

Tensor Study of Quantum Link Model

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1 Hamiltonian of QLM as a spin system

We want to study the Square Ice Hamiltonian

$$\mathcal{H} = \sum_{\square} (-f_{\square} + \lambda f_{\square}^2), \quad (1)$$

as the sum over all plaquettes:

$$f_{\square} = \sigma_{\mu_1}^+ \sigma_{\mu_2}^+ \sigma_{\mu_3}^- \sigma_{\mu_4}^- + \sigma_{\mu_1}^- \sigma_{\mu_2}^- \sigma_{\mu_3}^+ \sigma_{\mu_4}^+. \quad (2)$$

on a long cylindrical lattice

$$\Omega = \{\mu = (n, m) | n \in \{1, \dots, L_x\}, m \in \{1, \dots, L_y\}\} \quad (3)$$

displayed in ??.

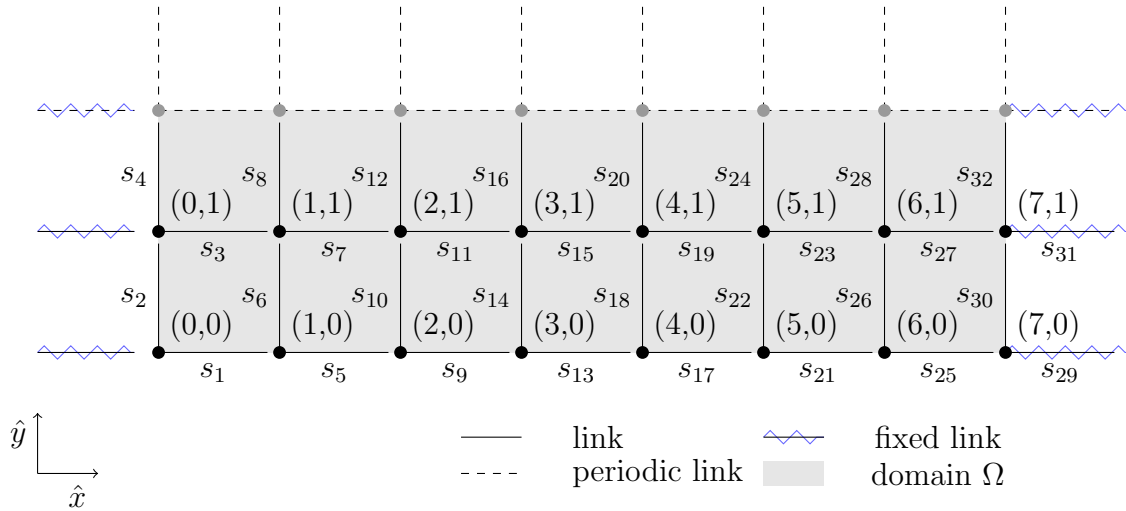


Figure 1: Definition of the computational mesh

In the conventional up/down $s^\pm \in \mathbb{R}^2$ ($[1\ 0]/[0\ 1]$) basis the link operators σ^\pm are pauli matrices :

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (4)$$

In all our lattices $L_y \ll L_x$. For now we fix $L_y = 2$ as in ???. Before explaining the computations we want to point out some properties of the Hamiltonian.

1.1 Mathematical Properties of the Quantum Link Model

Gauss Law: The Hamiltonian \mathcal{H} in ?? commutes with the *vertex operator* G_μ , which counts the number of in and outgoing arrows at vertex μ . We can therefore fix the total charge at each vertex with the *Gauss law constraint*:

$$G_\mu = 0 \quad \text{for all} \quad \mu \in \Omega, \quad (5)$$

$$G_\mu := \sum_{\hat{i} \in \{\hat{x}, \hat{y}\}} (s_{\nu - \hat{i}/2} - s_{\nu + \hat{i}/2}). \quad (6)$$

Winding Numbers

$$W_y = \frac{1}{2L_y} \sum_{\mu} E_{\mu, x} \quad (7)$$

Fluxes

1.2 Hilbert-Space

In the absence of the ice rule eq.(?) the hilbertspace becomes $2^{2 \cdot L_x L_y}$ dimensional and the linear combination of every state is given by:

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_{L_x}} A_{i_1, i_2, \dots, i_{L_x}} |i_1\rangle |i_2\rangle \dots |i_{L_x}\rangle \quad (8)$$

where $i_n = 1, 2, \dots, 2^{2L_y}$ labels the corresponding quantum state at site n . For the $L_y = 2$ we thus have 16 different quantum states at each site $|i_n\rangle = |(s_1, s_2, s_3, s_4)\rangle$, where $s_i \in \{0, 1\}$ labels the i th spin in the local basis drawn in ?. The 16 different combinations in the set can be explicitly written down:

$$\left\{ \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \dots, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \right\} \quad (9)$$

The number of elements in the set will be also referred to as local hilbertspace dimension D .

2 Computational Basis

For the MPS we have to rewrite the Hamiltonian of the system in the nearest neighbour setting. The local Hamiltonian $H_{n,n+1}$ thus defines the interaction between the states at site $|i_n\rangle$ and $|i_{n+1}\rangle$. The Hamilton operator (??) consists of 4 terms. Where on each site we have $m = 1, \dots, L_y$ possible interactions. Thus the hamiltonian consists of $4L_y$ Kronecker products:

$$H_{n,n+1} = \sum_{j=1}^4 \sum_{m=1}^{L_y} h_{\sqsubset,n,m}^{(j)} \otimes h_{\sqsupset,n+1,m}^{(j)} \quad (10)$$

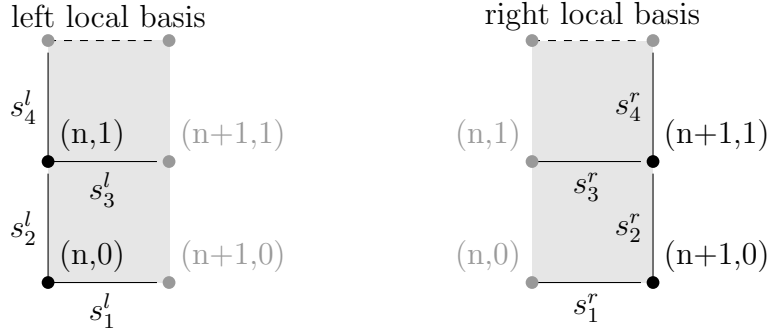


Figure 2: Definition of the computational mesh

To identify the different local interaction terms in the Hamilton operator (??) with (??) we rewrite the plaquette-operator into our computational basis $|i_n\rangle$. A plaquette operator defines our nearest neighbor interaction between state $|i_n\rangle$ and $|i_{n+1}\rangle$

$$f_{\square} = f_{\sqsubset,n,m} \otimes f_{\sqsupset,n,m} + h.c. \quad (11)$$

$$f_{\sqsubset,n,m} = \sigma_{r,n,m+1}^- \sigma_{v,n,m+1}^- \sigma_{r,n,m}^+ \quad (12)$$

$$f_{\sqsupset,n+1,m} = \sigma_{l,n+1,m+1}^+ \sigma_{v,n+1,m+1}^+ \sigma_{l,n+1,m}^- \quad (13)$$

Comparing this to (??) yields:

$$h_{\sqsubset,n,m}^{(1)} = -f_{\sqsubset,n,m} \quad h_{\sqsupset,n+1,m}^{(1)} = f_{\sqsupset,n+1,m} \quad (14)$$

$$h_{\sqsubset,n,m}^{(2)} = -f_{\sqsubset,n,m}^\dagger \quad h_{\sqsupset,n+1,m}^{(2)} = f_{\sqsupset,n+1,m}^\dagger \quad (15)$$

$$h_{\sqsubset,n,m}^{(3)} = \lambda f_{\sqsubset,n,m}^\dagger f_{\sqsubset,n,m} \quad h_{\sqsupset,n+1,m}^{(3)} = f_{\sqsupset,n+1,m}^\dagger f_{\sqsupset,n+1,m} \quad (16)$$

$$h_{\sqsubset,n,m}^{(4)} = \lambda f_{\sqsubset,n,m} f_{\sqsubset,n,m}^\dagger \quad h_{\sqsupset,n+1,m}^{(4)} = f_{\sqsupset,n+1,m} f_{\sqsupset,n+1,m}^\dagger \quad (17)$$

$$(18)$$

For example in our $L_y = 2$ system we get 64×64 size Operators :

$$h_{\sqsubset,n,m}^{(1)} = -\sigma^+ \otimes \sigma^- \otimes \sigma^+ \otimes I_2 \otimes I_2 \otimes I_2 \in \mathbb{R}^{2^6, 2^6} \quad (19)$$

$$h_{\sqsupset,n,m}^{(1)} = I_2 \otimes I_2 \otimes \sigma^+ \otimes I_2 \otimes \sigma^- \otimes \sigma^+ \in \mathbb{R}^{2^6, 2^6} \quad (20)$$

$$(21)$$

Note that this already inherits the periodicity in \hat{y} . For the choosen up/down ($[1\ 0]/[0\ 1]$) basis the link operators are given by:

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (22)$$

$$f_{\square}^2 = \sigma_{\mu_1}^+ \sigma_{\mu_1}^- \sigma_{\mu_2}^+ \sigma_{\mu_2}^- \sigma_{\mu_3}^+ \sigma_{\mu_3}^- \sigma_{\mu_4}^+ \sigma_{\mu_4}^- + hc \quad (23)$$

If we define p_+ and p_- as:

$$p_+ = \frac{\mathbb{1} + \sigma^z}{2} ; p_- = \frac{\mathbb{1} - \sigma^z}{2} \quad (24)$$

I have:

$$f_{\square}^2 = p_{\mu_1}^+ p_{\mu_2}^+ p_{\mu_3}^- p_{\mu_4}^- + p_{\mu_1}^- p_{\mu_2}^- p_{\mu_3}^+ p_{\mu_4}^+ \quad (25)$$

2.1 Todos

- Hamiltonian in external magnetic field, $\phi_{\square} \in \mathbb{R}$. Therefore we define the generalized plaquette operator

$$f(\phi_{\square}) := u_{\square} e^{i\phi_{\square}} + u_{\square}^{\dagger} e^{-i\phi_{\square}} \quad (26)$$

and plug it in (??)

- Winding number operators

$$W_y = \quad (27)$$

3 Boundary Conditions

It is useful to discuss the role of boundary conditions in the lattice set-up.

4 Order Parameters

To detect the phase transitions, we study the so-called sublattice magnetization ($\mathcal{M}_A, \mathcal{M}_B$) which are defined as follows:

$$\mathcal{M}_A(x) = \mathbb{P}_{x,\mu}^+ \mathbb{P}_{x+\mu,\nu}^+ \mathbb{P}_{x+\nu,\mu}^- \mathbb{P}_{x,\nu}^- - \mathbb{P}_{x,\mu}^- \mathbb{P}_{x+\mu,\nu}^- \mathbb{P}_{x+\nu,\mu}^+ \mathbb{P}_{x,\nu}^+ \quad (28)$$

where $\mathbb{P}_{x,\mu}^+$ and $\mathbb{P}_{x,\mu}^-$ are the projection operators on the spin components $S^z = \pm \frac{1}{2}$ respectively.

5 Numerical Results and Simulation Parameters

Table 1: Parameter sets for all Simulations

Parameters	Simulation 1	Simulation 2
Vertical grid size L_x	20,40,60,100,200	60
Horizontal grid size L_y	2	2
Coupling λ	$[-4.0, -3.5, -3.0, \dots, -1.0]$	-1.0
Magnetic field angle θ	0	$\theta_k = \frac{\pi k}{4}, k = 0, 1, \dots, 8$

Figure 3: Extrapolation of the bond dimension

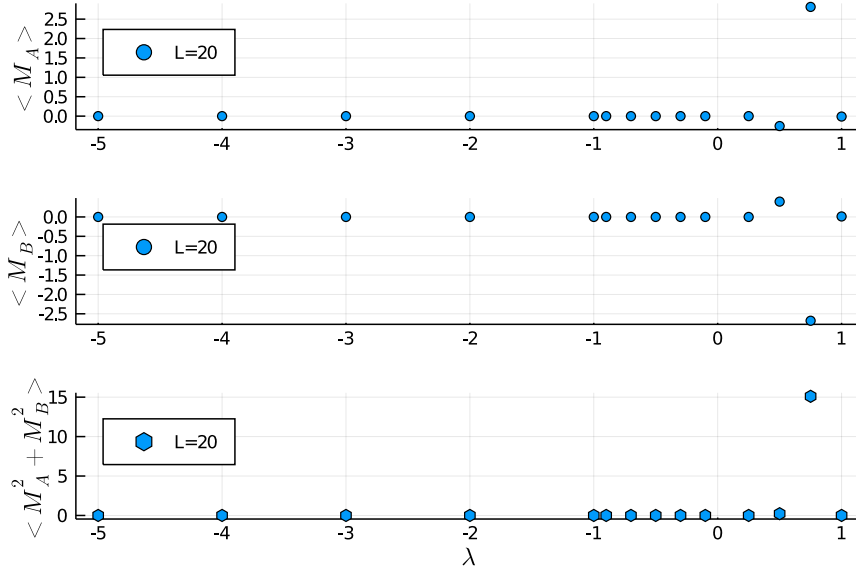


Figure 4: Chess operators

6 Von-Neumann entanglement entropy

Let us suppose we have the ground state of a gapped model on a lattice V described by the density matrix ρ . The von Neumann entropy is defined as:

$$S(\rho) = -\text{Tr}(\rho \log(\rho)) \quad (29)$$

The entropy of the ground-state is zero since it is a product state. We can not state this for subset of the system. We define a subset A of V such that $B := V/A$. We define the reduced density matrix of the sub-system as:

$$\rho_A = \text{Tr}_B(\rho) \quad (30)$$

We define the von-Neumann entropy of the subsystem A as:

$$S(\rho_A) = -\text{Tr}(\rho_A \log_2(\rho_A)) \quad (31)$$

Now, the entropy $S(\rho_A)$ is null if the subsystems A and B are product states. This is not true if there is quantum correlations between A and B . Quantum correlations can lead to non-vanishing values of $S(\rho_A)$. In fact, the von-Neumann entropy is an index of the entanglement for pure states. This is also why the von-Neumann entropy is also called entanglement entropy.

7 Matrix product states

We define the wavefunction of a quantum state as [?]:

$$|\psi\rangle = \sum_{j_1, \dots, j_n} c_{j_1, \dots, j_n} |j_1\rangle \otimes \dots \otimes |j_n\rangle \quad (32)$$

The matrix product state (MPS) Ansatz defines c_{j_1, \dots, j_n} as:

$$c_{j_1, \dots, j_n} = \sum_{\alpha, \beta, \dots, \gamma} A_{\alpha, \beta, j_1}^1 A_{\beta, \delta, j_2}^2 \dots A_{\gamma, \alpha, j_n}^N \quad (33)$$

We can now make a comparison between the number of parameters there are in the exact description and the MPS Ansatz. If we have a system of n spin physical dimension d we have $\mathcal{O}(d^n)$ parameters in the exact description. If we decide to truncate the dimension of the greek (i.e. $\alpha \beta \dots$) to be at most D (D is usually called *bond dimension* in the literature) indexes in the definition of the MPS Ansatz we have $\mathcal{O}(ndD^2)$ parameters.

7.1 Gauge degree of freedom

A MPS is defined univocally but the tensors $A^{(i)}$. On the other the set of tensors $A^{(i)}$ that define a generic Ψ is not unique. Ψ is defined as the contraction of the tensors $A^{(i)}$. Given an element of $Gl_D(\mathbb{C})$ M , a MPS is invariant under the insertions:

$$A_{\alpha, \beta}^{(i)} A_{\beta, \gamma}^{(i+1)} = A_{\alpha, \beta}^{(i)} M_{\beta, \delta} M_{\delta, \xi}^{-1} A_{\xi, \gamma}^{(i+1)} \quad (34)$$

At this point it is very important to remind the reader a fundamental tool in linear algebra: The singular value decomposition (SVD). Given a generic rectangular matrix N it is always possible to find matrices U, S, V such that:

$$N = U S V^\dagger \quad (35)$$

U is a matrix containing the left singular vectors of N . Since U has orthonormal columns it is also unitary $UU^\dagger = U^\dagger U = 1$. S is a diagonal matrix with non-negative entries. Those numbers s_a are called the singular values of N . The number of non-zero singular values is the rank of N . V^\dagger is a matrix that contains the right singular vectors. In the same way as U , V^\dagger has orthonormal columns it is also unitary $VV^\dagger = V^\dagger V = 1$. The singular values contained in S has a lot of interesting

properties. Let us suppose we have a state $|\psi\rangle$. For any partition A and B of the Hilbert space in which $|\psi\rangle$ is defined it is always possible to write:

$$|\psi\rangle = \sum_{\alpha, \beta} c_{\alpha, \beta} |\alpha\rangle_A |\beta\rangle_B \quad (36)$$

If perform a SVD of the matrix c in ??, we can write:

$$|\psi\rangle = \sum_{\alpha, \beta} \sum_{s_a} U_{\alpha, s_a} S_{s_a, s_a} V_{s_a, \beta}^\dagger |\alpha\rangle_A |\beta\rangle_B \quad (37)$$

We can absorb U and V in A and B due to their orthonormality in those spaces write:

$$|\psi\rangle = \sum_{s_a} s_a |\alpha\rangle_A |\beta\rangle_B \quad (38)$$

In this decomposition it is trivial to derive the reduced density matrix for the sub-system A in ??:

$$\rho_A = \sum_{s_a} s_a^2 (|\alpha\rangle\langle\alpha|)_A \quad (39)$$

The von-Neumann entanglement entropy can be computed directly from here:

$$S(\rho_A) = -\text{Tr}(\rho_A \log_2(\rho_A)) = -\sum_a s_a^2 \log_2 s_a^2 \quad (40)$$

7.2 Canonical form

Fixing those matrices M or, more generally, fixing M such that the MPS satisfies certain relations is referred to as *fixing a gauge*. Two particular gauge, called *canonical forms* are particularly useful when computing expectation values of operators (i.e. the Hamiltonian H of a quantum system). Those gauge consist into choosing the matrices M such that the tensors $A^{(i)}$ satisfy the following relations:

$$\sum_{\beta=1}^D \sum_{s=1}^d \left(A_{\alpha, \beta}^{[s](i)} \right)^* A_{\beta, \gamma}^{[s](i)} = \delta_{\alpha, \gamma} \quad (41)$$

$$\sum_{\beta=1}^D \sum_{s=1}^d A_{\alpha, \beta}^{[s](i)} \left(A_{\beta, \gamma}^{[s](i)} \right)^* = \delta_{\alpha, \gamma} \quad (42)$$

If a MPS satisfies the relation in ?? it is called to be in the *left canonical form*. If a MPS satisfies the relation in ?? it is called to be in the *right canonical form*.

There is also a very useful notation introduced by [?] that highlights the singular values of the matrices of a MPS:

$$|\psi\rangle = \sum_{s_1, \dots, s_N} U^{s_1} S_1 U^{s_2} S_2 \dots U^{s_N} S_N |s_1, \dots, s_N\rangle \quad (43)$$

7.3 Computation of the Von-Neumann entropy in the MPS formalism

Let us suppose we have a spin chain of local Physical dimension d and N sites described by a MPS in the *left canonical form*. The partition function ρ is defined as:

$$\rho = \sum_{s_1, \dots, s_N}^d \sum_{s'_1, \dots, s'_N}^d \text{Tr} \left[M^{1, s_1, s'_1} M^{2, s_2, s'_2} \dots M^{N, s_N, s'_N} \right] |s_1, \dots, s_N\rangle \langle s'_1, \dots, s'_N| \quad (44)$$

where:

$$M^{i, s_i, s'_i} = A^{[s_i](i)} \otimes \left(A^{[s'_i](i)} \right)^\dagger \quad (45)$$

We now partition the system in two sub-system A and B . A includes all the sites up to k and B its complementary. $\rho(A)$, defined as in ??, can now be written as:

$$\tilde{\rho}_A^{[l]} = \text{Tr}_B(\rho) = \sum_{s_1, \dots, s_l}^d \sum_{s'_1, \dots, s'_l}^d A^{1, s_1} \dots A^{l, s_l} \rho_{[A]}^{(l)} \left(A^{1, s'_1} \right)^\dagger \dots \left(A^{l, s'_l} \right)^\dagger |s_1, \dots, s_l\rangle \langle s'_1, \dots, s'_l| \quad (46)$$

where $\rho_{[A]}^{(l)}$ is defined as:

$$\rho_{[A]}^{(l)} = \sum_{s_{l+1}, \dots, s_N}^d \sum_{s'_{l+1}, \dots, s'_N}^d A^{l+1, s_{l+1}} \dots A^{N, s_N} \left(A^{l+1, s'_{l+1}} \right)^\dagger \dots \left(A^{N, s'_N} \right)^\dagger \quad (47)$$

?? denotes a recursive relation:

$$\rho_{[A]}^{(l+1)} = A^{l+1, s_{l+1}} \rho_{[A]}^{(l)} \left(A^{l+1, s'_{l+1}} \right)^\dagger \quad (48)$$

We can always rewrite a MPS such in the form of ??. From this form it is trivial to derive the von-Neumann entanglement entropy in the same fashion as in ??. We just need to identify:

$$|\alpha\rangle_A = \sum_{s_1, \dots, s_l} U^{s_1} S_1 U^{s_2} S_2 \dots S_{l-1} U^{s_l} |s_1, \dots, s_l\rangle \quad (49)$$

$$|\alpha\rangle_B = \sum_{s_{l+1}, \dots, s_N} U^{s_{l+1}} S_{l+1} U^{s_{l+2}} S_{l+2} \dots U^{s_N} S_N |s_{l+1}, \dots, s_N\rangle \quad (50)$$

At this point we can write:

$$\rho_A = \sum_a s_a^2 (|\alpha\rangle \langle \alpha|)_A = \sum_a (S_l)_{a,a} (|\alpha\rangle \langle \alpha|)_A \quad (51)$$

Since we have the coefficients of the reduced density matrix ρ_A we can compute the von-Neumann entropy as:

$$S(\rho_A) = -\text{Tr}(\rho_A \log_2(\rho_A)) = -\sum_a (S_l)_{a,a}^2 \log_2 (S_l)_{a,a}^2 \quad (52)$$