consider the graph with vertex and edge set as defined in (3.3.9) and (3.3.10) with $d = 1$. To each edge $\{\,\mathbf{i},\mathbf{j}\,\} \in \mathbb{T}_N$, attach a Poisson process on $[0,\beta]$ with intensity u such that Poisson processes for different edges are independent. Let $(\Omega,\mathcal{F},\mathbb{P})$ be the probability state space of these processes and let $\mathbb{E}[\cdot]$ be the corresponding expectation. Then for any realization $\omega \in \Omega$, we have that

$$\omega = ((e_1,t_1),\ldots,(e_k,t_k)) \tag{3.3.11}$$

where the times $0 < t_1 < \ldots < t_k < \beta$ are uniformly distributed and the edges are chosen uniformly in $\mathbb{T}_N$, To each realization, we have cycles simply defined in Figure (3.3.1), but have cumbersome definition.

To each edge process, denote the corresponding measure as $d\nu_{\mathbf{ij}}(\omega)$.

Denote by $\sigma(t) : \mathcal{V} \to \{\,-\frac{1}{2},\frac{1}{2}\,\}^{|\mathcal{V}|}$ the spin configuration corresponding to ω at t.

An event on the edge $\langle \mathbf{i}, \mathbf{j} \rangle$ is called a '**bridge**' at t if

$$\sigma_{\mathbf{i}}(t-) = \sigma_{\mathbf{j}}(t+) \qquad \text{and} \qquad \sigma_{\mathbf{j}}(t-) = \sigma_{\mathbf{i}}(t+) \tag{3.3.12}$$

A cycle $\gamma : [0, L] \longrightarrow \mathcal{V} \times [0, \beta]$ is a closed trajectory with $\gamma(s) = (\mathbf{i}(s), t(s))$ satisfying:

1. γ is piece-wise continuous i.e. $\mathbf{i}(s)$ is a constant if γ is continuous on $I \subset [0, L]$ and $\frac{d}{ds}t(s) = 1$ in I.

2. s is a point of discontinuity if and only if at the time $t(s)$ (with corresponding edge $e(s)$), there a '**bridge**'. Hence, $e(s) = (\gamma(s-), \gamma(s+))$.

The length of the cycle is the smallest positive number L such that $\gamma(0) = \gamma(L)$. This can be seen as the vertical legs in Figure (3.3.1), hence, it is a multiple of β. Denote $\mathcal{C}(\omega)$ as the collection of cycles in ω. Thus, $|\mathcal{C}(\omega)|$ is the number of cycles in ω.

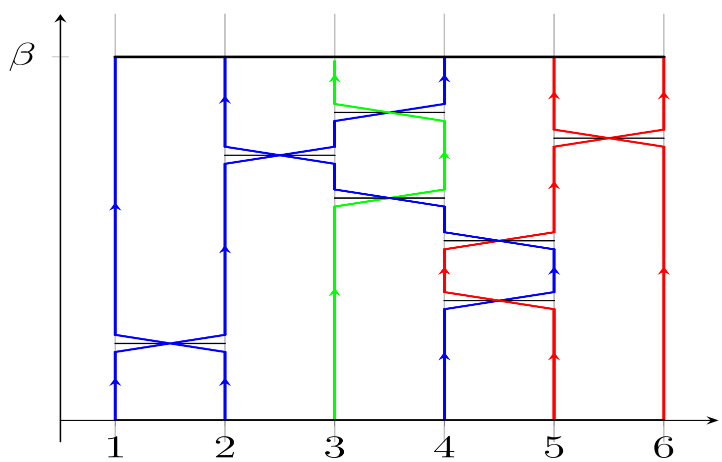

Figure 3.3.1: Configuration ω showing different cyclces.
$\mathcal{C}(\omega) = \{\, (1, 4, 2, 1), (3), (5, 6, 5) \,\}$ and each cycle is represented by the different colors.

Corollary 3.3.3 *Let* $B = \sum_{e\in\mathcal{E}} B_e$ *where* B_e *is an operator on the edge* e, *and* A, *any matrix on* $\mathcal{H}_{\mathcal{G}}$. *Then*

$$e^{\beta(A+B)} = \int_\Omega e^{t_1 A} B_{e_1} e^{(t_2-t_1)A} B_{e_2} \cdots B_{e_k} e^{(\beta-t_k)A}\, \mathrm{d}\nu_{\mathcal{E}}(\omega), \tag{3.3.13}$$

where $\omega = ((e_1,t_1),\ldots,(e_k,t_k))$ *is a sample point of the probability space* $\Omega = \bigcup_{k=0}^{\infty}\{((e_1,t_1),\ldots,(e_k,t_k)) : e_1,\ldots,e_k \in \mathcal{E}\,,\ 0 < t_1 < t_2 < \cdots < t_k < \beta\}$.

Proof:

$$\begin{aligned}\int e^{t_1 A} B_{e_1} e^{(t_2-t_1)A} B_{e_2} \cdots B_{e_k} e^{(\beta-t_k)A}\, \mathrm{d}\nu_{\mathcal{E}}(\omega) &= \sum_{k\geq 0} \int e^{t_1 A} B_{e_1} e^{(t_2-t_1)A} B_{e_2} \cdots B_{e_k} e^{(\beta-t_k)A}\, \mathrm{d}\nu_{\mathcal{E}}(\omega) \\ &= \sum_{k\geq 0} \int_{0<t_1<\cdots<t_k<\beta} e^{t_1 A} B e^{(t_2-t_1)A} B \cdots B e^{(\beta-t_k)A}\, \mathrm{d}t_1 \cdots \mathrm{d}t_k \\ &= e^{\beta(A+B)}\end{aligned} \tag{3.3.14}$$

Remark 3.3.4 *The second equation is as a result of integrating over each time interval* $(t_s, t_{s+1}]$, $s = 0,\ldots,k$ $(s_{k+1} = \beta)$ *and across each edge in* $e \in \mathcal{E}$ *while the last sum is gotten after a change of variable* $\bar{t_i} = t/\beta$ *and comparing the right hand side of* (3.3.2).

Let $T_{\mathbf{ij}}$ be the operator that flips the spins at sites $\mathbf{i}$ and $\mathbf{j}$. Then by direct calculation,

$$T_{\mathbf{ij}} = \frac{1}{2}\mathbb{1}_{\mathbf{ij}} + 2(S^x_{\mathbf{i}} S^x_{\mathbf{j}} + S^y_{\mathbf{i}} S^y_{\mathbf{j}} + S^z_{\mathbf{i}} S^z_{\mathbf{j}}) \tag{3.3.15}$$

Next, we express the partition function (3.3.7) in terms of the probability measure for the cycle representation. This representation is only true for the ferromagnetic regime i.e. $\Delta = 1$ in (3.3.4).

Theorem 3.3.5 (Tóth's representation [17, Theorem. 3.3]) . *For the ferromagnetic Hamiltonian,*

$$Z_{\mathcal{G},1}(\beta) = e^{-\frac{\beta}{4}|\mathcal{E}|} \int 2^{|\mathcal{C}(\omega)|} \mathrm{d}\nu_{\mathcal{E}}(\omega) \tag{3.3.16}$$

Remark 3.3.6 *The probability measure for the cycle representation is hence written as*

$$\mathrm{d}\nu_{\mathcal{E}}^{\mathcal{C}}(\omega) = (Z_{\mathcal{G},\Delta}(\beta))^{-1} e^{-\frac{\beta}{4}|\mathcal{E}|} 2^{|\mathcal{C}(\omega)|} \mathrm{d}\nu_{\mathcal{E}}(\omega) \tag{3.3.17}$$

3.3.3 The Aizenman-Nachtergaele's representation and ANTU for the XXZ model

Aizenman-Nachtergaele's representation

Here, we consider the case the antiferromagnetic Hamiltonian i.e. $\Delta = -1$ in (3.3.4). The Hamiltonian (3.3.4) becomes

$$H_{\mathcal{G},-1} := -\sum_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} (S_{\mathbf{i}}^x S_{\mathbf{j}}^x + S_{\mathbf{i}}^y S_{\mathbf{j}}^y - S_{\mathbf{i}}^z S_{\mathbf{j}}^z) \tag{3.3.18}$$

Lemma 3.3.7 *The two-site operator* $\vec{S}_i \cdot \vec{S}_j := S_{\mathbf{i}}^x S_{\mathbf{j}}^x + S_{\mathbf{i}}^y S_{\mathbf{j}}^y + S_{\mathbf{i}}^z S_{\mathbf{j}}^z$ *is*

(a.) self-adjoint

(b.) has eigenvalue $\frac{1}{4}$ *of multiplicity 3 with corresponding orthonormal eigenvectors* $|\frac{1}{2}, \frac{1}{2}\rangle$, $|-\frac{1}{2}, -\frac{1}{2}\rangle$ *and* $\frac{1}{\sqrt{2}}(|\frac{1}{2}, -\frac{1}{2}\rangle + |-\frac{1}{2}, \frac{1}{2}\rangle)$[1] , *and eigenvalue* $-\frac{3}{4}$ *of multiplicity 1 with corresponding eigenvector* $\frac{1}{\sqrt{2}}(|\frac{1}{2}, -\frac{1}{2}\rangle - |-\frac{1}{2}, \frac{1}{2}\rangle)$[2].

[1] These are referred to as triplet states by Physicists
[2] referred to as the singlet state.

Proof: The proof of (a) is true from the self-adjoint property of the Pauli matrices. To prove (b), observe that $\vec{S}_i \cdot \vec{S}_j$ is a 4×4 matrix. Hence, the result follows from Linear algebra calculuations.

Remark 3.3.8 *The eigenvector corresonding to* $-\frac{3}{4}$ *is called 'Singlet state' while the orthonormal eigenvectors corresponding to eigenvalue* $\frac{1}{4}$ *are called the 'Triplet states'.*

For all $r \in \{\frac{1}{2}, -\frac{1}{2}\}$, let $P_{\mathbf{ij}}$ be the operator defined below:

$$P_{\mathbf{ij}} |r, r\rangle = 0, \qquad P_{\mathbf{ij}} |r, -r\rangle = \tfrac{1}{2}(|r, -r\rangle - |-r, r\rangle) \tag{3.3.19}$$

Notice that $\frac{1}{2}P_{\mathbf{ij}}$ is the projection onto the singlet state in Lemma (3.3.7). Using the identities that for all $r, s \in \{\frac{1}{2}, -\frac{1}{2}\}$,

$$S^x_{\mathbf{i}} S^x_{\mathbf{j}} |r, s\rangle = \tfrac{1}{4} |-r, -s\rangle, \qquad S^y_{\mathbf{i}} S^y_{\mathbf{j}} |r, s\rangle = -rs |-r, -s\rangle, \qquad \text{and} \qquad S^z_{\mathbf{i}} S^z_{\mathbf{j}} |r, s\rangle = rs |r, s\rangle, \tag{3.3.20}$$

we have that

$$P_{\mathbf{ij}} = \frac{1}{4}\mathbb{1}_{\mathbf{ij}} - (S^x_{\mathbf{i}} S^x_{\mathbf{j}} + S^y_{\mathbf{i}} S^y_{\mathbf{j}} + S^z_{\mathbf{i}} S^z_{\mathbf{j}}) \tag{3.3.21}$$

Consider the bipartite graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ (for $\mathcal{V}$ and $\mathcal{E}$ as defined in (3.3.9) and (3.3.10) respectively). Let $\mathcal{V}_A$ and $\mathcal{V}_B$ be a partition on $\mathcal{V}$, and for any $\{\mathbf{i}, \mathbf{j}\} \in \mathcal{E}$, $\mathbf{i} \in \mathcal{V}_A$ and $\mathbf{j} \in \mathcal{V}_B$.

For any fixed time t, let $\sigma(t) : \mathcal{V} \to \{-\frac{1}{2}, \frac{1}{2}\}^{|\mathcal{V}|}$ be the spin configuration corresponding to the realization ω at t. An event on the edge $\{\mathbf{i}, \mathbf{j}\}$ is called a '**cul-de-sac**' at t if

$$\sigma_{\mathbf{i}}(t-) = -\sigma_{\mathbf{j}}(t-) \qquad \text{and} \qquad \sigma_{\mathbf{i}}(t+) = -\sigma_{\mathbf{j}}(t+) \tag{3.3.22}$$

A **loop** $\gamma : [0, L] \longrightarrow \mathcal{V} \times [0, \beta]$ is a closed trajectory with $\gamma(s) = (\mathbf{i}(s), t(s))$ satisfying:

1. γ is piecewise continuous i.e. $\mathbf{i}(s)$ is a constant if γ is continuous on $I \subseteq [0, L]$ and

$$\frac{\mathrm{d}}{\mathrm{d}s}t(s) = \begin{cases} 1 & \text{if} \quad \mathbf{i}(s) \in \mathcal{V}_A \\ -1 & \text{if} \quad \mathbf{i}(s) \in \mathcal{V}_B \end{cases} \tag{3.3.23}$$

2. s is a point of discontinuity if and only if at the time $t(s)$ (with corresponding edge $e(s)$), there a '**cul-de-sac**' event. Hence, $e(s) = (\gamma(s-), \gamma(s+))$.

The smallest positive number L such that $\gamma(0) = \gamma(L)$ is defined as the **loop length**. It is the sum of the vertical legs as seen in Figure (3.3.2) but not a multiple of β (unlike the case of cycles) since the orientation is not fixed (e.g. the length of the blue loop is 2β plus the height of the blue box between vertices 3 and 4 in Figure (3.3.2)). Denote $\mathcal{L}(\omega)$ as the collection of loops in ω. Thus, $|\mathcal{L}(\omega)|$ is the number of loops in ω.

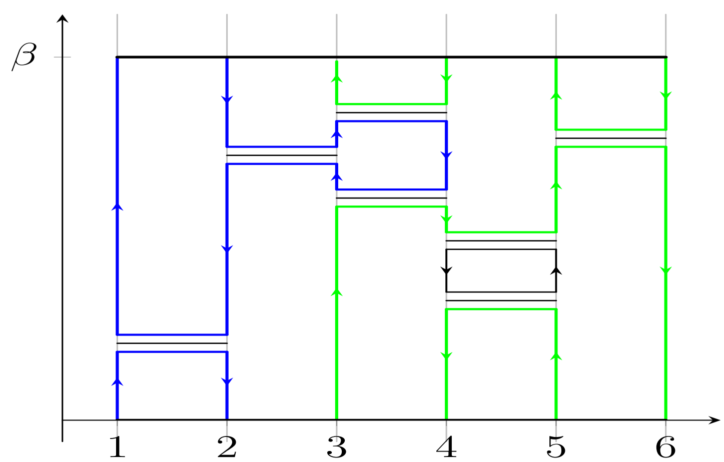

Figure 3.3.2: Configuration ω showing two loops $(1, 2, 1), (3, 6, 5, 4, 3)$, each cycle is represented by the colors blue and green respectively.

Assumuing the notation

$$(-1)^{\mathbf{i}} = \begin{cases} 1, & \text{if} \quad \mathbf{i} \in \mathcal{V}_A \\ -1 & \text{if} \quad \mathbf{i} \in \mathcal{V}_B \end{cases}, \tag{3.3.24}$$

we have the following representation for the antiferromagnet

Theorem 3.3.9 (Aizenman-Nachtergaele's representation [17, Theorem. 3.4]) *Let $\mathcal{G}$ be the bipartite graph described above and consider the antiferromagnetic Hamiltonan* (3.3.18) *(i.e.* $\Delta = -1$*). The partition function and the two-point correlation function are given by*

$$Z_{\mathcal{G},-1}(\beta) = e^{-\beta|\mathcal{E}|} \int 2^{|\mathcal{L}(\omega)|} \mathrm{d}\nu_{\mathcal{E},\frac{\beta}{2}}(\omega), \tag{3.3.25}$$

$$\mathrm{Tr}(S^z_{\mathbf{i}} S^z_{\mathbf{j}} e^{-\beta H_{\mathcal{G},-1}}) = \begin{cases} \frac{1}{4}(-1)^{\mathbf{i}}(-1)^{\mathbf{j}} e^{-\beta|\mathcal{E}|} \int 2^{\mathcal{L}(\omega)} \mathrm{d}\nu_{\mathcal{E},\frac{\beta}{2}} & \textit{if} \quad \gamma_{\mathbf{i}} = \gamma_{\mathbf{j}} \\ 0 & \textit{if} \quad \gamma_{\mathbf{i}} \neq \gamma_{\mathbf{j}} \end{cases} \tag{3.3.26}$$

Aizenman-Nactergaele-Toth-Ueltschi's (ANTU) representation

The combination of both the ferromagnetic and the antiferromagnetic loops in the same representation appeared first in [34]. In [34], two special Hamiltonians were considered, but here, we consider the relevant Hamiltonian for the spin-1/2 case (another Hamiltonian compatible with spin-1 Hamiltonian is given in [34]).

For $\{ \mathbf{i}, \mathbf{j} \} \in \mathcal{E}$, let $Q_{\mathbf{ij}}$ the operator with matrix elements

$$\langle a, b | Q_{\mathbf{i},\mathbf{j}} | c, d \rangle = \delta_{a,b}\delta_{c,d}, \qquad \forall\, a, b, c, d \in \{ -\tfrac{1}{2}, \tfrac{1}{2} \} \tag{3.3.27}$$

We then consider the Hamiltonian

$$H_{\mathcal{G},u} = -\sum_{\langle \mathbf{i},\mathbf{j} \rangle \in \mathcal{E}} (uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}} - 1) \tag{3.3.28}$$

with $T_{\mathbf{ij}}$ as defined in (3.3.15).

Let $\sigma(t) : \mathcal{V} \to \{ -\frac{1}{2}, \frac{1}{2} \}^{|\mathcal{V}|}$ be the spin configuration corresponding to the realization ω at t. An event on the edge $\{\mathbf{i},\mathbf{j}\}$ is called a '**dead-end**' at t if

$$\sigma_{\mathbf{i}}(t-) = \sigma_{\mathbf{j}}(t-) \qquad \text{and} \qquad \sigma_{\mathbf{i}}(t+) = \sigma_{\mathbf{j}}(t+) \tag{3.3.29}$$

For each edge $\{\mathbf{i},\mathbf{j}\} \in \mathcal{E}$, we consider two independent Poisson processes describing '**bridges**' and '**dead-ends**' on $\mathbb{R}$ with respective rates $\frac{1}{2}(1-u)$ and $\frac{1}{2}u$ respectively. Let $(\Omega, \mathcal{F}_u, \mathbb{P}_u)$ be a probability space supporting these processes, and let $\mathbb{E}_u[\cdot]$ denote the corresponding expectation. As before, we regard $\omega \in \Omega$ as a realization of finte events on $\mathcal{E} \times [0,\beta]$ i.e. $w = ((e_1,t_1),(e_2,t_2),\ldots,(e_k,t_k))$ for increasing times $0 < t_1 < \cdots < t_k < \beta$. Denote the measure associated with these processes as $\mathrm{d}\nu_\beta(\omega)$.

Following the notation in [9], let $\Sigma_{\mathcal{V}} = \{-\frac{1}{2},\frac{1}{2}\}^{|\mathcal{V}|}$, $\Sigma_{\mathcal{V},\beta}$ be the set of all piecewise constant functions $\sigma(\cdot) : [0,\beta] \to \Sigma_{\mathcal{V}}$, and let $\Sigma_{\mathcal{V},\beta}(\omega) \subset \Sigma_{\mathcal{V},\beta}$ denote satisfying the following:

- For any $\mathbf{i} \in \mathcal{V}$, consider the set of arrival times of all Poisson processes $\mathrm{d}\nu^F_{\mathbf{ij}}$ and $\mathrm{d}\nu^{AF}_{\mathbf{ij}}$ for all $\mathbf{j}$ such that $\{\mathbf{i},\mathbf{j}\} \in \mathcal{E}$. For $\epsilon > 0$, $\sigma_{\mathbf{i}}(\cdot)$ is constant on the interval $[t-\epsilon, t+\epsilon)$ if the set of all these times and $[t-\epsilon, t+\epsilon)$ are disjoint.
- We say $\sigma(\cdot)$ is **'compatible with'** ω if $\sigma(\cdot) \in \Sigma_{\mathcal{V},\beta}(\omega)$.

Finally, let $\Sigma^{\text{per}}_{\mathcal{V},\beta}(\omega) \subset \Sigma_{\mathcal{V},\beta}(\omega)$ be the set consisting of functions satisfying periodic-time condition $\sigma(0) = \sigma(\beta)$ for each $\mathbf{i} \in \mathcal{V}$. In this setting, graphs are decomposed entirely into loops as seen in Figure(3.3.3) (graphs are decomposed entirely into cycles as seen in Figure(3.3.1)). Each loop is a trajectory of a specific spin-value. Hence, $|\Sigma^{\text{per}}_{\mathcal{V},\beta}(\omega)| = 2^{|\mathcal{L}(\omega)|}$ (In the Cycle representation, $|\Sigma^{\text{per}}_{\mathcal{V},\beta}(\omega)| = 2^{|\mathcal{C}(\omega)|}$).

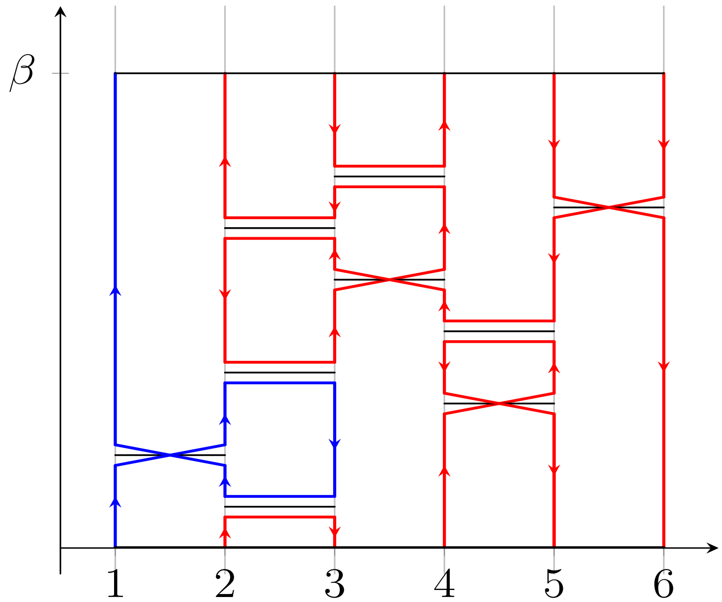

Figure 3.3.3: Configuration ω showing both brideges and dead-ends in the same realization ω.

Theorem 3.3.10 *For all $u \in [0,1]$, we have*

$$Z_{\mathcal{G},u}(\beta) = \int_{\Omega} 2^{|\mathcal{L}(\omega)|} \mathrm{d}\nu_\beta(\omega) \tag{3.3.30}$$

Proof: Using the Trotter's product formula in (3.3.1) and trivial asymptotics, we have

$$e^{-\beta H_{\mathcal{G},u}} = \left(\lim_{N\to\infty} \prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} e^{\frac{\beta}{N}}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}} - 1) \right)^N \tag{3.3.31}$$

$$= \lim_{N\to\infty} \left(\prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} \left[1 - \frac{\beta}{N} + \frac{\beta}{N}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}}) \right] \right)^N \tag{3.3.32}$$

Therefore,

$$\operatorname{Tr} e^{-\beta H_{\mathcal{G},u}} = \lim_{N\to\infty} \sum_{\sigma^{(0)}} \langle \sigma^{(0)}| \left(\prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} \left[1 - \frac{\beta}{N} + \frac{\beta}{N}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}}) \right] \right)^N |\sigma^{(0)}\rangle \tag{3.3.33}$$

By inserting the identity $\mathbb{1} = \sum_\sigma |\sigma\rangle \langle\sigma|$ after each product in the N products ($(N-1)$ times), we have

$$\operatorname{Tr} e^{-\beta H_{\mathcal{G},u}} = \lim_{N\to\infty} \sum_{\sigma^{(0)},\ldots,\sigma^{(N-1)}} \langle \sigma^{(0)}| \prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} \left(1 - \frac{\beta}{N} + \frac{\beta}{N}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}}) \right) |\sigma^{(1)}\rangle \cdots$$
$$\cdots \langle \sigma^{(N-1)}| \prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} \left(1 - \frac{\beta}{N} + \frac{\beta}{N}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}}) \right) |\sigma^{(0)}\rangle \tag{3.3.34}$$

$$= \lim_{N\to\infty} \sum_{\sigma^{(0)},\ldots,\sigma^{(N-1)}} \prod_{i=0}^{N-1} \langle \sigma^{(i)}| \prod_{\langle \mathbf{i},\mathbf{j}\rangle \in \mathcal{E}} \left(1 - \frac{\beta}{N} + \frac{\beta}{N}(uT_{\mathbf{ij}} + (1-u)Q_{\mathbf{ij}}) \right) |\sigma^{(i+1)}\rangle \tag{3.3.35}$$

Each sum is over $\sigma^{(i)} \in \{-\frac{1}{2}, \frac{1}{2}\}^{|\mathcal{V}|}$ and we have used the notaion $\sigma^{(N)} = \sigma^{(0)}$. Recall that the operator $T_{\mathbf{ij}}$ describes the '**bridge**' events while $Q_{\mathbf{ij}}$ describes the '**dead-end**' events. Therefore the inner product in the last equation equals 1 if and only if $\sigma^{(i+1)}(0) = \sigma^{(i)}$ and 0 otherwise for each $\sigma^{(i+1)} \in \Sigma^{\text{per}}_{\mathcal{V},\beta}(\omega)$. Hence,

$$\operatorname{Tr} e^{-\beta H_{\mathcal{G},u}} = \int_\Omega \sum_{\sigma(\cdot)\in\Sigma^{\text{per}}_{\mathcal{V},\beta}(\omega)} 1 \, \mathrm{d}\nu_\beta(\omega) \tag{3.3.36}$$

$$= \int_\Omega 2^{|\mathcal{L}(\omega)|} \mathrm{d}\nu_\beta(\omega) \tag{3.3.37}$$

3.4 The Feynman-Kac measure

Let $\{\psi^+, \psi^-\}$ be the canonical orthonormal basis in $\mathbb{C}^2$. For any $\tau \in \{-1, 1\}^{\mathcal{V}}$, define the Ising basis vector

$$\Psi_{\mathcal{V}}(\tau) = \bigotimes_{\mathbf{i} \in \mathcal{V}} \psi_{\mathbf{i}}^{\tau_{\mathbf{i}}} \tag{3.4.1}$$

From (3.3.4),

$$H_{\mathcal{G},\Delta} = H_{\mathcal{G},1} - (\Delta - 1) \sum_{\langle i,j \rangle \in \mathcal{E}} S_i^z S_j^z \tag{3.4.2}$$

This is a perfect expression for a Feynman-Kac type of expansion. Therefore by a similar proof of the Feynman-Kac Formula [7, Theorem. 6.3.7] using (3.3.1) and (3.3.13), we have that

$$e^{-\beta H_{\mathcal{G},\Delta}} \Psi(\tau) = e^{-\frac{\beta}{4}|\mathcal{E}|} \int \Psi(\omega(\beta)) \cdot \mathbb{1}_{\{\tau\}}(\omega(0)) \cdot e^{\frac{(\Delta-1)}{4} \int_0^\beta U_{\mathcal{G}}(\omega(t)) \mathrm{d}t} \mathrm{d}\nu_{\mathcal{E}}^F(\omega) \tag{3.4.3}$$

where $U_{\mathcal{G}}(\tau) = \sum_{\{\mathbf{i},\mathbf{j}\} \in \mathcal{E}} \tau_{\mathbf{i}} \tau_{\mathbf{j}}$ and $\omega(t)$ is the spin configuration immediately after arrival time t corresponding to ω.

Therefore, the partition function in the Feynman-Kac representation is given as

$$Z_{\mathcal{G},\Delta}(\beta) = \mathrm{Tr}(e^{-\beta H_{\mathcal{G},\Delta}}) = \sum_{\tau \in \Sigma_{\mathcal{V}}} \langle \Psi(\tau), e^{-\beta H_{\mathcal{G},\Delta}} \Psi(\tau) \rangle \tag{3.4.4}$$

$$= e^{-\frac{\beta}{4}|\mathcal{E}|} \int \sum_{\tau \in \Sigma_{\mathcal{V}}} \mathbb{1}_{\{\tau\}}(\omega(\beta)) \cdot \mathbb{1}_{\{\tau\}}(\omega(0)) \cdot e^{\frac{(\Delta-1)}{4} \int_0^\beta U_{\mathcal{G}}(\omega(t)) \mathrm{d}t} \mathrm{d}\nu_{\mathcal{E}}^F(\omega) \tag{3.4.5}$$

$$= e^{-\frac{\beta}{4}|\mathcal{E}|} \int \sum_{\sigma(\cdot) \in \Sigma_{\mathcal{V},\beta}^{\mathrm{per}}(\omega)} e^{\frac{(\Delta-1)}{4} \int_0^\beta U_{\mathcal{G}}(\sigma(t)) \mathrm{d}t} \mathrm{d}\nu_{\mathcal{E}}^F(\omega) \tag{3.4.6}$$

Equation (3.4.6) is a consequence of the fact that the summand in (3.4.5) is non-zero if and only if we have functions, $\sigma(\cdot)$ compatible with ω, satisfying periodic-time condition $\sigma(0) = \sigma(\beta)$ (i.e $\sigma(\cdot) \in \Sigma^{\mathrm{per}}_{\mathcal{V},\beta}(\omega)$).

Therefore, for any operator P on $\mathcal{H}_{\mathcal{V}}$ with adjoint $P^{\dagger}$,

$$\mathrm{Tr}(Pe^{-\beta H_{\mathcal{G},\Delta}}) = e^{-\frac{\beta}{4}|\mathcal{E}|} \int \sum_{\tau \in \Sigma_{\mathcal{V}}} \langle P^{\dagger}\Psi(\tau), \Psi(\omega(\beta))\rangle \cdot \mathbb{1}_{\{\tau\}}(\omega(0)) \cdot e^{\frac{(\Delta-1)}{4}\int_0^{\beta} U_{\mathcal{G}}(\omega(t))\mathrm{d}t} \mathrm{d}\nu^F_{\mathcal{E}}(\omega) \tag{3.4.7}$$

3.4.1 Lower bound for EFP

Lemma 3.4.1 *Suppose the dimension $d \in \mathbb{N}$ is fixed and $\Delta < -1$, there exist constants $c_1, C > 0$ such that,*

$$\mathrm{Tr}\left(\mathbf{Q}_L e^{-\beta H_{\mathcal{G},\Delta}}\right) \geq Ce^{-c_1 \beta L^d} \tag{3.4.8}$$

Proof: Applying (B.2.2) to any configuration $\Psi_{\mathcal{V}}(\tau)$, we have that

$$\langle \Psi_{\mathcal{V}}(\tau), e^{-\beta H_{\Delta}} \Psi_{\mathcal{V}}(\tau)\rangle \geq e^{-\beta \langle \Psi_{\mathcal{V}}(\tau), H_{\mathcal{G},\Delta}\Psi_{\mathcal{V}}(\tau)\rangle} \tag{3.4.9}$$

For a fixed τ (having all spins up in the sub-box $\mathbb{B}_L$),

$$\langle \Psi_{\mathcal{V}}(\tau), H_{\mathcal{G},\Delta}\Psi_{\mathcal{V}}(\tau)\rangle = \langle \Psi_{\mathcal{V}}(\tau), H_1 \Psi_{\mathcal{V}}(\tau)\rangle - \frac{(\Delta-1)}{4} U_{\mathcal{G}}(\tau)$$

$$= -\frac{1}{2}\sum_{\{\mathbf{i},\mathbf{j}\} \in \mathcal{E}} \langle \Psi_{\mathcal{V}}(\tau), T_{i,j}\Psi_{\mathcal{V}}(\tau)\rangle + \frac{1}{4}|\mathcal{E}| + \frac{(1-\Delta)}{4} U_{\mathcal{G}}(\tau)$$

$$= -\frac{1}{2}|\mathcal{E}(F)| + \frac{(|\mathcal{E}(F)| + |\mathcal{E}(AF)|)}{4} + \frac{(1-\Delta)}{4}(|\mathcal{E}(F)| - |\mathcal{E}(AF)|)$$

$$\leq \frac{|\mathcal{E}| - |\mathcal{E}(F)|}{4} - \frac{\Delta}{4}|\mathcal{E}(F)|$$

where $\mathcal{E}(F)$ is the set of ferromagnetic edges in $\mathcal{E}$ and $\mathcal{E}(AF)$ is the set of antiferromagnetic edges in $\mathcal{E}$. Let $\mathcal{E}(L)$ be the set of edges having all spins up on the sub-box $\mathbb{B}_L$. Since $\mathcal{E}(L) \subseteq \mathcal{E}(F)$, there exists constants $\tilde{c_1} \geq 0$, $\tilde{c_2} \geq 1$ (depending on τ) and $c_2 \geq 1$ such that $|\mathcal{E}| - |\mathcal{E}(L)| \leq \tilde{c_1}\,|\mathcal{E}|$, and $|\mathcal{E}(F)| \leq \tilde{c_2}\,|\mathcal{E}(L)|$.

Therefore,

$$\langle \Psi_{\mathcal{V}}(\tau), H_{\mathcal{G},\Delta}\Psi_{\mathcal{V}}(\tau)\rangle \leq \tilde{c}(\tau)\,|\mathcal{E}(L)| \leq \tilde{c}(\tau)L^d \tag{3.4.10}$$

where $\tilde{c}(\tau) := \left(\tilde{c_1} - \frac{\Delta}{4}\tilde{c_2}\right) dc_2 > 0$ since $\Delta < -1$.

Therefore,

$$\langle \Psi_{\mathcal{V}}(\tau), e^{-\beta H_{\mathcal{G},\Delta}}\Psi_{\mathcal{V}}(\tau)\rangle \geq e^{-c_1\beta L^d} \tag{3.4.11}$$

where $c_1 := \min\{\, \tilde{c(\tau)} : \tau \in \{\pm 1\}^{|\mathcal{V}|}\,\}$.

Hence the result where C is number of configurations having all spins up on the sub-box $\mathbb{B}_L$.

Lemma 3.4.2 *For a fixed $d \in \mathbb{N}$, the partition function satisfies*

$$Z_{\mathcal{G},\Delta}(\beta) \leq e^{c_3\beta L^d} \tag{3.4.12}$$

Proof: The proof follows trivially from [29, Eqn. (1)],

where $c_3 := 3/4 + |\Delta - 1|/2$.

Theorem 3.4.3 *Suppose $d \in \mathbb{N}$ is fixed. For $\Delta < -1$, there are constants $c, C \in (0,\infty)$ such that, whenever $L \leq \frac{N}{2}$,*

$$\langle \mathbf{Q}_L\rangle \geq Ce^{-c\beta L^d} \tag{3.4.13}$$

Proof: *Combining Lemma* (3.4.1) *and Lemma* (3.4.2)*, setting $c := c_1 + c_3$ and C as in the proof of* (3.4.1) *proves the result.*

3.4.2 Upper bound for EFP

For the upper bound, a similar result using the grahical representations technique is shown. Majorly, the Feymann-Kac is combined with the Tóth's representation and then estimating using large deviation bounds. The results here are quite similar to [9] with slight modifications.

Assume N is even. Define the configuration $\tau^{(L,N)}$ as follows:

$$\tau_{\mathbf{i}}^{L,N} = (-1)^{\lfloor \frac{2i_1-1}{2L} \rfloor + \cdots + \lfloor \frac{2i_d-1}{2L} \rfloor} \tag{3.4.14}$$

and the rank-1 projection

$$\hat{\mathbf{Q}}_{N,L} = |\Psi_N(\tau^{(L,N)})\rangle \langle \Psi_N(\tau^{(L,N)}| \tag{3.4.15}$$

The operator $\hat{\mathbf{Q}}_{N,L}$ is called the 'Universal Contour'. The definitions of $\tau^{(L,N)}$ and $\hat{\mathbf{Q}}_{N,L}$ seem cumbersome but it's quite clear from the Figure (3.4.1).

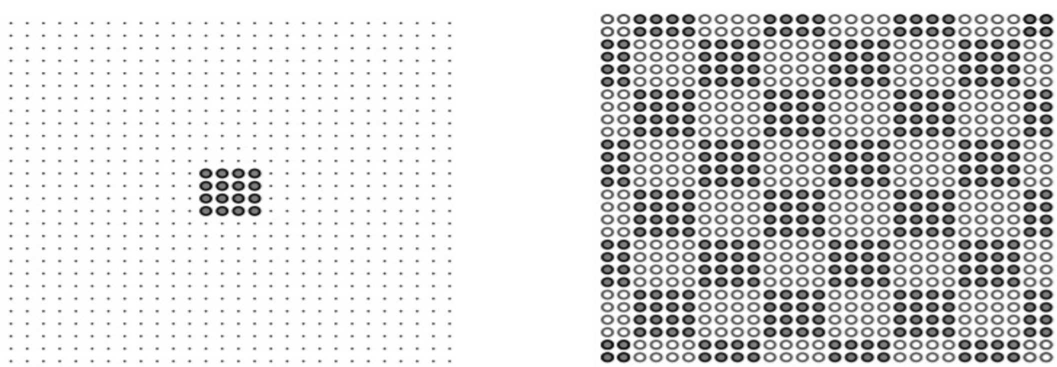

Figure 3.4.1: On the left is an example of $\mathbf{Q}_L$ (projection unto all spins up in the box $\mathbb{B}_L$) for $L = 4$, and $d = 2$ while on the right is the 'Universal Contour' $\hat{\mathbf{Q}}_{N,L}$ with $N = 28$. The black circles represents the up-spins while the white circles represent the down-spins. The dots represent sites without a projector.

Following the ideas in [9], $\mathbf{Q}_L$ is disseminated in space (along the direction of the outward orthonormal vectors). There may be some loss in the dissemination e.g. as seen in Fig (3.4.1) since N may not be a multiple of L. This loss does not have much effect since we will frequently consider cases where N is much larger than L. Estimating $\mathbf{Q}_L$ from above leads to getting an upper bound for $\hat{\mathbf{Q}}_L$ as seen below.

Lemma 3.4.4 ([9, Lemma. 3.2]) *Suppose $\Delta \leq 0$. For fixed L satisfying $L \leq N/2$,*

$$\mathbf{EFP}_{\mathrm{L}}(\mathrm{N}, \beta) = \langle \mathbf{Q}_{\mathrm{L}} \rangle_{\mathrm{N},\Delta,\beta} \leq \left(\langle \hat{\mathbf{Q}}_{\mathrm{N,L}} \rangle_{\mathrm{N},\Delta,\beta} \right)^{1/\mathrm{K}} \tag{3.4.16}$$

where $K = 2^{d(\log_2(N/L+1))}$.

Remark 3.4.5 *The proof is done by repeatedly applying the Cauchy-Schwarz theorem in the direction each normal vector where the n number of repetitions is $n = \lfloor \log_2(N/L) \rfloor$.*

Now, we have a projection $\hat{\mathbf{Q}}_{N,L}$ which maps to a specificed spin configuration on all $\mathbb{T}_N$. Considering the Feyman-Kac represetation, the next thing is to disseminate $\hat{\mathbf{Q}}_{N,L}$ in time. This is done by using Generalized Hölder's inequality (Chessboard Estimate). The method is to re-impose the projection $\hat{\mathbf{Q}}_{N,L}$ every $\beta/2n$ units of 'time'. The result is given below

Proposition 3.4.6 ([9, Prop. 3.4]) *For any positive integer n,*

$$\langle \hat{\mathbf{Q}}_{N,L} \rangle_{N,\Delta,\beta} \leq \left(\frac{\mathrm{Tr}[(\hat{\mathbf{Q}}_{N,L}\, e^{\beta H/(2n)})^{2n}]}{Z_{\mathcal{G},\Delta}(\beta)} \right)^{1/(2n)} \tag{3.4.17}$$

By inserting the identity $\mathbb{1} = \sum_{\Psi_V} |\Psi_V\rangle \langle \Psi_V|$, $(2n-1)-$times (where $\{ \mid \Psi_V \rangle \}$ are the energy eigenvectors) in the numerator of (3.4.17), we have

$$\mathrm{Tr}[(\hat{\mathbf{Q}}_{N,L}\ e^{\beta H/(2n)})^{2n}] = \left(\langle \Psi_V(\tau^{L,N}), e^{-\beta H/(2n)} \Psi_V(\tau^{L,N}) \rangle\right)^{2n} \tag{3.4.18}$$

Therefore (3.4.17) becomes

$$\langle \hat{\mathbf{Q}}_{N,L} \rangle_{N,\Delta,\beta} \leq \frac{\mathrm{Tr}[\hat{\mathbf{Q}}_{N,L}\ e^{-\beta H/(2n)}]}{(Z_{\mathcal{G},\Delta}(\beta))^{1/(2n)}} \tag{3.4.19}$$

For ease of calculation, define

$$\mathrm{Num}_{\beta,N,L,n} = e^{-(\beta/(2n))(|\mathcal{E}|/4)}\ \mathrm{Tr}[\hat{\mathbf{Q}}_{N,L}\ e^{\beta H/(2n)}] \tag{3.4.20}$$

$$\mathrm{Den}_{\beta,N,L,n} = e^{-(\beta/(2n))(|\mathcal{E}|/4)}\ \ (Z_{\mathcal{G},\Delta}(\beta))^{1/(2n} \tag{3.4.21}$$

Therefore,

$$\langle \hat{\mathbf{Q}}_{N,L} \rangle_{N,\Delta,\beta} \leq \frac{\mathrm{Num}_{\beta,N,L,n}}{\mathrm{Den}_{\beta,N,L,n}} \tag{3.4.22}$$

Pre-multiplying by $e^{-(\beta/(2n))(|\mathcal{E}|/4)}$ is crucial in estimating the partition function to obtain the (3.4.24).

To get an upper bound for (3.4.17), we need to get an upper bound for $\mathrm{Num}_{\beta,N,L,n}$ and a lower bound for $\mathrm{Den}_{\beta,N,L,n}$. A lower bound for $\mathrm{Den}_{\beta,N,L,n}$ was found using variational method:

Lemma 3.4.7 ([9, Lemma, 3.6]) *For any graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and any $\Delta \in \mathbb{R}$, $\beta > 0$, we have*

$$Z_{\mathcal{G},\Delta}(\beta) e^{-\beta|\mathcal{E}|/4} = \mathrm{Tr}\left[e^{-\beta(H_{\mathcal{G},\Delta}+(1/4)|\mathcal{E}|)}\right] \geq 1 \tag{3.4.23}$$

Moreover,

$$\mathrm{Den}_{\beta,N,L,n} = \left(e^{-\beta|\mathcal{E}|/4}\ Z_{\mathcal{G},\Delta}(\beta)\right)^{1/(2n)} \geq 1 \tag{3.4.24}$$

Upper bound on Num **using large deviation bounds**

Setting $P = \hat{\mathbf{Q}}_{N,L}$ in (3.4.7) and applying (3.4.20), we have

$$\mathrm{Num}_{\beta,N,L,n} = e^{-\beta|\mathcal{E}|/(4n)}\mathbb{E}_1\left[\sum_{\sigma(\cdot)\in\Sigma_{\mathcal{V},\beta/(2n)}(\omega)} \mathbb{1}_{\{\,\sigma(0)=\sigma(\beta/(2n))=\tau^{L,N}\,\}}\cdot\exp\left(\frac{\Delta-1}{4}\int_0^{\beta/(2n)} U_{\mathcal{G}}(\sigma(t))\mathrm{dt}\right)\right] \tag{3.4.25}$$

We hence have the following result:

Proposition 3.4.8 *For any* $\Delta < 1$ *and* $L \geq 4(3^d)$,

$$\mathrm{Num}_{\beta,N,L,n} \leq e^{-(1/8)(1-\Delta)dN^d\delta T} + e^{-[(\Delta/4)+(M\ln M-M+1)]dN^d\delta T} \tag{3.4.26}$$

where $\delta T = \beta/(2n)$ *and* $M = 7L/(2592d(6^d)\delta T)$.

Observe that in (3.4.25), estimating the term in the exponential uniformly (independent of L) totally removes the dependency of the inequality on L. This leads to a trivial result (i.e. $\mathrm{Num}_{\beta,L,N,n}$ is less than some exponentially large term). Furthermore, at the times $t = 0$ and $t = \beta/(2n)$, $U_{\mathcal{G}}(\sigma(t)) = U_{\mathcal{G}}(\tau^{L,N})$. By definition of $U_{\mathcal{G}}(\cdot)$ and for large L, we have that $U_{\mathcal{G}}(\tau^{L,N}) \approx |\mathcal{E}(\mathbb{T}_N)|$ since for $\{\,\mathbf{i},\mathbf{j}\,\} \in \mathcal{E}$, $\tau_{\mathbf{i}}^{L,N} = \tau_{\mathbf{j}}^{L,N}$ except for $\mathbf{i}$ and $\mathbf{j}$ spanning neighboring blocks. Hence to get the right dependecy on L for times $0 < t < \beta/(2n)$, we need to account for the hopping of spins allowed by the stochastic process associated with $\mathbb{E}_1$.

For $\Delta < 1$, $|\mathcal{E}(\mathbb{T})|$ is interpreted as the maximum possible energy of the ferromagnetic Ising potential which therefore leads to exponential suppression in (3.4.25). The idea to prove large deviation bound is hence, quite straightforward. Since the stocahstic process allows spins to hop between neighboring blocks and we do not expect too many arrivals of events $\mathrm{d}\nu_{\mathbf{i},\mathbf{j}}^{F}(\omega)$, then for times $t \in (0, \beta/(2n))$, the spin configurations $\sigma(t)$ will still have relatively low energy (approximately $|\mathcal{E}(\mathbb{T}_N)|$ for large L) for the ferromagnetic Ising potential. Therefore leading to an exponential suppression in the antiferromagnetic Ising Gibbs state.

In the complimentary event that the stochastic process allows enough 'bridges' such that the ground state of the Ising antiferromagnet is attained, then the exponential weight in the Ising Gibbs state is exponentially large. But the large deviation bound for this rare event (B.2) has a nonlinear decay rate which dominates the linear growth rate of this exponential.

Proof of Proposition (3.4.8)**:** Define a '**block**' to be a maximally connected set of sites $\mathbf{i} \in \mathbb{T}_N$ satisfying the condition $\tau_{\mathbf{i}}^{L,N} = \tau_{\mathbf{j}}^{L,N}$. Let

$$\mathcal{F} = \{ \{ \mathbf{i}, \mathbf{j} \} \in \mathcal{E}(\mathbb{T}_N) : \tau_{\mathbf{i}}^{L,N} \neq \tau_{\mathbf{j}}^{L,N} \} \tag{3.4.27}$$

i.e. any edge $\{ \mathbf{i}, \mathbf{j} \} \in \mathcal{F}$ spans two adjacent blocks.

Some blocks have full size L^d while there also may exist partial blocks at a distance less than L from one of the two faces of $\mathbb{B}_N$ in either the $+$ or the $-$ side of that cordinate direction (see Fig.(3.4.2)).

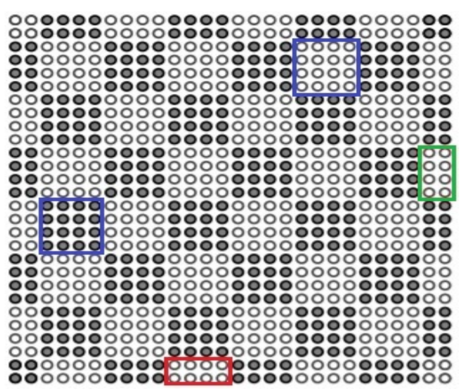

Figure 3.4.2: Example of a contour $\tau^{L,N}$ with blocks where $L = 4,$, $d = 2$ and $N = 28$. The Blue blocks are full blocks while the red and green blocks are partial blocks. The red box is at a distance 2 from the down face while green box is at a distance 2 from the right face.

Considering this, we see that

$$|F| \leq dL^{d-1}\left(\frac{N}{L}+2\right)^d \tag{3.4.28}$$

Therefore,

$$|\mathcal{F}| \leq L^{d-1}\left(\frac{1}{L}+\frac{2}{N}\right)^d |\mathcal{E}(\mathbb{T}_N)| \tag{3.4.29}$$

Since $N \geq L$, we have that $|\mathcal{F}| \leq 3^d L^{-1} |\mathcal{E}(\mathbb{T}_N)|$. Therefore,

$$|\mathcal{E}(\mathbb{T}_N)| - U_N(\tau^{L,N}) \leq 2\,|\mathcal{F}| \leq 2(3^d)L^{-1}\,|\mathcal{E}(\mathbb{T}_N)| \tag{3.4.30}$$

At times $t \in \{\,0, \beta/(2n)\,\}$, only the edges $\{\,\mathbf{i},\mathbf{j}\,\} \in \mathcal{F}$ satisfy the condition $\sigma_{\mathbf{i}}(t) = -\sigma_{\mathbf{j}}(t)$. We will show that with high probability at times between 0 and $\beta/(2n)$, most antiferromagnetic edges are close to $\mathcal{F}$. As as result of this we give an easy bound on the number of vertices at a short distance from $\mathcal{F}$.

For any positive integer r, define $\mathcal{V}_r$ to be the set of all sites $\mathbf{i} \in \mathbb{T}_N$ satisfying the condition: $\mathbf{i}$ is in a block $\Lambda \subset \mathbb{T}_N$, and has a distance less than or equal to r from $\mathbb{T}_N \setminus \Lambda$. For instance,

$$|\mathcal{V}_1| = \{\,\mathbf{i} \in \mathbb{T}_N : \exists\, \mathbf{j} \in \mathbb{T}_N \ \text{ such that } \ \{\,\mathbf{i},\mathbf{j}\,\} \in \mathcal{F}\,\} \tag{3.4.31}$$

Since for any edge in $\mathcal{F}$, there are least $2r$ sites from distance less than or equal to r (r sites on the separate blocks), then

$$|\mathcal{V}_r| \leq 2r\,|\mathcal{F}| \leq 2r(3^d)L^{-1}\,|\mathcal{E}(\mathbb{T}_N)| = 2dr(3^d)L^{-1}N^d \leq 6^d r L^{-1} N^d \tag{3.4.32}$$

We then proceed to the remainder of the proof.

For eadch time $t \in [0, \beta/(2n)]$ define $X(t)$ to be the number of sites $\mathbf{i}$ such that

$\tau_{\mathbf{i}}^{L,N} \neq \sigma_{\mathbf{i}}(t)$. Then

$$\left|U_N(\sigma(t)) - U_N(\tau^{L,N})\right| \leq 4dX(t). \tag{3.4.33}$$

and by (3.4.30), we have that

$$|\mathcal{E}(\mathbb{T}_N)| - 2(3^d)L^{-1}\,|\mathcal{E}(\mathbb{T}_N)| - U_N(\sigma(t)) \leq 4dX(t) \tag{3.4.34}$$

Let $\mathcal{A}$ be the set of events ω with fewer bridges, such that for all times $t \in [0, \beta/(2n)]$, we have $X(t) \leq N^d/8$. On $\mathcal{A}$,

$$\mathbb{1}_{\{\,\sigma(0)=\sigma(\beta/(2n))=\tau^{L,N}\,\}} \exp\left(-\frac{1-\Delta}{4}\int_0^{\beta/(2n)} U_N(\sigma(t))dt\right) \leq e^{-\beta/(16n)(1-\Delta)(1-4(3^d)L^{-1})|\mathcal{E}(\mathbb{T}_N)|} \tag{3.4.35}$$

This is a good bound for the kind result we expect.

Now to get a similar bound on $\mathcal{A}^c$, suppose there exists $\mathbf{i}$ such that $\mathbf{i} \in \mathbb{T}_N \setminus \mathcal{V}_r$ and $\sigma_{\mathbf{i}}(t) \neq \tau_{\mathbf{i}}^{L,N}$ at some time t. Then, $\mathbf{i}$ is in a block and the $\sigma_{\mathbf{i}}(t)$ is opposite to that of the block. Thus, in time $[0, t]$, there must be a path from some neighboring block via bridge arrivals of $\mathrm{d}\nu_{\mathbf{ij}}^F(\omega)$ to bring the oppositely oriented spin to site $\mathbf{i}$, and there is another path in time $(t, \beta/(2n)]$ that returns the spin $\sigma_{\mathbf{i}}(t)$ to that of the block. Since $\mathbf{i}$ is at a distance more r from $\mathcal{F}$, then there are at least $2r$ arrivals of $\mathrm{d}\nu_{\mathbf{ij}}^F(\omega)$ associated to these two paths.

As a result of this, there are at least $r(X(t) - |\mathcal{V}_r|)$ total arrivals of $\mathrm{d}\nu_{\mathbf{ij}}^F(\omega)$ in the interval $[0, \beta/(2n)]$. The factor of 2 has been removed since a given arrival of $\mathrm{d}\nu_{\mathbf{ij}}^F(\omega)$ could contribute to two different paths for two different vertices $\mathbf{i}, \mathbf{j}$ (since an edge has two point vertices). On $\mathcal{A}^c$, we have that $X(t) > N^d/8$ for some time t. Choosing $r = L/(6^{d+2})$ on $\mathcal{A}^c$ and by (3.4.32), we get that there are at least $7LN^d/((2592)6^d)$ arrivals of $\mathrm{d}\nu_{\mathbf{ij}}^F(\omega)$ in the time interval $[0, \beta/(2n)]$.

For a Poisson random variable $\mathcal{N}$, (B.2) implies that

$$\mathbf{P}(\mathcal{N} \geq M\mathbf{E}(\mathcal{N})) \leq e^{-(M \ln M - M + 1)\mathbf{E}(\mathcal{N})}, \qquad M \geq 1 \tag{3.4.36}$$

Recall that for $\mathrm{d}\nu^F_{\mathbf{ij}}(\omega)$ in the time interval $[0, \beta/(2n)]$, the total expectation of all arrivals is $|\mathcal{E}(\mathbb{T}_N)|\, \delta T$ where $\delta T = \beta/(2n)$. Therefore

$$\mathbb{P}_1(\mathcal{A}^c) \leq e^{-(M \ln M - M + 1) dN^d \delta T}, \tag{3.4.37}$$

where $\mathbb{P}_1$ is the Probability with respect to arrivals of $\mathrm{d}\nu^F_{\mathbf{ij}}(\omega)$ and $M = 7L/(2592d(6^d)\delta T)$.

Combining this with (3.4.35), (3.4.37) and the uniform upper bound

$$\mathbb{1}_{\{\,\sigma(0)=\sigma(\beta/(2n))=\tau^{L,N}\,\}} \exp\left(-\frac{1-\Delta}{4} \int_0^{\beta/(2n)} U_N(\sigma(t)) dt \right) \leq e^{(1/4)(1-\Delta) dN^d \delta T} \tag{3.4.38}$$

gives the result.

Remark 3.4.9 *As mentioned earlier the non-linear decay rate in* (3.4.37) *dominates the linear growth rate in* (3.4.38) *to give the expected exponential bound for events in* $\mathcal{A}^c$. *Also, to get the result,* $\mathbb{P}_1(\mathcal{A})$ *has been trivially bounded by 1.*

We therefore give a bound on the expectation of the universal contour:

Theorem 3.4.10 *For each* $\Delta < 1$*, there exists* $L_0 \in \mathbb{N}$*, and* $\tilde{c}$*,* $\tilde{C} > 0$ *such that for all* $L \geq L_0$*, we have*

$$\langle \hat{\mathbf{Q}}_{N,L} \rangle_{N,\Delta,\beta} \leq Ce^{-cN^d \min(L,\beta)} \tag{3.4.39}$$

Proof of Theorem (3.4.10)**:** Combining (3.4.22), Lemma (3.4.7) and Proposition (3.4.8). Choose $\varepsilon > 0$ (dependent on n) with $M = 7L/(2592d(6^d)\varepsilon \min(\beta, L))$ is large enough such that $M \ln M - M + 1 \geq (1/8)(1 - 3\Delta)$ and $M \geq 1$. Then, we have that

$$\mathrm{Num}_{\beta,N,L,n} \leq 2e^{-(1/8)(1-\Delta)dN^d\varepsilon\min(\beta,L)} \tag{3.4.40}$$

Defining $\tilde{c} := (1/8)(1-\Delta)d\varepsilon$ yields the desired result.

CHAPTER 4

OUTLOOK

There is interest in the community to further study the area law for bipartite entanglement entroopy. With randomness, an area law is expected to hold as seen in [19], and [5] (in the spin 1/2 case). The Combes -Thomas estimate used in this research is not a sufficient condition to achieve the area law, as it gives dependency of the subsystem size. Some other expectation decay bounds may be needed in order to get the desired bounds. Also, questions concerning the study the free XXZ quantum spin model defined on a ring with the aim of showing a logarithmically corrected area law for the bipartite entanglement entropy of eigenstates belonging to the first energy band above the vacuum ground state seem important.

For emptiness formation probability, the greatest interest is among combinatorialist whose work is different than the rough bounds presented here. But there are some interesting questions:

1. For the Heisenberg (or Schrödinger) dynamics in real time, how does the emptiness formation probability observable evolve. (Note: this thesis considers imaginary time dynamics.)

2. In the presence of a phase transition with multiple pure states, how does the choice of a ground state affect the emptiness formation probability.

References

[1] H. Abdul-Rahman, C. Fischbacher and G. Stolz: Entanglement bounds in the XXZ quantum spin chain, Ann. Henri Poincaré **21**, 2327-2366, (2020).

[2] L. Adame, L. M. Rivera and A. Trujillo-Negrete: Hamiltonicity of the Double Vertex Graph and the Complete Double Vertex Graph of some Join Graphs (2020).

[3] M. Aisenman and B. Nachtergaele: Geometric aspects of quantum spin states. *Commun. Math. Phys.* **164**, 1, 17-63 (1994).

[4] V. Beaud and S. Warzel: Low-energy Fock space localization for attractive hard-core particles in disorder, Ann. Henri Poincaré **18**, 3143-3166 (2017).

[5] V. Beaud and S. Warzel: Bounds on the entanglement entropy of droplet states in the XXZ spin chain, J. Math. Phys. **59**, 012109 (2018).

[6] M. Biskup: Reflection Positivity and Phase Transitions in Lattice Spin Models, Los Angeles, CA 90095-1555 (2009).

[7] O. Bratteli and D. Robinson: Operator Algebras and Quantum Statistical Mechanics 2, second edition (1997).

[8] W. Carballosa, R. Fabila-Monroy, J. Leaños and L. M. Rivera, *Regularity and planarity of tokenvgraphs*, Discuss. Math. Graph Theory **37** (2017), 573–586.

[9] N. Crawford, S. Ng, and S. Starr: Emptiness formation probability. *Commun. in Math. Phys.* **345**, 881–922 (2016).

[10] A. Elgart, A. Klein and G. Stolz, *Many-body localization in the droplet spectrum of the random XXZ quantum spin chain*, J. Funct. Anal. **275** (2018), 211–258

[11] A. Elgart, A. Klein and G. Stolz, *Manifestations of dynamical localization in the disordered XXZ spin chain*, Comm. Math. Phys. **361** (2018), 1083–1113

[12] C. Fischbacher: A Schrödinger Operator Approach to Higher Spin XXZ Systems on General Graphs, Analytic trends in Mathematical physics, Contemp. Math. **741**, 83–103 (2020).

[13] C. Fischbacher and G. Stolz: Droplet states in quantum XXZ spin systems on general graphs, J. Math. Phys. **59**, 051901 (2018).

[14] C. Fischbacher and R. Schulte: Lower Bound to the Entanglement Entropy of the XXZ Spin Ring, *arXiv:2007.00735*

[15] B. Pfirsch and A. V. Sobolev, Formulas of Szegő type for the periodic Schrödinger operator, *Commun. Math. Phys.* **358**, 675–704 (2018).

[16] J. Fröhlich, R. Israel, E.H Lieb, B. Simaon. Phase transitions and reflection positivity. I. General theory and long range lattice models. Commun.Math. Phys. 62, 1–34 (1978).

[17] C. Goldschmidt, D. Ueltschi, and P. Windridge: Quantum Heisenberg models and their probabilistic representations (2011).

[18] B. Hall: Lie groups, Lie algebras and representations; An elementary introduction, second edition (2015).

[19] M. B. Hastings: An area law for one-dimensional quantum systems, J. Stat. Mech. **08024** (2007).

[20] A. Klein, *private communication*, (2020).

[21] V. Korepin, N. Bogoliubov, & A. Izergin, A: Quantum Inverse Scattering Method and Correlation Functions, Cambridge Monographs on Mathematical Physics, . Cambridge, Cambridge University Press (1993).

[22] H. Leschke, A. V. Sobolev and W. Spitzer, Scaling of Rényi entanglement entropies of the free Fermi-gas ground state: A rigorous proof, *Phys. Rev. Lett.* **112**, 160403–1–5 (2014).

[23] H. Leschke, A. V. Sobolev and W. Spitzer, Trace formulas for Wiener-Hopf operators with applications to entropies of free fermionic equilibrium states, *J. Funct. Anal.* **273**, 1049–1094 (2017).

[24] J. Mulherkar, B. Nachtergaele, R. Sims and S. Starr, *Isolated Eigenvalues of the Ferromagnetic Spin-J XXZ Chain with Kink Boundary Conditions*, J. Stat. Mech. **2008**, P01016.

[25] P. Müller, L. Pastur and R. Schulte, How much delocalisation is needed for an enhanced area law of the entanglement entropy?, *Commun. Math. Phys.* **376**, 649–679 (2020).

[26] P. Müller and R. Schulte, Stability of the enhanced area law of the entanglement entropy, *Ann. Henri Poincaré* **21**, 3639–3658 (2020).

[27] Y. Ouyang, Computing spectral bounds of the Heisenberg ferromagnet from geometric consideratios. J. Math. Phys. **60**(7), 071901 (2019).

[28] L. M. Rivera and A. L. Trujillo-Negrete, Hamiltonicity of token graphs of fan graphs, Art Discr. Appl. Math., **1**, #P07 (2018).

[29] D. W. Robinson, Statistical Mechanics of Quantum Spin Systems, *Commun. Math. Phys.* **6**, 151–160 (1967).

[30] S. Starr, Some properties for the low-lying spectrum of the ferromagnetic, quantum XXZ spin system, PhD Thesis, UC Davis, 2001

[31] G. Stolz, Aspects of the Mathematical Theory of Disordered Quantum Spin Chains, Analytic trends in Mathematical physics, Contemp. Math. **741**, 163–197 (2020).

[32] J. Weidmann: Lineare Operatoren in Hilberträumen, Teil I Grundlagen, Verlag B.G. Teubner, Stuttgart/Leipzig/Wiesbaden, 2000 (German).

[33] B. Tóth: Improved lower bounds on the thermodynamical pressure of the spin 1/2 Heisenberg ferromagnet. *Lett. Math Phys.* **54**, no. 8, 083301 (2013).

[34] D. Ueltschi: Random loop representations for quantum spin systems. *J. Math. Phys.* **54**, no. 8, 083301 (2013).

[35] M. M. Wolf, Violation of the entropic area law for fermions, *Phys. Rev. Lett.* **96**, 010404–1–4 (2006).

APPENDIX A

AUXILIARY RESULTS FOR ENTANGLEMENT ENTROPY

A.1 Proof of the distance formula

Lemma A.1.1 *The graph distance $d^N(X,Y)$ from X to Y is given by* (2.2.23)*.*

Proof: Let $\delta^N(X,Y) := \sum_{i=1}^N |x_i - y_i|$. To prove that $\delta^N(X,Y)$ is a lower bound of the graph distance $d^N(X,Y)$, we first show that $\mathbf{m}_X \sim \mathbf{m}_Y$ if and only if $\delta^N(X,Y) = 1 \ \forall\, X, Y \in \mathbb{S}_L^N$.

For $X, Y \in \mathbb{S}_L^N$, where $X = (x_1, x_2, \ldots, x_N)$, $Y = (y_1, y_2, \ldots, y_N)$, suppose $d^N(X,Y) = 1$. By (2.2.23), there exists $k_0 \in \{1, 2, \ldots, N\}$ such that $|x_{k_0} - y_{k_0}| = 1$ and $x_k = y_k \ \ \forall\, k \in \{1, 2, \ldots, N\} \setminus \{k_0\}$. Define $j_0 := x_{k_0}$. Therefore $y_{k_0} = j_0 \pm 1$. Now, let $\mathbf{m}_X$ and $\mathbf{m}_Y$ be the occupation number functions corresponding to X and Y respectively. Without loss of generality, let $y_{k_0} = j_0 + 1$ and suppose that $\mathbf{m}_X(j_0) = r, \ \ r \in \{1, \ldots, 2J\}$. Then $\mathbf{m}_Y(j_0) = r - 1$, since $y_{k_0} \neq j_0$. Hence, $\mathbf{m}_X(j_0) - \mathbf{m}_Y(j_0) = r - (r-1) = 1$. Also, suppose $\mathbf{m}_Y(j_0+1) = s, \ \ s \in \{\, 1, \ldots, 2J \,\}$, then $\mathbf{m}_X(j_0+1) = s - 1$, since $y_{k_0} = j_0 + 1$. Therefore, $\mathbf{m}_X(j_0+1) - \mathbf{m}_Y(j_0+1) = s - 1 - s = -1$ and $\mathbf{m}_X(j) = \mathbf{m}_Y(j), \ \ \forall\, j \in \{1, \ldots L\} \setminus \{j_0, j_0+1\}$. Hence, $\mathbf{m}_X \sim \mathbf{m}_Y$.

Conversely, suppose $\mathbf{m}_X \sim \mathbf{m}_Y$. By (2.2.9), there exists a unique $j_0 \in \{1, \ldots, L - 1\}$ such that $\mathbf{m}_X(j_0) - \mathbf{m}_Y(j_0) = \pm 1, \quad \mathbf{m}_X(j_0+1) - \mathbf{m}_Y(j_0+1) = \mp 1$ and $\mathbf{m}_X(j) = \mathbf{m}_Y(j) \ \ \forall\, j \in \{1, \ldots, L\} \setminus \{j_0, j_0+1\}$. Without loss of generality, suppose $\mathbf{m}_X(j_0) - \mathbf{m}_Y(j_0) = 1$ and $\mathbf{m}_X(j_0+1) - \mathbf{m}_Y(j_0+1) = -1$. Using the same definitions as before that $j_0 := x_{k_0}$ and $\mathbf{m}_X(j_0) = r$, let $\mathbf{m}_X(j_0+1) = s'$, i.e. $s' = s - 1$ where $\mathbf{m}_Y(j_0+1) = s$. Let $i_1 = \min\{\, k : x_k = j_0 \,\}$, then $x_k = j_0$ for $k = i_1, \ldots, i_1 + (r-1)$ and $x_k = j_0 + 1$ for $k = i_1 + r, \ldots, i_1 + r + (s'-1)$. Therefore,

$$\begin{aligned} \delta^N(X,Y) = \sum_{j=1}^N |x_j - y_j| &= 0 + \cdots + 0 + |x_{i_1+(r-1)} - y_{i_1+(r-1)}| + 0 + \cdots + 0 \\ &= |j_0 - (j_0+1)| = 1 \end{aligned} \tag{A.1.1}$$

$\implies \quad \delta^N(X,Y) = 1.$

It then follows from the triangle inequality that $\delta^N(X,Y)$ is a lower bound of the graph distance.

To prove equality, it suffices to show that there exists a path from X to Y such that the length of the path is $\delta^N(X,Y)$. Let $X, Y \in \mathbb{S}_L^N$ and $i_0 = \min\{k \in \{1, \dots N\} : x_k \neq y_k\}$. Without loss of generality, suppose $x_{i_0} < y_{i_0}$. Consider the path

$$\begin{aligned} Y = (\dots, y_{i_0-1}, y_{i_0}, y_{i_0+1}, \dots) &\longrightarrow Y_1 = (\dots, y_{i_0-1}, y_{i_0} - 1, y_{i_0+1}, \dots) \\ \longrightarrow Y_2 = (\dots, y_{i_0-1}, y_{i_0} - 2, y_{i_0+1}, \dots) \cdots &\longrightarrow Y_{y_{i_0} - x_{i_0}} = (\dots, y_{i_0-1}, x_{i_0}, y_{i_0+1}, \dots) . \end{aligned} \tag{A.1.2}$$

The case $x_{i_0} > y_{i_0}$ is similar by switching the roles of X and Y. Notice that $\mathbf{m}_Y \sim \mathbf{m}_{Y_1} \sim \mathbf{m}_{Y_2} \sim \cdots \sim \mathbf{m}_{Y_{y_{i_0} - x_{i_0}}}$ and the length of this path is $|x_{i_0} - y_{i_0}|$. Define $i_1 := \min\{k \in \{i_0 + 1, \dots, N\} : x_k \neq y_k$. Repeating the above process for $x_{i_1} < y_{i_1}$ (with a similar case for $x_{i_1} > y_{i_1}$), we get another path of length $|x_{i_1} - y_{i_1}|$. Since $N < \infty$, the process ends at some $i_s \leq n$ such that $i_s := \min\{k \in \{i_0 + s, \dots, N\} : x_k \neq y_k\}$ and repeating the process for x_{i_s} yields a path of length $|x_{i_s} - y_{i_s}|$. Therefore, we have a path from X to Y of length

$$|x_{i_0} - y_{i_0}| + |x_{i_1} - y_{i_1}| + \cdots + |x_{i_s} - y_{i_s}|$$

$$= \sum_{j:1\le j<i_0} |x_j - y_j| + |x_{i_0} - y_{i_0}| + \sum_{j:i_0<j<i_1} |x_j - y_j| + |x_{i_1} - y_{i_1}| + \cdots$$

$$+ \sum_{j:i_{s-1}<j<i_s} |x_j - y_j| + |x_{i_s} - y_{i_s}| + \sum_{j:i_s<j\le N} |x_j - y_j|$$

$$= \sum_{j=1}^{N} |x_j - y_j| = d^N(X,Y)\,, \tag{A.1.3}$$

which finishes the proof.

A.2 Auxiliary results concerning the interaction potential

A.2.1 Proof of Proposition (2.2.5)

Proof: Firstly, note that for any $\mathbf{m} \in \mathbf{M}_L^N$ one gets

$$V(\mathbf{m}) = \sum_{j=1}^{L-1} [J(\mathbf{m}(j) + \mathbf{m}(j+1)) - \mathbf{m}(j)\mathbf{m}(j+1)] + J(\mathbf{m}(1) + \mathbf{m}(L)) \tag{A.2.1}$$

$$= 2J \sum_{j=1}^{L} \mathbf{m}(j) - \sum_{j=1}^{L-1} \mathbf{m}(j)\mathbf{m}(j+1) = 2JN - \sum_{j=1}^{L-1} \mathbf{m}(j)\mathbf{m}(j+1)\,, \tag{A.2.2}$$

which shows that finding minimizers of the potential is equivalent to finding maximizers of $Q_N(\mathbf{m}) := \sum_{j=1}^{L-1} \mathbf{m}(j)\mathbf{m}(j+1)$. From the explicit form of Q_N, it is obvious that if $\mathrm{supp}(\mathbf{m})$ is not a discrete interval, i.e. if there exists a $j_0 \notin \mathrm{supp}(\mathbf{m})$ with $\min \mathrm{supp}(\mathbf{m}) < j_0 < \max \mathrm{supp}(\mathbf{m})$, then $\mathbf{m}$ cannot be a maximizer of Q_N. Hence, from now on, we will only consider $\mathbf{m} \in \mathbf{M}_L^N$ such that $\mathrm{supp}(\mathbf{m})$ is a discrete interval and w.l.o.g. let us assume $\mathrm{supp}(\mathbf{m}) = \{1, 2, \ldots, k\}$ for some $k \in \mathbb{N}$. For a proof by contradiction, let us now assume that there is an $\mathbf{m} \in \mathbf{M}_L^N$ which maximizes Q_N but is not of the form (2.2.16) or (2.2.17). Note that since $N \ge 4J$ and $\mathbf{m}(j) \le 2J$ for every $j \in \{1, 2, \ldots, k\}$, this implies that $k \ge 3$. Note that for $k = 3$, we get

$$Q_N(\mathbf{m}) = \mathbf{m}(1)\mathbf{m}(2) + \mathbf{m}(2)\mathbf{m}(3) = \mathbf{m}(2)(N - \mathbf{m}(2))\,, \tag{A.2.3}$$

where we have used that $\mathbf{m}(3) = N - \mathbf{m}(1) - \mathbf{m}(2)$ for the last equation. Now, observe that since $N \geq 4J$, the maximal possible value for Q_N is only attained if $\mathbf{m}(2) = 2J$, which shows that for $k = 3$, any maximizer of Q_N has to be of the form (2.2.16) or (2.2.17). Hence, from now on, we will only consider the case $k \geq 4$. Let us now distinguish a few different cases and show that for each of these cases, if $\mathbf{m}$ is not of the form (2.2.16) or (2.2.17), then we can construct another $\widehat{\mathbf{m}} \in \mathbf{M}_L^N$ such that $Q_N(\widehat{\mathbf{m}}) > Q_N(\mathbf{m})$ – a contradiction to $\mathbf{m}$ maximizing Q_N:

First case: $\mathbf{m}(1) > \mathbf{m}(2)$. In this case, we set $\widehat{\mathbf{m}}(1) := \mathbf{m}(2), \widehat{\mathbf{m}}(2) := \mathbf{m}(1)$ and for every other j, we define $\widehat{\mathbf{m}}(j) := \mathbf{m}(j)$. This yields

$$Q_N(\widehat{\mathbf{m}}) - Q_N(\mathbf{m}) = (\mathbf{m}(1) - \mathbf{m}(2)) \cdot \mathbf{m}(3) > 0\,, \tag{A.2.4}$$

which shows that $\mathbf{m}$ cannot maximize Q_N in this case.

Second case: $\mathbf{m}(1) \leq \mathbf{m}(2)$, and it is not true that $\mathbf{m}(2) = \mathbf{m}(3) = 2J$. We split this second case into two subcases:

First subcase: $\mathbf{m}(2) < \mathbf{m}(3)$. In this case, we define the configuration $\widehat{\mathbf{m}}$ by setting $\widehat{\mathbf{m}}(1) := \mathbf{m}(1) - 1, \widehat{\mathbf{m}}(2) := \mathbf{m}(2) + 1$ and for every other j, we define $\widehat{\mathbf{m}}(j) := \mathbf{m}(j)$. This yields

$$Q_N(\widehat{\mathbf{m}}) - Q_N(\mathbf{m}) = (\mathbf{m}(1) - 1) + \mathbf{m}(3) - \mathbf{m}(2) \geq \mathbf{m}(3) - \mathbf{m}(2) > 0, \tag{A.2.5}$$

which shows that $\mathbf{m}$ cannot maximize Q_N in this case.

Second subcase: $\mathbf{m}(2) \geq \mathbf{m}(3)$. Note that since we are in the Second case, it is not possible that $\mathbf{m}(3) = 2J$. We then define the configuration $\widehat{\mathbf{m}}$ by setting $\widehat{\mathbf{m}}(1) := \mathbf{m}(1) - 1, \widehat{\mathbf{m}}(3) := \mathbf{m}(3) + 1$ and for every other j, we define $\widehat{m}(j) := \mathbf{m}(j)$.

We then get

$$Q_N(\widehat{\mathbf{m}}) - Q_N(\mathbf{m}) = \mathbf{m}(4) > 0\,, \tag{A.2.6}$$

which shows that $\mathbf{m}$ is not a maximizer of Q_N.

Third case: $\mathbf{m}(2) = \mathbf{m}(3) = 2J$. Note that in this case, we must have $k \geq 5$, since otherwise $\mathbf{m}$ would be of the form (2.2.16) or (2.2.17). Let $k_0 \in \{4, \ldots, k-1\}$ be the smallest number for which $\mathbf{m}(k_0) \neq 2J$. (Again, note that such a k_0 must exist, since otherwise $\mathbf{m}$ would be of the form (2.2.16) or (2.2.17).) In particular, this means that $\mathbf{m}(k_0 - 1) = 2J$ and $\mathbf{m}(k_0 + 1) > 0$. Now, define $\widehat{\mathbf{m}}(1) := \mathbf{m}(1) - 1, \widehat{\mathbf{m}}(k_0) := \mathbf{m}(k_0) + 1$ and for every other j, we set $\widehat{\mathbf{m}}(j) := \mathbf{m}(j)$. We then find

$$Q_N(\widehat{\mathbf{m}}) - Q_N(\mathbf{m}) = \mathbf{m}(k_0 + 1) > 0\,, \tag{A.2.7}$$

which shows that $\mathbf{m}$ cannot be a maximizer of Q_N.

Since these three cases exhaust all possibilities and from (2.2.16) or (2.2.17), $V_{N,0} = 4J^2$. This finishes the proof.

A.2.2 Proof of Lemma 2.5.2

Proof Let $Z = (z_1, z_2, \ldots, z_{j+k}) \in \mathbb{S}^{j+k}_{L,K}$ be such that $d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K}) = d^{j+k}(X \vee Y, Z)$. Now, introduce the configurations $Z' = (z_1, z_2, \ldots, z_j) \in \mathbb{S}^j_L$ and $Z'' = (z_{j+1}, \ldots, z_{j+k}) \in \mathbb{S}^k_L$. Moreover, let $\mathbf{m}_{Z'}$ and $\mathbf{m}_{Z''}$ denote the corresponding occupation number functions. Note that $\mathbf{m}_{Z'}(i) = 0$ for $i > z_j$ as well as $\mathbf{m}_{Z''}(i) = 0$ for $i < z_j$. Moreover, note that $\mathbf{m}_{Z'}(z_j) + \mathbf{m}_{Z''}(z_j) \leq 2J$. It follows that $V(\mathbf{m}_{Z'}) \leq$

$V(\mathbf{m}_{Z'}+\mathbf{m}_{Z''})$, i.e. $V(Z') \le V(Z)$ and thus $Z' \in \mathbb{S}^j_{L,K}$. To see this, observe that

$$V(\mathbf{m}_{Z'}+\mathbf{m}_{Z''}) = V(\mathbf{m}_{Z'}) + (2J - \mathbf{m}_{Z'}(z_j-1))\mathbf{m}_{Z''}(z_j) + (2J - (\mathbf{m}_{Z'}(z_j)+\mathbf{m}_{Z''}(z_j))\mathbf{m}_{Z''}(z_j+1) + \sum_{i=z_j+1}^{L-1}(2J-\mathbf{m}_{Z''}(i))\mathbf{m}_{Z''}(i+1) \ge V(\mathbf{m}_{Z'})\,, \tag{A.2.8}$$

where we used that since $\mathbf{m}_{Z'}, \mathbf{m}_{Z''} \in \mathbf{M}_L$, one has $\mathbf{m}_{Z'}(i), \mathbf{m}_{Z''}(i) \le 2J$ for any $i \in \{1,2,\ldots,L\}$ and moreover that $\mathbf{m}_{Z'}(z_j)+\mathbf{m}_{Z''}(z_j) \le 2J$. Now, if in addition $z_j \le \ell$, this would imply $Z' \in \mathbb{S}^j_{\Lambda_\ell,K}$ and since – trivially – $d^j(X, \mathbb{S}^j_{\Lambda_\ell,K}) \le d^j(X,Z') \le d^{j+k}(X \vee Y, Z' \vee Z'') = d^{j+k}(X\vee Y, \mathbb{S}^{j+k}_{L,K})$ this shows (2.5.2) for the case $z_j \le \ell$. If $z_j > \ell$, we need to modify our argument. If $z_1 > \ell$, we construct the occupation number function $\mathbf{g} \in \mathbf{M}^j_{\Lambda_\ell}$ as follows:

$$\mathbf{g}(i) := \begin{cases} 2J & \text{if} \quad \ell - \lfloor \frac{j}{2J} \rfloor + 1 \le i \le \ell \\ j(\text{mod } 2J) & \text{if} \quad \ell - \lfloor \frac{j}{2J} \rfloor \end{cases} . \tag{A.2.9}$$

Let $X_\mathbf{g} \in \mathbb{S}^j_{\Lambda_\ell}$ denote the multiset associated with $\mathbf{g}$. Note that $X_\mathbf{g}$ is of the form (2.2.16) or (2.2.17) and thus, by Proposition 2.2.5 we have $X_\mathbf{g} \in \mathbb{S}^j_{\Lambda_\ell,K}$. Therefore, $d^j(X, \mathbb{S}^j_{\Lambda_\ell,K}) \le d^j(X, X_\mathbf{g}) \le d^j(X,Z') \le d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K})$ (where the second inequality is due to the fact that $x_i \le g_i \le \ell < z_i,\;\; i = 1,\ldots,j$). So, from now on, we may assume that $z_1 \le \ell$ and thus let $j_0 := \max\{i \in \{1,2,\ldots,j\} : z_i \le \ell\}$ be the index of the last particle of Z' that still lies in Λ_ℓ. We now split $Z' = Z'_{\Lambda_\ell} \vee Z'_{\Lambda_\ell^c}$, where $Z'_{\Lambda_\ell} = (z_1,\ldots,z_{j_0})$ and $Z'_{\Lambda_\ell^c} = (z_{j_0+1},\ldots,z_j)$. Let $\mathbf{m}_{Z'_{\Lambda_\ell}} \in \mathbf{M}^{j_0}_{\Lambda_\ell}$ be the occupation number function associated to Z'_{Λ_ℓ}. Lastly, let $j_c := j - j_0$ be the number of particles in $Z'_{\Lambda_\ell^c}$. We then distinguish the following two cases:

Case 1: $j_c + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell) + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell-1) \ge 4J$.

Define $r_0 := \max\{k \in \{1,\ldots,\ell-2\} : \sum_{s=k}^{\ell}(2J - \mathbf{m}_{Z'_{\Lambda_\ell}}(s)) \ge j_c\}$ and let

$\mu = j_c - \sum_{s=r_0+1}^{\ell}(2J - \mathbf{m}_{Z'_{\Lambda_\ell}}(s))$. We construct the occupation number function $\mathbf{c} \in \mathbf{M}^j_{\Lambda_\ell}$ as follows:

$$\mathbf{c}(i) := \begin{cases} \mathbf{m}_{Z'_{\Lambda_\ell}}(i) & \text{if} \quad 1 \leq i \leq r_0 - 1 \\ \mathbf{m}_{Z'_{\Lambda_\ell}}(i) + \mu & \text{if} \quad i = r_0 \\ 2J & \text{if} \quad r_0 + 1 \leq i \leq \ell \end{cases} \tag{A.2.10}$$

In other words, the particles in $Z'_{\Lambda_\ell^c}$ are used to "fill up" each site of configuration $\mathbf{m}_{Z'_{\Lambda_\ell}}$ to its maximal occupation number $2J$ – starting from $\ell, \ell-1$, etc. until the j_c particles in $Z'_{\Lambda_\ell^c}$ have been exhausted (cf. Figure A.2.1). Note that the choice $\mathbf{c}(\ell) = \mathbf{c}(\ell-1) = 2J$ is following the same principle and is due to the assumption $j_c + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell) + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell-1) \geq 4J$.

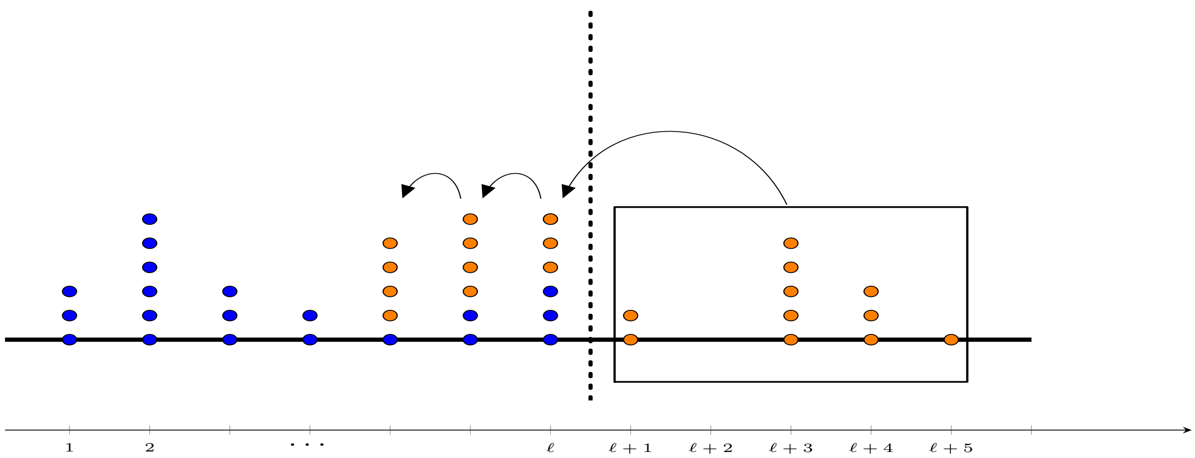

Figure A.2.1: Picture showing the construction of configuration $\mathbf{c}$, by moving the $j_c = 11$ particles in Λ_ℓ^c such that they fill up each site to its maximum occupation number $2J = 6$ starting at ℓ to the left (here: from ℓ to $\ell - 2$).

We now make the following observations: Firstly, let $X_{\mathbf{c}} \in \mathbb{S}^j_{\Lambda_\ell}$ denote the multiset corresponding to $\mathbf{c}$. Then, by construction, it is clear that $d^j(X, X_{\mathbf{c}}) \leq d^j(X, Z')$. Secondly, let $s_0 = \min\{s \in \{1, 2, \ldots, \ell-2\} : \forall t \in \{s+1, \ldots, \ell\} : \mathbf{c}(t) = 2J\}$. If $s_0 = 1$, then $X_{\mathbf{c}}$ is a minimizer configuration with $\mathbf{c}(i) =$

$2J \quad \forall\, i = 2, \ldots, \ell$ and hence, $X_{\mathbf{c}} \in \mathbb{S}^j_{\Lambda_\ell, K}$. Since $x_i \le c_i \le z_i, \;\; i = 1, \ldots, j$, we get

$$d^j(X, X_{\mathbf{c}}) = \sum_{i=1}^{j} (c_i - x_i) \le \sum_{i=1}^{j} (z_i - x_i) \le d^j(X, Z') \tag{A.2.11}$$

and therefore, $d^j(X, \mathbb{S}^j_{\Lambda_\ell, K}) \le d^j(X, X_{\mathbf{c}}) \le d^j(X, Z') \le d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K})$ for the case $s_0 = 1$.

Now for $s_0 \neq 1$, define $\mathbf{c}'' := \mathbf{c} \cdot 1_{\{s_0, \ldots, \ell\}}$, $\mathbf{c}' := \mathbf{c} - \mathbf{c}''$, $\mathbf{d}'' := \mathbf{m}_{Z'} \cdot 1_{\{s_0, \ldots, L\}}$ and $\mathbf{d}' := \mathbf{m}_{Z'} - \mathbf{d}''$. Then, observe that $\mathbf{c}(s_0) \ge \mathbf{m}_{\mathbb{Z}'_{\Lambda_\ell}}(s_0)$ and moreover that $\mathbf{c}(s) = \mathbf{m}_{\mathbb{Z}'_{\Lambda_\ell}}(s)$ for every $s < s_0$. Consequently, we get $\mathbf{c}' = \mathbf{d}'$. Observe that $\mathbf{c}''$ is of the form (2.2.16) or (2.2.17) and thus $V(\mathbf{c}'') = 4J^2$. Moreover, by Proposition 2.2.5, we have $V(\mathbf{c}'') \le V(\mathbf{d}'')$. Consequently, we get

$$V(\mathbf{c}) = V(\mathbf{c}') - \mathbf{c}(s_0 - 1)\mathbf{c}(s_0) + V(\mathbf{c}'') \le V(\mathbf{d}') - \mathbf{m}_{Z'_{\Lambda_\ell}}(s_0 - 1)\mathbf{m}_{Z'_{\Lambda_\ell}}(s_0) + V(\mathbf{d}'') = V(\mathbf{m}_{Z'}) \le K. \tag{A.2.12}$$

This shows that $X_{\mathbf{c}} \in \mathbb{S}^j_{\Lambda_\ell, K}$. Since $d^j(X, \mathbb{S}^j_{\Lambda_\ell, K}) \le d^j(X, X_{\mathbf{c}}) \le d^j(X, Z') \le d^{j+k}(X \vee Y, \mathbb{S}^{j+k}_{L,K})$, this shows the assertion for Case 1.

Case 2: $j_c + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell) + \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell - 1) < 4J$. Firstly, let us define the following two quantities:

$$\xi' := \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell - 1) + \sum_{k \in \mathbb{N}: \ell + 2k - 1 \le L} \mathbf{m}_{Z'_{\Lambda^c_\ell}}(\ell + 2k - 1) \tag{A.2.13}$$

$$\xi'' := \mathbf{m}_{Z'_{\Lambda_\ell}}(\ell) \qquad + \sum_{k \in \mathbb{N}: \ell + 2k \le L} \mathbf{m}_{Z'_{\Lambda^c_\ell}}(\ell + 2k) \quad \text{and observe that} \tag{A.2.14}$$

$$\sum_{i=\ell-1}^{L-1} \mathbf{m}_{Z'}(i)\mathbf{m}_{Z'}(i+1) \le \xi'\xi''\,, \tag{A.2.15}$$

since the left hand side of (A.2.15) is a sum over a subset of the (non–negative) cross–terms one obtains when expanding the product $\xi'\xi''$. Moreover, note that the assumption for being in Case 2 is equivalent to $\xi' + \xi'' < 4J$. Next, we define the occupation number function $\mathbf{e} \in \mathbb{S}^j_{\Lambda_\ell}$ as follows:

$$\mathbf{e}(i) := \begin{cases} \min\{2J, \xi''\} + \max\{\xi' - 2J, 0\} & \text{if} \quad i = \ell \\ \min\{2J, \xi'\} + \max\{\xi'' - 2J, 0\} & \text{if} \quad i = \ell - 1 \\ \mathbf{m}_{Z'_{\Lambda_\ell}}(i) & \text{if} \quad i \in \{1, 2, \ldots, \ell - 2\} \,. \end{cases} \tag{A.2.16}$$

Let us now show that $V(\mathbf{e}) \leq V(\mathbf{m}_{Z'})$. To this end, observe that

$$V(\mathbf{m}_{Z'}) - V(\mathbf{e}) = \mathbf{m}_{Z'}(\ell-2)(\mathbf{e}(\ell-1) - \mathbf{m}_{Z'}(\ell-1)) + \mathbf{e}(\ell-1)\mathbf{e}(\ell) - \sum_{i=\ell-1}^{L-1} \mathbf{m}_{Z'}(i)\mathbf{m}_{Z'}(i+1) \tag{A.2.17}$$

$$\geq \mathbf{e}(\ell-1)\mathbf{e}(\ell) - \xi'\xi'' \,, \tag{A.2.18}$$

where we used $\mathbf{e}(\ell-1) \geq \mathbf{m}_{Z_{\Lambda_\ell}}(\ell-1)$ and (A.2.15). Since $\xi' + \xi'' < 4J$, there are only three possible cases:

(i) $\xi'' > 2J$ and $\xi' \leq 2J$

(ii) $\xi'' \leq 2J$ and $\xi' > 2J$

(iii) $\xi' \leq 2J$ and $\xi'' \leq 2J$.

We will only discuss Cases (i) and (iii); Case (ii) follows from an argument similar to Case (i). If we are in Case (i), this means $\mathbf{e}(\ell) = 2J$ and $\mathbf{e}(\ell-1) = \xi' + \xi'' - 2J$. Hence, by (A.2.18), we get

$$V(\mathbf{m}_{Z'}) - V(\mathbf{e}) \geq 2J(\xi' + \xi'' - 2J) - \xi'\xi'' = (2J - \xi')(\xi'' - 2J) \geq 0 \,. \tag{A.2.19}$$

For Case (iii), we have $\mathbf{e}(\ell) = \xi''$ and $\mathbf{e}(\ell-1) = \xi'$ and thus get – again by (A.2.18) – the estimate

$$V(\mathbf{m}_{Z'}) - V(\mathbf{e}) \geq \xi'\xi'' - \xi'\xi'' = 0\,. \tag{A.2.20}$$

Hence, we have shown $V(\mathbf{e}) \leq V(\mathbf{m}_{Z'})$. Now, let $X_{\mathbf{e}} \in \mathbb{S}^j_{\Lambda_\ell}$ denote the multiset associated to $\mathbf{e}$. If we can show that $d^j(X, X_{\mathbf{e}}) \leq d^j(X, Z')$, this will prove (2.5.2) for the Case 2. Now, to see this, we firstly define the configuration $\mathbf{f} \in \mathbf{M}^j_{\Lambda_\ell}$ as follows

$$\mathbf{f}(i) := \begin{cases} \min\{2J, \mathbf{m}_{Z'}(\ell) + j_c\} & \text{if} \quad i = \ell \\ \mathbf{m}_{Z'}(\ell-1) + \max\{\mathbf{m}_{Z'}(\ell) + j_c - 2J, 0\} & \text{if} \quad i = \ell - 1 \\ \mathbf{m}_{Z'}(i) & \text{if} \quad i \in \{1, 2, \ldots, \ell-2\}\,, \end{cases} \tag{A.2.21}$$

which means that configuration $\mathbf{f}$ is obtained by adding the particles in Z'_{Λ_c} to the configuration $\mathbf{m}_{Z'}$ – starting at site ℓ and any possibly remaining particles to site $\ell - 1$. Let $X_{\mathbf{f}} = (f_1, f_2, \ldots, f_j) \in \mathbb{S}^j_{\Lambda_\ell}$ be the multiset associated to $\mathbf{f}$ and let $p = \min\{i : z_i > \ell\}$ and $\xi = \max\{\, i : z_i \leq \ell - 2\,\}$ (note that ξ exists since if $z_1 > \ell - 2$ and $j_c < 4J - \mathbf{m}_{Z'}(\ell-1) - \mathbf{m}_{Z'}(\ell)$, then we would have $j = j_0 + j_c < 4J$, a contradiction). Again, we distinguish two cases:

(a) If $j_c \leq 2J - \mathbf{m}_{Z'}(\ell)$, then $z_i = f_i$ for $1 \leq i \leq p-1$ and $f_i = \ell$ for $p \leq i \leq j$. Then,

$$
\begin{aligned}
d^j(X, Z') &= \sum_{i=1}^{p-1} |x_i - z_i| + \sum_{i=p}^{j} (z_i - x_i) \\
&= \sum_{i=1}^{p-1} |x_i - z_i| + \sum_{i=p}^{j} (z_i - f_i) + \sum_{i=p}^{j} (f_i - x_i) \\
&= \sum_{i=1}^{p-1} |x_i - f_i| + \sum_{i=p}^{j} |z_i - f_i| + \sum_{i=p}^{j} |f_i - x_i| \\
&= d^j(X, X_{\mathbf{f}}) + \sum_{i=j-j_c+1}^{j} |z_i - f_i| \geq d^j(X, X_{\mathbf{f}}) + j_c
\end{aligned}
\tag{A.2.22}
$$

(b) If $j_c > 2J - \mathbf{m}_{Z'}(\ell)$, let $\eta = j_c - (2J - \alpha_1)$, where $\alpha_1 = \mathbf{m}_{Z'}(\ell)$ and $\alpha_2 = \mathbf{m}_{Z'}(\ell - 1)$. Then, observe that

$$
\begin{cases}
f_i = z_i, & 1 \leq i \leq \xi + \alpha_2 \\
f_i = \ell - 1, & \xi + \alpha_2 + 1 \leq i \leq \xi + \alpha_2 + n \\
f_i = \ell, & i > \xi + \alpha_2 + \eta \\
z_i = \ell, & \xi + \alpha_2 + 1 \leq i \leq p - 1
\end{cases}
\tag{A.2.23}
$$

Hence,

$$
d^j(X, Z') = \sum_{i=1}^{\xi+\alpha_2} |x_i - z_i| + \sum_{i=\xi+\alpha_2+1}^{p-1} |x_i - z_i| + \sum_{i=p}^{j} (z_i - x_i)
$$

$$
\begin{aligned}
&= \sum_{i=1}^{\xi+\alpha_2} |x_i - z_i| + \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} (z_i - x_i) + \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} (z_i - x_i) \\
&\qquad + \sum_{i=p}^{j} (z_i - f_i) + \sum_{i=p}^{j} (f_i - x_i)
\end{aligned}
$$

$$= \sum_{i=1}^{\xi+\alpha_2} |x_i - f_i| + \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} (z_i - f_i) + \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} (f_i - x_i) + \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} (z_i - f_i)$$
$$+ \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} (f_i - x_i) + \sum_{i=p}^{j} (z_i - f_i) + \sum_{i=p}^{j} (f_i - x_i)$$

$$= \sum_{i=1}^{\xi+\alpha_2} |x_i - f_i| + \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} |f_i - x_i| + \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} |f_i - x_i| + \sum_{i=p}^{j} |f_i - x_i|$$
$$+ \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} |z_i - f_i| + \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} |z_i - f_i| + \sum_{i=p}^{j} |z_i - f_i|$$

$$\begin{aligned} &= d^j(X, X_{\mathbf{f}}) + \sum_{i=\xi+\alpha_2+1}^{\xi+\alpha_2+\eta} |z_i - f_i| + \sum_{i=\xi+\alpha_2+\eta+1}^{p-1} |z_i - f_i| + \sum_{i=p}^{j} |z_i - f_i| \\ &\geq d^j(X, X_{\mathbf{f}}) + \sum_{i=p}^{j} |z_i - f_i| \\ &\geq d^j(X, X_{\mathbf{f}}) + (j - p + 1) = d^j(X, X_{\mathbf{f}}) + j_c \end{aligned} \tag{A.2.24}$$

Moreover, since $\mathbf{e}(i) \neq \mathbf{f}(i)$ only if $i = \ell - 1, \ell$, this implies

$$d^j(X_{\mathbf{e}}, X_{\mathbf{f}}) = |\mathbf{f}(\ell) - \mathbf{e}(\ell)| \leq j_c \, . \tag{A.2.25}$$

We therefore get

$$d^j(X, X_{\mathbf{e}}) \leq d^j(X, X_{\mathbf{f}}) + d^j(X_{\mathbf{f}}, X_{\mathbf{e}}) \leq d^j(X, X_{\mathbf{f}}) + j_c \leq d^j(X, Z') \; , \tag{A.2.26}$$

and thus, we have shown (2.5.2) for Case 2.

This finishes the proof.

APPENDIX B

AUXILIARY RESULTS FOR EMPTINESS FORMATION PROBABILITY

B.1 Equivalence to the Antiferromagnetic XXZ and Reflection positivity

Suppose N is even. Then, we may decompose $\mathbb{B}_N$ into two halves;

For a fixed $\nu \in \{1, \ldots, d\}$, define

$$V_- = \{\, \mathbf{i} = (i_1, \ldots, i_d) \in \{0, \ldots, N-1\}^d : \; i_\nu \in \{1, \ldots, N/2\} \,\} \tag{B.1.1}$$

$$V_+ = \{\, \mathbf{i} = (i_1, \ldots, i_d) \in \{0, \ldots, N-1\}^d : \; i_\nu \in \{N/2+1, \ldots, N\} \,\} \tag{B.1.2}$$

Moreover, define $\mathcal{H}_+ := \ell^2(C(V_+))$ and $\mathcal{H}_- = \ell^2(C(V_-))$ where $C(\mathbb{B}_N)$ is the set of all function $\sigma = (\sigma_\mathbf{i})_{\mathbf{i} \in V_\pm}$. Hence, we may associate $\mathcal{H}(\mathbb{B}_N) = \mathcal{H}_- \otimes \mathcal{H}_+$.

Hence, a function $f_- \in \mathcal{H}_-$ ($f_+ \in \mathcal{H}_+$) is supported on the vertex set V_- (V_+ respectively). We therefore define the function $(f_- \otimes f_+) \in \mathcal{H}(\mathbb{B}_N)$ as follows: given $\sigma \in C(\mathbb{B}_N)$ such that

$$\sigma^\pm = (\sigma_\mathbf{i})_{\mathbf{i} \in V_\pm}, \tag{B.1.3}$$

$$(f_- \otimes f_+)(\sigma) = f_-(\sigma^-) f_+(\sigma^+) \tag{B.1.4}$$

Define the reflection $R : V_\pm \to V_\mp$, a reflection by the plane (passing through no sites) between V_- and V_+:

$$R(i_1, \ldots, i_{\nu-1}, i_\nu, i_{\nu+1}, \ldots, i_d) = (i_1, \ldots, i_{\nu-1}, i_\nu, N-1-i_\nu, i_{\nu+1}, \ldots, i_d) \tag{B.1.5}$$

We then define the isomorphism $\mathcal{R} : C(V_-) \to C(V_+)$ as

$$\mathcal{R}((\sigma_\mathbf{i})_{\mathbf{i} \in V_-}) = (\tau_\mathbf{i})_{\mathbf{i} \in V_+}, \quad \tau_\mathbf{i} = \sigma_{R(\mathbf{i})} \tag{B.1.6}$$

Define the unitary transformation $F : \mathcal{H}_- \to \mathcal{H}_+$ by

$$Ff((\sigma_{\mathbf{i}})_{\mathbf{i}\in V_-}) = f((\tau_{\mathbf{i}})_{\mathbf{i}\in V_+}) \tag{B.1.7}$$

Finally, define a C^*-algebra isomorphism $\theta : \mathcal{B}(\mathcal{H}_+) \to \mathcal{B}(\mathcal{H}_+)$ by

$$\theta(A) = FAF^*, \quad A \in \mathcal{B}(\mathcal{H}_-) \tag{B.1.8}$$

We then extend the C^*-algebra isomorphism to $\mathcal{B}(\mathcal{H}_- \otimes \mathcal{H}_+)$ by

$$\tilde{\theta}(A \otimes \mathbb{1}_{\mathcal{H}_+}) = \mathbb{1}_{\mathcal{H}_-} \otimes \theta(A) \tag{B.1.9}$$

Lemma B.1.1 *The Hamiltonian in* (3.3.4) *is unitarily equivalent to the Antiferromagnetic XXZ Hamiltonian. Moreover, for some* $K \in \mathbb{N}$ *there are operators* $B, C_1, \dots C_K$ *of the form* $S \otimes \mathbb{1}_{\mathcal{H}_+}$, $S \in \mathcal{B}(\mathcal{H}_+)$, *such the Antiferromagnetic XXZ Hamiltonian can be expressed as*

$$B + \tilde{\theta}(B) - \sum_{r=1}^{K} C_r \tilde{\theta}(C_r) \tag{B.1.10}$$

Proof: *Define* $U : \mathcal{H}_+ \to \mathcal{H}_+$ *given by*

$$Uf(\sigma) = f(-\sigma), \qquad f \in \mathcal{H}_+ \tag{B.1.11}$$

where $\sigma = (\sigma_{\mathbf{j}})_{\mathbf{j}\in V_+}$, $-\sigma = (-\sigma_{\mathbf{j}})_{\mathbf{j}\in V_+}$ *and* $\sigma_{\mathbf{j}} \in \left\{ \left| \pm\frac{1}{2} \right\rangle \right\}$.

Let $\{\delta_\tau : \tau \in C(V_+)\}$ *be the orthonormal basis of* $\ell^2(C(V_+)$ *where*

$$\delta_\tau(\sigma) = \begin{cases} 1, & \text{if } \sigma = \tau \\ \\ 0, & \text{if } \sigma \neq \tau \end{cases} \tag{B.1.12}$$

Then $U = U^* = U^{-1}$ *and also,*

$$US^x_{\mathbf{j}}U = S^x_{\mathbf{j}}, \qquad US^y_{\mathbf{j}}U = -S^y_{\mathbf{j}}, \quad \text{and} \quad US^z_{\mathbf{j}}U = -S^z_{\mathbf{j}} \tag{B.1.13}$$

Recall that $US^x_{\mathbf{j}}U := U(\mathbb{1} \otimes \cdots \otimes S^x_{\mathbf{j}} \otimes \cdots \mathbb{1})U$ *for tensors only on* V_+.

The operator $\mathcal{U} := I_{\mathcal{H}_-} \otimes U$ *is a unitary transformation on the* $\ell^2(C(\mathcal{V}))$ *and satisfies* $\mathcal{U} = \mathcal{U}^* = \mathcal{U}^{-1}$. *Moreover, for* $i \in V_-$ *and* $j \in V_+$, *we have that*

$$\begin{aligned} \mathcal{U}h^{\Delta}_{ij}\mathcal{U} &= -S^x_i S^x_j + S^y_i S^y_j + \Delta S^z_i S^z_j \\ &= -S^x_i S^x_j - (iS_i)^y (iS^y_j) + \Delta S^z_i S^z_j \end{aligned} \tag{B.1.14}$$

Where the second equation is needed in order to make the right hand side a sum of real operators (since S^y_i *and* S^y_j *are not real operators).*

For the case $\Delta < 0$ *and* $R(i) = j$, *we have that*

$$\mathcal{U}h^{\Delta}_{ij}\mathcal{U} = -\sum_{k=1}^{3} D^k_i \tilde{\theta}(D^k_i) \tag{B.1.15}$$

where $D^1 = S^x,\ D^2 = S^y$ *and* $D^3 = \sqrt{-\Delta}\, S^z$.

If $i, j \in V_+$, *then* $\mathcal{U}h^{\Delta}_{ij}\mathcal{U} = h^{\Delta}_{ij}$. *Therefore, enumerating the pairs* $\{\, i, j \,\}$ *with* $j = R(i)$

and $\{i,j\} \in \mathcal{E}$ *as* $\{i_1, j_1\}, \ldots, \{i_K, j_K\}$*, we have*

$$\mathcal{U} H_{\mathcal{G},\Delta} \mathcal{U} = B + \tilde{\theta}(B) - \sum_{r=1}^{K} \sum_{k=1}^{3} D_{i_r}^{k} \tilde{\theta}(D_{i_r}^{k}) \tag{B.1.16}$$

where

$$B = \sum_{\{i,j\} \in \mathcal{E}(V_-)} h_{i,j}^{\Delta} \tag{B.1.17}$$

Hence by Theorem (B.1.3)*,* $H_{\mathcal{G},\Delta}$ *is unitarily equivalent to a reflection positive Hamiltonian.*

Let $\mathcal{B}_{\mathbb{R}}(\mathcal{H}_-)$ be the set of bounded "real"[1] operators on $\mathcal{H}_-$.

Lemma B.1.2 *The tracial state, defined as* $\langle \cdot \rangle = \mathrm{Tr}[\cdot] / \mathrm{Tr}[\mathbb{1}]$ *is reflection positive.*

Proof:

Let $\mathcal{A} := A \otimes \mathbb{1}_{\mathcal{H}_+}, \;\; A \in \mathcal{B}(\mathcal{H}_-)$.

$$\mathrm{Tr}[\mathcal{A}\tilde{\theta}(\mathcal{A})] = \mathrm{Tr}[A \otimes \theta(A)] \tag{B.1.18}$$

$$= \sum_{\sigma \in C(\mathbb{B}_N)} \langle g_{(\sigma)}, (A \otimes \theta(A)) g_{(\sigma)} \rangle \tag{B.1.19}$$

$$= \sum_{\sigma \in C(\mathbb{B}_N)} \langle g_{(\sigma)^-}, A g_{(\sigma)^-} \rangle_{\mathcal{H}_-} \cdot \langle g_{(\sigma)^+}, \theta(A) g_{(\sigma)^+} \rangle_{\mathcal{H}_+} \tag{B.1.20}$$

$$= \sum_{\sigma \in C(\Lambda_-)} \langle g_{(\sigma)}, A g_{(\sigma)} \rangle_{\mathcal{H}_-} \sum_{\sigma \in C(\Lambda_+)} \langle F^* g_{(\sigma)}, A F^* g_{(\sigma)} \rangle_{\mathcal{H}_+} \tag{B.1.21}$$

Since R is a bijection and by the definition of F, the sums in the last equation are

[1] An operator A is said to be real if $\langle g_\sigma, A g_{\sigma'} \rangle \in \mathbb{R}$ for all $\sigma, \sigma' \in C(\Lambda_+)$

equal. Hence,

$$\mathrm{Tr}[\mathcal{A}\tilde{\theta}(\mathcal{A})] = \left(\mathrm{Tr}_{\mathcal{H}_-[A]}\right)^2 \geq 0 \tag{B.1.22}$$

where the last inequality is as a result of the fact that A is real.

Theorem B.1.3 ([16, Thm. 2.1], [6, Cor. 5.4]) *If $-H = B+\tilde{\theta}(B)+\sum_{j=1}^{K} C_j\tilde{\theta}(C_j)$ (or more generally $B + \theta(B) + \int C(x)\tilde{\theta}[C(x)]d\rho(x)$ for a positive measure $d\rho$) with $B, C_1, \ldots C_K$ of the form $S \otimes \mathbb{1}_{\mathcal{H}_+}$, $S \in \mathcal{B}(\mathcal{H}_+)$, and if $\langle\cdot\rangle_0$ is generalized reflection positive, then*

$$\langle\cdot\rangle_H = \frac{\langle A e^{-\beta H}\rangle_0}{\langle e^{-\beta H}\rangle_0}, \quad \beta > 0 \tag{B.1.23}$$

is generalized reflection positive.

The proof of the theorem can also be found in [9, Thm. A.6]

B.2 Large deviation bounds

We start with a large deviation bound for a Poisson random variable. Suppose that X is a Poisson random variable with mean value $\lambda > 0$. Then for any number $a \geq 0$, we have

$$\mathbf{P}(\mathsf{X} \geq a) \ = \ \mathbf{P}(e^{t\mathsf{X}} \geq e^{at})\,, \tag{B.2.1}$$

for any $t > 0$. Using Chernoff bounds, this gives the inequality

$$\mathbf{P}(\mathsf{X} \geq a) \ \leq \ \frac{\mathbf{E}[e^{t\mathsf{X}}]}{e^{at}} \ = \ e^{\lambda(e^t-1)-at}\,. \tag{B.2.2}$$

For $a \geq \lambda$, we may take $t = \ln(a/\lambda)$ to obtain

$$\forall a \geq \lambda\,, \qquad \mathbf{P}(\mathsf{X} \geq a) \ \leq \ \exp\left(a - \lambda - a\ln\left(\frac{a}{\lambda}\right)\right)\,. \tag{B.2.3}$$

Note that we assume that $0 < \lambda \leq a$. But if we introduce a new variable κ such that

$$a - \lambda \;=\; \kappa\lambda\,, \tag{B.2.4}$$

then this gives

$$\forall \kappa \geq 0\,, \qquad \mathbf{P}(\mathsf{X} \geq (1+\kappa)\lambda) \;\leq\; \exp\left(-\left((1+\kappa)\ln(1+\kappa) - \kappa\right)\lambda\right)\,, \tag{B.2.5}$$

which is the bound that we most commonly use. We frequently take λ to be large, and actually often $\lambda = n$ for an integer $n \in \mathbb{N}$ which is large.

Remark B.2.1 *We can, just as easily, obtain large deviation bounds for binomial random variables. But unless we discretize time, the underlying variables for all the graphical representations are continuous, and hence Poisson point processes.*

Note, that the exact calculation shows that, still for a Poisson random variable X with mean value λ, we have

$$\mathbf{P}(\mathsf{X} = 0) \;=\; e^{-\lambda}\,. \tag{B.2.6}$$

This is occassionally useful when $\lambda > 0$.

Next, we give an operator version of the Jensen inequality

Theorem B.2.2 *Let $f : \mathbb{R} \to \mathbb{R}$ be a convex funtion and suppose $A : \mathbb{C}^n \to \mathbb{C}^n$ is a positive semi-definite matrix. Then, for any normalized vector $x \in \mathbb{C}^n$, we have*

$$f(\langle x, Ax\rangle) \leq \langle x, f(A)x\rangle \tag{B.2.7}$$

where $f(A)$ is defined by functional calculus.

Proof: By spectral decomposition,

$$\langle x, f(A)x\rangle = \left\langle x, \left(\sum_{i=1}^{n} f(a_i)\mathrm{P}_{\mathrm{a_i}}\right) x\right\rangle \tag{B.2.8}$$

$$= \sum_{i=1}^{n} f(a_i)\left\langle x, \mathrm{P}_{\mathrm{a_i}}\mathrm{x}\right\rangle \tag{B.2.9}$$

$$\geq f\left(\sum_{i=1}^{n} a_i \left\langle x, \mathrm{P}_{\mathrm{a_i}}\mathrm{x}\right\rangle\right) \tag{B.2.10}$$

$$= f(\langle x, A, x\rangle) \tag{B.2.11}$$

Remark B.2.3 *Jensen inequaity has been applied in equation* (B.2.10)