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

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

as the sum over all plaquettes:

$$f_{\square} = \sigma^+_{\mu_1}\sigma^+_{\mu_2}\sigma^-_{\mu_3}\sigma^-_{\mu_4} + \sigma^-_{\mu_1}\sigma^-_{\mu_2}\sigma^+_{\mu_3}\sigma^+_{\mu_4}. \tag{2}$$

on a long cylindrical lattice

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

displayed in fig. 1.

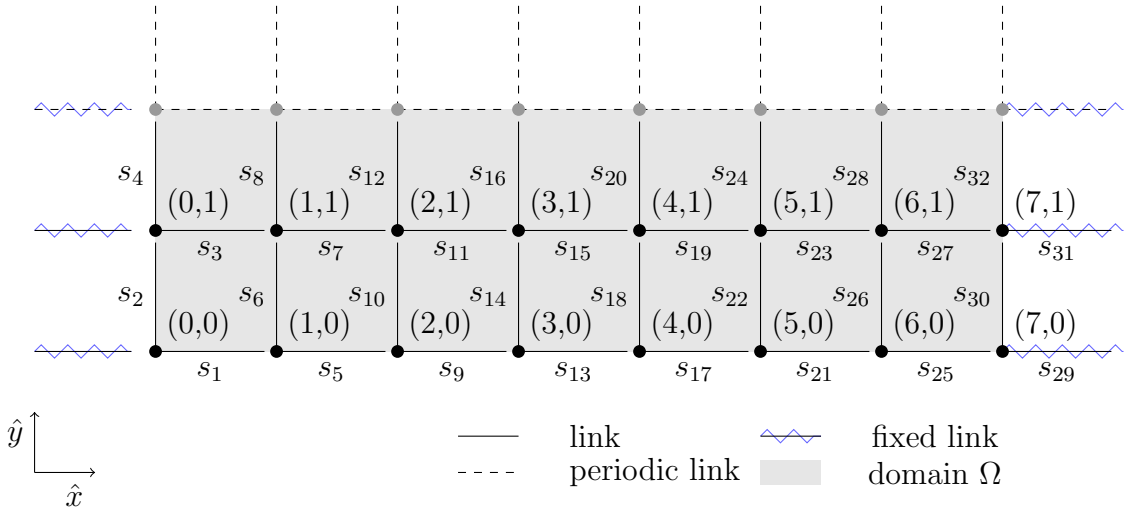

Figure 1: Definition of the computational mesh

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

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

In all our lattices $L_y \ll L_x$. For now we fix $L_y = 2$ as in fig. 1. 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 eq. (1) 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*:

$$G_\mu = 0 \qquad \text{for all} \qquad \mu \in \Omega\,, \tag{5}$$

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

Winding Numbers

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

Fluxes

1.2 Hilbert-Space

In the absence of the ice rule eq.(5) the hilbertspace becomes $2^{2\cdot L_x L_y}$ dimensional and the linear combination of every state is given by:

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_{L_x}} A_{i_1,i_2,\ldots,i_{L_x}} |i_1\rangle|i_2\rangle\ldots|i_{L_x}\rangle \tag{8}$$

where $i_n = 1, 2, \ldots, 2^{2L_y}$ 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 ith spin in the local basis drawn in fig. 2. The 16 different combinations in the set can be explicitly written down:

$$\left\{ \begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \begin{pmatrix}1\\0\\1\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\1\end{pmatrix}, \ldots, \begin{pmatrix}0\\0\\0\\1\end{pmatrix}, \begin{pmatrix}0\\0\\0\\0\end{pmatrix} \right\} \tag{9}$$

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 (1) consists of 4 terms. Where on each site we have $m = 1, \ldots, L_y$ possible interactions. Thus the hamiltonian consists of $4L_y$ Kronecker products:

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

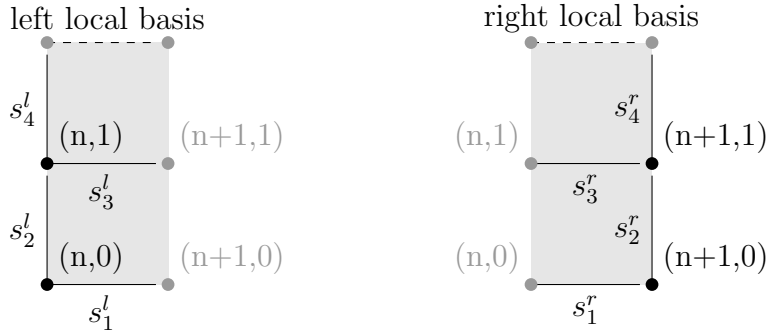

Figure 2: Definition of the computational mesh

To identify the different local interaction terms in the Hamilton operator (10) with (1) 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 $|i_{n+1}\rangle$

$$f_{\square} = f_{\sqsubset,n,m} \otimes f_{\sqsupset,n,m} + h.c. \tag{11}$$
$$f_{\sqsubset,n,m} = \sigma^-_{r,n,m+1}\sigma^-_{v,n,m+1}\sigma^+_{r,n,m} \tag{12}$$
$$f_{\sqsupset,n+1,m} = \sigma^+_{l,n+1,m+1}\sigma^+_{v,n+1,m+1}\sigma^-_{l,n+1,m} \tag{13}$$

Comparing this to (10) yields:

$$h^{(1)}_{\sqsubset,n,m} = -f_{\sqsubset,n,m} \qquad h^{(1)}_{\sqsupset,n+1,m} = f_{\sqsupset,n+1,m} \tag{14}$$
$$h^{(2)}_{\sqsubset,n,m} = -f^\dagger_{\sqsubset,n,m} \qquad h^{(2)}_{\sqsupset,n+1,m} = f^\dagger_{\sqsupset,n+1,m} \tag{15}$$
$$h^{(3)}_{\sqsubset,n,m} = \lambda f^\dagger_{\sqsubset,n,m} f_{\sqsubset,n,m} \qquad h^{(3)}_{\sqsupset,n+1,m} = f^\dagger_{\sqsupset,n+1,m} f_{\sqsupset,n+1,m} \tag{16}$$
$$h^{(4)}_{\sqsubset,n,m} = \lambda f_{\sqsubset,n,m} f^\dagger_{\sqsubset,n,m} \qquad h^{(4)}_{\sqsupset,n+1,m} = f_{\sqsupset,n+1,m} f^\dagger_{\sqsupset,n+1,m} \tag{17}$$
$$\tag{18}$$

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

$$h^{(1)}_{\sqsubset,n,m} = -\sigma^+ \otimes \sigma^- \otimes \sigma^+ \otimes I_2 \otimes I_2 \otimes I_2 \in \mathbb{R}^{2^6,2^6} \tag{19}$$
$$h^{(1)}_{\sqsupset,n,m} = I_2 \otimes I_2 \otimes \sigma^+ \otimes I_2 \otimes \sigma^- \otimes \sigma^+ \in \mathbb{R}^{2^6,2^6} \tag{20}$$
$$\tag{21}$$

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

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

$$f_{\square}^2 = \sigma_{\mu_1}^+ \sigma_{\mu_1}^- \, \sigma_{\mu_2}^+ \sigma_{\mu_2}^- \, \sigma_{\mu_3}^- \sigma_{\mu_3}^+ \, \sigma_{\mu_4}^- \sigma_{\mu_4}^+ \; + hc \tag{23}$$

If we define $p+$ and $p+$ as:

$$p+ = \frac{\mathbb{1} + \sigma^z}{2} \; ; \; p- = \frac{\mathbb{1} - \sigma^z}{2} \tag{24}$$

I have:

$$f_{\square}^2 = p_{\mu_1}^+ p_{\mu_2}^+ p_{\mu_3}^- p_{\mu_4}^- \; + p_{\mu_1}^- p_{\mu_2}^- p_{\mu_3}^+ p_{\mu_4}^+ \tag{25}$$

2.1 Todos

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

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

  and plug it in (1)

- Winding number operators

  $$W_y = \tag{27}$$

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 $(\mathcal{M}_{\mathrm{A}}, \mathcal{M}_{\mathrm{B}})$ which are defined as follows:

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

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	$[-4.0, -3.5, -3.0, \ldots, -1.0]$	-1.0
Magnetic field angle θ	0	$\theta_k = \frac{\pi}{4}k, k = 0, 1, \ldots, 8$

Figure 3: Extrapolation of the bond dimension

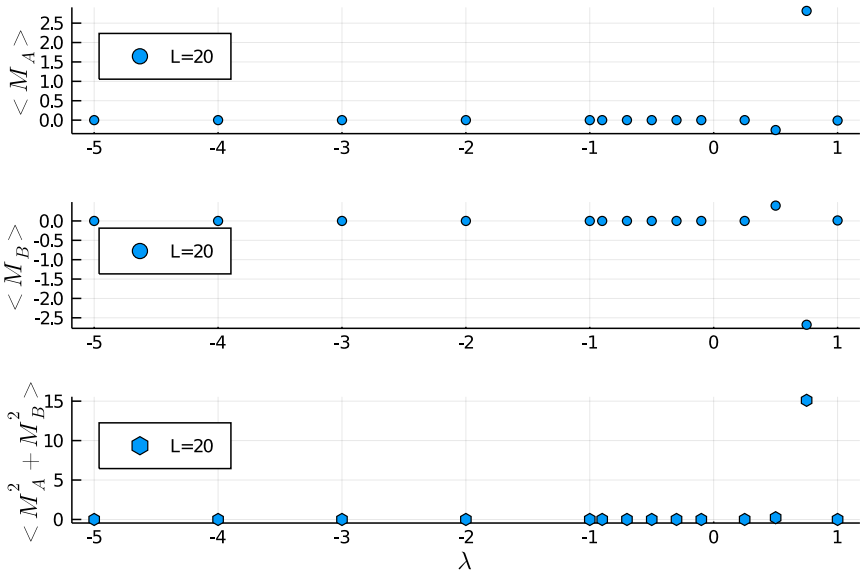

Figure 4: Chess operators

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:

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

At zero temperature, the entropy of the ground state is zero for any gapped Hamiltonian [**?**]. 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:

$$\rho_A = Tr_B(\rho) \tag{30}$$

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

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

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 a 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 wave-function of a quantum state as [**?**]:

$$|\psi\rangle = \sum j_1, ..., j_n c_{j_1,...,j_n} |j_1\rangle \otimes ... \otimes |j_n\rangle \tag{32}$$

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

$$c_{j_1,...,j_n} = \sum_{\alpha,\beta,\,...\,,\gamma} A^1_{\alpha,\beta,j_1} A^2_{\beta,\delta,j_2} ... A^N_{\gamma,\alpha,j_n} \tag{33}$$

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. $\alpha\,\beta\,...$) 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 a element of $Gl_D(\mathbb{C})$ M, a MPS is invariant under the insertions:

$$A^{(i)}_{\alpha,\,\beta} A^{(i+1)}_{\beta,\,\gamma} = A^{(i)}_{\alpha,\,\beta} M_{\beta,\,\delta} M^{-1}_{\delta,\,\xi} A^{(i+1)}_{\xi,\,\gamma} \tag{34}$$

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

$$N = U\,S\,V^\dagger \tag{35}$$

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 sigular values contained in S has 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:

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

If perform a SVD of the matrix c in eq. (36), we can write:

$$|\psi\rangle = \sum_{\alpha,\,\beta} \sum_{s_a} U_{\alpha,\,s_a} S_{s_a,\,s_a} V^{\dagger}_{s_a,\,\beta} \, |\alpha\rangle_A \, |\beta\rangle_B \tag{37}$$

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

$$|\psi\rangle = \sum_{s_a} s_a \, |\alpha\rangle_A \, |\beta\rangle_B \tag{38}$$

In this decoposition it is trivial to derive the reduced density matrix for the subsystem A in eq. (30):

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

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

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

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:

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

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

If a MPS satisfies the relation in eq. (41) it is called to be in the *left canonical form*. If a MPS satisfies the relation in eq. (42) 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:

$$|\psi\rangle = \sum_{s_1,\,\ldots\,,\,s_N} U^{s_1} S_1 U^{s_2} S_2 \ldots U^{s_N} S_N \, |s_1,\,\ldots\,,\,s_N\rangle \tag{43}$$

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:

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

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 eq. (30), can now be written as:

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

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

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

eq. (47) denotes a recursive relation:

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

We can always rewrite a MPS such in the form of eq. (43). From this form it is trivial to derive the von-Neumann entanglement entropy in the same fashion as in eq. (52). We just need to identify:

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

$$|\alpha\rangle_B = \sum_{s_1,\dots,s_N} U^{s_{l+1}} S_{l+1} U^{s_{l+2}} S_{l+2} \dots U^{s_N} S_N |s_{l+1},\dots,s_N\rangle \quad (50)$$

At this point we can write:

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

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

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