Dimerization and Néel order in different quantum spin chains through a shared loop representation

Michael Aizenman, Hugo Duminil-Copin, Simone Warzel*

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Abstract: The ground states of the spin-S antiferromagnetic chain H_{AF} with a projection-based interaction and the spin-1/2 XXZ-chain H_{XXZ} at anisotropy parameter $\Delta = \cosh(\lambda)$ share a common loop representation in terms of a two-dimensional functional integral which is similar to the classical planar Q-state Potts model at $\sqrt{Q} = 2S+1 = 2\cosh(\lambda)$. The multifaceted relation is used here to directly relate the distinct forms of translation symmetry breaking which are manifested in the ground states of these two models: dimerization for H_{AF} at all $S > 1/2$, and Néel order for H_{XXZ} at $\lambda > 0$. The results presented include: i) a translation to the above quantum spin systems of the results which were recently proven by Duminil-Copin-Li-Manolescu for a broad class of two-dimensional random-cluster models, and ii) a short proof of the symmetry breaking in a manner similar to the recent structural proof by Ray-Spinka of the discontinuity of the phase transition for $Q > 4$. Altogether, the quantum manifestation of the change between $Q = 4$ and $Q > 4$ is a transition from a gapless ground state to a pair of gapped and extensively distinct ground states.

1 Introduction

The focus of this work is the structure of the ground states in two families of antiferromagnetic quantum spin chains, each of which includes the spin-1/2 Heisenberg anti-ferromagnet as a special case. In the infinite volume limit, with the exception of their common root, in both cases the systems exhibit symmetry breaking at the level of ground states. The physics underlying the phenomenon is different. In one case it is extensive quantum frustration which causes dimerization expressed here in spacial energy oscillations. In the other case, the Hamiltonian is frustration free, and the symmetry breaking is expressed in long-range Néel order. Yet, in mathematical terms both phenomena are analyzable through a common random loop representation. Curiously, a similar loop system appears also as the auxiliary scaffoldings of a classical planar Q-state Potts models for which the symmetry breaking relates to a discontinuity in the order parameter.

The models under consideration have been studied extensively, and hence the specific results we discuss may be regarded as known, at one level or another. The techniques which have been applied for the purpose include numerical works, Bethe ansatz calculations [1, 8, 9, 10, 11, 26], and cluster

*Corresponding author

expansions [29]. The validity of Bethe ansatz calculations for similar systems has recently received support through a careful mathematical analysis [19]. The results presented here are based on non-perturbative structural arguments. They may be worth presenting since in the models considered here such arguments allow full characterization of the conditions under which the symmetry breaking occurs, as well as other qualitative features of the model's grounds states. The relation between the models may be of intrinsic interest. At the mathematical level it plays an essential role in the non-perturbative proof of symmetry breaking which is the main result presented here.

1.1 Antiferromagnetic $SU(2S+1)$ invariant spin chains with projection based interaction

The first family of models concerns the quantum spin chain of spin-S operators $\mathbf{S}_u := (S_u^x, S_u^y, S_u^z)$ with the antiferromagnetic Hamiltonian

$$H_{\mathrm{AF}}^{(L)} = \sum_{u=-L+1}^{L-1} \begin{cases} [2\mathbf{S}_u \cdot \mathbf{S}_{u+1} - 1/2] & \text{for } S = 1/2, \\ -(2S+1) P_{u,u+1}^{(0)} & \text{for } S \geq 1/2, \end{cases} \tag{1.1}$$

with $P_{u,u+1}^{(0)}$ the orthogonal projection onto the singlet state of spins on neighboring sites $u, (u+1) \in \Lambda_L := \{-L+1, \ldots, L\}$. When referring to such local operators in the context of the product Hilbert space $\mathcal{H}_L := \bigotimes_{v=-L+1}^{L} \mathbb{C}^{2S+1}$, they are to be understood as acting as the identity on the other components of the product. This model was studied by Affleck [1], Batchelor and Barber [8, 9], Klümper [26], Aizenman and Nachtergaele [5], and more recently Ueltschi and Nachtergaele [29].

For $S = 1/2$, in which case the two formulations agree, this system is just the Heisenberg anti-ferromagnet, for which the $L = 1$ ground state $P^{(0)} = |D_1\rangle\langle D_1|$ is the maximally entangled state

$$|D_1\rangle := (|+,-\rangle - |-,+\rangle)/\sqrt{2}\,. \tag{1.2}$$

The more general expression of the rank-one projection is:

$$P_{u,v}^{(0)} \;:=\; 1\,[|\boldsymbol{S}_u + \boldsymbol{S}_v| = 0] = \frac{1}{2s+1} \sum_{m,m'=-S}^{S} (-1)^{m-m'} \left|m,-m\rangle_{u,v}\langle m',-m'\right|, \tag{1.3}$$

where $|m\rangle_u$ are the eigenstates of S_u^z, for which $S_u^z|m\rangle_u = m|m\rangle_u$, $m \in \{-S, -S+1, \ldots, S\})$[1]. Here and in the following, the subscripts on the vectors indicate on which tensor component of $\mathcal{H}_L$ they act.

Each of the two-spin interaction terms in (1.1) is minimized in the state in which the two spins are coherently intertwined into the unique state in which $|\mathbf{S}_u + \mathbf{S}_v| = 0$. However, a spin cannot be locked into such a state with both its neighbours simultaneously. This effect, which results in the spin-Peierls instability, is purely quantum as there is no such restriction for classical spins. Classical spin models exhibit frustration when placed on a non-bipartite graph with antiferromagnetic interactions, and also on arbitrary graphs under suitably mixed interactions. Such geometric frustration is then shared by their quantum counterparts.

The naive pairing depicted in Fig. 1 suggests that in finite volume the ground-states' local energy density may not be homogeneous and have a bias triggered by the boundary conditions, i.e. the parity

[1] The projection $P_{u,v}^{(0)}$ can also be expressed as a polynomial of degree $2S$ in $\boldsymbol{S}_u \cdot \boldsymbol{S}_v$, for instance $P_{u,v}^{(0)} = -\boldsymbol{S}_u \cdot \boldsymbol{S}_v + 1/4$ for $S = 1/2$ and $P_{u,v}^{(0)} = 1 - (\boldsymbol{S}_u \cdot \boldsymbol{S}_v)^2$ for $S = 1$.

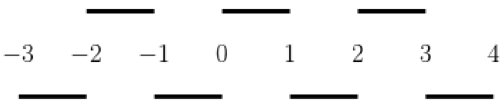

Figure 1: The natural pairing in $\Lambda_L = \{-L+1, \ldots, L-1, L\}$ for $L = 3$ and $L = 4$. Notice the difference at $u = 0$.

of L. Indeed, through approximations, numerical simulations, or the probabilistic representation of [5] (our preferred method), one may see that the local energy density of the corresponding finite-volume ground states $\langle \cdot \rangle_L^{(\mathrm{gs})}$ is not homogeneous and satisfies

$$(-1)^L \big[\langle P_{2n,2n+1} \rangle_L^{(\mathrm{gs})} - \langle P_{2n-1,2n} \rangle_L^{(\mathrm{gs})} \big] \; > \; 0 \, . \tag{1.4}$$

An interesting question is whether this bias persists in the limit $L \to \infty$, in which case in the infinite-volume limit the system has (at least) two distinct ground states, for which the expectation values of local observables F are given by

$$\langle F \rangle_{\mathrm{even}} \; := \; \lim_{\substack{L\to\infty \\ L \mathrm{even}}} \langle F \rangle_L^{(\mathrm{gs})} \qquad \text{and} \qquad \langle F \rangle_{\mathrm{odd}} \; := \; \lim_{\substack{L\to\infty \\ L \mathrm{odd}}} \langle F \rangle_L^{(\mathrm{gs})} \, , \tag{1.5}$$

where the limit is interpreted in the weak sense, i.e. with F being any (fixed) local bounded operator. These are generated by products of spin operators

$$F_U := \prod_{j=1}^{k} S_{u_j}^{\alpha_j} \, , \quad u_j \in U \, , \quad \alpha_j \in \{x, y, z\} \tag{1.6}$$

which are supported in some bounded set $U \subset \mathbb{Z}$. In finite-volume, their (imaginary) time-evolved counterparts are given by

$$F_U^{(L)}(t) := \; e^{-tH_{\mathrm{AF}}^{(L)}} \; F_U \; e^{tH_{\mathrm{AF}}^{(L)}} \, .$$

The corresponding truncated correlations also converge, e.g. for any fixed $t \in \mathbb{R}$,

$$\langle F_U(t); F_V \rangle_{\mathrm{even}} := \lim_{\substack{L\to\infty \\ L \mathrm{even}}} \langle F_U^{(L)}(t) F_V \rangle_L^{(\mathrm{gs})} - \langle F_U^{(L)}(t) \rangle_L^{(\mathrm{gs})} \langle F_V \rangle_L^{(\mathrm{gs})} \, , \tag{1.7}$$

and similarly for $\langle F_U(t); F_V \rangle_{\mathrm{odd}}$.

The separate convergence of the limits (1.5) or (1.7) was established in [5] through probabilistic techniques which are enabled by the loop representation which is presented below. This representation also led to the following dichotomy.[2]

Proposition 1.1 (cf. Thm. 6.1 in [5]). *For each value of $S \in \mathbb{N}/2$ one of the following holds true:*

1. *The two ground states $\langle \cdot \rangle_{even}$ and $\langle \cdot \rangle_{odd}$ are distinct, each invariant under the 2-step shift, each being the 1-step shift of the other. Furthermore, their translation symmetry breaking is manifested in energy oscillations, namely, for every $n \geq \mathbb{N}$*

$$\langle P_{2n,2n+1}^{(0)} \rangle_{even} - \langle P_{2n-1,2n}^{(0)} \rangle_{even} > 0 \, . \tag{1.8}$$

[2] This version of the AN dichotomy is a bit more carefully crafted than in the original work, as the two options stated there need not be mutually exclusive. However, as (1.10) shows, ipso-facto they are.

2. *The even and odd ground states coincide, and form a translation invariant ground state* $\langle \cdot \rangle$ *with slowly decaying correlations, satisfying*

$$\sum_{v \in \mathbb{Z}} |v| \, |\langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_v \rangle| = \infty \,. \tag{1.9}$$

For $S = 1/2$ the second alternative is known to hold [20]. In this case the model reduces to the quantum Heisenberg antiferromagnet, for which Bethe [7] predicted the low-energy spectrum exactly by means of his famous ansatz. In the converse direction, dimerization in this model was established for $S \geq 8$ [29] through a cluster expansion. The gap between these results is closed here through a structural proof that for all $S > 1/2$ the first option holds (regardless of the parity of $2S$).

Theorem 1.2. *For all* $S > 1/2$*:*

1. *the even and odd ground-states, defined by* (1.5)*, differ. They are translates of each other, and exhibit the energy oscillation* (1.8)*.*

2. *there exist* $C = C(S), \xi = \xi(S) < \infty$ *such that for all* $U, V \subset \mathbb{Z}$ *with distance* $\mathrm{dist}(U,V)$ *and any* $t \in \mathbb{R}$*:*

$$|\langle F_U(t); F_V \rangle_{even}| \;\leq\; C\, e^{-(\mathrm{dist}(U,V)+|t|)/\xi} \,. \tag{1.10}$$

The proof draws on the progress which was recently made in the study of the related loop models. In [19], the loop representation of the critical Q-state Potts model on the square lattice with $Q > 4$ was proved to have two distinct infinite-volume measures under which the probability of having large loops is decaying exponentially fast (see [27] for the case of large Q). The result was extended in [17, Theorem 1.4] to a slightly modified version of the loop model that will be redefined in this paper and connected to the spin chains (there, the model is not defined in terms of loops but in terms of percolation, as in Section 6). More recently, Ray and Spinka [30] provided an alternative proof of the non-uniqueness of the infinite-volume measures on the square lattice.

In this article, the inspiring proof of Ray-Spinka is extended to our context to provide a new proof of item 1. We believe that this proof is more transparent and conceptual than the one in [17], and that even though the technique does not directly lead to 2., it illustrates perfectly the interplay between the quantum and classical realms. In fact, a careful analysis of the proofs in the paper of [17] shows that the argument there relies on two pillars: a theorem proving a stronger form of Proposition 1.1 (see also [18, 20] for versions on the square lattice), in which 1. is proved to imply 2., and an argument relying on the Bethe Ansatz showing that 1. indeed occurs. The adaptation of the Ray-Spinka argument enables us to prove 1. directly without using the Bethe Ansatz, so that the argument in this paper replace half of the argument in [17], and that combined with the other half it also implies 2.

Let us finally note that under the dimerization scenario, which is now established for its full range ($S > 1/2$), other physically interesting features follow:

1. *Spectral gap:* As was argued already in [5, Theorem 7.1], the exponential decay of truncated correlations (1.10) in the t-direction implies a non-vanishing spectral gap in the excitation spectrum above the even and odd ground-states.

2. *Excess spin operators:* When the decay of correlations is fast enough so that (1.9) does not hold, in particular under (1.10), in the even/odd states the spins are organized into tight neutral clusters. That is manifested in the tightness of the distribution of the block spins $S^z_{[a,b]} = \sum_{u\in[a,b]} S^z_u$ (in a sense elaborated in [4]). That is equivalent to the existence of the excess spin operators $\widehat{S}^z_u$ with which

$$\sum_{u=1}^{k} S^z_u = \widehat{S}^z_u(0) - \widehat{S}^z_u(k) \tag{1.11}$$

and such that $\widehat{S}^z_u(k)$ commutes with the spins in $(-\infty, k]$. The quantity $\widehat{S}^z_u(k)$ can be interpreted as the total spin in $[k, \infty)$, and constructed as $\lim_{\varepsilon\downarrow 0} \sum_{v>u} e^{-\varepsilon|u-v|} S^z_v$ (in the strong-resolvent sense), cf. [5, Sec. 6]. As was further discussed in [6], the excess spins play a role in the classification of the topological properties of the gapped ground-state phases.

3. *Entanglement entropy:* Another general implication of the exponential decay of correlations is a so-called area law (which for chains equates to the boundedness) of the entanglement entropy of the ground-states, see [13] for details.

1.2 The $S = 1/2$ antiferromagnetic XXZ spin chain

The second model discussed in this paper is the anisotropic XXZ spin-1/2 chain with the Hamiltonian

$$H^{(L)}_{\mathrm{XXZ}} := -\frac{1}{2} \sum_{v=-L+1}^{L-1} \left[\tau^x_v \tau^x_{v+1} + \tau^y_v \tau^y_{v+1} - \Delta\, (\tau^z_v \tau^z_{v+1} - 1)\right] \tag{1.12}$$

acting on the Hilbert space $\mathcal{H}_L := \bigotimes_{v=-L+1}^{L} \mathbb{C}^2$. It consists of Pauli spin matrices on $\mathbb{C}^2$ which are denoted by (τ^x, τ^y, τ^z) to avoid confusion. It is convenient to present the anisotropy parameter as

$$\Delta := \cosh(\lambda) > 1\,. \tag{1.13}$$

Throughout the paper and unless stated otherwise explicitly, we will take $\lambda \geq 0$ the non-negative solution of (1.13).

The sign and the magnitude of $\Delta > 1$ favor antiferromagnetic order in the ground state. The negative sign in front of the terms involving the x- and y-component of the Pauli spin matrices can be flipped through the unitary transformation $U_L = \exp\left(i\frac{\pi}{4}\sum_u (-1)^u \tau^z_u\right)$. It renders the Hamiltonian in the manifestly antiferromagnetic form

$$U_L H^{(L)}_{\mathrm{XXZ}} U^*_L = \frac{1}{2} \sum_{v=-L+1}^{L-1} \left[\boldsymbol{\tau}_v \cdot \boldsymbol{\tau}_{v+1} + (\Delta - 1)\, \tau^z_v \tau^z_{v+1} - \Delta\right]\,. \tag{1.14}$$

The antiferromagnetic XXZ chain has been the subject of many works. Following Lieb's work on interacting Bose gas [28], Yang and Yang gave a justification for the Bethe Ansatz solution of the ground state in a series of papers [35, 36] in 1966. The ground state has long-range order with two period-2 states in the thermodynamic limit, which exhibit non-vanishing Néel order. The Néel order vanishes in the limit $\Delta \downarrow 1$. Since the exact solution is not very transparent, there has been interest in obtaining qualitative information by other means, e.g. expansions and other rigorous methods. These typically apply only for large Δ.

Our motivation for returning to the XXZ spin chain is that it emerges very naturally in the analysis of the thermal and ground states of the model H_{AF}. Furthermore, the relation between the two facilitates the proof of the symmetry breaking stated in Theorem 1.2. In the converse relation, this relation is used here to established symmetry breakdown in the form of Néel order of the XXZ ground state(s) for all $\Delta > 1$.

To prove the translation symmetry breaking we consider the pair of finite-volume ground states for the Hamiltonian (1.12) with an added boundary field,[3] i.e.

$$H_{\text{XXZ}}^{(L,\text{bc})} := H_{\text{XXZ}}^{(L)} + \sinh(\lambda)(-1)^L \, \frac{\tau_{-L+1}^z - \tau_L^z}{2} \times \begin{cases} +1 & \text{for bc} = + \\ -1 & \text{for bc} = - \end{cases} . \tag{1.15}$$

As a preparatory statement let us state:

Proposition 1.3. *For any $\Delta \geq 1$, in the limit $L \to \infty$ with L even, the finite-volume ground states of the XXZ-spin system with the above boundary terms converge to states $\langle \cdot \rangle_+$ and $\langle \cdot \rangle_-$. Regardless of whether the two agree, each is a one-step shift of the other. The two states are different if and only if they exhibit Néel order, in the sense for all n:*

$$(-1)^n \langle \tau_n^z \rangle_+ = -(-1)^n \langle \tau_n^z \rangle_- = M_{Néel} \tag{1.16}$$

at some $M_{Néel} \neq 0$.

Similarly to Proposition 1.1, this statement is proven here through the FKG inequality which is made applicable in a suitable loop representation. We postpone its proof to Section 6, next to the place where it is applied. Following is the XXZ-version of the symmetry breaking statement.

Theorem 1.4. *For any $\Delta > 1$ the construction described in Proposition 1.3 yields two different ground states of infinite XXZ-spin chain which differ by a one step shift and satisfy* (1.16)*.*

Theorem 1.4 is proven in Section 6 together with Theorem 1.2. In each case the symmetry breaking is initially established through the expectation value of a conveniently defined quasi-local observable. The conclusion is then boosted to the more easily recognizable statements presented in the theorems through the preparatory statements of Proposition 1.3 and respectively Proposition 1.1
.

1.3 Seeding the ground states

Infinite-volume ground-states can be approached through their intrinsic properties (such as the energy-minimizing criterion) or, constructively, as limits of finite-volume ground-state expectation value functionals. To establish their non-uniqueness, we shall consider different sequences of finite volume ground-states, and establish convergence of the expectation value functionals to limits which are extensively different. Equivalently, it suffices to construct a single limiting ground state which does not have the Hamiltonian's translation symmetry. A shift (or another symmetry operation) produces then another ground state. We shall take the latter path in the discussion of both models.

[3] One may expect that in case there is Néel order any antisymmetric boundary field would flip the ground state into one of the extremal states. However the proof of that is simpler for the case the field's magnitude is at least $|\sinh(\lambda)|$.

The finite-volume ground states will be constructed through limits of the form

$$\langle F\rangle_L^{(\mathrm{gs})} = \lim_{\beta\to\infty} \frac{\langle \Psi_L | e^{-\beta H_L/2} F e^{-\beta H_L/2} | \Psi_L\rangle}{\langle \Psi_L | e^{-\beta H_L} | \Psi_L\rangle} \,. \tag{1.17}$$

with $|\Psi_L\rangle$ a convenient *seeding vector*. To assure that the limiting functional corresponds to a ground state (or *the* ground state if it is unique) one needs to verity that this vector is not annihilated by the ground-state projection operator $P_L^{(\mathrm{gs})}$. That will be established by verifying that

$$\frac{\langle \Psi_L | P_L^{(\mathrm{gs})} | \Psi_L\rangle}{\dim P_L^{(\mathrm{gs})}} = \lim_{\beta\to\infty} \frac{\langle \Psi_L | e^{-\beta H_L} | \Psi_L\rangle}{\mathrm{tr}\, e^{-\beta H_L}} > 0\,. \tag{1.18}$$

Our choice of the seeding vectors is primarily guided not by the condition (1.18), which is generically satisfied, but rather by the goal of a transparent expression for the expectation value functional.

In view of the quantum frustration effect, a natural seed vector for the construction of a ground-state for the Hamiltonian $H_{\mathrm{AF}}^{(L)}$ on an even collection of spins in $\Lambda_L = \{-L+1, \ldots, L\}$ is the dimerized state

$$\begin{aligned} |D_L\rangle \;&:=\; \bigotimes_{j=1}^{L} \Big(\sum_{m=-S}^{S} (-1)^m \, |m, -m\rangle_{-L+2j-1, -L+2j} \Big) \\ &=\; U_L \bigotimes_{j=1}^{L} \Big(\sum_{m=-S}^{S} |m, -m\rangle_{-L+2j-1, -L+2j} \Big) \,. \end{aligned} \tag{1.19}$$

The role of the gauge transformation

$$U_L := \exp\Big(i \tfrac{\pi}{2} \sum_u (-1)^u S_u^z \Big) \,, \tag{1.20}$$

expressed in the standard z-basis of the joint eigenstates of S_u^z, $u\in\Lambda_L$, is to ensure non-negativity of the matrix-elements of $U_L^* e^{-\beta H_{\mathrm{AF}}^{(L)}} U_L$ in the z-basis. This will enable a probabilistic loop representation of this semigroup presented in Section 2. From this representation, we will also see that (1.18) is valid for the seed state $\Psi_L = D_L$ at any finite L, cf. (3.10) below. The standard Perron-Frobenius argument is not applicable in this case.

Applying the semigroup operator $e^{-\beta H_L/2}$ to $|D_L\rangle$, one gets the expectation-value functional which assigns to each local observable F the value

$$\langle F\rangle_{L,\beta}^{(\mathrm{AF})} \;:=\; \frac{\langle D_L | e^{-\beta H_{\mathrm{AF}}^{(L)}/2} F e^{-\beta H_{\mathrm{AF}}^{(L)}/2} | D_L\rangle}{\langle D_L | e^{-\beta H_{\mathrm{AF}}^{(L)}} | D_L\rangle} \,, \tag{1.21}$$

and which converges as $\beta\to\infty$ to a ground-state expectation $\langle F\rangle_L^{(\mathrm{gs})}$. It is the above expectation-value functional which we study in the proof of Theorem 1.2 by probabilistic means.

To study the Néel order of the XXZ-Hamiltonian we find it convenient to focus on the sequence of constant parity, say even L, and use as seed in (1.17) the vector

$$|N_\lambda^{(L)}\rangle \;=\; \bigotimes_{j=1}^{L} \Big(e^{-\lambda/2} |+,-\rangle_{-L+2j-1,-L+2j} + e^{\lambda/2} |-,+\rangle_{-L+2j-1,-L+2j} \Big) \tag{1.22}$$

which is indexed by λ. Using it, the state $\langle\cdot\rangle_+$ of Proposition 1.3 is presentable as the double limit

$$\langle F\rangle_+^{(\mathrm{XXZ})} = \lim_{\substack{L\to\infty\\ L\mathrm{even}}} \lim_{\beta\to\infty} \langle F\rangle_{L,\beta,\lambda}^{(\mathrm{XXZ},+)} \tag{1.23}$$

of

$$\langle F\rangle_{L,\beta,\lambda}^{(\mathrm{XXZ},+)} := \frac{\langle N_\lambda^{(L)}| e^{-\beta H_{\mathrm{XXZ}}^{(L,+)}/2}\, F\, e^{-\beta H_{\mathrm{XXZ}}^{(L,+)}/2} |N_\lambda^{(L)}\rangle}{\langle N_\lambda^{(L)}| e^{-\beta H_{\mathrm{XXZ}}^{(L,+)}} |N_\lambda^{(L)}\rangle} \,. \tag{1.24}$$

For the state $\langle\cdot\rangle_-^{(\mathrm{XXZ})}$, we reverse the sign in front of λ in (1.22), and apply the operator $H_{\mathrm{XXZ}}^{(L,-)}$.

Note that for fixed $L \in 2\mathbb{N}$, the limit $\beta \to \infty$ in (1.23) converges to the finite-volume ground-state of $H_{\mathrm{XXZ}}^{(L,+)}$, which is found in the subspace

$$S_{\mathrm{tot}}^z := \sum_{u=-L+1}^{L} \tau_u^z/2 = 0 \tag{1.25}$$

where it is unique. This follows from a standard Perron-Frobenius argument, which is enabled here by the positivity and transitivity of the semigroup on that subspace. As a consequence, the finite-volume ground-state can be constructed through the limit $\beta \to \infty$ starting from any non-negative seed vector with $S_{\mathrm{tot}}^z = 0$. The vectors $N_\lambda^{(L)}$ with $\lambda \in \mathbb{R}$ arbitrary are examples of such seed vectors and the limit (1.23) does not depend on the choice of λ in the seed (but still depends on λ through $H_{\mathrm{XXZ}}^{(L,+)}$.)

Next we start the detailed discussion by recalling the probabilistic loop representations of the states described above. The construction is included here mainly to keep the paper reasonably self-contained, since it is already contained in [5].

2 Functional integral representation of the thermal states

2.1 The general construction

Thermal states of d-dimensional quantum systems can always be expressed in terms of a $(d+1)$-dimensional functional integral. When the integrand can be expressed in positive terms, the result is a relation with a statistic-mechanical system in dimension $d+1$. General discussion of this theme and applications for specific purposes can be found e.g. in [2, 5, 14, 21, 22, 33, 34]. Our aim in this section is to present this relation for the models discussed here.

As a starting point, let us note the following elementary identity, in which the power expansion of $e^{\beta K}$, which is valid for any bounded operator K, is cast in probabilistic terms:

$$e^{\beta(K-1)} = \sum_{n=0}^{\infty} e^{-\beta} \int_{0<t_1<\cdots<t_n<\beta} K_{t_n}\ldots K_{t_1} dt_1 \ldots dt_n = \int \mathcal{T}(\prod_{t\in\omega} K_t)\ \rho_{[0,\beta]}(d\omega)\,. \tag{2.1}$$

In the last expression, the sequence of times is presented as a random point subset $\omega = (t_1,\ldots,t_n) \subset [0,\beta]$ distributed as a Poisson process on $[0,\beta]$ with intensity measure dt. The Poisson probability distribution is denoted here by $\rho_{[0,\beta]}(d\omega)$. Attached to each point $t \in \omega$ is a copy of the operator K labelled by t. The factors K_t are rearranged according to their time label, which is denoted using the time ordering operator $\mathcal{T}$. The integral reproduces the familiar power series.

For operators which are given by sums of (local) terms, as in our case

$$H_\Lambda = - \sum_{b \in \mathcal{E}(\Lambda)} K_b \tag{2.2}$$

with K_b indexed by the edge-set $\mathcal{E}(\Lambda)$ of a graph Λ, the identity (2.1) has the following extension

$$e^{\beta \sum_{b\in\mathcal{E}(\Lambda)}(K_b - 1)} \quad = \quad \int K_{b_{|\omega|}, t_{|\omega|}} \cdot \ldots \cdot K_{b_2,t_2} \cdot K_{b_1,t_1} \; \rho_{\Lambda \times [0,\beta]}(d\omega) \tag{2.3}$$

where ω are the configurations of a Poisson point process over $\mathcal{E}(\Lambda) \times [0, \beta]$, which may be depicted as collections of rungs of a random multicolumnar ladder net whose rungs are listed as $\{(b_j, t_j)\}$ in increasing order of t. We denote by $\Omega_{\Lambda,\beta}$ the space of such configurations, and by $\rho_{\Lambda\times[0,\beta]}(d\omega)$ the Poisson process with intensity measure dt along the collection of vertical columns $\cup_{b\in\mathcal{E}(\Lambda)}\{b\} \times [0, \beta]$.

Given an orthonormal basis $\{|\alpha\rangle\}$ of the Hilbert space in which these operators operate, one has

$$\begin{aligned} \langle\alpha'|\mathcal{T}\Big(\prod_{(b,t)\in\omega} K_{b,t}\Big)|\alpha\rangle \quad &= \quad \sum_{\widetilde{\alpha}} \mathbb{1}[\omega, \widetilde{\alpha}] \; \mathbb{1}\left[{}^{\alpha(t_{|\omega|})=\alpha'}_{\;\;\alpha(0)=\alpha}\right] \; W(\alpha', \alpha) \\ W(\alpha', \alpha) \quad &:= \quad \prod_{j=1}^{|\omega|} \langle \alpha(t_j + 0)|\, K_{b_j,t_j} \,|\alpha(t_j - 0)\rangle \end{aligned} \tag{2.4}$$

where $\widetilde{\alpha}$ is summed over functions $\widetilde{\alpha} : [0, \beta] \mapsto \{|\alpha\rangle\}$ which are constant between the transition times $0 < t_1 < \ldots < t_{|\omega|} < \beta$, and the consistency constraint is expressed in the indicator function $\mathbb{1}[\omega, \alpha]$.

Applying this representation, one gets

$$\mathrm{tr}\, e^{\beta \sum_{b\in\mathcal{E}(\Lambda)}(K_b - 1)} \quad = \quad \int \sum_{\widetilde{\alpha}:\, \alpha(\beta)=\alpha(0)} \mathbb{1}[\omega, \widetilde{\alpha}] \;\; W(\alpha(0), \alpha(0)) \;\, \rho_{\Lambda\times[0,\beta]}(d\omega). \tag{2.5}$$

The left side is obviously non-negative. If a basis of vectors $|\alpha\rangle$ can be found in which also the matrix elements of K_b are all non-negative, then (2.4) yields a functional integral for the quantum partition function in which the integration is over $(\omega, \widetilde{\alpha})$ which resembles a "classical" statistic mechanical system in $d + 1$ dimensions (with $\alpha(t)$ a time dependent configuration which changes at random times).

In that case one also gets a potentially useful decomposition of the thermal state:

$$\frac{\mathrm{tr}\, e^{-\beta H_\Lambda} F}{\mathrm{tr}\, e^{-\beta H_\Lambda}} = \int \mathbb{E}\,(F|\omega)\, \mu_{\Lambda\times[0,\beta]}(d\omega) \tag{2.6}$$

with

$$\begin{aligned} \mathbb{E}\,(F|\omega) &= \mathrm{tr}\, \mathcal{T}\Big(F \prod_{(b,t)\in\omega} K_{b,t}\Big) \Big/ \,\mathrm{tr}\, \mathcal{T}\Big(\prod_{(b,t)\in\omega} K_{b,t}\Big) \\ \mu_{\Lambda\times[0,\beta]}(d\omega) &= \frac{1}{\text{Norm.}}\, \mathrm{tr}\, \Big[\mathcal{T}\Big(\prod_{(b,t)\in\omega} K_{b,t}\Big)\Big] \; \rho_{\Lambda,\times[0,\beta]}(d\omega)\,. \end{aligned} \tag{2.7}$$

The functional $F \mapsto \mathbb{E}\,(F|\omega)$ was dubbed in [5] a quasi-state. It does not possess the full positivity of a quantum state on all observables, but is a proper state on the sub-algebra of observables which are diagonal in the basis in which the interaction terms K_b are all non-negative.

A similar decomposition is valid for states $\langle\Psi|e^{-\beta H_\Lambda/2}Fe^{-\beta H_\Lambda/2}|\Psi\rangle$, which are seeded by vectors Ψ with non-negative overlaps with the above base vectors. For that it is pictorially convenient to cyclicly shift the time interval to $[-\beta/2,\beta/2]$, and consider ω given by the Poisson process over the set

$$\Lambda_{L,\beta} := \Lambda_L \times [-\beta/2,\beta/2], \tag{2.8}$$

whose law is denoted by $\rho_{\Lambda_{L,\beta}}$.

Such non-negative functional integral representations of quantum states are associated with Gibbs states of a classical statistic mechanical systems. Under this correspondence, non-uniqueness of the ground states of a d-dimensional quantum spin system, in the infinite-volume limit, is associated with a first-order phase transition (at a non-zero temperature) of the corresponding $d+1$ dimensional classical system.

2.2 A potential-like extension

We shall use also an extension of the above expressions to operators of the form

$$H_\Lambda = -\sum_{b\in\mathcal{E}(\Lambda)} K_b - V \tag{2.9}$$

with V an operator which is diagonal in the basis $\{|\alpha\rangle\}$, with $V|\alpha\rangle = V(\alpha)|\alpha\rangle$. In a manner reminiscent of the way that potential appears in the Feynman-Kac formula, one has

$$\langle\alpha'|e^{\beta\sum_{b\in\mathcal{E}(\Lambda)}(K_b-1)+V}|\alpha\rangle = \int \sum_{\substack{\widetilde{\alpha}:\,\alpha(0)=\alpha \\ \alpha(\beta)=\alpha'}} \mathbb{1}[\omega,\widetilde{\alpha}]\;\; W(\alpha(0),\alpha(0))\, e^{\int_{-\beta/2}^{\beta/2} V(\alpha(t))\,dt}\, \rho_{\Lambda\times[0,\beta]}(d\omega). \tag{2.10}$$

as can be deduced from (2.4), e.g. using the Lie-Trotter product formula.

3 Loop measures associated with $H_{\mathbf{AF}}$

3.1 The $H_{\mathbf{AF}}$ seeded states

The positivity assumption does hold in the case of the two families of quantum spin chains considered here. Under the unitary (gauge) transformation $U_L := \exp\left(i\frac{\pi}{2}\sum_u(-1)^v S_u^z\right)$, the interaction terms of $H_{\mathrm{AF}}^{(L)}$ acquire positive matrix elements in the standard basis of the joint eigenstates of $(S_u^z)_{u\in\Lambda_L}$

$$U_L^* P_{uv}^{(0)} U_L = \frac{1}{2S+1}\sum_{m,m'=-S}^{S} \big|m,-m\rangle_{u,v}\langle m',-m'\big| \ . \tag{3.1}$$

In this basis, the factors $K_b = (2S+1)U_L^* P_{uv}^{(0)} U_L$ which appear in (2.3) reduce to constraints imposing the condition that before and after each rung the two spins at its edges add to zero. To compute the global effect of that, one may replace each rung by a pair of "infinitesimally separated" lines, and then decompose the graph into non-crossing loops, as indicated in Fig. 2.

By elementary considerations [5], it follows that for each rung configuration ω drawn on $\Lambda_{L,\beta}$:

$$\langle D_L|\,\mathcal{T}\Big(\prod_{(b,t)\in\omega} K_{b,t}\Big)\,|D_L\rangle \;=\; (2S+1)^{N_\ell(\omega)}\,, \tag{3.2}$$

where $N_\ell(\omega)$ is the number of loops into which the set of lines decomposes when the vertical lines are turned into columns through "capping" them at $t = \pm\beta/2$ over every other column starting with the left-most, cf. Fig. 2. Depending on the parity of L, the capping rule thus follows the two pairings in Fig. 1.

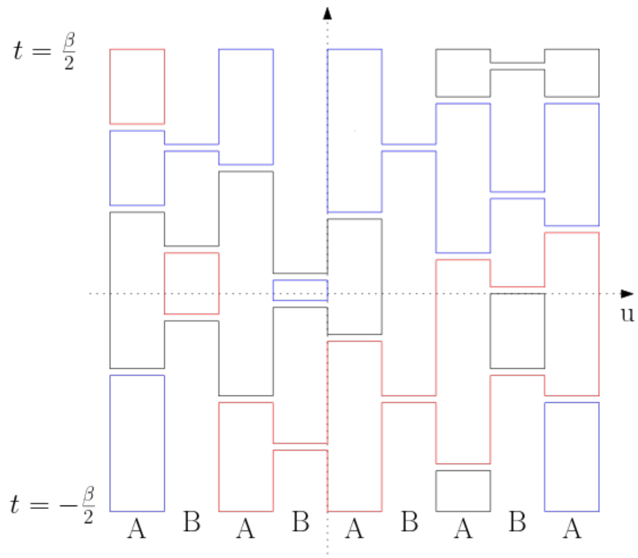

Figure 2: A configuration of randomly placed horizontal rungs in case $L = 5$, and its collection of loops obtained from alternating boundary conditions at $t = \pm\beta/2$. The rungs act as u-turns for the loops. Each of these loops is assigned independently one value $m \in \{-S, \dots, S-1, S\}$ depicted here in terms of three colors corresponding to $S = 1$.

More generally, as is detailed in [5] the matrix elements $\langle \boldsymbol{\sigma}' | \mathcal{T} \left(\prod_{(b,t)\in\omega} K_{b,t} \right) | \boldsymbol{\sigma} \rangle$ are given by the sum over configurations of functions $\sigma : \Lambda_{L,\beta} \mapsto \{-S, -S+1, \dots, S\}$ for which $\sigma(x,t)$ is constant in time, except for encounters with the rungs of ω at which the above constrains are satisfied, and which at $t = \pm\beta/2$ agree with $|\boldsymbol{\sigma}\rangle$ and $|\boldsymbol{\sigma}'\rangle$ correspondingly.

Adapting the quasi-state decomposition to the above seeded states, one gets:

Proposition 3.1 (cf. Prop. 2.1 in [5])**.** *For the expectation value* (1.21) *corresponding to the seed vector* $|D_L\rangle$ *and any observable* F*:*

$$\langle F \rangle_{L,\beta} = \int \mathbb{E}\left(F|\omega\right) \mu_{L,\beta}(d\omega), \tag{3.3}$$

where

$$\mathbb{E}\left(F|\omega\right) := \frac{1}{(2S+1)^{N_\ell(\omega)}} \langle D_L | \mathcal{T}\Big(\prod_{\substack{(b,t)\in\omega \\ t\in[0,\beta/2)}} (2S+1) P_b(t) \Big) \, F \, \mathcal{T}\Big(\prod_{\substack{(b,t)\in\omega \\ t\in[-\beta/2,0)}} (2S+1) P_b(t) \Big) |D_L\rangle \tag{3.4}$$

and

$$\mu_{L,\beta}(d\omega) := \frac{1}{Norm.} \sqrt{Q}^{N_\ell(\omega)} \rho_{\Lambda_{L,\beta}}(d\omega) \qquad at \ \sqrt{Q} = 2S+1\,. \tag{3.5}$$

Behind the complicated looking formula (3.4) is a simple rule which is particularly easy to describe for observables F which are functions of the spins S_u^z. The conditional expectation conditioned on ω is obtained by averaging the value of F over spin configurations which vary independently between the loops of ω. On each loop the spins are constrained to assume only two values, changing the sign upon each U-turn.

Following are some instructive examples:

1. For each ω
$$\mathbb{E}\left(S_u^x S_v^x|\omega\right) = \mathbb{E}\left(S_u^z S_v^z|\omega\right) = (-1)^{u-v}\, C_S\ \mathbb{1}[(u,0) \overset{\omega}{\leftrightarrow} (v,0)] \tag{3.6}$$
where $C_S = \sum_{m=-S}^{S} m^2/(2S+1)^2$ and the space-time points $(u,0) \overset{\omega}{\leftrightarrow} (v,0)$ denotes the condition that $(u,0)$ and $(v,0)$ lie on the same loop of ω.

2. For the projection operator defined by (1.3)
$$\begin{aligned}\mathbb{E}[(2S+1)P_{u,v}^{(0)}|\omega] &= \begin{cases} 1 & \text{if } (u,0) \overset{\omega}{\leftrightarrow} (v,0) \\ (2S+1)^{-1} & \text{if not} \end{cases} \\ &= \Big(1 + 2S\ \mathbb{1}[\,(u,0) \overset{\omega}{\leftrightarrow} (v,0)\,]\Big)/(2S+1)\,. \end{aligned} \tag{3.7}$$

3.2 The H_{AF} thermal equilibrium states

The above representation has a natural extension to the thermal Gibbs states, for which the expectation value functional is given by
$$\frac{\operatorname{tr} F e^{-\beta H_{\rm AF}^{(L)}}}{\operatorname{tr} e^{-\beta H_{\rm AF}^{(L)}}}\,. \tag{3.8}$$
In this case the above construction yields a representation in terms of random loop decomposition of $\Lambda_{L,\beta}$ constructed with the time-periodic boundary conditions, with loops continuing directly from $t = \pm\beta/2$. And if the quantum Hamiltonian $H_{AF}^{(L)}$ is taken with periodic boundary conditions then also the spacial coordinate is periodic, i.e. the loops are over a torus. Similarly as in (3.2) one gets
$$\operatorname{tr} \mathcal{T}\Big(\prod_{(b,t)\in\omega} K_{b,t}\Big) = \ (2S+1)^{N_\ell^{\rm per}(\omega)}\,, \tag{3.9}$$
where $N_\ell^{\rm per}(\omega)$ is the number of loops into which the set of lines decomposes with the time-periodic boundary condition under which $t = \pm\beta/2$ are identified.

With this adjustment in the assignment of loops to rung configurations, the state's representation in terms of the loop system with the probability distribution (3.5) remains valid also in the presence of periodicity of either the temporal or spacial direction. This point should be borne in mind in the discussion which follows. In the pseudo spin representation, which is described next, a distinction will appear between the weights of winding versus contractable loops.

From (3.9) and (3.2) we also obtain the inequality
$$\frac{\langle D_L|e^{-\beta H_{\rm AF}^{(L)}}|D_L\rangle}{\operatorname{tr} e^{-\beta H_{\rm AF}^{(L)}}} = \frac{\int \sqrt{Q}^{N_\ell(\omega)} \rho_{\Lambda_{L,\beta}}(d\omega)}{\int \sqrt{Q}^{N_\ell^{\rm per}(\omega)} \rho_{\Lambda_{L,\beta}}(d\omega)} \geq \frac{1}{\sqrt{Q}^L}\,. \tag{3.10}$$

Indeed, for fixed rung configuration ω, the loops in the denominator are constructed on the time-periodic version of $\Lambda_{L,\beta}$ and the loops in the numerator arise in the capped version of $\Lambda_{L,\beta}$. Since the addition of a rung changes the number of loops by ± 1 (depending on whether the two points were already connected by a loop or not), we have $|N_\ell(\omega) - N_\ell^{\text{per}}(\omega)| \leq L$ and hence the lower bound in (3.10) follows.

4 The loop representation of the anisotropic XXZ-model

4.1 A modified 4-edge presentation of the XXZ interaction

We shall now show that the loop measure which appeared quite naturally in the representation of the ground states of $H_{\text{AF}}^{(L)}$ plays a similar role also for the $H_{\text{XXZ}}^{(L)}$ spin system. Preparing for that, we rewrite the Hamiltonian of the XXZ chain in terms of the slightly modified local interactions consisting of the two-spin operators $K_{v,v+1}$ whose non-vanishing matrix-elements in the joint eigenbasis $|\pm,\pm\rangle$ of (τ_v^z, τ_{v+1}^z) are

$$\begin{aligned} &\langle +,-|K_{v,v+1}|-,+\rangle = \langle -,+|K_{v,v+1}|+,-\rangle = 1, \\ &\langle +,-|K_{v,v+1}|+,-\rangle = e^{-\lambda}, \quad \langle -,+|K_{v,v+1}|-,+\rangle = e^{\lambda}\,. \end{aligned} \tag{4.1}$$

The action of $K_{v,v+1}$ is depicted in Fig. 3 in terms of the the four edge configurations with the weights:

$$W_a = 1\,, \quad W_b = 1\,, \quad W_c = e^{-\lambda}\,, \quad W_d = e^{\lambda}\,. \tag{4.2}$$

In this representation of $H_{\text{XXZ}}^{(L)}$, the local interaction terms are no longer invariant under spacial reflection, but their sum differs from the more symmetric expression (1.12) only in a boundary term – in fact the one which was included in (1.15) due to this correspondence. Furthermore, this boundary term does not appear in the operators' periodic version

$$H_{\text{XXZ}}^{(L,\text{per})} := -\frac{1}{2} \sum_{v=-L+1}^{L} \left[\left(\tau_v^x \tau_{v+1}^x + \tau_v^y \tau_{v+1}^y \right) + \cosh(\lambda) \left(1 - \tau_v^z \tau_{v+1}^z \right) \right] , \tag{4.3}$$

where the sum extends also to the edge connecting L and $-L+1 \equiv L+1$. Following is the exact statement.

Lemma 4.1. *For any $L \in \mathbb{N}$ and $\lambda \in \mathbb{R}$:*

$$H_{XXZ}^{(L)} + \sinh(\lambda)\ \frac{\tau_{-L+1}^z - \tau_L^z}{2} \ = \ - \sum_{v=-L+1}^{L-1} K_{v,v+1} \quad (\ := K^{(L)}\ ) \tag{4.4}$$

Furthermore, taken with the periodic boundary conditions the two operators agree without the boundary term:

$$H_{XXZ}^{(L,per)} \ = \ - \sum_{v=-L+1}^{L-1} K_{v,v+1} - K_{L,-L+1} \quad (\ := K^{(L,per)}\ )\,. \tag{4.5}$$

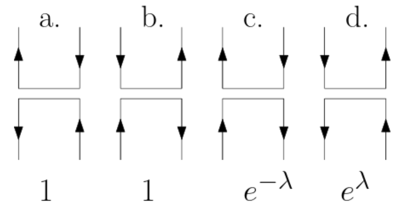

Figure 3: The matrix elements of the two-spin operators $K_{v,v+1}$, and their weights. These weights can be reinterpreted in terms of weights $e^{\lambda/4}$ for each left U-turn and $e^{-\lambda/4}$ for each right U-turn of the τ-oriented loop lines.

Proof of Lemma 4.1. The action of the sum of the first two edges (a. and b.) agrees with that of $\left[\tau_v^x\tau_{v+1}^x + \tau_v^y\tau_{v+1}^y\right]/2$, which represent the local x- and y-terms in (1.12). The local z-terms in (1.12) and (4.3) agree with the action of the last two edges (c. and d.) in Fig. 3. However, their weight in (1.12) and (4.3) is $\cosh(\lambda)$ for both edges c. and d.. The fact that the summation of these edges over all edges in the non-periodic box Λ_L yields the same result up to a boundary term is checked by noting that for a given spin configuration $\boldsymbol{\tau}$ the difference between these two cases can be expressed in terms of the number of up- and down-turns, $n_\uparrow^{(L)}(\boldsymbol{\tau})$, $n_\downarrow^{(L)}(\boldsymbol{\tau})$, over the edges of Λ_L:

$$\begin{aligned} K^{(L)} + H_{\mathrm{XXZ}}^{(L)} &= e^{\lambda} n_\uparrow^{(L)}(\boldsymbol{\tau}) + e^{-\lambda} n_\downarrow^{(L)}(\boldsymbol{\tau}) + \sum_{v=-L+1}^{L-1} \cosh(\lambda) \frac{\tau_v^z\tau_{v+1}^z - 1}{2} \\ &= e^{\lambda} n_\uparrow^{(L)}(\boldsymbol{\tau}) + e^{-\lambda} n_\downarrow^{(L)}(\boldsymbol{\tau}) - \cosh(\lambda)\big(n_\uparrow^{(L)}(\boldsymbol{\tau}) + n_\downarrow^{(L)}(\boldsymbol{\tau})\big) \\ &= \sinh(\lambda)\big(n_\uparrow^{(L)}(\boldsymbol{\tau}) - n_\downarrow^{(L)}(\boldsymbol{\tau})\big) . \end{aligned} \tag{4.6}$$

The proof of (4.4) is completed by noting that $n_\uparrow^{(L)}(\boldsymbol{\tau}) - n_\downarrow^{(L)}(\boldsymbol{\tau}) = (\tau_L^z - \tau_{-L+1}^z)/2$. In the periodic case, this boundary term drops out. □

4.2 A link between the $H_{\mathbf{XXZ}}$ and $H_{\mathbf{AF}}$ loop measures

Applying the general procedure to the operator $e^{-\beta H_{\mathrm{XXZ}}^{(L,+)}/2}$ written as $e^{\beta K^{(L)}/2}$ we obtain a representation of states in terms a functional integral over configurations $\vec{\omega} = (\omega, \tau)$ with binary-valued functions

$$\tau : \Lambda_{L,\beta} \to \{-1, 1\}$$

whose values may change only at the rungs of ω, consistently with the edges depicted in Fig. 3. The local condition implies that the allowed functions τ are consistent with the loop structure of ω: Along each loop of ω the function τ is aligned with either its clockwise of counterclockwise orientation. We denote by $\mathbb{1}[\omega, \tau]$ the indicator function expressing this consistency condition.

Theorem 4.2. *For $\lambda \geq 0$, any L even and β, the expectation value of any function of τ^z in the state defined in* (1.23) *is given by*

$$\langle f(\tau^z)\rangle_{L,\beta,\pm\lambda}^{(XXZ,\pm)} = \int \mathbb{E}_\pm\left(f|\omega\right)\mu_{L,\beta}(d\omega) \tag{4.7}$$

with $\mu_{L,\beta}$ the measure defined in (3.5) *at*

$$\sqrt{Q} = e^{\lambda} + e^{-\lambda} \tag{4.8}$$

and the normalized expectation value

$$\mathbb{E}_{\pm}\left(f|\omega\right) = \frac{1}{\sqrt{Q}^{N_\ell(\omega)}} \sum_{\tau} \mathbb{1}[\omega,\tau]\ W_{\pm}(\omega,\tau)\ f(\tau(\cdot,0)) \tag{4.9}$$

with the weights

$$W_{\pm}(\omega,\tau) := \Big(\prod_{+\ell} e^{\pm\lambda}\Big)\Big(\prod_{-\ell} e^{\mp\lambda}\Big), \tag{4.10}$$

where the product is over $(+)$ *and* $(-)$ *oriented loops* ℓ *of* (ω,τ)*.*

Proof. We spell the proof in the case $+$. Proceeding as described in Section 2, we get

$$\frac{\langle N_+^{(L)}|e^{-\beta H_{XXZ}^{(L,+)}/2}\, f(\tau^z)\, e^{-\beta H_{XXZ}^{(L,+)}/2}|N_+^{(L)}\rangle}{\langle N_+^{(L)}|e^{-\beta H_{XXZ}^{(L,+)}}|N_+^{(L)}\rangle} = \frac{\int\sum_\tau \mathbb{1}[\omega,\tau]\widetilde{W}_+(\omega,\tau)f(\tau(\cdot,0))\rho_{\Lambda_{L,\beta}}(d\omega)}{\int\sum_\tau \mathbb{1}[\omega,\tau]\widetilde{W}_+(\omega,\tau)\rho_{\Lambda_{L,\beta}}(d\omega)} \tag{4.11}$$

with weights given by the product over all rungs of ω in terms the four types $\#(\tau,b)\in\{a.,b.,c.,d.\}$ listed in (4.2) (cf. Fig. 3):

$$\widetilde{W}_+(\omega,\tau) \quad = \quad \prod_{b\in\omega} W_{\#(\tau,b)}. \tag{4.12}$$

Lumping the factors by the loops of ω, for each loop which does not reach the upper and lower boundary of the box $\Lambda_{L,\beta}$, one gets the total of $e^{+\lambda}$ per counter-clockwise $(+)$ and $e^{-\lambda}$ per clockwise $(-)$ oriented loop. In that case $\widetilde{W}_+(\omega,\tau)$ reduces to the above defined $W_+(\omega,\tau)$. Furthermore, with our choice of the seed vector $|N_+^{(L)}\rangle$ that is also true of the loops which are reflected from the upper and/or the lower boundary.

Summing over the $2^{N_\ell(\omega)}$ possible loop orientations one gets, for each ω

$$\sum_\tau \mathbb{1}[\omega,\tau]\ W_{\pm}(\omega,\tau) = (e^{\lambda}+e^{-\lambda})^{N_\ell(\omega)} = \sqrt{Q}^{N_\ell(\omega)}. \tag{4.13}$$

Thus, the average in (4.11) is over (ω,τ) with the joint distribution whose marginal distribution of ω is the normalized probability measure

$$\frac{1}{\text{Norm.}}(e^{\lambda}+e^{-\lambda})^{N_\ell(\omega)}\rho_{\Lambda_{L,\beta}}(d\omega) = \mu_{L,\beta}(d\omega)\,, \tag{4.14}$$

with the conditional distribution of τ conditioned on ω stated in (4.9). $\square$

It may be instructive to pause here and compare the different perspectives on the above loop measure. Starting from the analysis of the two different quantum spin chains we arrive at a common system of random rung configurations ω, whose probability distribution in both models takes the form

$$\mu_{L,\beta}(d\omega) = \sqrt{Q}^{N_\ell(\omega)}\rho_{\Lambda_{L,\beta}}(d\omega)/\text{Norm.} \quad \text{at} \quad 2S+1 \;=\; \sqrt{Q} \;=\; e^{\lambda}+e^{-\lambda} \tag{4.15}$$

with $\rho_{\Lambda_{L,\beta}}(d\omega)$ a Poisson measure of intensity one. The factor $\sqrt{Q}^{N_\ell(\omega)}$, by which the measure is tilted, appears through the summation over another degree of freedom, at which point the models differ. More explicitly, in the different systems this common factor is variably decomposed as

$$\begin{aligned}
\sqrt{Q}^{N_\ell(\omega)} &= \sum_\sigma \mathbb{1}[\omega,\sigma] && (H_{\mathrm{AF}}) \\
&= \sum_\tau \mathbb{1}[\omega,\tau] \quad \prod_{b\in\omega} W_{\#(\tau,b)} && (H_{\mathrm{XXZ}})
\end{aligned} \tag{4.16}$$

where the summations are over functions

$$\begin{aligned}
\sigma : \Lambda_L &\mapsto \{-S, -S+1, \ldots, S\} \quad (\text{with } (2S+1) = \sqrt{Q}), \\
\tau : \Lambda_L &\mapsto \{-1, +1\} \quad\quad\quad\quad (\text{with } e^{\lambda} + e^{-\lambda} = \sqrt{Q}) \ .
\end{aligned} \tag{4.17}$$

The indicator functions impose the consistency condition requiring σ or τ to be consistent with the loop structure of ω, i.e. a switch of signs at each U-turn and otherwise be constant along each vertical segment.

Thus, the above system of the random *oriented loop* described by $\vec{\omega} = (\omega, \tau)$ can be presented in two equivalent forms:

1. Locally: as a 4-edge model of random oriented lines with the weights listed in Fig. 3.

2. Globally: by the following two characteristics of its probability distribution $\widehat{\mu}_{L,\beta,\lambda}$:

   i) ω has the probability distribution $\mu_{L,\beta}$ which is tilted relative to the Poisson process $\rho_{\Lambda_{L,\beta}}(d\omega)$ by the factor $\sqrt{Q}^{N_\ell(\omega)}$

   ii) conditioned on ω, the conditional distribution of τ corresponds to independent assignments of orientation to the loops of ω, at probabilities $e^{\pm\lambda}/[e^{\lambda} + e^{-\lambda}]$ depending on whether the loop is anticlockwise (+) or cklockwise (−) oriented.

   To emphasise the fact that the measure $\widehat{\mu}_{L,\beta,\lambda}$ changes under a change of the sign of $\lambda \in \mathbb{R}$, we keep track of it in the notation.

The above local to global relation is reminiscent of the Baxter-Kelland-Wu [12] correspondence between the Q-state Potts model and the 6-vertex model, which followed the analysis of Temperley and Lieb [32].

In the context of the XXZ-operator, the loop picture carries a particularly simple implication for sites at the boundary of Λ_L, where the relation of $\tau(u,t)$ to loop's helicity is unambiguous. One gets, for the finite volume ground states:

$$\langle \tau(u,0)\rangle_{L,\beta} = \begin{cases} -\tanh(\lambda) & u = -L+1, \\ +\tanh(\lambda) & u = L, \end{cases} \tag{4.18}$$

regardless of the value of L and $\beta > 0$.

4.3 The XXZ-Hamiltonian with the periodic boundary conditions

The measure on τ (when restricted to $t = 0$) of the joint distribution $\widehat{\mu}_{L,\beta,\lambda}$ on oriented loops was shown to agree with the seeded expectation value of z-spins in the XXZ-Hamiltonian with boundary term on Λ_L. This relation takes a simpler form for the XXZ-Hamiltonian with periodic boundary conditions (4.3) and its tracial state.

Define similarly the 4-edges measure $\widehat{\mu}^{\rm per}_{L,\beta,\lambda}$ on $\Lambda_{L,\beta}$, where one considers periodic boundary conditions in both space and time direction.

Theorem 4.3. *The marginal distribution of $\widehat{\mu}^{per}_{L,\beta,\lambda}$ on orientations τ coincides with the quantum expectation of the XXZ-model's tracial state, i.e. for any finite collection of space-time points (u_j, t_j) which are ordered $t_1 < t_2 < \cdots < t_N$:*

$$\frac{tr\left(e^{-(\beta-t_N)H^{(L,per)}_{XXZ}} P_{u_N}(\sigma_N) e^{-(t_N-t_{N-1})H^{(L,per)}_{XXZ}} \cdots P_{u_1}(\sigma_1)\ e^{-t_1 H^{(L,per)}_{XXZ}}\right)}{tr\left(e^{-\beta H^{(L,per)}_{XXZ}}\right)} =$$

$$= \int \prod_{j=1}^{N} 1\left[\tau(u_j,t_j) = \sigma_j\right]\ \widehat{\mu}^{per}_{L,\beta,\lambda}(d\vec{\omega})\,. \quad (4.19)$$

where $\sigma_j \in \{-1, 1\}$ are prescribed spin values and $P_u(\sigma) := 1\left[\tau^z_u = \sigma\right]$ stands for the projection operator onto states with σ as the z-component of the spin at u.

Proof. The proof proceeds by plugging the operator $K^{(L,\rm per)}$ from (4.5) into the loop representation (2.3) for each of the factors $\exp[(t_j - t_{j-1})H^{(L,\rm per)}_{\rm XXZ}]$ in the time-ordered product in the numerator. The operator $K^{(L,\rm per)}$ produces exactly the weights of the 4-edges model with spatially periodic boundary conditions. The projection operators $P_{u_j}(\sigma_j)$ inserted behind each factor $\exp[(t_j - t_{j-1})K^{(L,\rm per)}]$ fixes the spin-value to σ_j at the particular instance (u_j, t_j) in space-time. Evaluating the trace in the joint eigenbasis of τ^z_u will enforce periodic boundary conditions of the oriented loops also in the time direction. □

Since the right-side in (4.19) depends on λ only through the anisotropy parameter $\cosh(\lambda)$ entering the periodic XXZ-Hamiltonian, the distribution of the pseudo-spins is easily seen to exhibit the following symmetry, which will play a crucial role in our proof of dimerization (Theorem 1.2).

Corollary 4.4. *Under $\widehat{\mu}^{per}_{L,\beta,\lambda}$, the marginal distribution of τ is a symmetric function of λ.*

4.4 Further symmetry considerations

As a preparatory step towards the proof of Néel order, let us discuss the symmetries of the oriented loop's distribution. We start by denoting three mappings on the space of functions $\tau(u, t)$ which are defined by

$$\begin{aligned} \mathcal{S}[\tau](u,t) &= \tau(u-1,t) && \text{one-step shift} \\ F[\tau](u,t) &= -\tau(u,t) && \text{spin flip} \\ R[\tau](u,t) &= \tau(-u+1,-t) && \text{space}\times\text{time reflection w.r.t. } (1/2,0) \end{aligned} \quad (4.20)$$

and extend the last two to a similarly defined action on the un-oriented edge configuration ω.

The following is a simple but very helpful observation.

Theorem 4.5. *For each finite L, β, and λ, the above joint probability distribution of (ω, τ) is invariant under $R \circ F$. Furthermore, in any accumulation point of such measures (e.g. limit $L \to \infty$ with L of a fixed parity) which is invariant under the two-step shift ($\mathcal{S}^2$), the magnetization satisfies*

$$\langle \tau(u,0) \rangle_{(L,\beta)} = (-1)^u M \tag{4.21}$$

for some $M \in [-1, 1]$.

To avoid confusion let us stress that (4.21) does not yet establish existence of Néel order. For that, one needs to show that $M \neq 0$.

Proof. The first statement follows readily from the above i)-ii) characterization of the measure, as under reflections the distribution of ω is invariant, but the loop's orientational preference is inverted.

To prove the second statement we combine the above symmetry with the assumed two-step shift invariance. These imply

$$\tau(2,0) \ = \ [\mathcal{S}^2 \circ (R \circ F\tau)](2,0) \ = \ (R \circ F\tau)](0,0) = -\tau(1,0)\,. \tag{4.22}$$

The full oscillation (4.21) follows by another application of invariance under the double shift $\mathcal{S}^2$. □

5 The quantum loops system's critical percolation structure

5.1 An FKG-type structure

The probability distribution (3.5) is reminiscent of the loop representation of the planar Q-state random-cluster models. For details on the random-cluster model itself, we refer to the monograph [24] and the lecture notes [16] (for recent developments).

As in that case, it is relevant to recognize here the presence of a self-dual A/B-percolation model. To formulate it, we partition any rectangle $\Lambda_{L,\beta} \subset \mathbb{Z} \times \mathbb{R}$ into a union of vertical columns of width 1 over the edges of Λ_L, labelled alternatively as A and B,

$$A := \{(2n, 2n+1)\}_{n \in \mathbb{Z}}\,, \quad B := \{(2n-1, 2n)\}_{n \in \mathbb{Z}}\,, \tag{5.1}$$

with the column over $(0, 1)$ marked as A. Rungs ω are then distributed in the edge columns with respect to the probability measure $\mu_{L,\beta}$.

These rungs serve a dual role. We interpret each as a cut in the column over which it lies and at the same time a bridge linking the two domains which are touched by its endpoints. To visualize the

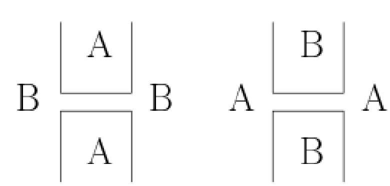

Figure 4: The rungs of ω both connect and, in the dual sense, disconnect: those placed over A strips decrease the A connectivity; those over B strips increase it, and vice versa.

A- and B-connected components, also called A- and B-*clusters*, which result from this convention it is convenient to think of each rung as having a small (infinitesimal) width and being bounded by a pair of segments, as is indicated in Fig. 4.

Thus, associated with each configuration ω is a decomposition of $\Lambda_{L,\beta}$ into A-clusters and B-clusters, with A-clusters bounded by B-clusters, and vice versa. In the topological sense this percolation model is self dual. Also, the probability distribution is symmetric, except possibly for asymmetry introduced by boundary conditions. As is explained below, this implies that the percolation model is at its phase transition point. The transition can be continuous, as is the case for independent percolation ($Q = 1$), or discontinuous as in models with Q large enough. This distinction is tied in with the existence or not of symmetry breaking in the ground states of the two quantum models discussed here.

The similarity with the random-cluster measures led [5] to introduce a partial order ($\prec$) on the space of rung configurations in which A-connection is monotone increasing and B-connection is monotone decreasing. More explicitly, labelling the rungs as of A- or B-type: $\omega_1 \prec \omega_2$ if the A-connections in ω_1 are all holding in ω_2. This notion is useful since the measures $\mu_{L,\beta}$ satisfy the Fortuin-Kasteleyn-Ginibre (FKG) lattice condition which enables powerful monotonicity arguments. The FKG structure was used in the proof of the AN-dichotomy [5] stated in Proposition 1.1. Here, we will use the following facts. First, it implies the FKG inequality stating, for every events E and F that are *increasing* (meaning that their indicator functions are increasing for $\prec$):

$$\mu_{L,\beta}[E \cap F] \geq \mu_{L,\beta}[E]\mu_{L,\beta}[F]. \tag{5.2}$$

Another implication of the FKG lattice condition is the monotonicity in so-called boundary conditions. Here, the boundary conditions are imposed by the structure of the underlying graph $\Lambda_{L,\beta}$, so we wish to draw a comparison with the random-cluster model. The construction with rungs at the top and bottom capping the loops implies that when L is odd, the complement of the box $\Lambda_{L,\beta}$ is treated as B-connected, while when L is even it is A-connected. Borrowing the language of the random-cluster model, we see that our capping procedure used in the construction of $\mu_{L,\beta}$ can be understood as enforcing B-wired or A-wired boundary conditions depending on the parity of L. To stress the type of the boundary condition and to draw an even more direct link to the standard theory of random-cluster models, in this section we write $\mu^{\#}_{L,\beta}$ instead of $\mu_{L,\beta}$, with $\# = A$ if L is even, and $\# = B$ if L is odd.

Now, consider $L \geq \ell$ with ℓ even and $\beta \geq t$. The measure $\mu^{A}_{\ell,t}$ can be seen as the measure $\mu^{\#}_{L,\beta}$ (with # equal to A or B depending on L even or odd, or equal to per if one wishes) in which we place the so-called A-*cutter*, since either the points in $\Lambda_{\ell,t}$ were already A-connected within $\Lambda_{\ell,t}$ or, in case their A-connection ran through the complement of $\Lambda_{\ell,t}$, this will still be true due to the fact that the boundary conditions render this complement into a single A-cluster. The monotonicity in boundary conditions therefore implies that for an increasing event E depending on rungs in $\Lambda_{\ell,t}$ only,

$$\mu^{\#}_{L,\beta}(E) \leq \mu^{A}_{\ell,\beta}(E)\,. \tag{5.3}$$

Likewise, if ℓ is odd and one uses a B-*cutter* to cut out a smaller box, one gets

$$\mu^{B}_{\ell,\beta}(E) \leq \mu^{\#}_{L,\beta}(E). \tag{5.4}$$

5.2 Results based on the percolation analysis

By the monotonicity in the domain, the above FKG structure implies the convergence of the extremal measures, i.e. along increasing sequences of A- or B-wired boundary conditions:

$$\begin{aligned} \mu^A &:= \lim_{\substack{L\to\infty \\ L \text{ even}}} \lim_{\beta\to\infty} \mu^A_{L,\beta} \\ \mu^B &:= \lim_{\substack{L\to\infty \\ L \text{ odd}}} \lim_{\beta\to\infty} \mu^B_{L,\beta} \,, \end{aligned} \tag{5.5}$$

in the weak sense of convergence of probability measures on the configuration spaces of rungs on $\mathbb{Z} \times \mathbb{R}$.

To present the full resolution of the question posed by the dichotomy, we start with the following preparatory statements.

Theorem 5.1. *Let $Q = (e^\lambda + e^{-\lambda})^2 \geq 1$. Regardless of whether the loop measures μ^A, μ^B coincide:*

1. *each measure is supported on configurations with only closed loops, i.e. there is no infinite boundary line,*
2. *the convergence extends to that of the joint distribution of (ω, τ), i.e. of the ordered loop lines,*
3. *for the limiting measures the conditional distribution of τ, conditioned on ω, is given by the same rule as in finite volume: at given ω the loops are oriented independently of each other with probabilities $e^{\pm\lambda}/[e^\lambda + e^{-\lambda}]$, with $(-)$ for clockwise and $(+)$ for counter-clockwise orientation.*

In case the measures coincide ($\mu^A = \mu^B$), then

4. *the limiting state is supported on configurations in which there is no infinite A-clusters or B-clusters, and instead each point is surrounded by an infinite family of nested loops,*
5. *the loop measures with the periodic boundary conditions in both temporal and spacial direction $\mu^{per}_{L,\beta}$ converge to the shared limit as $L, \beta \to \infty$.*

The proof of this theorem will follow standard arguments in percolation theory that must still be adapted to the current context.

5.3 Proofs

We begin with three statements that will play important roles. The first one deals with ergodic properties of μ^A and μ^B. Let $\mathcal{S}_x$ be a translation by $x \in \mathbb{Z} \times \mathbb{R}$. This translation induces a shift $\mathcal{S}_x\omega$ and $\mathcal{S}_x E$ of a configuration and an event. Furthermore, an event E is *invariant under translations* if for any $x \in \mathbb{Z} \times \mathbb{R}$, $\mathcal{S}_x E = E$. A measure μ is *invariant under translations* if $\mu[\mathcal{S}_x E] = \mu[E]$ for any event E and any $x \in \mathbb{Z} \times \mathbb{R}$. The measure is *ergodic* if any event invariant under translation has probability 0 or 1.

Lemma 5.2. *The measures μ^A and μ^B are invariant under spacial translations by $2\mathbb{Z}$ and any time-translation. They are ergodic separately with respect to each of these sub-groups.*

Proof. We will treat the case of μ^A only, as the case of μ^B is similar. By inclusion-exclusion, it is sufficient to consider an increasing event E depending on rungs in $\Lambda_{\ell,t}$. Let $L, k, \ell \in 2\mathbb{N}$ with $L \geq \ell + k$ and $\beta \geq t + s$. The comparison between boundary conditions implies that for $x = (k, s)$,

$$\mu^A_{L+k,\beta+s}[E] \leq \mu^A_{L,\beta}[\mathcal{S}_x E] \leq \mu^A_{L-k,\beta-s}[E].$$

Letting L, β tend to infinity implies the invariance under translations.

Any event can be approximated by events depending on rungs in $\Lambda_{\ell,t}$ for some ℓ, t, hence the ergodicity follows from mixing, i.e. from the property that for any events E and F depending on finite sets,

$$\lim_{\substack{|x|\to\infty \\ x=(k,s),\, k \text{ even}}} \mu^A[E \cap \mathcal{S}_x F] = \mu^A[E]\mu^A[F]. \tag{5.6}$$

Observe that again by inclusion-exclusion, it is sufficient to prove the equivalent result for E and F increasing. Let us give ourselves these two increasing events E and F depending on rungs in $\Lambda_{\ell,t}$ only. The FKG inequality and the invariance under translations of μ^A imply that for sufficiently large $x = (k, s)$ with k even:

$$\mu^A[E \cap \mathcal{S}_x F] \geq \mu^A[E]\mu^A[\mathcal{S}_x F] = \mu^A[E]\mu^A[F].$$

In the other direction, fix $\varepsilon > 0$ and choose $L = L(\varepsilon)$ and $\beta = \beta(\varepsilon)$ so large than $\mu^A_{L,\beta}[E] \leq \mu^A[E] + \varepsilon$ and $\mu^A_{L,\beta}[F] \leq \mu^A[F] + \varepsilon$. If $x = (k, s)$ with $2\ell < k < L - \ell$, then $\Lambda_{\ell,t}$ and its translate by x do not intersect. Thus, the FKG inequality enables to put a unique A-cluster cluster in the complement of $\Lambda_{\ell,t}$ and $\mathcal{S}_x\Lambda_{\ell,t}$ disconnecting the two areas so that

$$\mu^A[E \cap \mathcal{S}_x F] \leq \mu^A_{L,\beta}[E \cap \mathcal{S}_x F] + 2\varepsilon \leq \mu^A_{L,\beta}[E]\mu^A_{L,\beta}[F] + 2\varepsilon \leq \mu^A[E]\mu^A[F] + 5\varepsilon.$$

The result therefore follows by taking x to infinity, and then ε to 0. □

The second statement is the following important theorem.

Theorem 5.3. *For any $Q \geq 1$ and $\# \in \{A, B\}$, one of the two following properties occur:*

- $\mu^\#[(1/2, 0)$ *is A-connected to infinity*$] = 0$ *or*
- $\mu^\#[\exists$ *a unique infinite A-cluster*$] = 1$.

This result was first proved in [3] for Bernoulli percolation. It was later obtained via different types of arguments. The beautiful argument presented here is due to Burton and Keane [15]. We now adapt this argument and only sketch it as it is by now presented in various different forms (see e.g. [16]).

Proof. We present the proof for μ^A, since the proof for μ^B is the same. Let $E_{\leq 1}$, $E_{<\infty}$ and $E_{=\infty}$ be the events that there are no more than one, finitely many and infinitely many infinite A-clusters respectively. We first show that there cannot be finitely many, but strictly more than one infinite A-cluster.

Assume that $\mu^A[E_{<\infty}] > 0$. Choose L and β large enough that $\mu^A[F] \geq \frac{1}{2}\mu^A[E_{<\infty}] > 0$, where F is the event that all (there may be none) the infinite A-clusters of $(\mathbb{Z} \times \mathbb{R}) \setminus \Lambda_{L,\beta}$ intersect $\Lambda_{L,\beta}$. Since F is independent of the rungs in $\Lambda_{L,\beta}$ and that one may easily see that conditioned on F, there is a positive probability that the event G that the configuration of rungs in $\Lambda_{L,\beta}$ is such that all the boundary vertices of $\Lambda_{L,\beta}$ are A-connected in $\Lambda_{L,\beta}$, we find that

$$\mu^A[E_{\le 1}] \ge \mu^A[F \cap G] > 0.$$

By ergodicity, this means that $\mu^A[E_{\le 1}] = 1$, a fact which concludes the proof that $E_{<\infty} \setminus E_{\le 1}$ has zero probability. We now exclude the possibility of an infinite number of infinite clusters.

Assume by contradiction that $\mu^A[E_{=\infty}] > 0$. Consider $\Lambda = \Lambda_{L_0,\beta_0}$ so that

$$\mu^A[K \text{ infinite } A\text{-clusters of } \mathbb{Z} \times \mathbb{R} \setminus S \text{ intersect } S] \ge \tfrac{1}{2}\mu^A[E_{=\infty}] > 0, \tag{5.7}$$

where $K = K(d)$ is large enough that three vertices x, y, z of $\partial\Lambda$ at a Euclidean distance at least three of each other that are A-connected to infinity in the complement of Λ. Using a configuration in this event, with positive conditional probability, one may force that the configuration in Λ is such that the event T_0 that $B_0 := \{0\} \times (0, 1]$ intersects an A-cluster $\mathcal{C}$ such that $\mathcal{C} \setminus B_0$ contains at least three distinct infinite A-clusters, is occurring. We deduce that

$$\mu^A[T_0] > 0. \tag{5.8}$$

It is also classical (see the version of Burton-Keane for random-cluster models on $\mathbb{Z}^d$) that the number of $x \in \mathbb{Z}^2$ such that $\mathcal{S}_x T_0$ is occurring is bounded by the number of A-clusters intersecting $\partial\Lambda_{L,\beta}$, whose expectation is itself bounded by $C(\beta+L)\mu^A[\mathsf{N}_0]$, where N_0 is the number of A-clusters intersecting B_0. This gives

$$\mu^A[T_0] \le \mu^A[\mathsf{N}_0]\frac{C(\beta + L)}{\beta L}.$$

Using the FKG inequality, it is quite elementary to show that $\mu^A[\mathsf{N}_0] < \infty$, and therefore letting L and β tend to infinity at the same speed implies that $\mu^A[T_0] = 0$, which contradicts (5.8), and therefore the assumption $\mu^A[E_{=\infty}] > 0$. This concludes the proof. □

We finish by a third lemma.

Lemma 5.4. *All B-clusters are finite μ^A-almost surely.*

By duality, μ^B-almost surely all the A-clusters are finite almost surely.

Proof. Assume by contradiction that $\mu^A[\exists \text{ infinite } B\text{-cluster}] = 1$ and fix L, β so that

$$\mu^A[\Lambda_{L,\beta} \text{ is } B\text{-connected to infinity}] \ge 1 - \tfrac{1}{10^4} \tag{5.9}$$

and the probability that the top, bottom, left and right of the boundary of $\Lambda_{L,\beta}$ are B-connected to infinity in the complement of $\Lambda_{L,\beta}$ are the same (simply fix L_0, β_0 large enough to get (5.9), and then increase L_0 and/or β_0 in order to obtain L, β).

Since a path from infinity to $\Lambda_{L,\beta}$ ends up either on the top, bottom, left or right of it, the FKG inequality implies (through the square-root trick) that

$$\mu^A[\text{top of } \Lambda_{L,\beta} \ B\text{-connected to infinity outside } \Lambda_{L,\beta}] \ge 1 - \tfrac{1}{10^{4/4}} = 1 - \tfrac{1}{10},$$

and similarly for the right, bottom and top. Now, assume that the top and bottom are B-connected to infinity, and the left and right (more precisely the A-lines on the left and right of the respective boundaries) are A-connected to infinity (the probability of the latter is larger than the probability that there exists a B-connection since under μ^A the A-clusters dominate the B-ones[4]). The union bound implies that this happens with probability $1-\frac{4}{10}>0$. Yet, the finite-energy property also implies that conditionally on this event, the rungs in $\Lambda_{L,\beta}$ are such that no boundary vertex of $\Lambda_{L,\beta}$ are A-connected using paths in $\Lambda_{L,\beta}$, implying that there exist two infinite A-clusters with positive μ^A-probability. But this contradicts the fact, proved in the previous statement, that there is zero or one infinite A-cluster. □

We are now in a position to prove the main theorem of this section.

Proof of Theorem 5.3. Property 1 is a direct consequence of the fact that μ^A does not possess any infinite B-cluster. It also means that when fixing a finite set, and taking L and β large enough, no loop intersecting the finite set reaches the boundary of $\Lambda_{L,\beta}$ or winds around the vertical direction. By construction, we deduce that all these loops are oriented in an independent fashion described in the previous section. As a consequence, Properties 2 and 3 follow trivially. Property 4 is a direct consequence of $\mu^A=\mu^B$, so that the distribution of the A- and B-clusters is the same under μ^A. In particular, there is no infinite A- or B-cluster, which immediately implies Property 4. Finally, if the two measures are equal, $\mu^{\mathrm{per}}_{L,\beta}$ stochastically dominates $\mu^B_{L,\beta}$ and is stochastically dominated by $\mu^A_{L,\beta}$. Since these measures converge to the same measure $\mu^A=\mu^B$, so does $\mu^{\mathrm{per}}_{L,\beta}$. □

6 Proofs of symmetry breaking

We now have the tools for a structural proof of the different forms of symmetry breaking in the models considered here. We start with the translation symmetry breaking in the limiting distribution of the random loop measure for all $Q>4$. This is then used to conclude dimerization in the ground states of the H_{AF} spin chains with $S>1/2$, and Néel order in the ground states of spin 1/2 XXZ-chain at $\Delta>1$. These results can be obtained through the rigorous analysis of the Bethe ansatz along the lines of Duminil et.al. [19], which yields also more quantitative information. However, for a shorter and somewhat more transparent proof we present an analog of the argument which was recently developed by Ray and Spinka [30] in the context of the 6-vertex/Q-state random-cluster model on $\mathbb{Z}^2$.

6.1 Translation symmetry breaking for the loop measure at $Q>4$

As in [23, 30] we shall make an essential use of a random height function $h:(\mathbb{R}\setminus\mathbb{Z})\times\mathbb{R}\to\mathbb{Z}$, which in our case is assigned the configurations of $\vec{\omega}=(\omega,\tau)$. The function is piecewise constant with discontinuities at lines supporting the loops of ω. Along the horizontal line $t=0$ it is defined by:

$$h_{\vec{\omega}}(-1/2,0):=0,\qquad h_{\vec{\omega}}(u,0):=\begin{cases}\displaystyle\sum_{n\in(-1/2,u)\cap\mathbb{Z}}\tau(n,0) & \text{if } u\geq 0,\\ \displaystyle\sum_{n\in(u,-1/2)\cap\mathbb{Z}}-\tau(n,0) & \text{if } u<-1\,.\end{cases}\tag{6.1}$$

More generally, the value of $h_{\vec{\omega}}(u,t)$ at any point off the grid of loop lines of ω is the sum of the flux of τ across an arbitrary simple path from $(1/2,0)$ to (u,t), counted with the sign of the-cross

[4]By symmetry the B-clusters under μ^A are distributed as the A-clusters under μ^B, which by FKG is dominated by μ^A.

product of the direction of τ with the curve's tangent at the point of crossing. When the crossing occurs at vertical rungs of ω the height function increases by 0 or ± 2, depending on the nature of the rung and the direction of crossing. Thus, along any generic smooth curve the function increases by ± 1 upon crossing a loop, depending on the direction of crossing.

An essential property of the height function is that for any (ω, τ) the values of $h_{\vec{\omega}}(u,t)$ at generic points can be read from just the pseudo spin function τ. It will be used in the proof of the following auxilliary statement.

Lemma 6.1. *For any $Q > 4$, let $\widehat{\mu}$ be a probability measure on the systems of oriented loops over $\mathbb{Z} \times \mathbb{R}$, described by the variables $\vec{\omega} = (\omega, \tau)$, with the properties:*

1. *$\widehat{\mu}$ almost surely the loop configurations corresponding to ω consist of only finite loops.*
2. *conditioned on ω the loops are oriented independently of each other clockwise $(-)$ or counter-clockwise $(+)$, with the probabilities $e^{\pm\lambda}/[e^{-\lambda} + e^{+\lambda}]$, correspondingly,*
3. *the marginal distribution of the τ variables is invariant under a global reversal of orientation $(\lambda \mapsto -\lambda)$.*

Then the event

$$\mathcal{N} := \{\ (1/2, 0) \text{ is encircled by an infinite number of loops of } \omega\} \tag{6.2}$$

has zero measure.

Proof. The proof is by contradiction. Let $\alpha_k = (u_k, t_k)$ be a sequence of points with $|\alpha_k| \nearrow \infty$ each of which lies on a level set of $h_{\vec{\omega}}$ which includes a path winding around $(-1/2, 0)$. The values of $h(\alpha_k)$ are given by the sum of loop orientations over those loops of ω which separate α_k from $(-1/2, 0)$. For $Q > 4$, these orientations are given by a sequence of iid ± 1 valued random variables, of the non-zero mean $\tanh(\lambda)$. It readily follows that almost surely the following limit exist and satisfies

$$\lim_{k\to\infty} h_{\vec{\omega}}(\alpha_k) = \begin{cases} \operatorname{sign}(\lambda)\,\infty & (\omega,\tau) \in \mathcal{N} \\ \text{a finite value} & (\omega,\tau) \notin \mathcal{N} \end{cases} . \tag{6.3}$$

From this one may deduce that the probability distribution of $\lim_{k\to\infty} h(\alpha_k)$ is:

$$\lim_{k\to\infty} h_{\vec{\omega}}(\alpha_k) = \begin{cases} \operatorname{sign}(\lambda)\,\infty & \text{with probability } \widehat{\mu}(\mathcal{N}) \\ \text{a finite value} & \text{with probability } [1 - \widehat{\mu}(\mathcal{N})] \end{cases} . \tag{6.4}$$

The level sets of $h_{\vec{\omega}}$ can be determined from just τ (i.e. ignoring ω) and, under the assumption made here its distribution does not change under the flip $\lambda \to -\lambda$. Hence (6.4) yields a contradiction unless $\widehat{\mu}(\mathcal{N}) = 0$. □

From this we shall now deduce three symmetry breaking statements. The first concerned just the loop measure, but in the statement's proof we make use of the measure's significance for the two quantum spin models.

Theorem 6.2. *For all $Q > 4$ (equivalently $S > 1/2$): the loop measures corresponding to the even and odd ground-states $\langle\cdot\rangle_{even}$ and $\langle\cdot\rangle_{odd}$ of (1.5) differ.*

Proof. Assume the two loop measures coincide. Then by Theorem 5.1 (4) the event $\mathcal{N}$ occurs with probability 1 with respect to the common probability measure.

However, by Theorem 5.1 (5), under the above assumption these measures describe also the limiting distribution of ω corresponding to the ground state of the periodic operator $H_{XXZ}^{(L,per)}$ in the limit $L \to \infty$, which for concreteness' sake we take to be along $2\mathbb{Z}$ and with λ being the positive solution of (4.8). However, as was noted in Corollary 4.4 the periodic boundary condition state is actually an even function of λ. It follows that the limiting state satisfied all the assumption made in Lemma 6.1, and hence the event $\mathcal{N}$ is of probability zero.

The contradiction between the two implications of the above assumption implies that the measures are distinct. □

6.2 Dimerization for $S > 1/2$

Next, we extract from the above probabilistic statement a proof of dimerization in the quantum H_{AF} spin chain.

Proof of Theorem 1.2. 1. From Theorem 6.2 we already know that for any $S > 1/2$ the loop measures associated with the states $\mu^A \equiv \langle\cdot\rangle_{even}$ and $\mu^B \equiv \langle\cdot\rangle_{odd}$ are different. Theorem 5.3 allows to identify the difference in percolation terms: in both cases there is almost surely a unique infinite connected cluster, which is of type A in one and B in the other. More explicitly,

$$\mu^A\left[(u+1/2,0) \leftrightarrow \infty\right] = \mu^B\left[(u-1/2,0) \leftrightarrow \infty\right] = \begin{cases} 0 & \text{for } u \text{ odd} \\ p_\infty > 0 & \text{for } u \text{ even} \end{cases} . \tag{6.5}$$

However, that leaves still the challenge to determine whether this difference between the two measures and, in each, between the even and odd sites, can be detected in terms of a physical observable, i.e. the expectation value of some function of the spin degrees of freedom.

The question was addressed in [5] where it is shown (see also the next section for a similar reasoning) that:

i) since the two limiting distributions of ω are related by the FKG inequality, if they differ then the difference is manifested also in the more elementary connectivity probability to lie on the same loop, and in particular for even sites $u = 2n$:

$$\mu^A\left[(2n,0)\leftrightarrow(2n+1,0)\right]\right] \;>\; \mu^A\left[(2n-1,0)\leftrightarrow(2n,0)\right]\right]. \tag{6.6}$$

ii) combining (6.6) with (3.7) one learns that

$$\langle P^{(0)}_{2n,2n+1}\rangle_{even} \;>\; \langle P^{(0)}_{2n-1,2n}\rangle_{even} \tag{6.7}$$

with the opposite inequality for the odd state. Thus the differences in the two states are detectable and extensive.

2. Theorem 7.2 of [5] bounds the truncated quantum correlations from above in terms of the correlations

$$\min_{\#\in\{A,B\}} \mu^{\#}[(\boldsymbol{u},t) \text{ and } (\boldsymbol{v},0) \text{ belong to the same cluster}] \tag{6.8}$$

of the underlying loop measures for every $\boldsymbol{u} \in U \pm 1/2$ and $\boldsymbol{v} \in V \pm 1/2$. Now, the percolation model considered in Section 1.3 of [17] corresponds exactly to our model here.[5] The fifth bullet of Theorem. 1.5 of [17] thus implies, with the notation of our paper, that there exists $c = c(q) > 0$ such that for every $n \geq 1$,

$$\mu^B[(\tfrac{1}{2}, 0) \text{ belongs to a } A\text{-cluster reaching } \partial\Lambda_{n,n}] \leq \exp[-cn]. \tag{6.9}$$

Since for $\boldsymbol{u} \in U \pm 1/2$ and $\boldsymbol{v} \in V \pm 1/2$ to be connected to each other, there must exist a path from $\boldsymbol{u}$ to the translate of $\partial\Lambda_{n,n}$ by $\boldsymbol{u}$, where $n = \max\{|t|, |\boldsymbol{u} - \boldsymbol{v}| - 1\}$, we deduce that all the quantities in (6.8) are smaller than $C\exp[-(\text{dist}(U,V) + |t|)/\xi]$ for some small enough constant $\xi = \xi(q) > 0$. □

6.3 Néel order for $\Delta = \cosh(\lambda) > 1$

Turning to the ground states of the XXZ-spin system, let us recall the notation. Let $\lambda > 0$ be the positive solution of (1.13), and denote by $\widehat{\mu}^A_{+\lambda}$ the even limit (cf. (5.5)) of the measure on the enhanced system of the variables (ω, τ), in which the winding probabilities of loops of ω are $e^{\pm\lambda}/(e^{\lambda} + e^{-\lambda})$, with $(+)$ winding corresponding to the counterclockwise and $(-)$ the clockwise orientation. The corresponding state on (just) the spin variables, is denoted $\langle \tau(u, 0) \rangle_+$. These are to be contrasted with $\widehat{\mu}^A_-$ and $\langle \tau(u, 0) \rangle_-$. The superscript may be omitted, but it should be remembered that in both $+$ and $-$ cases, the limit $L \to \infty$ is taken over the even sequence.

Proof of Theorem 1.4. As we saw, the probability distribution of ω under the two measures $\widehat{\mu}^A_{\pm\lambda}$ agree with that of the corresponding H_{AF} system. Hence, in both cases there is positive probability $p_\infty > 0$ that $(1/2, 0)$ belongs to an infinite connected cluster. When that happens, the sign of $\tau(0, 0)$ coincides with the winding sign of the loop which passes through $(0, 0)$. Thus the spin $\tau(0, 0)$ takes the values $\pm$ with probabilities $e^{\pm\lambda}/(e^{\lambda} + e^{-\lambda})$. The same holds true for any even site $u = 2n$. Consequently, for any $n \in \mathbb{Z}$:

$$\begin{aligned}\int \tau(2n, 0) \cdot \mathbb{1}[(2n + 1/2, 0) \leftrightarrow \infty]\, \widehat{\mu}^A_+(d\vec{\omega}) &= \tanh(\lambda)\, p_\infty \\ &= -\int \tau(2n, 0) \cdot \mathbb{1}[(2n + 1/2, 0) \leftrightarrow \infty]\, \widehat{\mu}^A_-(d\vec{\omega})\,. \end{aligned} \tag{6.10}$$

Since $p_\infty > 0$, we deduce that $\widehat{\mu}^A_+$ and $\widehat{\mu}^A_-$ are different.

To that let us add the observation that percolation with respect to ω corresponds to percolation along a level set of the height function which is readable from τ. Hence the observable which distinguishes the two states is in principle a functional of the physically meaningful spin function. We conclude that also the states $\langle \cdot \rangle_+$ and $\langle \cdot \rangle_-$ are different, and hence the infinite XXZ-spin system has at least two different ground states.

A remaining challenge is to simplify the distinction between the two states, as was done in step (ii) of the above proof of Theorem 1.2. For the XXZ-model that can be deduced using the last statement in Proposition 1.3. It allows to conclude from (6.10) (and the previously established fact that $p_\infty > 0$) that for any $u \in \mathbb{Z}$

$$\langle \tau(u, 0) \rangle_+ \neq \langle \tau(u, 0) \rangle_- \,. \tag{6.11}$$

[5] One may be surprised by the fact that the Poisson point process there has intensity 1 and q depending on the column. This comes from the fact that the Radon-Nikodym derivative is expressed in [17] as q to the number of A-clusters, which can be shown, using Euler's formula, to be expressed in terms of $\sqrt{q}$ to the number of loops if one changes the intensity of the Poisson point process to 1 in every column.

This also implies the non-vanishing of the Néel order parameter M of (4.21). $\square$

In the last step, leading to (6.11), we invoked an "FKG boost" whose full discussion was postponed in order to streamline the presentation of the main results. Following is its proof.

Proof of Proposition 1.3 . The convergence of each of the two finite-volume ground states in the limit $L \to \infty$, with L limited to even values, is based on the FKG monotonicity of the percolation model discussed in the previous section, which is common to the two systems discussed here.

It remains to establish that for the XXZ system at any $\Delta \geq 1$, the states $\langle \cdot \rangle_+$ and $\langle \cdot \rangle_-$ are either equal or of different magnetization, satisfying (6.11). In the proof we shall again employ the FKG inequality but do so in a different setup than used above. This time it will be in the context of an Ising-like representation of the distribution of the staggered spins

$$\kappa(u,t) \;=\; (-1)^u \tau(u,t)\,. \tag{6.12}$$

In terms of these variables the ground states of XXZ-system take the form of an annealed Gibbs equilibrium state of a ferromagnetic Ising model, and the two boundary conditions correspond to $(+)$ and correspondingly $(-)$ fields applied along the "vertical" part of the boundary.

To present the ground states in this form we start with the following preparatory steps:

1) Rewrite the XXZ Hamiltonian of (1.14), with the boundary term of (1.15), as the spin-1/2 version of the H_{AF} operator with an added anti-ferromagnetic coupling of strength $\delta = \Delta - 1$. I.e., for any even L:

$$U_L H^{(L,\pm)}_{\mathrm{XXZ}} U_L^* = \frac{1}{2} \sum_{v=-L+1}^{L-1} \left[\boldsymbol{\tau}_v \cdot \boldsymbol{\tau}_{v+1} + \pm \delta \tau^z_v \tau^z_{v+1} - \Delta \cdot \mathbb{1} \right] + \frac{\sinh(\lambda)}{2} [\tau^z_{-L+1} - \tau^z_L]\,. \tag{6.13}$$

2) For each even L and choice of the $\pm$ sign, construct the ground state of this operator, applying the hybrid representation (2.10), with the δ term treated as a potential (V) added to the $\Delta = 1$ operator, and starting from the seed state $|N_0^{(L)}\rangle$ of (1.22) with $\lambda = 0$.

We are particularly interested in operators which arise from functionals of τ, or equivalently of κ (the two being related by (6.12)). Taking the limits indicated in (1.23), we get

$$\langle F \rangle_\pm \;=\; \lim_{\substack{L\to\infty \\ L \text{ even}}} \lim_{\beta\to\infty} \langle F \rangle^{(\mathrm{XXZ},\pm)}_{L,\beta,0} \tag{6.14}$$

with the Feynman-Kac type functional integral

$$\langle F \rangle^{(\mathrm{XXZ},\pm)}_{L,\beta,0} \;=\; \frac{\int \mathbb{E}^\pm_{L,\beta}\left[F|\omega\right] \; Z^\pm_{L,\beta}(\omega)\, \rho_{L,\beta}(d\omega)}{\int Z^\pm_{L,\beta}(\omega)\, \rho_{L,\beta}(d\omega)} =: \int \mathbb{E}^\pm_{L,\beta}\left[F|\omega\right] \; \mu_{L,\beta}(d\omega) \tag{6.15}$$

with

$$\begin{aligned} Z^\pm_{L,\beta}(\omega) \;&:= \sum_\kappa \mathbb{1}[\omega,\kappa] \; \exp\Big(- \int_{-\beta/2}^{\beta/2} V_\pm(t)\, dt \Big)\,, \\ \mathbb{E}^\pm_{L,\beta}\left[F|\omega\right] \;&:= \frac{1}{Z^\pm_{L,\beta}(\omega)} \sum_\tau \mathbb{1}[\omega,\kappa] \; \exp\Big(- \int_{-\beta/2}^{\beta/2} V_\pm(t)\, dt \Big) \; F[\kappa]\,, \end{aligned} \tag{6.16}$$

where, in a slight abuse of notation, we denote by $\mathbb{1}[\omega,\kappa]$ the consistency indicator function which is inherited from $\mathbb{1}[\omega,\tau]$ through the correspondence (6.12), and the potential is

$$V_\pm(t) \ := -\sum_{u=-L+1}^{L-1} \kappa(u,t)\ \kappa(u+1,t) \mp \frac{\sinh(\lambda)}{2}\left[\kappa(-L+1,t)+\kappa(L,t)\right] . \tag{6.17}$$

It is now important to note that in terms of κ the consistency condition translated into the constraint that $\kappa(u,t)$ is constant along each of the loops of ω. Thus, for a given ω the function $\kappa(u,t)$ is fully characterized by the collection of binary variables $\{\kappa_\gamma\}$ indexed by the loops of ω. Furthermore, the potential $V_\pm(t)$ is expressible as a ferromagnetic pair interaction among the values of this collection of observables.

By the general FKG property of the ferromagnetic Ising measures, for each ω the $(+)$ and $(-)$ measures $\mathbb{E}^\pm_{L,\beta}\left[\cdot|\omega\right]$ admit a monotone coupling (this is referred to as Strassen's theorem). That is, there exists a joint probability distribution $\hat\nu_\omega(\kappa_+,\kappa_-)$, with marginals given by the two measures $\mathbb{E}^\pm_{L,\beta}\left[\cdot|\omega\right]$ and which is supported on pairs of configurations satisfying

$$\kappa_+(u,t) \geq \kappa_-(u,t) \quad \forall (u,t)\in\Lambda_{L,\beta}\,. \tag{6.18}$$

In terms of such a coupling, for any functional $F[\kappa]$:

$$\mathbb{E}^+_{L,\beta}\left[F[\kappa]\,|\omega\right] - \mathbb{E}^-_{L,\beta}\left[F[\kappa]\,|\omega\right] = \sum_{\kappa_+,\kappa_-}\left(F[\kappa_+]-F[\kappa_-]\right)\hat\nu_\omega(\kappa_+,\kappa_-)\,. \tag{6.19}$$

and for $F[\kappa]$ monotone non-decreasing the terms on the right are all non-negative.

In studying the limit $L,\beta\to\infty$ it is convenient to measure the distance of the two induced measures within rectangular space-time domains of the form $B_{K,T}=[-K,K]\times[-T,T]$, through the Wasserstein-type metric

$$W_{K,T}\big(\langle\cdot\rangle^{(\mathrm{XXZ},+)}_{L,\beta,0},\langle\cdot\rangle^{(\mathrm{XXZ},-)}_{L,\beta,0}\big) = \int\Big\{\inf_{\nu_\omega}\Big[\sum_{u=-K}^{K}\int_{-T}^{T}|\kappa_+(u,t)-\kappa_-(u,t)|\,dt\Big]\nu_\omega(\kappa_+,\kappa_-)\Big\}\mu_{L,\beta}(d\omega) \tag{6.20}$$

where ν_ω ranges over couplings of the two measures $\mathbb{E}^\pm_{L,\beta}\left[\cdot|\omega\right]$.

For the monotone coupling the absolute value can be dropped, in which case the integral reduces to the simple difference in expectation values of κ. One cannot do better than that since $|X|\leq X$, and thus

$$W_{K,T}\big(\langle\cdot\rangle^{(\mathrm{XXZ},+)}_{L,\beta,0},\langle\cdot\rangle^{(\mathrm{XXZ},-)}_{L,\beta,0}\big) = \sum_{u=-K}^{K}\int_{-T}^{T}[\langle\kappa(u,t)\rangle^{(\mathrm{XXZ},+)}_{L,\beta,0}-\langle\kappa(u,t)\rangle^{(\mathrm{XXZ},-)}_{L,\beta,0}]\,dt\,. \tag{6.21}$$

In the infinite volume limit, in which the mean value of $\kappa(u,t)$ is translation invariant, one gets

$$\begin{aligned}\lim_{\substack{L\to\infty\\ L\text{even}}}\lim_{\beta\to\infty} W_{K,T}\big(\langle\cdot\rangle^{(\mathrm{XXZ},+)}_{L,\beta,0},\langle\cdot\rangle^{(\mathrm{XXZ},-)}_{L,\beta,0}\big) &= |B_{K,T}|\,[\langle\kappa(0,0)\rangle_+-\langle\kappa(0,0)\rangle_-] \\ &= 4(2K+1)\,T\,\langle\tau(0,0)\rangle_+\,. \end{aligned}\tag{6.22}$$

We learn that if $\langle\tau(0,0)\rangle_+=0$ then for any $K,T<\infty$ the Wasserstein distance between the restrictions of the two measures to the box $B_{K,T}$ tends to zero. It follows that if the measures converge, as we know to be the case here, then they have a common limit.

In other words, if for some measurable functional of τ, $\langle F\rangle_+ \neq \langle F\rangle_-$, then we may conclude that also $\langle \tau(0,0)\rangle_+ \neq \langle \tau(0,0)\rangle_-$. In view of the relation between the two states the latter is equivalent to

$$\langle \tau(0,0)\rangle_+ \neq 0\,. \tag{6.23}$$

□

Postscript – quantum degrees of freedom as emergent features

The analysis presented here provides another example where the categorical distinction between classical and quantum physics is blurred. We started with two quantum spin chains and moved on to their relation with a common random loop model. An alternative presentation could have started from the random loop model, based on the random rung configurations ω, which is of independent interest in probability theory and statistical mechanics and then proceed by recognising that this system's features can be best understood through emergent quantum degrees of freedom.

The utility of such crossings of the quantum/classical divide has been noted before: In one direction, the thermodynamics of the planar Ising model are best explained in terms of emergent quantum degrees of freedom, among which are Bruria Kaufmann's spinors [25] and Lieb-Mattis-Schultz fermions [31]. In the other direction one finds Feynman-Kac functional integral representations for thermal states of quantum particle system in terms of classical functional integrals, and analogous formulas for quantum spin chains, such as employed in [2, 5, 14, 21, 22, 33, 34].

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Michael Aizenman
Departments of Physics and Mathematics
Princeton University
Princeton, NJ 08544, USA

Hugo Duminil-Copin
IHES, 91440 Bures-sur-Yvette, France
and
Dpt. de Mathématiques, Université de Geneve
1211 Geneve 4, Switzerland

Simone Warzel
Munich Center for Quantum Science and Technology, and
Zentrum Mathematik, TU München
85747 Garching, Germany
warzel@ma.tum.de