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Explicit properties of the simplest inhomogeneous Matrix-Product-State including the Riemann metric of the MPS manifold

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We consider the simplest inhomogeneous Matrix-Product-State for an open chain of N quantum spins that involves only two angles per site and two angles per bond with the following direct physical meanings. The two angles associated to the site k are the two Bloch angles that parametrize the two orthonormal eigenvectors of the reduced density matrix ρ_k of the spin k alone. The two angles associated to the bond $(k, k + 1)$ parametrize the entanglement properties of the Schmidt decomposition across the bond $(k, k + 1)$. Explicit results are given for the reduced density matrix $\rho_{k, k+1}$ of two consecutive sites that is needed to evaluate the energy of two-body Hamiltonians, and for the reduced density matrix $\rho_{k, k+r}$ of two sites at distance r that is needed to evaluate the spin-spin correlations at distance r . The global structure of the MPS manifold as parametrized by these $(4N - 2)$ angles is then characterized by its explicit Riemann metric. Finally, the generalizations to any tree-like structure without loops and to the chain with periodic boundary conditions are discussed.

I. INTRODUCTION

The difficulty in studying systems with a large number N of quantum spins comes from the exponential growth of the size of the Hilbert space $\mathcal{N} = 2^N$. The exact representation of a ket in the tensor Pauli basis

$$|\psi_N\rangle = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \dots \sum_{S_N=\pm 1} c_{S_1, \dots, S_N} |\sigma_1^z = S_1\rangle |\sigma_2^z = S_2\rangle \dots |\sigma_N^z = S_N\rangle \quad (1)$$

involves $\mathcal{N} = 2^N$ complex coefficients c_{S_1, \dots, S_N} , i.e. $2\mathcal{N}$ real parameters. The normalization $\langle \psi_N | \psi_N \rangle = 1$ and the removal of the global phase with no physical meaning allows to reduce by two the number of parameters, so that the total number of real parameters needed to parametrize the ket grows exponentially with N as

$$P_N^{full} = 2\mathcal{N} - 2 = 2(2^N - 1) \quad (2)$$

The key idea of the whole Tensor Network field (see the reviews [1–11] and references therein) is that in most physical problems, the big tensor c_{S_1, \dots, S_N} may be decomposed in terms of elementary small tensors that can be assembled in various ways in order to adapt to the geometry and to the entanglement properties of the problem under focus. Indeed the notion of entanglement between the different regions has emerged as the central idea and has completely changed the perspective on many-body quantum systems (see the reviews [12–17] and references therein). In particular for one-dimensional quantum spin chains, the Matrix-Products-States (MPS) are well adapted to describe non-critical states displaying area-law entanglement [1–11], i.e. for most ground-states of local Hamiltonians [18]. In the Vidal canonical form of MPS [19], the coefficients c_{S_1, \dots, S_N} of Eq. 1 are decomposed into

$$c_{S_1, \dots, S_N} = \sum_{\alpha_1=1}^D \sum_{\alpha_2=1}^D \dots \sum_{\alpha_{N-1}=1}^D \Gamma_{1, \alpha_1}^{[1]S_1} \lambda_{\alpha_1}^{[1,2]} \Gamma_{\alpha_1, \alpha_2}^{[2]S_2} \lambda_{\alpha_2}^{[2]} \dots \lambda_{\alpha_{N-1}}^{[N-1, N]} \Gamma_{\alpha_{N-1}, 1}^{[N]S_N} \quad (3)$$

where the D variables $\lambda_{\alpha_k=1, \dots, D}^{[k, k+1]}$ associated to the bond $(k, k + 1)$ are the Schmidt coefficients associated to the Schmidt decomposition of the MPS across the bond $(k, k + 1)$, while the tensor $\Gamma_{\alpha_{k-1}, \alpha_k}^{[k]S_k}$ associated to the site k represents some appropriate transformation within the local Hilbert space of the site k . The number of parameters in the MPS grows only linearly in N (instead of the exponential growth of Eq. 2) and these MPS parameters can be optimized numerically to obtain the best approximation within the some given MPS manifold. This variational point of view can be seen as a reformulation of the Density-Matrix-RG algorithm [20–22]. More generally, the Tensor Network activity has been mostly oriented towards the production of extremely powerful numerical algorithms, based on the variational optimization of the whole Tensor Network and where the numerical precision can be systematically improved by increasing the bond dimension D .

In the field of disordered spin chains, area-law states are even more important since they appear not only for non-critical ground-states of generic local random Hamiltonians but also for excited states in Many-Body-Localized phases [23–29]. While in pure systems, the translational invariance allows to choose the same elementary matrix with a finite number of parameters in the MPS and to apply the transfer-matrix formalism to compute all physical

observables (see the reviews [1–11] and references therein), the presence of disorder breaks the translational invariance and one needs to consider inhomogeneous MPS, where the parameters of the elementary tensors can adapt to the local disorder variables. In the present paper, we will thus focus on the simplest inhomogeneous Matrix-Product-States of bond dimension $D = 2$ that involves only two real parameters per site and two real parameters per bond, so that the number of real parameters for an open chain of N spins and $(N - 1)$ bonds will grow linearly with respect to the size N as

$$P_N^{MPS} = 2N + 2(N - 1) = 4N - 2 \quad (4)$$

In addition, these parameters will have a very direct physical meaning, since the bond variables will be related to the entanglement across the bond as in the Vidal canonical form of Eq. 3 even if we will use a different choice of gauge fixing for the Schmidt decomposition, while the sites variables will be the Bloch angles that parametrize the eigenvectors of the single-site reduced density matrices. Our goal will be to compute explicitly the properties of this simplest inhomogeneous MPS.

The paper is organized as follows. In section II, we describe the specific choice of gauge fixing for the Schmidt decomposition and introduce the useful notations for the whole paper. In section III, we explain the parametrization of the simplest inhomogeneous Matrix-Product-States and analyze its basic properties. In section IV, we study the reduced density matrix of an interval in the bulk, whereas its diagonalization is given in Appendix A. In section V, we discuss the optimization of the MPS parameters to approximate the ground-state of local Hamiltonian with one-body and two-body terms. In section VI, we obtain the reduced density matrix of two sites at distance r and evaluate the spin-spin correlations. In section VII, we compute the Riemann metric of the MPS manifold. Finally, we describe the generalization of the simple MPS to an arbitrary tree-like structure without loops in section VIII, and the generalization to the chain with periodic boundary conditions in section IX. Section X summarizes our conclusions.

II. PRESENT CHOICE OF GAUGE FIXING FOR THE SCHMIDT DECOMPOSITION

A. Schmidt decomposition for a state in the tensor product of two Hilbert spaces of dimension D

In this section, we focus on a quantum state $|\psi\rangle$ in the tensor product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, where the two Hilbert spaces \mathcal{H}_A and \mathcal{H}_B have the same dimension D . The diagonalization of the reduced density matrices

$$\begin{aligned} \rho_A &= \text{Tr}_{\{B\}}(|\psi\rangle\langle\psi|) = \sum_{\alpha=1}^D p_\alpha |A_\alpha\rangle\langle A_\alpha| \\ \rho_B &= \text{Tr}_{\{A\}}(|\psi\rangle\langle\psi|) = \sum_{\alpha=1}^D p_\alpha |B_\alpha\rangle\langle B_\alpha| \end{aligned} \quad (5)$$

involve the same real positive weights $p_\alpha \geq 0$ normalized to unity

$$\sum_{\alpha=1}^D p_\alpha = 1 \quad (6)$$

while the corresponding eigenvectors $|A_\alpha\rangle$ and $|B_\alpha\rangle$ form orthonormal basis of A and B respectively

$$\begin{aligned} \langle A_\alpha | A_{\alpha'} \rangle &= \delta_{\alpha\alpha'} \\ \langle B_\alpha | B_{\alpha'} \rangle &= \delta_{\alpha\alpha'} \end{aligned} \quad (7)$$

The new basis $|A_\alpha\rangle$ can be obtained from the initial basis of A by a unitary matrix of size $D \times D$ that contains a priori D^2 real parameters. However each ket $|A_\alpha\rangle$ for $\alpha = 1, \dots, D$ contains a global phase that disappears from the projector $|A_\alpha\rangle\langle A_\alpha|$ appearing in the reduced density matrix of Eq. 5, so the D projectors $|A_\alpha\rangle\langle A_\alpha|$ can be parametrized with only $(D^2 - D)$ parameters. Similarly, the D projectors $|B_\alpha\rangle\langle B_\alpha|$ can be parametrized with only $(D^2 - D)$ parameters.

So together, the two reduced density matrices ρ_A and ρ_B of Eq. 5 involve $(D - 1)$ real parameters for the D weights p_α normalized to unity (Eq 6), $(D^2 - D)$ real parameters for the D projectors $|A_\alpha\rangle\langle A_\alpha|$ in A and $(D^2 - D)$ real parameters for the D projectors $|B_\alpha\rangle\langle B_\alpha|$ in B , so that the total number of real parameters contained in the pair (ρ_A, ρ_B) is

$$P^{(\rho_A, \rho_B)} = (D - 1) + 2(D^2 - D) = 2D^2 - D - 1 \quad (8)$$

The comparison with the total number of real parameters needed to parametrize the ket $|\psi\rangle$ in the Hilbert space of dimension $D \times D$ (Eq 2)

$$P^{full} = 2(D^2 - 1) = 2D^2 - 2 \quad (9)$$

yields that the number of missing parameters to reconstruct the ket $|\psi\rangle$ reduces to

$$P^{missing} = P^{full} - P^{(\rho_A, \rho_B)} = D - 1 \quad (10)$$

These $(D - 1)$ missing parameters are the phases $\phi_\alpha \in [0, 2\pi[$ for $\alpha = 2, \dots, D$ that are needed to write the Schmidt decomposition in the present gauge fixing, where we have already chosen the phases of the eigenvectors $|A_\alpha\rangle$ and $|B_\alpha\rangle$ as explained above

$$|\psi\rangle = \sum_{\alpha=1}^D \sqrt{p_\alpha} e^{i\phi_\alpha} |A_\alpha\rangle \otimes |B_\alpha\rangle \equiv \sum_{\alpha=1}^D \lambda_\alpha |A_\alpha\rangle \otimes |B_\alpha\rangle \quad (11)$$

so in the present paper, the Schmidt values λ_α in front of the tensor product $|A_\alpha\rangle \otimes |B_\alpha\rangle$ will be complex numbers

$$\lambda_\alpha \equiv \sqrt{p_\alpha} e^{i\phi_\alpha} \quad (12)$$

except for the first phase that will be chosen to vanish

$$\phi_{\alpha=1} = 0 \quad (13)$$

in order to fix the global phase of the ket of Eq. 11.

Here it should be stressed that the Schmidt decomposition is usually formulated via the Singular Value Decomposition of matrices, where the Schmidt values are real positive $\lambda_\alpha^{usual} = \sqrt{p_\alpha}$, i.e. the phases $e^{i\phi_\alpha}$ introduced above are actually included in the eigenvectors $|A_\alpha\rangle$ and $|B_\alpha\rangle$. In the present paper however, it will be more convenient to choose the global phases of the eigenvectors as explained above, and to work with complex Schmidt values as in Eq. 12, in order to avoid the gauge freedom and the gauge redundancy that exist in the usual definition of Matrix-Product-States. Let us now describe in detail what this gauge fixing means for the dimension $D = 2$, since it will be the basic building block of the MPS studied in the further sections.

B. Example with the dimension $D = 2$

Here A corresponds to a single spin with the Pauli basis $|\sigma_1^z = \pm\rangle$, and B corresponds to a single spin with the Pauli basis $|\sigma_2^z = \pm\rangle$. The Schmidt decomposition of Eq. 11 contains only $D = 2$ terms, and it will be more convenient to label them with $\alpha = \pm$ (instead of $\alpha = 1, 2$). The two weights normalized to unity $p_+ + p_- = 1$ can be parametrized by the single angle $\theta \in [0, \frac{\pi}{2}]$ (if one chooses the ordering $p_+ \geq p_-$)

$$\begin{aligned} p_+ &= \cos^2\left(\frac{\theta}{2}\right) = \frac{1 + \cos\theta}{2} \\ p_- &= \sin^2\left(\frac{\theta}{2}\right) = \frac{1 - \cos\theta}{2} \end{aligned} \quad (14)$$

The two complex Schmidt values of Eq. 12 are then parametrized in terms of two angles (θ, ϕ)

$$\begin{aligned} \lambda_+ &= \cos\left(\frac{\theta}{2}\right) \\ \lambda_- &= \sin\left(\frac{\theta}{2}\right) e^{i\phi} \end{aligned} \quad (15)$$

leading to the following Schmidt decomposition in the present gauge fixing

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |\tau_1^z = +\rangle \otimes |\tau_2^z = +\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi} |\tau_1^z = -\rangle \otimes |\tau_2^z = -\rangle \quad (16)$$

where $|\tau_k^z = \pm\rangle$ should be the two eigenvectors of the reduced density matrix ρ_k for $k = 1, 2$. It is convenient to parametrize the eigenvector $|\tau_k^z = +\rangle$ by the usual Bloch angles $\theta_k \in [0, \pi]$ and $\phi_k \in [0, 2\pi[$, while the orthogonal

eigenvector $|\tau_k^z = -\rangle$ will correspond to the opposite point on the Bloch sphere with Bloch angles $(\pi - \theta_k)$ and $(\phi_k + \pi)[2\pi]$

$$\begin{aligned} |\tau_k^z = +\rangle &\equiv |\theta_k, \phi_k\rangle = \cos \frac{\theta_k}{2} |\sigma_k^z = +\rangle + \sin \frac{\theta_k}{2} e^{i\phi_k} |\sigma_k^z = -\rangle \\ |\tau_k^z = -\rangle &\equiv |\pi - \theta_k, \phi_k + \pi\rangle = \sin \frac{\theta_k}{2} |\sigma_k^z = +\rangle - \cos \frac{\theta_k}{2} e^{i\phi_k} |\sigma_k^z = -\rangle \end{aligned} \quad (17)$$

From the point of view of Pauli operators, the ket change of basis from $|\sigma_k^z = \pm\rangle$ to $|\tau_k^z = \pm\rangle$ corresponds to the change from the initial Pauli basis $(1, \sigma_k^z, \sigma_k^x, \sigma_k^y)$ to the new Pauli basis $(1, \tau_k^z, \tau_k^x, \tau_k^y)$

$$\begin{aligned} \tau_k^z &= \cos \theta_k \sigma_k^z + \sin \theta_k [\cos \phi_k \sigma_k^x + \sin \phi_k \sigma_k^y] \\ \tau_k^x &= \sin \theta_k \sigma_k^z - \cos \theta_k [\cos \phi_k \sigma_k^x + \sin \phi_k \sigma_k^y] \\ \tau_k^y &= \sin \phi_k \sigma_k^x - \cos \phi_k \sigma_k^y \end{aligned} \quad (18)$$

It will be convenient to denote by R_k the reciprocal 3×3 rotation matrix

$$\begin{pmatrix} \sigma_k^z \\ \sigma_k^x \\ \sigma_k^y \end{pmatrix} = R_k \begin{pmatrix} \tau_k^z \\ \tau_k^x \\ \tau_k^y \end{pmatrix} = \begin{pmatrix} \cos \theta_k & \sin \theta_k & 0 \\ \sin \theta_k \cos \phi_k & -\cos \theta_k \cos \phi_k & \sin \phi_k \\ \sin \theta_k \sin \phi_k & -\cos \theta_k \sin \phi_k & -\cos \phi_k \end{pmatrix} \begin{pmatrix} \tau_k^z \\ \tau_k^x \\ \tau_k^y \end{pmatrix} \quad (19)$$

and to denote its matrix elements by R_k^{ab} with $a = z, x, y$ and $b = z, x, y$

$$\sigma_k^a = \sum_{b=z,x,y} R_k^{ab} \tau_k^b \quad (20)$$

In terms of the new Pauli basis $(1, \tau_k^z, \tau_k^x, \tau_k^y)$, the reduced density matrix for the spin k is diagonal and involves only the two operator $(1, \tau_k^z)$

$$\rho_k = p_+ |\tau_k^z = +\rangle \langle \tau_k^z = +| + p_- |\tau_k^z = -\rangle \langle \tau_k^z = -| = \frac{1}{2} (1 + \cos \theta \tau_k^z) \quad (21)$$

while the full density matrix for the two spins computed from Eq 16

$$\begin{aligned} \rho_{1,2} \equiv |\psi\rangle \langle \psi| &= \left(\frac{1 + \cos \theta}{2} \right) \left(\frac{1 + \tau_1^z}{2} \right) \left(\frac{1 + \tau_2^z}{2} \right) + \left(\frac{1 - \cos \theta}{2} \right) \left(\frac{1 - \tau_1^z}{2} \right) \left(\frac{1 - \tau_2^z}{2} \right) \\ &+ \frac{\sin \theta}{2} \left[e^{-i\phi} \left(\frac{\tau_1^x + i\tau_1^y}{2} \right) \left(\frac{\tau_2^x + i\tau_2^y}{2} \right) + e^{i\phi} \left(\frac{\tau_1^x - i\tau_1^y}{2} \right) \left(\frac{\tau_2^x - i\tau_2^y}{2} \right) \right] \\ &= \frac{1}{4} [1 + \cos \theta (\tau_1^z + \tau_2^z) + \tau_1^z \tau_2^z + \sin \theta \cos \phi (\tau_1^x \tau_2^x - \tau_1^y \tau_2^y) + \sin \theta \sin \phi (\tau_1^x \tau_2^y + \tau_1^y \tau_2^x)] \end{aligned} \quad (22)$$

involves only the 8 operators that commute with $\tau_1^z \tau_2^z$ among the 16 operators of the tensor basis $\tau_1^a \otimes \tau_2^b$ with $a = 0, x, y, z$ and $b = 0, x, y, z$. In the next section, the exact decomposition of Eq. 16 for $N = 2$ spins is used as the building block to construct the simplest approximation for the ket $|\psi_N\rangle$ for an open chain of N spins via a Matrix-Product-State of Schmidt dimension $D = 2$.

III. SIMPLEST MATRIX-PRODUCT-STATE FOR AN OPEN CHAIN OF N SPINS

In this section, the gauge fixing described in the previous section is used to build the simplest Matrix-Product-State for an open chain of N spins in terms of $(4N - 2)$ parameters with a clear physical meaning.

A. Parametrization of the MPS ket $|\psi\rangle$ in terms of $(4N - 2)$ angles

For each spin $k = 1, \dots, N$, two Bloch angles θ_k and ϕ_k will be used to parametrize the new appropriate local basis $|\tau_k^z = \pm\rangle$ as in Eq. 17. For each bond $(k, k + 1)$ with $k = 1, \dots, N - 1$, two angles $\theta_{k+\frac{1}{2}}$ and $\phi_{k+\frac{1}{2}}$ will be used to

parametrize the two complex Schmidt values as in Eq 15

$$\begin{aligned}\lambda_{k,k+1}^+ &\equiv \cos\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) \\ \lambda_{k,k+1}^- &\equiv \sin\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) e^{i\phi_{k+\frac{1}{2}}}\end{aligned}\quad (23)$$

With these $(4N - 2)$ angles, the following Matrix-Product-State is constructed by adapting the Vidal canonical form recalled Eq. 3 to the present gauge fixing

$$\begin{aligned}|\psi\rangle &= \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{N-1}=\pm} |\tau_1^z = \alpha_1\rangle \lambda_{1,2}^{\alpha_1} |\tau_2^z = \alpha_1\alpha_2\rangle \lambda_{2,3}^{\alpha_2} |\tau_3^z = \alpha_2\alpha_3\rangle \lambda_{3,4}^{\alpha_3} \dots \\ &\dots |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \lambda_{k,k+1}^{\alpha_k} |\tau_{k+1}^z = \alpha_k\alpha_{k+1}\rangle \dots |\tau_{N-1}^z = \alpha_{N-2}\alpha_{N-1}\rangle \lambda_{N-1,N}^{\alpha_{N-1}} |\tau_N^z = \alpha_{N-1}\rangle \\ &= \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{N-1}=\pm} \left[\prod_{k=1}^{N-1} \lambda_{k,k+1}^{\alpha_k} \right] \left[\prod_{k=1}^N |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \right]\end{aligned}\quad (24)$$

with the following convention for the boundary conditions on the last line

$$\begin{aligned}\alpha_0 &= 1 \\ \alpha_N &= 1\end{aligned}\quad (25)$$

Eq. 24 represents the simplest generalization beyond the mean-field product state of the $|\tau_k^z = +\rangle$ (that would corresponds to the Schmidt values $\lambda_{k,k+1}^+ = 1$ and $\lambda_{k,k+1}^- = 0$)

$$|\psi^{MF}\rangle = |\tau_1^z = +\rangle |\tau_2^z = +\rangle \dots |\tau_N^z = +\rangle \quad (26)$$

where one introduces quantum fluctuations on each site via the opposite ket $|\tau_k^z = -\rangle$, and where one introduces entanglement on each bond via the Schmidt values $\lambda_{k,k+1}^- \neq 0$ of Eq. 23.

B. Corresponding Matrix-Product-Operator form of the full density matrix ρ

Using the same convention for the boundary conditions as in Eq. 25

$$\begin{aligned}\beta_0 &= 1 \\ \beta_N &= 1\end{aligned}\quad (27)$$

the MPS state of Eq. 24 translates into the following Matrix-Product-Operator form for the full density matrix

$$\rho = |\psi\rangle \langle\psi| = \sum_{\substack{\alpha_1=\pm \\ \beta_1=\pm}} \dots \sum_{\substack{\alpha_{N-1}=\pm \\ \beta_{N-1}=\pm}} \left[\prod_{k=1}^{N-1} \Lambda_{k,k+1}^{\alpha_k, \beta_k} \right] \left[\prod_{k=1}^N O_k^{\alpha_{k-1}\alpha_k, \beta_{k-1}\beta_k} \right] \quad (28)$$

with the following notations. The variables $\Lambda_{k,k+1}^{\alpha, \beta}$ associated to the bond $(k, k+1)$ involve two indices $\alpha = \pm$ and $\beta = \pm$ and read in terms of the complex Schmidt values of Eq. 23

$$\Lambda_{k,k+1}^{\alpha, \beta} \equiv \lambda_{k,k+1}^{\alpha} \overline{\lambda_{k,k+1}^{\beta}} \quad (29)$$

i.e. they correspond to the following four values in terms of the two angles of Eq. 23

$$\begin{aligned}\Lambda_{k,k+1}^{+,+} &= \left| \lambda_{k,k+1}^+ \right|^2 = \cos^2\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) = \frac{1 + \cos\left(\theta_{k+\frac{1}{2}}\right)}{2} \\ \Lambda_{k,k+1}^{-,-} &= \left| \lambda_{k,k+1}^- \right|^2 = \sin^2\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) = \frac{1 - \cos\left(\theta_{k+\frac{1}{2}}\right)}{2} \\ \Lambda_{k,k+1}^{+,-} &= \lambda_{k,k+1}^+ \overline{\lambda_{k,k+1}^-} = \cos\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) e^{-i\phi_{k+\frac{1}{2}}} = \frac{\sin\left(\theta_{k+\frac{1}{2}}\right)}{2} e^{-i\phi_{k+\frac{1}{2}}} \\ \Lambda_{k,k+1}^{-,+} &= \lambda_{k,k+1}^- \overline{\lambda_{k,k+1}^+} = \sin\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) e^{i\phi_{k+\frac{1}{2}}} \cos\left(\frac{\theta_{k+\frac{1}{2}}}{2}\right) = \frac{\sin\left(\theta_{k+\frac{1}{2}}\right)}{2} e^{i\phi_{k+\frac{1}{2}}}\end{aligned}\quad (30)$$

that can be summarized by

$$\Lambda_{k,k+1}^{\alpha,\beta} = \delta_{\alpha,\beta} \left(\frac{1 + \alpha \cos(\theta_{k+\frac{1}{2}})}{2} \right) + \delta_{\alpha,-\beta} \left(\frac{\sin(\theta_{k+\frac{1}{2}}) \left[\cos(\phi_{k+\frac{1}{2}}) - i\alpha \cos(\phi_{k+\frac{1}{2}}) \right]}{2} \right) \quad (31)$$

The operators $O_k^{T,T'}$ associated to the site k involve two indices $T = \pm 1$ and $T' = \pm$

$$O_k^{T,T'} \equiv |\tau_k^z = T\rangle \langle \tau_k^z = T'| \quad (32)$$

i.e. these four operators correspond to the two projectors that can be rewritten in terms of $(1, \tau_k^z)$

$$\begin{aligned} O_k^{+,+} &= |\tau_k^z = +\rangle \langle \tau_k^z = +| = \frac{1 + \tau_k^z}{2} \\ O_k^{-,-} &= |\tau_k^z = -\rangle \langle \tau_k^z = -| = \frac{1 - \tau_k^z}{2} \end{aligned} \quad (33)$$

and to the two ladder operators that can be rewritten in terms of (τ_k^x, τ_k^y)

$$\begin{aligned} O_k^{+,-} &= |\tau_k^z = +\rangle \langle \tau_k^z = -| = \tau_k^+ = \frac{\tau_k^x + i\tau_k^y}{2} \\ O_k^{-,+} &= |\tau_k^z = -\rangle \langle \tau_k^z = +| = \tau_k^- = \frac{\tau_k^x - i\tau_k^y}{2} \end{aligned} \quad (34)$$

that can be summarized by

$$O_k^{T,T'} = |\tau_k^z = T\rangle \langle \tau_k^z = T'| = \delta_{T,T'} \left(\frac{1 + T\tau_k^z}{2} \right) + \delta_{T,-T'} \left(\frac{\tau_k^x + iT\tau_k^y}{2} \right) \quad (35)$$

These operators could be rewritten in terms of the two angles (θ_k, ϕ_k) and of the initial Pauli basis $(1, \sigma_k^z, \sigma_k^x, \sigma_k^y)$ using Eq 18, but in the present paper it will be more convenient to do all the calculations in the basis τ .

Plugging the explicit forms of Eq. 31 and Eq. 35 into Eq. 28, one obtains the more explicit Matrix-Product-Operator form of the full density matrix

$$\begin{aligned} \rho &= \sum_{\substack{\alpha_1=\pm \\ \beta_1=\pm}} \dots \sum_{\substack{\alpha_{N-1}=\pm \\ \beta_{N-1}=\pm}} \left(\prod_{k=1}^N \left[\delta_{\alpha_{k-1}\alpha_k, \beta_{k-1}\beta_k} \left(\frac{1 + \alpha_{k-1}\alpha_k\tau_k^z}{2} \right) + \delta_{\alpha_{k-1}\alpha_k, -\beta_{k-1}\beta_k} \frac{\tau_k^x + i\alpha_{k-1}\alpha_k\tau_k^y}{2} \right] \right) \\ &\left(\prod_{k=1}^{N-1} \left[\delta_{\alpha_k, \beta_k} \left(\frac{1 + \alpha_k \cos(\theta_{k+\frac{1}{2}})}{2} \right) + \delta_{\alpha_k, -\beta_k} \left(\frac{\sin(\theta_{k+\frac{1}{2}}) \left[\cos(\phi_{k+\frac{1}{2}}) - i\alpha_k \cos(\phi_{k+\frac{1}{2}}) \right]}{2} \right) \right] \right) \end{aligned} \quad (36)$$

C. Schmidt decomposition across the bond $[k, k+1]$

The Schmidt decomposition of the ket of Eq. 24 with respect to the bond $[k, k+1]$ reads

$$|\psi\rangle = \sum_{\alpha=\pm} |\Phi_\alpha^{[1,\dots,k]}\rangle \lambda_{k,k+1}^\alpha |\Phi_\alpha^{[k+1,\dots,N]}\rangle \quad (37)$$

where the two complex Schmidt values $\lambda_{k,k+1}^\pm$ have been given in Eq 23, while the corresponding orthonormalized Schmidt eigenvectors $|\Phi_\pm^{[1,\dots,k]}\rangle$ of the Left part $[1, 2, \dots, k]$ and the corresponding orthonormalized Schmidt eigenvectors $|\Phi_\pm^{[k+1,\dots,N]}\rangle$ of the Right part $[k+1, \dots, N]$

$$\begin{aligned} \langle \Phi_\alpha^{[1,\dots,k]} | \Phi_\beta^{[1,\dots,k]} \rangle &= \delta_{\alpha\beta} \\ \langle \Phi_\alpha^{[k+1,\dots,N]} | \Phi_\beta^{[k+1,\dots,N]} \rangle &= \delta_{\alpha\beta} \end{aligned} \quad (38)$$

read

$$\begin{aligned}
|\Phi_\alpha^{[1,\dots,k]}\rangle &\equiv \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{k-1}=\pm} |\tau_1^z = \alpha_1\rangle \lambda_{1,2}^{\alpha_1} |\tau_2^z = \alpha_1\alpha_2\rangle \lambda_{2,3}^{\alpha_2} |\tau_3^z = \alpha_2\alpha_3\rangle \lambda_{3,4}^{\alpha_3} \dots \lambda_{k-1,k}^{\alpha_{k-1}} |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \\
&= \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{k-1}=\pm} \left[\prod_{n=1}^{k-1} \lambda_{n,n+1}^{\alpha_n} \right] \left[\prod_{n=1}^{k-1} |\tau_n^z = \alpha_{n-1}\alpha_n\rangle \right] |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \\
|\Phi_\alpha^{[k+1,\dots,N]}\rangle &\equiv \sum_{\alpha_{k+1}=\pm} \dots \sum_{\alpha_{N-1}=\pm} |\tau_{k+1}^z = \alpha\alpha_{k+1}\rangle \lambda_{k+1,k+2}^{\alpha_{k+1}} \dots |\tau_{N-1}^z = \alpha_{N-2}\alpha_{N-1}\rangle \lambda_{N-1,N}^{\alpha_{N-1}} |\tau_N^z = \alpha_{N-1}\alpha_N\rangle \\
&= \sum_{\alpha_{k+1}=\pm} \dots \sum_{\alpha_{N-1}=\pm} \left[\prod_{n=k+1}^{N-1} \lambda_{n,n+1}^{\alpha_n} \right] |\tau_{k+1}^z = \alpha\alpha_{k+1}\rangle \left[\prod_{n=k+2}^N |\tau_n^z = \alpha_{n-1}\alpha_n\rangle \right]
\end{aligned} \tag{39}$$

and satisfy the recurrences

$$\begin{aligned}
|\Phi_\alpha^{[1,\dots,k]}\rangle &\equiv \sum_{\alpha_{k-1}=\pm} |\Phi_{\alpha_{k-1}}^{[1,\dots,k-1]}\rangle \lambda_{k-1,k}^{\alpha_{k-1}} |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \\
|\Phi_\alpha^{[k,\dots,N]}\rangle &= \sum_{\alpha_k=\pm} |\tau_k^z = \alpha\alpha_k\rangle \lambda_{k,k+1}^{\alpha_k} |\Phi_{\alpha_k}^{[k+1,\dots,N]}\rangle
\end{aligned} \tag{40}$$

The Schmidt decomposition of Eq. 37 for the MPS across the bond $[k, k+1]$ translates into the following decomposition for the density matrix

$$\rho = |\psi\rangle\langle\psi| = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left(|\Phi_\alpha^{[1,\dots,k]}\rangle\langle\Phi_\beta^{[1,\dots,k]}| \right) \Lambda_{k,k+1}^{\alpha,\beta} \left(|\Phi_\alpha^{[k+1,\dots,N]}\rangle\langle\Phi_\beta^{[k+1,\dots,N]}| \right) \tag{41}$$

The reduced density matrices of the Left part $[1, \dots, k]$ and of the Right part $[k+1, \dots, N]$ read

$$\begin{aligned}
\rho_{[1,\dots,k]} &= \sum_{\alpha=\pm} \Lambda_{k,k+1}^{\alpha,\alpha} |\Phi_\alpha^{[1,\dots,k]}\rangle\langle\Phi_\alpha^{[1,\dots,k]}| \\
&= \left(\frac{1 + \cos(\theta_{k+\frac{1}{2}})}{2} \right) |\Phi_+^{[1,\dots,k]}\rangle\langle\Phi_+^{[1,\dots,k]}| + \left(\frac{1 - \cos(\theta_{k+\frac{1}{2}})}{2} \right) |\Phi_-^{[1,\dots,k]}\rangle\langle\Phi_-^{[1,\dots,k]}| \\
\rho_{[k+1,\dots,N]} &= \sum_{\alpha=\pm} \Lambda_{k,k+1}^{\alpha,\alpha} |\Phi_\alpha^{[k+1,\dots,N]}\rangle\langle\Phi_\alpha^{[k+1,\dots,N]}| \\
&= \left(\frac{1 + \cos(\theta_{k+\frac{1}{2}})}{2} \right) |\Phi_+^{[k+1,\dots,N]}\rangle\langle\Phi_+^{[k+1,\dots,N]}| + \left(\frac{1 - \cos(\theta_{k+\frac{1}{2}})}{2} \right) |\Phi_-^{[k+1,\dots,N]}\rangle\langle\Phi_-^{[k+1,\dots,N]}|
\end{aligned} \tag{42}$$

For the special case $k=1$ of the Schmidt decomposition across the bond $(1, 2)$, one obtains that the ket $|\tau_1^z = \pm\rangle$ corresponds to the Schmidt eigenvectors $|\Phi_\pm^{[1]}\rangle$

$$|\Phi_\pm^{[1]}\rangle \equiv |\tau_1^z = \pm\rangle \tag{43}$$

that diagonalize the reduced density matrix for the boundary spin $k=1$

$$\rho_1 = \frac{1}{2} \left[1 + \cos(\theta_{\frac{3}{2}}) \tau_1^z \right] \tag{44}$$

Similarly, the special case $k=N-1$, the Schmidt decomposition across the bond $(k, k+1) = (N-1, N)$ yields that the boundary ket $|\tau_N^z = \pm\rangle$ are directly the Schmidt eigenvectors

$$|\Phi_\pm^{[N]}\rangle \equiv |\tau_N^z = \pm\rangle \tag{45}$$

that diagonalize the reduced density matrix

$$\rho_N = \frac{1}{2} \left[1 + \cos(\theta_{N-\frac{1}{2}}) \tau_N^z \right] \tag{46}$$

D. Reduced density matrix ρ_k for the site k in the bulk ($k = 2, \dots, N-1$)

If one wishes to focus on the spin k with the simultaneous Schmidt decomposition with respect to the Left part $[1, \dots, k-1]$ and to the Right part $[k+1, \dots, N]$, Eq 24 becomes with Eq. 39

$$|\psi\rangle = \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} |\Phi_{\alpha_L}^{[1, \dots, k-1]}\rangle \lambda_{k-1, k}^{\alpha_L} |\tau_k^z = \alpha_L \alpha_R\rangle \lambda_{k, k+1}^{\alpha_R} |\Phi_{\alpha_R}^{[k+1, \dots, N]}\rangle \quad (47)$$

leading to the full density matrix

$$\rho = |\psi\rangle \langle \psi| = \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1, \dots, k-1]}\rangle \langle \Phi_{\beta_L}^{[1, \dots, k-1]}| \right) \Lambda_{k-1, k}^{\alpha_L, \beta_L} O_k^{\alpha_L \alpha_R, \beta_L \beta_R} \Lambda_{k, k+1}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+1, \dots, N]}\rangle \langle \Phi_{\beta_R}^{[k+1, \dots, N]}| \right) \quad (48)$$

The orthonormalization of the Schmidt eigenvectors (Eq 38) yields that the trace over the Left part $[1, \dots, k-1]$ imposes $\beta_L = \alpha_L$, while the trace over the Right part $[k+1, \dots, N]$ imposes $\beta_R = \alpha_R$, so that the reduced density matrix for the spin k alone reduces to

$$\rho_k = \text{Tr}_{\{1, \dots, k-1\}, \{k+1, \dots, N\}}(\rho) = \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} \Lambda_{k-1, k}^{\alpha_L, \alpha_L} O_k^{\alpha_L \alpha_R, \alpha_L \alpha_R} \Lambda_{k, k+1}^{\alpha_R, \alpha_R} \quad (49)$$

The explicit expressions of Eq. 31 and of Eq. 35 lead to the final result

$$\begin{aligned} \rho_k &= \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} \left(\frac{1 + \alpha_L \cos\left(\theta_{k-\frac{1}{2}}\right)}{2} \right) \left(\frac{1 + \alpha_L \alpha_R \tau_k^z}{2} \right) \left(\frac{1 + \alpha_R \cos\left(\theta_{k+\frac{1}{2}}\right)}{2} \right) \\ &= \frac{1}{2} \left[1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \tau_k^z \cos\left(\theta_{k+\frac{1}{2}}\right) \right] \end{aligned} \quad (50)$$

So the two ket $|\tau_k^z = \pm\rangle$ parametrized by the two Bloch angles (θ_k, ϕ_k) (Eq. 17) are the two eigenvectors of the reduced density matrix ρ_k with the corresponding eigenvalues

$$p_k^\pm = \frac{1}{2} \left[1 \pm \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{1}{2}}\right) \right] \quad (51)$$

that involve the angles $\theta_{k\pm\frac{1}{2}}$ of the two neighboring bonds.

E. Multifractality of the MPS components in the $\{\tau_k^z\}$ basis

The groundstate wavefunction of manybody quantum systems have been found to be generically multifractal, with many studies concerning the Shannon-Rényi entropies in quantum spin models [30–46], while multifractal properties have been also much studied recently in the field of Many-Body-Localization [47–50]. Of course this multifractal analysis depends on the basis, and a natural question is thus to determine what is the more appropriate basis in each context. Here since the ket $|\tau_k^z = \pm\rangle$ are the two eigenvectors of the one-site density matrix ρ_k (Eq 50), it is interesting to consider the expansion of the MPS of Eq 24 in this basis $\tau_k^z = \pm 1$ (instead of the expansion of Eq. 1 in the initial basis $\sigma_k^z = \pm 1$)

$$|\psi\rangle = \sum_{T_1=\pm 1} \sum_{T_2=\pm 1} \dots \sum_{T_N=\pm 1} \psi_{T_1, \dots, T_N} |\tau_1^z = T_1\rangle |\tau_2^z = T_2\rangle \dots |\tau_N^z = T_N\rangle \quad (52)$$

in order to characterize the statistics of the coefficients

$$\begin{aligned} \psi_{T_1, \dots, T_N} &= (\langle \tau_1^z = T_1 | \langle \tau_2^z = T_2 | \dots \langle \tau_N^z = T_N |) |\psi\rangle \\ &= \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{N-1}=\pm} \delta_{T_1, \alpha_1} \lambda_{1,2}^{\alpha_1} \delta_{T_2, \alpha_1 \alpha_2} \lambda_{2,3}^{\alpha_2} \delta_{T_3, \alpha_2 \alpha_3} \dots \lambda_{N-2, N-1}^{\alpha_{N-2}} \delta_{T_{N-1}, \alpha_{N-2} \alpha_{N-1}} \lambda_{N-1, N}^{\alpha_{N-1}} \delta_{T_N, \alpha_{N-1}} \\ &= \delta_{1, (T_1 T_2 \dots T_N)} \lambda_{1,2}^{T_1} \lambda_{2,3}^{(T_1 T_2)} \lambda_{3,4}^{(T_1 T_2 T_3)} \dots \lambda_{N-2, N-1}^{(T_1 T_2 \dots T_{N-2})} \lambda_{N-1, N}^{(T_1 T_2 \dots T_{N-1})} = \delta_{1, (T_1 T_2 \dots T_N)} \prod_{k=1}^{N-1} \lambda_{k, k+1}^{(T_1 T_2 \dots T_k)} \end{aligned} \quad (53)$$

Besides the global constraint $1 = T_1 T_2 \dots T_N$, these coefficients are thus simply given by the product of the complex Schmidt values $\lambda_{k,k+1}^{\alpha_k}$ (Eq 23) along the whole chain with the indices

$$\alpha_k = T_1 T_2 \dots T_k \quad (54)$$

The maximal weight $|\psi_{T_1, \dots, T_N}|^2$ corresponds to the case where each bond $[k, k+1]$ is in its biggest Schmidt value $\lambda_{k,k+1}^+$ corresponding to $T_k = +1$ for all k (i.e. the state of Eq. 26)

$$|\psi_{max}|^2 = |\psi_{++++\dots++++}|^2 = \prod_{k=1}^{N-1} |\lambda_{k,k+1}^+|^2 = \prod_{k=1}^{N-1} \cos^2 \left(\frac{\theta_{k+\frac{1}{2}}}{2} \right) = \prod_{k=1}^{N-1} \left[\frac{1 + \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right] \quad (55)$$

On the contrary, the minimal weight $|\psi_{T_1, \dots, T_N}|^2$ corresponds to the case where each bond $[k, k+1]$ is in its lowest Schmidt value $\lambda_{k,k+1}^-$: the two possibilities are thus $T_k = (-1)^k$, or $T_k = -(-1)^k$ for N even

$$|\psi_{min}|^2 = |\psi_{+-+-+\dots-}|^2 = |\psi_{-+-+-+\dots-}|^2 = \prod_{k=1}^{N-1} |\lambda_{k,k+1}^-|^2 = \prod_{k=1}^{N-1} \sin^2 \left(\frac{\theta_{k+\frac{1}{2}}}{2} \right) = \prod_{k=1}^{N-1} \left[\frac{1 - \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right] \quad (56)$$

More generally, the statistics of all the weights $|\psi_{T_1, \dots, T_N}|^2$ normalized to unity can be analyzed via the Inverse Participation Ratios $Y_q(N)$ where q is a continuous parameter

$$\begin{aligned} Y_q(N) &\equiv \sum_{T_1=\pm 1} \sum_{T_2=\pm 1} \dots \sum_{T_N=\pm 1} |\psi_{T_1, \dots, T_N}|^2 \\ &= \sum_{\alpha_1=\pm 1} \sum_{\alpha_2=\pm 1} \dots \sum_{\alpha_{N-1}=\pm 1} \prod_{k=1}^{N-1} |\lambda_{k,k+1}^{\alpha_k}|^{2q} = \prod_{k=1}^{N-1} \left(|\lambda_{k,k+1}^+|^{2q} + |\lambda_{k,k+1}^-|^{2q} \right) \\ &= \prod_{k=1}^{N-1} \left(\cos^{2q} \left(\frac{\theta_{k+\frac{1}{2}}}{2} \right) + \sin^{2q} \left(\frac{\theta_{k+\frac{1}{2}}}{2} \right) \right) = \prod_{k=1}^{N-1} \left(\left[\frac{1 + \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q + \left[\frac{1 - \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q \right) \end{aligned} \quad (57)$$

or equivalently with the corresponding Rényi entropies

$$\mathcal{S}_q(N) \equiv \frac{\ln Y_q(N)}{1-q} = \frac{1}{1-q} \sum_{k=1}^{N-1} \ln \left(\left[\frac{1 + \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q + \left[\frac{1 - \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q \right) \quad (58)$$

The leading extensive behavior of the Rényi entropies define the generalized fractal dimensions $0 \leq \mathcal{D}_q \leq 1$

$$S_q(N) \underset{N \rightarrow +\infty}{\propto} \mathcal{D}_q (N \ln 2) \quad (59)$$

so here one obtains that the generalized fractal dimensions

$$\mathcal{D}_q = \frac{1}{(1-q) \ln 2} \lim_{N \rightarrow +\infty} \left[\frac{1}{N} \sum_{k=1}^{N-1} \ln \left(\left[\frac{1 + \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q + \left[\frac{1 - \cos \left(\theta_{k+\frac{1}{2}} \right)}{2} \right]^q \right) \right] \quad (60)$$

correspond to the spatial average over $k = 1, \dots, N-1$ of some q -dependent function of the bond angles $\theta_{k+\frac{1}{2}}$.

This specific example suggests that in other contexts, it would be also interesting to analyze the multifractality in the basis that diagonalize the individual single-site reduced density matrices in order to avoid the arbitrariness of the choice of the basis and in order to characterize directly the global entanglement properties along the chain.

IV. REDUCED DENSITY MATRIX $\rho_{k,k+1, \dots, k+r}$ OF $(r+1)$ CONSECUTIVE SITES IN THE BULK

A. Simultaneous Schmidt decomposition across the two distant bonds $(k-1, k)$ and $(k+r, k+r+1)$

After considering the Schmidt decomposition across a single bond (Eq. 37) and across two neighboring bonds (Eq. 47), it is now interesting to focus on the simultaneous Schmidt decomposition across the two distant bonds $(k-1, k)$

and $(k+r, k+r+1)$ by rewriting Eq. 24 as

$$|\psi\rangle = \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} |\Phi_{\alpha_L}^{[1,\dots,k-1]}\rangle \lambda_{k-1,k}^{\alpha_L} |I_{\alpha_L,\alpha_R}^{[k,\dots,k+r]}\rangle \lambda_{k+r,k+r+1}^{\alpha_R} |\Phi_{\alpha_R}^{[k+r+1,\dots,N]}\rangle \quad (61)$$

where the four ket $|I_{\alpha_L=\pm,\alpha_R=\pm}^{[k,\dots,k+r]}\rangle$ associated to the interval $[k, \dots, k+r]$ read

$$|I_{\alpha_L,\alpha_R}^{[k,\dots,k+r]}\rangle \equiv \sum_{\alpha_k=\pm} \dots \sum_{\alpha_{k+r-1}=\pm} \left[\prod_{n=k}^{k+r-1} \lambda_{n,n+1}^{\alpha_n} \right] |\tau_k^z = \alpha_L \alpha_k\rangle \left[\prod_{n=k+1}^{k+r-1} |\tau_n^z = \alpha_{n-1} \alpha_n\rangle \right] |\tau_{k+r}^z = \alpha_{k+r-1} \alpha_R\rangle \quad (62)$$

Their scalar products can be computed using Eq. 31

$$\begin{aligned} \langle I_{\beta_L,\beta_R}^{[k,\dots,k+r]} | I_{\alpha_L,\alpha_R}^{[k,\dots,k+r]} \rangle &= \delta_{\beta_L\beta_R,\alpha_L\alpha_R} \prod_{n=k}^{k+r-1} \left[\sum_{\alpha_n=\pm} \lambda_{n,n+1}^{\alpha_n} \overline{\lambda_{n,n+1}^{(\beta_L\alpha_L)\alpha_n}} \right] = \delta_{\beta_L\beta_R,\alpha_L\alpha_R} \prod_{n=k}^{k+r-1} \left[\sum_{\alpha_n=\pm} \Lambda_{n,n+1}^{\alpha_n,(\beta_L\alpha_L)\alpha_n} \right] \\ &= \delta_{\beta_L\beta_R,\alpha_L\alpha_R} \\ &\prod_{n=k}^{k+r-1} \left[\sum_{\alpha_n=\pm} \left(\delta_{\alpha_L,\beta_L} \left(\frac{1 + \alpha_n \cos(\theta_{n+\frac{1}{2}})}{2} \right) + \delta_{\alpha_L,-\beta_L} \left(\frac{\sin(\theta_{n+\frac{1}{2}}) [\cos(\phi_{n+\frac{1}{2}}) - i\alpha_n \cos(\phi_{n+\frac{1}{2}})]}{2} \right) \right) \right] \\ &= \delta_{\beta_L\beta_R,\alpha_L\alpha_R} \prod_{n=k}^{k+r-1} \left[\delta_{\alpha_L,\beta_L} + \delta_{\alpha_L,-\beta_L} \sin(\theta_{n+\frac{1}{2}}) \cos(\phi_{n+\frac{1}{2}}) \right] \\ &= \delta_{\beta_L\beta_R,\alpha_L\alpha_R} [\delta_{\alpha_L,\beta_L} + \delta_{\alpha_L,-\beta_L} \omega_{k,k+r}] \end{aligned} \quad (63)$$

where we have introduced the notation

$$\omega_{k,k+r} \equiv \prod_{n=k}^{k+r-1} \left[\sin(\theta_{n+\frac{1}{2}}) \cos(\phi_{n+\frac{1}{2}}) \right] \quad (64)$$

This parameter will appear in various observables that involve the correlations between the sites k and $k+r$ separated by the distance r .

Eq. 63 means that these four ket are normalized

$$\langle I_{\alpha_L,\alpha_R}^{[k,\dots,k+r]} | I_{\alpha_L,\alpha_R}^{[k,\dots,k+r]} \rangle = 1 \quad (65)$$

and can be classified into the two following orthogonal subspaces :

(i) the subspace $\alpha_L\alpha_R = 1$ is generated by the two ket $|I_{+,+}^{[k,\dots,k+r]}\rangle$ and $|I_{-,-}^{[k,\dots,k+r]}\rangle$ whose overlap is given by Eq 64

$$\langle I_{-,-}^{[k,\dots,k+r]} | I_{+,+}^{[k,\dots,k+r]} \rangle = \omega_{k,k+r} \quad (66)$$

(ii) the subspace $\alpha_L\alpha_R = -1$ is generated by the two ket $|I_{+,-}^{[k,\dots,k+r]}\rangle$ and $|I_{-,+}^{[k,\dots,k+r]}\rangle$ whose overlap is also given by Eq. 64

$$\langle I_{-,+}^{[k,\dots,k+r]} | I_{+,-}^{[k,\dots,k+r]} \rangle = \omega_{k,k+r} \quad (67)$$

The comparison of Eq. 61 with the Schmidt decomposition across the single bond $(k-1, k)$ yields the following recursions for the Schmidt eigenvectors of the Right part

$$|\Phi_{\alpha}^{[k,\dots,N]}\rangle = \sum_{\alpha_R=\pm} |I_{\alpha,\alpha_R}^{[k,\dots,k+r]}\rangle \lambda_{k+r,k+r+1}^{\alpha_R} |\Phi_{\alpha_R}^{[k+r+1,\dots,N]}\rangle \quad (68)$$

while the comparison with the Schmidt decomposition across the single bond $(k+r, k+r+1)$ yields the following recursion for the Schmidt eigenvectors of the Right part

$$|\Phi_{\alpha}^{[1,\dots,k+r]}\rangle = \sum_{\alpha_L=\pm} |\Phi_{\alpha_L}^{[1,\dots,k-1]}\rangle \lambda_{k-1,k}^{\alpha_L} |I_{\alpha_L,\alpha}^{[k,\dots,k+r]}\rangle \quad (69)$$

that generalizes the recurrences of Eqs 40 concerning a difference of a single site.

The interval ket of Eq. 62 satisfy the following recurrences with respect to their leftmost spin k or with respect to the rightmost spin ($k+r$)

$$\begin{aligned} |I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle &= \sum_{\alpha=\pm} |\tau_k^z = \alpha_L \alpha\rangle \lambda_{k, k+1}^\alpha |I_{\alpha, \alpha_R}^{[k+1, \dots, k+r]}\rangle \\ |I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle &= \sum_{\alpha=\pm} |I_{\alpha_L, \alpha}^{[k, \dots, k+r-1]}\rangle \lambda_{k+r-1, k+r}^\alpha |\tau_{k+r}^z = \alpha \alpha_R\rangle \end{aligned} \quad (70)$$

and satisfy more generally the following decomposition with respect to any internal bond ($n, n+1$)

$$|I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle = \sum_{\alpha=\pm} |I_{\alpha_L, \alpha}^{[k, \dots, n]}\rangle \lambda_{n, n+1}^\alpha |I_{\alpha, \alpha_R}^{[n+1, \dots, k+r]}\rangle \quad (71)$$

The Schmidt decomposition of Eq. 61 for the MPS ket translates into the following decomposition for the full density matrix

$$\begin{aligned} \rho &= |\psi\rangle \langle \psi| = \sum_{\substack{\alpha_L=\pm, \alpha_R=\pm \\ \beta_L=\pm, \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1, \dots, k-1]}\rangle \langle \Phi_{\beta_L}^{[1, \dots, k-1]}| \right) \Lambda_{k-1, k}^{\alpha_L, \beta_L} \left(|I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle \langle I_{\beta_L, \beta_R}^{[k, \dots, k+r]}| \right) \Lambda_{k+r, k+r+1}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+r+1, \dots, N]}\rangle \langle \Phi_{\beta_R}^{[k+r+1, \dots, N]}| \right) \end{aligned} \quad (72)$$

Depending on the applications, it will be convenient to keep the interval operators $\left(|I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle \langle I_{\beta_L, \beta_R}^{[k, \dots, k+r]}| \right)$ in their global form in terms of the interval ket, or it will be more convenient to write their Matrix-Product-Operator form analogous to Eq. 28

$$\begin{aligned} |I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle \langle I_{\beta_L, \beta_R}^{[k, \dots, k+r]}| &= \sum_{\substack{\alpha_k=\pm \\ \beta_k=\pm}} \dots \sum_{\substack{\alpha_{k+r-1}=\pm \\ \beta_{k+r-1}=\pm}} \left[\prod_{n=k}^{k+r-1} \Lambda_{n, n+1}^{\alpha_n, \beta_n} \right] \\ &O_k^{(\alpha_L \alpha_k), (\beta_L \beta_k)} \left[\prod_{n=k+1}^{k+r-1} O_n^{(\alpha_{n-1} \alpha_n), (\beta_{n-1} \beta_n)} \right] O_{k+r}^{(\alpha_{k+r-1} \alpha_R), (\beta_{k+r-1} \beta_R)} \end{aligned} \quad (73)$$

B. Global properties of the reduced density matrix $\rho_{k, k+1, \dots, k+r}$ of the interval $[k, \dots, k+r]$

The reduced density matrix $\rho_{k, k+1, \dots, k+r}$ of the interval $[k, \dots, k+r]$ can be computed from the full density matrix of Eq. 72 by taking the trace over the Left part $[1, \dots, k-1]$ that imposes $\beta_L = \alpha_L$ and by taking the trace over the Right part $[k+r+1, \dots, N]$ that imposes $\beta_R = \alpha_R$

$$\rho_{k, k+1, \dots, k+r} \equiv \text{Tr}_{\{[1, \dots, k-1], [k+r+1, \dots, N]\}} (\rho) = \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} \Lambda_{k-1, k}^{\alpha_L, \alpha_L} \left(|I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle \langle I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}| \right) \Lambda_{k+r, k+r+1}^{\alpha_R, \alpha_R} \quad (74)$$

At the global level of the interval, this corresponds to the following weighted sum over the four projectors associated to the four ket of Eq. 62

$$\begin{aligned} \rho_{k, k+1, \dots, k+r} &= \Lambda_{k-1, k}^{+,+} |I_{+,+}^{[k, \dots, k+r]}\rangle \langle I_{+,+}^{[k, \dots, k+r]}| \Lambda_{k+r, k+r+1}^{+,+} + \Lambda_{k-1, k}^{-,-} |I_{-,-}^{[k, \dots, k+r]}\rangle \langle I_{-,-}^{[k, \dots, k+r]}| \Lambda_{k+r, k+r+1}^{-,-} \\ &+ \Lambda_{k-1, k}^{+,+} |I_{+,-}^{[k, \dots, k+r]}\rangle \langle I_{+,-}^{[k, \dots, k+r]}| \Lambda_{k+r, k+r+1}^{-,-} + \Lambda_{k-1, k}^{-,-} |I_{-,+}^{[k, \dots, k+r]}\rangle \langle I_{-,+}^{[k, \dots, k+r]}| \Lambda_{k+r, k+r+1}^{+,+} \end{aligned} \quad (75)$$

Note that this is not the spectral decomposition of the reduced density matrix $\rho_{k, k+1, \dots, k+r}$ as a consequence as the non-vanishing overlaps of Eq. 66 and of Eq. 67, but the diagonal form of $\rho_{k, k+1, \dots, k+r}$ is given in Appendix A.

C. Matrix-Product-Operator form of the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of the Interval $[k, \dots, k+r]$

Plugging the MPO form of Eq. 73 for the interval operators with the special values $\beta_L = \alpha_L$ and $\beta_R = \alpha_R$

$$\begin{aligned}
|I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}\rangle \langle I_{\alpha_L, \alpha_R}^{[k, \dots, k+r]}| &= \sum_{\substack{\alpha_k = \pm \\ \beta_k = \pm}} \dots \sum_{\substack{\alpha_{k+r-1} = \pm \\ \beta_{k+r-1} = \pm}} \left[\prod_{n=k}^{k+r-1} \Lambda_{n, n+1}^{\alpha_n, \beta_n} \right] \\
&O_k^{(\alpha_L \alpha_k), (\alpha_L \beta_k)} \left[\prod_{n=k+1}^{k+r-1} O_n^{(\alpha_{n-1} \alpha_n), (\beta_{n-1} \beta_n)} \right] O_{k+r}^{(\alpha_{k+r-1} \alpha_R), (\beta_{k+r-1} \alpha_R)}
\end{aligned} \tag{76}$$

into Eq. 74 leads to the MPO form

$$\rho_{k, k+1, \dots, k+r} = \sum_{\substack{\alpha_k = \pm \\ \beta_k = \pm}} \dots \sum_{\substack{\alpha_{k+r-1} = \pm \\ \beta_{k+r-1} = \pm}} \left[\prod_{n=k}^{k+r-1} \Lambda_{n, n+1}^{\alpha_n, \beta_n} \right] W_{[k]}^{\alpha_k, \beta_k} \left[\prod_{n=k+1}^{k+r-1} O_n^{(\alpha_{n-1} \alpha_n), (\beta_{n-1} \beta_n)} \right] W_{[k+r]}^{\alpha_{k+r-1}, \beta_{k+r-1}} \tag{77}$$

with the two modified operators for the spins k and $(k+r)$ at the boundaries of the interval $[k, \dots, k+r]$

$$\begin{aligned}
W_{[k]}^{\alpha_k, \beta_k} &\equiv \sum_{\alpha_L = \pm} \Lambda_{k-1, k}^{\alpha_L, \alpha_L} O_k^{(\alpha_L \alpha_k), (\alpha_L \beta_k)} \\
W_{[k+r]}^{\alpha_{k+r-1}, \beta_{k+r-1}} &\equiv \sum_{\alpha_R = \pm} O_{k+r}^{(\alpha_{k+r-1} \alpha_R), (\beta_{k+r-1} \alpha_R)} \Lambda_{k+r, k+r+1}^{\alpha_R, \alpha_R}
\end{aligned} \tag{78}$$

Using Eqs 31 and 35, one obtains their explicit expressions in terms of the Pauli operators and the angles

$$\begin{aligned}
W_{[k]}^{\alpha_k, \beta_k} &= \sum_{\alpha_L = \pm} \left(\frac{1 + \alpha_L \cos\left(\theta_{k-\frac{1}{2}}\right)}{2} \right) \left[\delta_{\alpha_k, \beta_k} \left(\frac{1 + \alpha_L \alpha_k \tau_k^z}{2} \right) + \delta_{\alpha_k, -\beta_k} \left(\frac{\tau_k^x + i \alpha_L \alpha_k \tau_k^y}{2} \right) \right] \\
&= \delta_{\alpha_k, \beta_k} \left(\frac{1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \alpha_k \tau_k^z}{2} \right) + \delta_{\alpha_k, -\beta_k} \left(\frac{\tau_k^x + i \cos\left(\theta_{k-\frac{1}{2}}\right) \alpha_k \tau_k^y}{2} \right)
\end{aligned} \tag{79}$$

and similarly

$$\begin{aligned}
W_{[k+r]}^{\alpha_{k+r-1}, \beta_{k+r-1}} & \\
= \delta_{\alpha_{k+r-1}, \beta_{k+r-1}} \left(\frac{1 + \cos\left(\theta_{k+r+\frac{1}{2}}\right) \alpha_{k+r-1} \tau_{k+r}^z}{2} \right) + \delta_{\alpha_{k+r-1}, -\beta_{k+r-1}} \left(\frac{\tau_{k+r}^x + i \cos\left(\theta_{k+r+\frac{1}{2}}\right) \alpha_{k+r-1} \tau_{k+r}^y}{2} \right)
\end{aligned} \tag{80}$$

These results will be used in the section V concerning the energy of two-body Hamiltonians where one needs the MPO form of $\rho_{k, k+1}$, and will be used in the section VI concerning the correlations between two spins at distance r .

V. OPTIMIZATION OF THE MPS TO APPROXIMATE GROUND STATES

The MPS $|\psi\rangle$ or equivalently the corresponding full density matrix $\rho = |\psi\rangle \langle \psi|$ allows to compute the energy associated to an Hamiltonian H via

$$E = \langle \psi | H | \psi \rangle = \text{Tr}(H\rho) \tag{81}$$

For a given local Hamiltonian, the goal is then to find the MPS parameters that minimize the energy in order to obtain the best approximation of the ground-state within the MPS manifold.

A. General Hamiltonian with one-body and two-body terms

Let us consider a general Hamiltonian with one-body and two-body terms

$$H = \sum_{k=1}^N h_k + \sum_{k=1}^{N-1} h_{k,k+1} \quad (82)$$

The one-body Hamiltonian h_k acting on the spin k can be expanded in the Pauli basis $\sigma_k^{x,y,z}$ with three coefficients $B_k^{x,y,z}$ that play the role of the three components of the local magnetic field

$$h_k = \sum_{a=x,y,z} B_k^a \sigma_k^a = B_k^x \sigma_k^x + B_k^y \sigma_k^y + B_k^z \sigma_k^z \quad (83)$$

while the two-body Hamiltonian $h_{k,k+1}$ acting on the two consecutive spins k and $(k+1)$ can be expanded in the Pauli basis of these two spins with up to nine couplings $J_{k+\frac{1}{2}}^{ab}$

$$h_{k,k+1} \equiv \sum_{a=x,y,z} \sum_{b=x,y,z} J_{k+\frac{1}{2}}^{ab} \sigma_k^a \sigma_{k+1}^b \quad (84)$$

As a consequence, the energy of Eq. 81 can be decomposed into

$$E = \sum_{k=1}^N e_k + \sum_{k=1}^{N-1} e_{k,k+1} \quad (85)$$

where the elementary contributions associated to h_k and $h_{k,k+1}$ involve only the reduced density matrix of a single spin ρ_k and the reduced density matrix of two neighboring spins $\rho_{k,k+1}$

$$\begin{aligned} e_k &= \text{Tr}(h_k \rho) = \text{Tr}_{\{k\}}(h_k \rho_k) \\ e_{k,k+1} &= \text{Tr}(h_{k,k+1} \rho) = \text{Tr}_{\{k,k+1\}}(h_{k,k+1} \rho_{k,k+1}) \end{aligned} \quad (86)$$

B. Contribution e_k of h_k

Since the reduced density matrix ρ_k of Eq. 50 only contains the operator τ_k^z

$$\rho_k = \frac{1}{2} \left[1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{1}{2}}\right) \tau_k^z \right] \quad (87)$$

with the convention $\cos\left(\theta_{\frac{1}{2}}\right) = 1 = \cos\left(\theta_{N+\frac{1}{2}}\right)$ to describe also the two boundary spins (Eqs 44 and 46), it is convenient to translate the one-body Hamiltonian h_k of Eq. 83 into the τ basis using Eq. 20

$$h_k = \sum_{a=x,y,z} B_k^a \sigma_k^a = \sum_{a=x,y,z} \tilde{B}_k^a \tau_k^a \quad (88)$$

The contribution e_k of Eq. 86 actually involves only the component

$$\tilde{B}_k^z = \cos \theta_k B_k^z + \sin \theta_k (\cos \phi_k B_k^x + \sin \phi_k B_k^y) \quad (89)$$

as a consequence of the specific form of Eq. 87

$$e_k = \text{Tr}_{\{k\}}(h_k \rho_k) = \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{1}{2}}\right) \tilde{B}_k^z \quad (90)$$

If one wishes to see the role of each initial magnetic field component B_k^a in the initial basis σ , one can decompose Eq. 90

$$e_k = \sum_{a=x,y,z} B_k^a e_k^a \quad (91)$$

into the following contributions

$$\begin{aligned} e_k^z &= \cos\left(\theta_{k-\frac{1}{2}}\right) [\cos \theta_k] \cos\left(\theta_{k+\frac{1}{2}}\right) \\ e_k^x &= \cos\left(\theta_{k-\frac{1}{2}}\right) [\sin \theta_k \cos \phi_k] \cos\left(\theta_{k+\frac{1}{2}}\right) \\ e_k^y &= \cos\left(\theta_{k-\frac{1}{2}}\right) [\sin \theta_k \sin \phi_k] \cos\left(\theta_{k+\frac{1}{2}}\right) \end{aligned} \quad (92)$$

C. Matrix-Product-Operator form of the reduced density matrix $\rho_{k,k+1}$ of two consecutive sites $(k, k+1)$

The Matrix-Product-Operator form of the reduced density matrix $\rho_{k,k+1}$ of two consecutive sites $(k, k+1)$ corresponds to the special case $r = 1$ in Eq. 77. Using the explicit forms of Eqs 31, 79 and 80, one obtains the MPO form

$$\begin{aligned}
\rho_{k,k+1} &= \sum_{\alpha=\pm} \sum_{\beta=\pm} \Lambda_{k,k+1}^{\alpha,\beta} W_{[k]}^{\alpha,\beta} W_{k+1}^{\alpha,\beta} \\
&= \sum_{\alpha=\pm} \sum_{\beta=\pm} \left[\delta_{\alpha,\beta} \left(\frac{1 + \alpha \cos(\theta_{k+\frac{1}{2}})}{2} \right) + \delta_{\alpha,-\beta} \left(\frac{\sin(\theta_{k+\frac{1}{2}})}{2} e^{-i\alpha\phi_{k+\frac{1}{2}}} \right) \right] \\
&\quad \left[\delta_{\alpha,\beta} \left(\frac{1 + \cos(\theta_{k-\frac{1}{2}})}{2} \alpha \tau_k^z \right) + \delta_{\alpha,-\beta} \left(\frac{\tau_k^x + i \cos(\theta_{k-\frac{1}{2}})}{2} \alpha \tau_k^y \right) \right] \\
&\quad \left[\delta_{\alpha,\beta} \left(\frac{1 + \cos(\theta_{k+\frac{3}{2}})}{2} \alpha \tau_{k+1}^z \right) + \delta_{\alpha,-\beta} \left(\frac{\tau_{k+1}^x + i \cos(\theta_{k+\frac{3}{2}})}{2} \alpha \tau_{k+1}^y \right) \right] \\
&= \sum_{\alpha=\pm} \left(\frac{1 + \alpha \cos(\theta_{k+\frac{1}{2}})}{2} \right) \left(\frac{1 + \alpha \cos(\theta_{k-\frac{1}{2}})}{2} \tau_k^z \right) \left(\frac{1 + \alpha \cos(\theta_{k+\frac{3}{2}})}{2} \tau_{k+1}^z \right) \\
&\quad + \frac{\sin(\theta_{k+\frac{1}{2}})}{2} \sum_{\alpha=\pm} \left(\cos(\phi_{k+\frac{1}{2}}) - i\alpha \sin(\phi_{k+\frac{1}{2}}) \right) \left(\frac{\tau_k^x + i\alpha \cos(\theta_{k-\frac{1}{2}})}{2} \tau_k^y \right) \left(\frac{\tau_{k+1}^x + i\alpha \cos(\theta_{k+\frac{3}{2}})}{2} \tau_{k+1}^y \right)
\end{aligned} \tag{93}$$

This factorized form with respect to the Pauli operators of the two spins can be expanded in order to perform the summation over $\alpha = \pm$ and one obtains the final result

$$\begin{aligned}
\rho_{k,k+1} &= \frac{1}{4} + \cos(\theta_{k+\frac{1}{2}}) \left[\cos(\theta_{k-\frac{1}{2}}) \frac{\tau_k^z}{4} + \cos(\theta_{k+\frac{3}{2}}) \frac{\tau_{k+1}^z}{4} \right] + \cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) \frac{\tau_k^z \tau_{k+1}^z}{4} \\
&\quad + \sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}}) \left[\frac{\tau_k^x \tau_{k+1}^x}{4} - \cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) \frac{\tau_k^y \tau_{k+1}^y}{4} \right] \\
&\quad + \sin(\theta_{k+\frac{1}{2}}) \sin(\phi_{k+\frac{1}{2}}) \left[\cos(\theta_{k+\frac{3}{2}}) \frac{\tau_k^x \tau_{k+1}^y}{4} + \cos(\theta_{k-\frac{1}{2}}) \frac{\tau_k^y \tau_{k+1}^x}{4} \right]
\end{aligned} \tag{94}$$

Again as in Eq. 22, it involves only the 8 operators that commute with $\tau_1^z \tau_2^z$ among the 16 operators of the tensor basis $\tau_1^a \otimes \tau_2^b$ with $a = 0, x, y, z$ and $b = 0, x, y, z$.

D. Contribution $e_{k,k+1}$ of $h_{k,k+1}$

Again it is convenient to translate the two-body Hamiltonian $h_{k,k+1}$ of Eq. 84 into the τ basis using Eq. 20

$$h_{k,k+1} \equiv \sum_{a=x,y,z} \sum_{b=x,y,z} J_{k+\frac{1}{2}}^{ab} \sigma_k^a \sigma_{k+1}^b = \sum_{a=x,y,z} \sum_{b=x,y,z} \tilde{J}_{k+\frac{1}{2}}^{ab} \tau_k^a \tau_{k+1}^b \tag{95}$$

with the effective couplings in the τ basis

$$\tilde{J}_{k+\frac{1}{2}}^{ab} = \sum_{a'=x,y,z} \sum_{b'=x,y,z} J_{k+\frac{1}{2}}^{a'b'} R_k^{a'a} R_{k+1}^{b'b} \tag{96}$$

Since the reduced density matrix of Eq. 94 involves only five terms containing two Pauli matrices, the contribution $e_{k,k+1}$ of Eq. 86 involve the corresponding five effective couplings

$$\begin{aligned}
e_{k,k+1} &= \cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) \tilde{J}_{k+\frac{1}{2}}^{zz} + \sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}}) \left[\tilde{J}_{k+\frac{1}{2}}^{xx} - \cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) \tilde{J}_{k+\frac{1}{2}}^{yy} \right] \\
&\quad + \sin(\theta_{k+\frac{1}{2}}) \sin(\phi_{k+\frac{1}{2}}) \left[\cos(\theta_{k+\frac{3}{2}}) \tilde{J}_{k+\frac{1}{2}}^{xy} + \cos(\theta_{k-\frac{1}{2}}) \tilde{J}_{k+\frac{1}{2}}^{yx} \right]
\end{aligned} \tag{97}$$

If one wishes to see the role of each initial coupling $J_{k+\frac{1}{2}}^{ab}$ in the initial basis σ , one can decompose Eq. 97

$$e_{k,k+1} = \sum_{a=x,y,z} \sum_{b=x,y,z} J_{k+\frac{1}{2}}^{ab} e_{k,k+1}^{ab} \quad (98)$$

into the corresponding contributions

$$\begin{aligned} e_{k,k+1}^{ab} &= \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) R_k^{az} R_{k+1}^{bz} + \sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \left[R_k^{ax} R_{k+1}^{bx} - \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) R_k^{ay} R_{k+1}^{by} \right] \\ &+ \sin\left(\theta_{k+\frac{1}{2}}\right) \sin\left(\phi_{k+\frac{1}{2}}\right) \left[\cos\left(\theta_{k+\frac{3}{2}}\right) R_k^{ax} R_{k+1}^{by} + \cos\left(\theta_{k-\frac{1}{2}}\right) R_k^{ay} R_{k+1}^{bx} \right] \end{aligned} \quad (99)$$

where the rotation coefficients R_k^{ab} involve the angles (θ_k, ϕ_k) of the site k (Eq. 19) while the rotation coefficients R_{k+1}^{ab} involve the angles $(\theta_{k+1}, \phi_{k+1})$ of the site $(k+1)$.

As examples, let us mention the three contributions $a = b$ that correspond to the three standard couplings $J_{k+1/2}^{zz}$, $J_{k+1/2}^{xx}$ and $J_{k+1/2}^{yy}$. The zz contribution involves only two terms

$$e_{k,k+1}^{zz} = \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) \cos\theta_k \cos\theta_{k+1} + \sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \sin\theta_k \sin\theta_{k+1} \quad (100)$$

while the xx and yy contributions involve the five terms of Eq. 99

$$\begin{aligned} e_{k,k+1}^{xx} &= \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) [\sin\theta_k \cos\phi_k] [\sin\theta_{k+1} \cos\phi_{k+1}] \\ &+ \sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \left([\cos\theta_k \cos\phi_k] [\cos\theta_{k+1} \cos\phi_{k+1}] - \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) \sin\phi_k \sin\phi_{k+1} \right) \\ &- \sin\left(\theta_{k+\frac{1}{2}}\right) \sin\left(\phi_{k+\frac{1}{2}}\right) \left(\cos\left(\theta_{k+\frac{3}{2}}\right) [\cos\theta_k \cos\phi_k] \sin\phi_{k+1} + \cos\left(\theta_{k-\frac{1}{2}}\right) \sin\phi_k [\cos\theta_{k+1} \cos\phi_{k+1}] \right) \end{aligned} \quad (101)$$

and

$$\begin{aligned} e_{k,k+1}^{yy} &= \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) [\sin\theta_k \sin\phi_k] [\sin\theta_{k+1} \sin\phi_{k+1}] \\ &+ \sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \left([\cos\theta_k \sin\phi_k] [\cos\theta_{k+1} \sin\phi_{k+1}] - \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{3}{2}}\right) \cos\phi_k \cos\phi_{k+1} \right) \\ &+ \sin\left(\theta_{k+\frac{1}{2}}\right) \sin\left(\phi_{k+\frac{1}{2}}\right) \left(\cos\left(\theta_{k+\frac{3}{2}}\right) [\cos\theta_k \sin\phi_k] \cos\phi_{k+1} + \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\phi_k [\cos\theta_{k+1} \sin\phi_{k+1}] \right) \end{aligned} \quad (102)$$

E. Optimization of the MPS parameters to minimize the energy

As explained above, the energy can be computed in terms of the $(4N-2)$ angles via the elementary contributions of Eq. 85, where e_k^a was found in Eq. 92 to depend only on the four angles $[\theta_{k-\frac{1}{2}}; \theta_k, \phi_k; \theta_{k+\frac{1}{2}}]$, while $e_{k,k+1}^{ab}$ was found in Eq. 99 to depend on the eight angles $[\theta_{k-\frac{1}{2}}; \theta_k, \phi_k; \theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}}; \theta_{k+1}, \phi_{k+1}; \theta_{k+\frac{3}{2}}]$. It is thus convenient to rewrite Eq. 85 with these explicit dependences

$$\begin{aligned} E &= \sum_{k=1}^N \sum_{a=x,y,z} B_k^a e_k^a \left(\theta_{k-\frac{1}{2}}; \theta_k, \phi_k; \theta_{k+\frac{1}{2}} \right) \\ &+ \sum_{k=1}^{N-1} \sum_{a=x,y,z} \sum_{b=x,y,z} J_{k+\frac{1}{2}}^{ab} e_{k,k+1}^{ab} \left(\theta_{k-\frac{1}{2}}; \theta_k, \phi_k; \theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}}; \theta_{k+1}, \phi_{k+1}; \theta_{k+\frac{3}{2}} \right) \end{aligned} \quad (103)$$

For $k = 1, \dots, N$, the optimizations with respect to the sites angles (θ_k, ϕ_k) for $k = 1, \dots, N$ only involve the terms related to $(e_{k-1,k}^{ab}, e_k^a, e_{k,k+1}^{ab})$ as expected

$$\begin{aligned} 0 &= \frac{\partial E}{\partial \theta_k} = \sum_{a=x,y,z} B_k^a \frac{\partial e_k^a}{\partial \theta_k} + \sum_{a=x,y,z} \sum_{b=x,y,z} \left[J_{k-\frac{1}{2}}^{ab} \frac{\partial e_{k-1,k}^{ab}}{\partial \theta_k} + J_{k+\frac{1}{2}}^{ab} \frac{\partial e_{k,k+1}^{ab}}{\partial \theta_k} \right] \\ 0 &= \frac{\partial E}{\partial \phi_k} = \sum_{a=x,y,z} B_k^a \frac{\partial e_k^a}{\partial \phi_k} + \sum_{a=x,y,z} \sum_{b=x,y,z} \left[J_{k-\frac{1}{2}}^{ab} \frac{\partial e_{k-1,k}^{ab}}{\partial \phi_k} + J_{k+\frac{1}{2}}^{ab} \frac{\partial e_{k,k+1}^{ab}}{\partial \phi_k} \right] \end{aligned} \quad (104)$$

For $k = 1, \dots, N-1$, the optimizations with respect to the bond angles $\phi_{k+\frac{1}{2}}$ only involve the term related to $(e_{k,k+1}^{ab})$

$$0 = \frac{\partial E}{\partial \phi_{k+\frac{1}{2}}} = \sum_{a=x,y,z} \sum_{b=x,y,z} J_{k+\frac{1}{2}}^{ab} \frac{\partial e_{k,k+1}^{ab}}{\partial \phi_{k+\frac{1}{2}}} \quad (105)$$

while the optimizations with respect to the bond angles $\theta_{k+\frac{1}{2}}$ involve the terms related to $(e_{k-1,k}^{ab}, e_k^a, e_{k,k+1}^{ab}, e_{k+1}^a, e_{k+1,k+2}^{ab})$

$$0 = \frac{\partial E}{\partial \theta_{k+\frac{1}{2}}} = \sum_{a=x,y,z} \left[B_k^a \frac{\partial e_k^a}{\partial \theta_{k+\frac{1}{2}}} + B_{k+1}^a \frac{\partial e_{k+1}^a}{\partial \theta_{k+\frac{1}{2}}} \right] + \sum_{a=x,y,z} \sum_{b=x,y,z} \left[J_{k-\frac{1}{2}}^{ab} \frac{\partial e_{k-1,k}^{ab}}{\partial \theta_{k+\frac{1}{2}}} + J_{k+\frac{1}{2}}^{ab} e_{k,k+1}^{ab} \frac{\partial e_{k,k+1}^{ab}}{\partial \theta_{k+\frac{1}{2}}} + J_{k+\frac{3}{2}}^{ab} e_{k+1,k+2}^{ab} \frac{\partial e_{k+1,k+2}^{ab}}{\partial \theta_{k+\frac{1}{2}}} \right] \quad (106)$$

VI. CORRELATIONS BETWEEN THE TWO SPINS $(k, k+r)$ AT DISTANCE r

To compute any correlations between the two spins k and $(k+r)$ at distance r , one needs the reduced density matrix $\rho_{k,k+r}$ of these two spins.

A. Reduced density matrix $\rho_{k,k+r}$ of the two spins $(k, k+r)$ at distance r

We have already computed $\rho_{k,k+1}$ for two consecutive spins in section VC, so in this section we focus only on the cases $r > 1$. It is convenient to use the MPO form of Eq 77 for the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of the whole interval $(k, k+1, \dots, k+r-1, k+r)$, and to compute the trace over all the interval spins $n = k+1, \dots, k+r-1$ using Eq. 35

$$\begin{aligned} \rho_{k,k+r} &= \text{Tr}_{\{k+1,\dots,k+r-1\}} (\rho_{k,k+1,\dots,k+r}) \quad (107) \\ &= \sum_{\substack{\alpha_k=\pm \\ \beta_k=\pm}} \dots \sum_{\substack{\alpha_{k+r-1}=\pm \\ \beta_{k+r-1}=\pm}} \left[\prod_{n=k}^{k+r-1} \Lambda_{n,n+1}^{\alpha_n,\beta_n} \right] W_{[k]}^{\alpha_k,\beta_k} \left[\prod_{n=k+1}^{k+r-1} \text{Tr}_{\{n\}} \left(O_n^{(\alpha_{n-1}\alpha_n),(\beta_{n-1}\beta_n)} \right) \right] W_{[k+r]}^{\alpha_{k+r-1},\beta_{k+r-1}} \\ &= \sum_{\substack{\alpha_k=\pm \\ \beta_k=\pm}} \dots \sum_{\substack{\alpha_{k+r-1}=\pm \\ \beta_{k+r-1}=\pm}} \left[\prod_{n=k}^{k+r-1} \Lambda_{n,n+1}^{\alpha_n,\beta_n} \right] W_{[k]}^{\alpha_k,\beta_k} \left[\prod_{n=k+1}^{k+r-1} \delta_{\beta_n,(\alpha_{n-1}\beta_{n-1})\alpha_n} \right] W_{[k+r]}^{\alpha_{k+r-1},\beta_{k+r-1}} \\ &= \sum_{\substack{\alpha_k=\pm \\ \beta_k=\pm}} \sum_{\alpha_{k+r-1}=\pm} W_{[k]}^{\alpha_k,\beta_k} W_{[k+r]}^{\alpha_{k+r-1},(\alpha_k\beta_k)\alpha_{k+r-1}} \Lambda_{k,k+1}^{\alpha_k,\beta_k} \Lambda_{k+r-1,k+r}^{\alpha_{k+r-1},(\alpha_k\beta_k)\alpha_{k+r-1}} \left[\prod_{n=k+1}^{k+r-2} \left(\sum_{\alpha_n=\pm} \Lambda_{n,n+1}^{\alpha_n,(\alpha_k\beta_k)\alpha_n} \right) \right] \end{aligned}$$

Replacing the boundary operators by their explicit forms of Eqs 79, 80

$$\begin{aligned} W_k^{\alpha_k,\beta_k} &= \delta_{\alpha_k,\beta_k} \left(\frac{1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \alpha_k \tau_k^z}{2} \right) + \delta_{\alpha_k,-\beta_k} \left(\frac{\tau_k^x + i \cos\left(\theta_{k-\frac{1}{2}}\right) \alpha_k \tau_k^y}{2} \right) \quad (108) \\ W_{k+r}^{\alpha_{k+r-1},(\alpha_k\beta_k)\alpha_{k+r-1}} &= \delta_{\alpha_k,\beta_k} \left(\frac{1 + \cos\left(\theta_{k+r+\frac{1}{2}}\right) \alpha_{k+r-1} \tau_{k+r}^z}{2} \right) + \delta_{\alpha_k,-\beta_k} \left(\frac{\tau_{k+r}^x + i \cos\left(\theta_{k+r+\frac{1}{2}}\right) \alpha_{k+r-1} \tau_{k+r}^y}{2} \right) \end{aligned}$$

replacing the bond variables by their explicit forms of Eq. 31

$$\begin{aligned} \Lambda_{k,k+1}^{\alpha_k,\beta_k} &= \delta_{\alpha_k,\beta_k} \left(\frac{1 + \alpha_k \cos\left(\theta_{k+\frac{1}{2}}\right)}{2} \right) + \delta_{\alpha_k,-\beta_k} \left(\frac{\sin\left(\theta_{k+\frac{1}{2}}\right)}{2} e^{-i\alpha_k \phi_{k+\frac{1}{2}}} \right) \\ \Lambda_{k+r-1,k+r}^{\alpha_{k+r-1},(\alpha_k\beta_k)\alpha_{k+r-1}} &= \delta_{\alpha_k,\beta_k} \left(\frac{1 + \alpha_{k+r-1} \cos\left(\theta_{k+r-\frac{1}{2}}\right)}{2} \right) + \delta_{\alpha_k,-\beta_k} \left(\frac{\sin\left(\theta_{k+r-\frac{1}{2}}\right)}{2} e^{-i\alpha_{k+r-1} \phi_{k+r-\frac{1}{2}}} \right) \quad (109) \end{aligned}$$

and replacing the last factor by its explicit form in terms of the overlap introduced in Eq. 66

$$\prod_{n=k+1}^{k+r-2} \left(\sum_{\alpha_n=\pm} \Lambda_{n,n+1}^{\alpha_n, (\alpha_k \beta_k) \alpha_n} \right) = \prod_{n=k+1}^{k+r-2} \left(\Lambda_{n,n+1}^{+, (\alpha_k \beta_k)} + \Lambda_{n,n+1}^{-, -(\alpha_k \beta_k)} \right) = \delta_{\alpha_k, \beta_k} + \delta_{\alpha_k, -\beta_k} \omega_{k+1, k+r-1} \quad (110)$$

with the convention

$$\omega_{k+1, k+1} = 1 \quad (111)$$

in order to describe also the special case $r = 2$ within the same formula, Eq 107 reduces to

$$\begin{aligned} \rho_{k, k+r} &= \left[\sum_{\alpha_k=\pm} \left(\frac{1 + \alpha_k \cos(\theta_{k-\frac{1}{2}}) \tau_k^z}{2} \right) \left(\frac{1 + \alpha_k \cos(\theta_{k+\frac{1}{2}})}{2} \right) \right] \\ &\left[\sum_{\alpha_{k+r-1}=\pm} \left(\frac{1 + \alpha_{k+r-1} \cos(\theta_{k+r+\frac{1}{2}}) \tau_{k+r}^z}{2} \right) \left(\frac{1 + \alpha_{k+r-1} \cos(\theta_{k+r-\frac{1}{2}})}{2} \right) \right] \\ &+ \sin(\theta_{k+\frac{1}{2}}) \omega_{k+1, k+r-1} \sin(\theta_{k+r-\frac{1}{2}}) \left[\sum_{\alpha_k=\pm} \left(\frac{\tau_k^x + i \alpha_k \cos(\theta_{k-\frac{1}{2}}) \tau_k^y}{2} \right) \left(\frac{\cos(\phi_{k+\frac{1}{2}}) - i \alpha_k \sin(\phi_{k+\frac{1}{2}})}{2} \right) \right] \\ &\left[\sum_{\alpha_{k+r-1}=\pm} \left(\frac{\tau_{k+r}^x + i \alpha_{k+r-1} \cos(\theta_{k+r+\frac{1}{2}}) \tau_{k+r}^y}{2} \right) \left(\frac{\cos(\phi_{k+r-\frac{1}{2}}) - i \alpha_{k+r-1} \sin(\phi_{k+r-\frac{1}{2}})}{2} \right) \right] \\ &= \left(\frac{1 + \cos(\theta_{k-\frac{1}{2}}) \tau_k^z \cos(\theta_{k+\frac{1}{2}})}{2} \right) \left(\frac{1 + \cos(\theta_{k+r-\frac{1}{2}}) \tau_{k+r}^z \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) \\ &+ \omega_{k, k+r} \left(\frac{\tau_k^x + \cos(\theta_{k-\frac{1}{2}}) \tau_k^y \tan(\phi_{k+\frac{1}{2}})}{2} \right) \left(\frac{\tau_{k+r}^x + \tan(\phi_{k+r-\frac{1}{2}}) \tau_{k+r}^y \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) \quad (112) \end{aligned}$$

One could of course expand to obtain the form analogous to Eq 94 for $\rho_{k, k+1}$, but the factorized form of Eq. 112 has a very direct physical meaning in terms of connected correlations.

B. Connected reduced density matrix $\rho_{k, k+r}^{\text{connected}}$ and physical meaning of $\omega_{k, k+r}$

Since the first contribution in the final result of Eq. 112 corresponds to the product of the one-point reduced density matrices ρ_k and ρ_{k+r} of Eq 50, it is useful to rewrite Eq. 112 with the difference

$$\begin{aligned} \rho_{k, k+r}^{\text{connected}} &\equiv \rho_{k, k+r} - \rho_k \rho_{k+r} \\ &= \omega_{k, k+r} \left(\frac{\tau_k^x + \cos(\theta_{k-\frac{1}{2}}) \tau_k^y \tan(\phi_{k+\frac{1}{2}})}{2} \right) \left(\frac{\tau_{k+r}^x + \tan(\phi_{k+r-\frac{1}{2}}) \tau_{k+r}^y \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) \quad (113) \end{aligned}$$

that shows clearly the physical meaning of the prefactor $\omega_{k, k+r}$ that governs the decay with the distance r via the multiplicative structure of Eq. 64.

C. Computation of the two-point connected correlations between the two sites $(k, k+r)$ at distance r

Any type of connected correlations with $a = x, y, z$ and $b = x, y, z$ between the two sites k and $(k+r)$ can be now computed from the reduced density matrix $\rho_{k, k+r}^{\text{connected}}$ of Eq. 113 via

$$\begin{aligned} C_{k, k+r}^{ab} &\equiv \langle \psi | \sigma_k^a \sigma_{k+r}^b | \psi \rangle - \langle \psi | \sigma_k^a | \psi \rangle \langle \psi | \sigma_{k+r}^b | \psi \rangle = \text{Tr}_{\{k, k+r\}} (\sigma_k^a \sigma_{k+r}^b \rho_{k, k+r}) - (\text{Tr}_{\{k\}} (\sigma_k^a \rho_k)) (\text{Tr}_{\{k+r\}} (\sigma_{k+r}^b \rho_{k+r})) \\ &= \text{Tr}_{\{k, k+r\}} (\sigma_k^a \sigma_{k+r}^b \rho_{k, k+r}^{\text{connected}}) \quad (114) \end{aligned}$$

The explicit form of Eq 113 and the rotation of Eq. 20 then yields

$$\begin{aligned}
C_{k,k+r}^{ab} &= \omega_{k,k+r} \text{Tr}_{\{k\}} \left[\sigma_k^a \left(\frac{\tau_k^x + \cos\left(\theta_{k-\frac{1}{2}}\right) \tau_k^y \tan\left(\phi_{k+\frac{1}{2}}\right)}{2} \right) \right] \\
&\text{Tr}_{\{k+1\}} \left[\sigma_{k+r}^b \left(\frac{\tau_{k+r}^x + \tan\left(\phi_{k+r-\frac{1}{2}}\right) \tau_{k+r}^y \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{2} \right) \right] \\
&= \omega_{k,k+r} \left(\frac{R_k^{ax} + \cos\left(\theta_{k-\frac{1}{2}}\right) \tan\left(\phi_{k+\frac{1}{2}}\right) R_k^{ay}}{2} \right) \left(\frac{R_{k+r}^{bx} + \tan\left(\phi_{k+r-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right) R_{k+r}^{by}}{2} \right) \quad (115)
\end{aligned}$$

For instance, the diagonal $a = b$ connected correlations read

$$\begin{aligned}
C_{k,k+r}^{zz} &= \omega_{k,k+r} \sin\theta_k \sin\theta_{k+r} \\
C_{k,k+r}^{xx} &= \omega_{k,k+r} \left[-\cos\theta_k \cos\phi_k + \cos\left(\theta_{k-\frac{1}{2}}\right) \tan\left(\phi_{k+\frac{1}{2}}\right) \sin\phi_k \right] \\
&\quad \left[-\cos\theta_{k+r} \cos\phi_{k+r} + \tan\left(\phi_{k+r-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right) \sin\phi_{k+r} \right] \\
C_{k,k+r}^{yy} &= \omega_{k,k+r} \left[\cos\theta_k \sin\phi_k + \cos\left(\theta_{k-\frac{1}{2}}\right) \tan\left(\phi_{k+\frac{1}{2}}\right) \cos\phi_k \right] \\
&\quad \left[\cos\theta_{k+r} \sin\phi_{k+r} + \tan\left(\phi_{k+r-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right) \cos\phi_{k+r} \right] \quad (116)
\end{aligned}$$

VII. RIEMANN METRIC FOR THE MPS MANIFOLD PARAMETRIZED BY THE $(4N - 2)$ ANGLES

The geometry of quantum states is a fascinating field (see the book [51] and references therein). The Riemann Fubini-Study metric for the tangent space can be introduced either for the ket $|\psi\rangle$ or for the density matrix $\rho = |\psi\rangle\langle\psi|$ with the same output for the metric [51], as it is well known for the Bloch sphere geometry of a single spin. The tangent space of MPS kets has been much studied, both for the detailed analysis of their geometric properties [52, 53] and for the applications to dynamical algorithms [54–59]. Here we have chosen instead the formulation in terms of the density matrix ρ in order to use the properties of the Hilbert-Schmidt inner product for operators that simplify some calculations, since our goal in this section is to compute explicitly the metric for the MPS manifold parametrized by the $(4N - 2)$ angles.

A. Reminder on the Hilbert-Schmidt inner product for operators

The Hilbert-Schmidt inner product between two operators X and Y

$$(X|Y)_{HS} \equiv \text{Tr}(X^\dagger Y) \quad (117)$$

allows to define the squared norm of an operator X

$$\|X\|_{HS}^2 \equiv (X|X)_{HS} = \text{Tr}(X^\dagger X) \quad (118)$$

and the squared distance between two operators X and Y

$$\|X - Y\|_{HS}^2 \equiv (X - Y|X - Y)_{HS} = \text{Tr}((X - Y)^\dagger (X - Y)) \quad (119)$$

The full density matrix $\rho = |\psi\rangle\langle\psi|$ satisfies

$$\begin{aligned}
\rho^\dagger &= \rho \\
\rho^2 &= \rho \\
\text{Tr}(\rho) &= 1
\end{aligned} \quad (120)$$

so its Hilbert-Schmidt squared norm is unity

$$\|\rho\|_{HS}^2 = \text{Tr}(\rho^\dagger \rho) = \text{Tr}(\rho^2) = \text{Tr}(\rho) = 1 \quad (121)$$

B. Notion of Tangent Space around the density matrix ρ

The MPS density matrix ρ is a function of the $(2N - 2)$ bond angles $(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}})$ with $k = 1, \dots, N - 1$ and of the $(2N)$ site angles (θ_k, ϕ_k) with $k = 1, \dots, N$. It will be momentarily convenient to relabel them by $(4N - 2)$ coordinates x^μ with $\mu = 1, \dots, 4N - 2$, for instance according to their appearance along the chain

$$\begin{aligned}\theta_k &\equiv x^{4k-3} \quad \text{for } k = 1, 2, \dots, N \\ \phi_k &\equiv x^{4k-2} \quad \text{for } k = 1, 2, \dots, N \\ \theta_{k+\frac{1}{2}} &\equiv x^{4k-1} \quad \text{for } k = 1, 2, \dots, N - 1 \\ \phi_{k+\frac{1}{2}} &\equiv x^{4k} \quad \text{for } k = 1, 2, \dots, N - 1\end{aligned}\tag{122}$$

Let us now consider how the full density matrix ρ changes when all the parameters are changed from x^μ to $x^\mu + dx^\mu$

$$d\rho = \sum_{k=1}^{N-1} \left[d\theta_{k+\frac{1}{2}} V_{\theta_{k+\frac{1}{2}}} + d\phi_{k+\frac{1}{2}} V_{\phi_{k+\frac{1}{2}}} \right] + \sum_{k=1}^{N-1} [d\theta_k V_{\theta_k} + d\phi_k V_{\phi_k}] \equiv \sum_{\mu=1}^{4N-2} dx^\mu V_{x^\mu}\tag{123}$$

The Tangent space around ρ is thus generated by the $(4N - 2)$ tangent operators

$$V_{x^\mu} \equiv \frac{\partial \rho}{\partial x^\mu}\tag{124}$$

The properties of the density matrix ρ summarized in Eq 120 yields that each tangent operator V_{x^μ} in Eq. 123 is hermitian

$$V_{x^\mu}^\dagger = V_{x^\mu}\tag{125}$$

has a vanishing trace

$$\text{Tr}(V_{x^\mu}) = 0\tag{126}$$

and is orthogonal to the density matrix ρ for the Hilbert-Schmidt inner-product

$$0 = \text{Tr}(\rho V_{x^\mu}) = (\rho | V_{x^\mu})_{HS}\tag{127}$$

C. Reminder on the Riemann Fubini-Study metric

The Riemann Fubini-Study metric [51] can be defined in terms of the Hilbert-Schmidt distance of Eq. 119 between ρ and $\rho + d\rho$ (Eq .123)

$$ds^2 = \|d\rho\|_{HS}^2 = \text{Tr}(d\rho d\rho) = \sum_{\mu=1}^{4N-2} \sum_{\nu=1}^{4N-2} g_{(x^\mu, x^\nu)} dx^\mu dx^\nu\tag{128}$$

where the metric coefficient $g_{(x^\mu, x^\nu)}$ between the coordinates x^μ and x^ν corresponds to the Hilbert-Schmidt inner product between their associated tangent operators V_{x^μ} and V_{x^ν}

$$g_{(x^\mu, x^\nu)} = \text{Tr}(V_{x^\mu} V_{x^\nu}) = (V_{x^\mu} | V_{x^\nu})_{HS}\tag{129}$$

In particular, the diagonal coefficients correspond to the squared norms of the tangent operators

$$g_{(x^\mu, x^\mu)} = \text{Tr}(V_{x^\mu} V_{x^\mu}) = \|V_{x^\mu}\|_{HS}^2\tag{130}$$

while the off-diagonal coefficients satisfy the symmetry $g_{(x^\mu, x^\nu)} = g_{(x^\nu, x^\mu)}$. In the following, our goal is thus to write explicitly the tangent operators associated to bonds angles and to sites angles and to compute the metric.

D. Tangent operators associated to the bonds angles $(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}})$

In the Schmidt decomposition of Eq. 41

$$\rho = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left(|\Phi_\alpha^{[1,\dots,k]} \rangle \langle \Phi_\beta^{[1,\dots,k]}| \right) \Lambda_{k,k+1}^{\alpha,\beta} \left(|\Phi_\alpha^{[k+1,\dots,N]} \rangle \langle \Phi_\beta^{[k+1,\dots,N]}| \right) \quad (131)$$

the only dependence with respect to the the two bond angles $(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}})$ is contained in the bond variables $\Lambda_{k,k+1}^{\alpha,\beta}$ of Eq. 31. So the tangent operators associated to these two angles read

$$\begin{aligned} V_{\theta_{k+\frac{1}{2}}} &\equiv \frac{\partial \rho}{\partial \theta_{k+\frac{1}{2}}} = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left(|\Phi_\alpha^{[1,\dots,k]} \rangle \langle \Phi_\beta^{[1,\dots,k]}| \right) \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \theta_{k+\frac{1}{2}}} \right] \left(|\Phi_\alpha^{[k+1,\dots,N]} \rangle \langle \Phi_\beta^{[k+1,\dots,N]}| \right) \\ V_{\phi_{k+\frac{1}{2}}} &\equiv \frac{\partial \rho}{\partial \phi_{k+\frac{1}{2}}} = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left(|\Phi_\alpha^{[1,\dots,k]} \rangle \langle \Phi_\beta^{[1,\dots,k]}| \right) \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \phi_{k+\frac{1}{2}}} \right] \left(|\Phi_\alpha^{[k+1,\dots,N]} \rangle \langle \Phi_\beta^{[k+1,\dots,N]}| \right) \end{aligned} \quad (132)$$

where the derivatives of the bond variables $\Lambda_{k,k+1}^{\alpha,\beta}$ of Eq. 31

$$\Lambda_{k,k+1}^{\alpha,\beta} = \delta_{\alpha,\beta} \left(\frac{1 + \alpha \cos(\theta_{k+\frac{1}{2}})}{2} \right) + \delta_{\alpha,-\beta} \left(\frac{\sin(\theta_{k+\frac{1}{2}})}{2} e^{-i\alpha\phi_{k+\frac{1}{2}}} \right) \quad (133)$$

read

$$\begin{aligned} \frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \theta_{k+\frac{1}{2}}} &= \delta_{\alpha,\beta} \left(\frac{-\alpha \sin(\theta_{k+\frac{1}{2}})}{2} \right) + \delta_{\alpha,-\beta} \left(\frac{\cos(\theta_{k+\frac{1}{2}})}{2} e^{-i\alpha\phi_{k+\frac{1}{2}}} \right) \\ \frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \phi_{k+\frac{1}{2}}} &= -i\alpha \delta_{\alpha,-\beta} \left(\frac{\sin(\theta_{k+\frac{1}{2}})}{2} e^{-i\alpha\phi_{k+\frac{1}{2}}} \right) \end{aligned} \quad (134)$$

Using the orthonormality of the Schmidt eigenvectors, one obtains that the conditions of vanishing trace (Eq 126) and orthogonality with the density matrix ρ (Eq. 127) correspond to the following local properties for the variables $\Lambda_{k,k+1}^{\alpha,\beta}$ of a single bond $(k, k+1)$

$$\begin{aligned} 0 &= \text{Tr}(V_{\theta_{k+\frac{1}{2}}}) = \sum_{\alpha=\pm} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\alpha}}{\partial \theta_{k+\frac{1}{2}}} \right] \\ 0 &= \text{Tr}(V_{\phi_{k+\frac{1}{2}}}) = \sum_{\alpha=\pm} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\alpha}}{\partial \phi_{k+\frac{1}{2}}} \right] \\ 0 &= \text{Tr}(\rho V_{\theta_{k+\frac{1}{2}}}) = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \theta_{k+\frac{1}{2}}} \right] \Lambda_{k,k+1}^{\beta,\alpha} \\ 0 &= \text{Tr}(\rho V_{\phi_{k+\frac{1}{2}}}) = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \phi_{k+\frac{1}{2}}} \right] \Lambda_{k,k+1}^{\beta,\alpha} \end{aligned} \quad (135)$$

E. Tangent operators associated to the site angles (θ_k, ϕ_k)

In the Schmidt decomposition of Eq. 48

$$\rho = \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]}| \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} O_k^{\alpha_L\alpha_R,\beta_L\beta_R} \Lambda_{k,k+1}^{\alpha_R,\beta_R} \left(|\Phi_{\alpha_R}^{[k+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+1,\dots,N]}| \right) \quad (136)$$

the only dependence with respect to the the two sites angles (θ_k, ϕ_k) is contained in the operators $O_k^{T,T'}$ of Eq 35 via the Pauli operators $\tau_k^{x,y,x}$ of Eq. 18. The derivatives of the Pauli operators $\tau_k^{x,y,x}$ with respect to the two angles (θ_k, ϕ_k) can be obtained from their expressions in the fixed σ basis (Eq. 18) and can be translated then back in the τ basis via Eq 19 in order to obtain the derivatives with respect to θ_k

$$\begin{aligned}\frac{\partial \tau_k^z}{\partial \theta_k} &= -\tau_k^x \\ \frac{\partial \tau_k^x}{\partial \theta_k} &= \tau_k^z \\ \frac{\partial \tau_k^y}{\partial \theta_k} &= 0\end{aligned}\tag{137}$$

and with respect to ϕ_k

$$\begin{aligned}\frac{\partial \tau_k^z}{\partial \phi_k} &= -\sin \theta_k \tau_k^y \\ \frac{\partial \tau_k^x}{\partial \phi_k} &= \cos \theta_k \tau_k^y \\ \frac{\partial \tau_k^y}{\partial \phi_k} &= \sin \theta_k \tau_k^z - \cos \theta_k \tau_k^x\end{aligned}\tag{138}$$

The derivatives of the operators Eq 35

$$O_k^{T,T'} = |\tau_k^z = T\rangle \langle \tau_k^z = T'| = \delta_{T,T'} \left(\frac{1 + T\tau_k^z}{2} \right) + \delta_{T,-T'} \left(\frac{\tau_k^x + iT\tau_k^y}{2} \right)\tag{139}$$

then read

$$\begin{aligned}\frac{\partial O_k^{T,T'}}{\partial \theta_k} &= \delta_{T,T'} \left(-\frac{T\tau_k^x}{2} \right) + \delta_{T,-T'} \left(\frac{\tau_k^z}{2} \right) \\ \frac{\partial O_k^{T,T'}}{\partial \phi_k} &= \delta_{T,T'} \left(-\frac{T \sin \theta_k \tau_k^y}{2} \right) + \delta_{T,-T'} \left(\frac{\cos \theta_k \tau_k^y + iT [\sin \theta_k \tau_k^z - \cos \theta_k \tau_k^x]}{2} \right)\end{aligned}\tag{140}$$

and appear in the tangent operators associated to the two sites angles (θ_k, ϕ_k)

$$\begin{aligned}V_{\theta_k} &\equiv \frac{\partial \rho}{\partial \theta_k} = \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]}\rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]}| \right) \Lambda_{k-1,k}^{\alpha_L, \beta_L} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \theta_k} \right] \Lambda_{k,k+1}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+1,\dots,N]}\rangle \langle \Phi_{\beta_R}^{[k+1,\dots,N]}| \right) \\ V_{\phi_k} &\equiv \frac{\partial \rho}{\partial \phi_k} = \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]}\rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]}| \right) \Lambda_{k-1,k}^{\alpha_L, \beta_L} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \phi_k} \right] \Lambda_{k,k+1}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+1,\dots,N]}\rangle \langle \Phi_{\beta_R}^{[k+1,\dots,N]}| \right)\end{aligned}\tag{141}$$

Here the conditions of vanishing trace (Eq 126) and orthogonality with the density matrix ρ (Eq. 127) translate into the local conditions

$$\begin{aligned}0 &= \text{Tr}(V_{\theta_k}) = \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \Lambda_{k-1,k}^{\alpha_L, \alpha_L} \left(\text{Tr}_{\{k\}} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \alpha_L \alpha_R}}{\partial \theta_k} \right] \right) \Lambda_{k,k+1}^{\alpha_R, \alpha_R} \\ 0 &= \text{Tr}(V_{\phi_k}) = \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \Lambda_{k-1,k}^{\alpha_L, \alpha_L} \left(\text{Tr}_{\{k\}} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \alpha_L \alpha_R}}{\partial \phi_k} \right] \right) \Lambda_{k,k+1}^{\alpha_R, \alpha_R} \\ 0 &= \text{Tr}(\rho V_{\theta_k}) = \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k-1,k}^{\beta_L, \alpha_L} \left(\text{Tr}_{\{k\}} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \theta_k} O_k^{\beta_L \beta_R, \alpha_L \alpha_R} \right] \right) \Lambda_{k,k+1}^{\alpha_R, \beta_R} \Lambda_{k,k+1}^{\beta_R, \alpha_R} \\ 0 &= \text{Tr}(\rho V_{\phi_k}) = \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k-1,k}^{\beta_L, \alpha_L} \left(\text{Tr}_{\{k\}} \left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \phi_k} O_k^{\beta_L \beta_R, \alpha_L \alpha_R} \right] \right) \Lambda_{k,k+1}^{\alpha_R, \beta_R} \Lambda_{k,k+1}^{\beta_R, \alpha_R}\end{aligned}\tag{142}$$

The two first conditions are trivially satisfied because the derivatives of the operators of Eq. 140 have zero trace

$$\begin{aligned}\mathrm{Tr}_{\{k\}} \left[\frac{\partial O_k^{T,T'}}{\partial \theta_k} \right] &= 0 \\ \mathrm{Tr}_{\{k\}} \left[\frac{\partial O_k^{T,T'}}{\partial \phi_k} \right] &= 0\end{aligned}\quad (143)$$

The third condition is also straightforward because the following trace over k vanishes

$$\mathrm{Tr}_{\{k\}} \left[\frac{\partial O_k^{T,T'}}{\partial \theta_k} O_k^{T',T} \right] = 0 \quad (144)$$

The trace appearing in the fourth condition does not vanish but reduces to

$$\mathrm{Tr}_{\{k\}} \left[\frac{\partial O_k^{T,T'}}{\partial \phi_k} O_k^{T',T} \right] = -iT(\cos \theta_k) \delta_{T,-T'} \quad (145)$$

so the fourth condition vanishes only as a consequence of the remaining sum over the indices $(\alpha_L, \alpha_R, \beta_L, \beta_R)$.

F. Metric within the sector of bonds angles $(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}})$ with $k = 1, \dots, N-1$

1. Metric coefficients between the two angles $(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}})$ associated to the same bond $(k, k+1)$

The tangent operators of Eq. 132 yields with Eq 134 that the two diagonal elements read

$$\begin{aligned}g(\theta_{k+\frac{1}{2}}, \theta_{k+\frac{1}{2}}) &= \mathrm{Tr} \left(V_{\theta_{k+\frac{1}{2}}} V_{\theta_{k+\frac{1}{2}}} \right) = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \theta_{k+\frac{1}{2}}} \right] \left[\frac{\partial \Lambda_{k,k+1}^{\beta,\alpha}}{\partial \theta_{k+\frac{1}{2}}} \right] = \frac{1}{2} \\ g(\phi_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}}) &= \mathrm{Tr} \left(V_{\phi_{k+\frac{1}{2}}} V_{\phi_{k+\frac{1}{2}}} \right) = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \phi_{k+\frac{1}{2}}} \right] \left[\frac{\partial \Lambda_{k,k+1}^{\beta,\alpha}}{\partial \phi_{k+\frac{1}{2}}} \right] = \frac{\sin^2 \left(\theta_{k+\frac{1}{2}} \right)}{2}\end{aligned}\quad (146)$$

while the off-diagonal element vanishes

$$g(\theta_{k+\frac{1}{2}}, \phi_{k+\frac{1}{2}}) = \mathrm{Tr} \left(V_{\theta_{k+\frac{1}{2}}} V_{\phi_{k+\frac{1}{2}}} \right) = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha,\beta}}{\partial \theta_{k+\frac{1}{2}}} \right] \left[\frac{\partial \Lambda_{k,k+1}^{\beta,\alpha}}{\partial \phi_{k+\frac{1}{2}}} \right] = 0 \quad (147)$$

2. Metric coefficients between the angles associated to the two bonds $(k, k+1)$ and $(k+r, k+r+1)$ with $r \geq 1$

In order to compare the tangent vectors of Eq. 132 associated to the bonds $(k, k+1)$ and $(k+r, k+r+1)$, it is convenient to rewrite them using the interval ket introduced in Eq. 62 as

$$\begin{aligned}V_{\theta_{k+\frac{1}{2}}} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \\ &\left(|\Phi_{\alpha_L}^{[1,\dots,k]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k]} | \right) \left[\frac{\partial \Lambda_{k,k+1}^{\alpha_L, \beta_L}}{\partial \theta_{k+\frac{1}{2}}} \right] \left(|I_{\alpha_L, \alpha_R}^{[k+1, \dots, k+r]} \rangle \langle I_{\beta_L, \beta_R}^{[k+1, \dots, k+r]} | \right) \Lambda_{k+r, k+r+1}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+r+1, \dots, N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1, \dots, N]} | \right) \\ V_{\theta_{k+r+\frac{1}{2}}} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \\ &\left(|\Phi_{\alpha_L}^{[1,\dots,k]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k]} | \right) \Lambda_{k,k+1}^{\alpha_L, \beta_L} \left(|I_{\alpha_L, \alpha_R}^{[k+1, \dots, k+r]} \rangle \langle I_{\beta_L, \beta_R}^{[k+1, \dots, k+r]} | \right) \left[\frac{\partial \Lambda_{k+r, k+r+1}^{\alpha_R, \beta_R}}{\partial \theta_{k+r+\frac{1}{2}}} \right] \left(|\Phi_{\alpha_R}^{[k+r+1, \dots, N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1, \dots, N]} | \right)\end{aligned}\quad (148)$$

Using the normalization of the interval ket (Eq 65), one obtains that all the off-diagonal elements vanish as a consequence of Eq. 135

$$\begin{aligned}
g(\theta_{k+\frac{1}{2}}, \theta_{k+r+\frac{1}{2}}) &= 0 \\
g(\phi_{k+\frac{1}{2}}, \phi_{k+r+\frac{1}{2}}) &= 0 \\
g(\theta_{k+\frac{1}{2}}, \phi_{k+r+\frac{1}{2}}) &= 0 \\
g(\phi_{k+\frac{1}{2}}, \theta_{k+r+\frac{1}{2}}) &= 0
\end{aligned} \tag{149}$$

So within the sector of bond angles, the metric has the nice property to be diagonal.

G. Metric within the sector of site angles (θ_k, ϕ_k) with $k = 1, \dots, N$

1. Metric coefficients between the two angles (θ_k, ϕ_k) associated to the same site (k)

The tangent operators of Eq. 141 yields with Eqs 140 that the two diagonal elements read

$$\begin{aligned}
g(\theta_k, \theta_k) &= \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k-1,k}^{\beta_L, \alpha_L} \Lambda_{k,k+1}^{\alpha_R, \beta_R} \Lambda_{k,k+1}^{\beta_R, \alpha_R} \text{Tr}_{\{k\}} \left(\left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \theta_k} \right] \left[\frac{\partial O_k^{\beta_L \beta_R, \alpha_L \alpha_R}}{\partial \theta_k} \right] \right) = \frac{1}{2} \\
g(\phi_k, \phi_k) &= \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k-1,k}^{\beta_L, \alpha_L} \Lambda_{k,k+1}^{\alpha_R, \beta_R} \Lambda_{k,k+1}^{\beta_R, \alpha_R} \text{Tr}_{\{k\}} \left(\left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \phi_k} \right] \left[\frac{\partial O_k^{\beta_L \beta_R, \alpha_L \alpha_R}}{\partial \phi_k} \right] \right) \\
&= \frac{1 - \cos^2 \left(\theta_{k-\frac{1}{2}} \right) \cos^2 \theta_k \cos^2 \left(\theta_{k+\frac{1}{2}} \right)}{2}
\end{aligned} \tag{150}$$

while the off-diagonal element vanishes

$$g(\theta_k, \phi_k) = \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k-1,k}^{\beta_L, \alpha_L} \Lambda_{k,k+1}^{\alpha_R, \beta_R} \Lambda_{k,k+1}^{\beta_R, \alpha_R} \text{Tr}_{\{k\}} \left(\left[\frac{\partial O_k^{\alpha_L \alpha_R, \beta_L \beta_R}}{\partial \theta_k} \right] \left[\frac{\partial O_k^{\beta_L \beta_R, \alpha_L \alpha_R}}{\partial \phi_k} \right] \right) = 0$$

Here one sees how the two neighboring bond angles $\theta_{k \pm \frac{1}{2}}$ modify the Bloch sphere metric of (θ_k, ϕ_k) that the spin k would have if it were isolated.

2. Metric coefficients between the angles associated to the two neighboring sites (k) and $(k+1)$

Here the appropriate common decomposition reads

$$\begin{aligned}
V_{\theta_k} &= \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha = \pm \\ \beta = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \left(|\Phi_{\alpha_L}^{[1, \dots, k-1]} \rangle \langle \Phi_{\beta_L}^{[1, \dots, k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L, \beta_L} \left[\frac{\partial O_k^{\alpha_L \alpha, \beta_L \beta}}{\partial \theta_k} \right] \Lambda_{k,k+1}^{\alpha, \beta} O_{k+1}^{\alpha \alpha_R, \beta \beta_R} \Lambda_{k+1,k+2}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+2, \dots, N]} \rangle \langle \Phi_{\beta_R}^{[k+2, \dots, N]} | \right) \\
V_{\theta_{k+1}} &= \sum_{\substack{\alpha_L = \pm \\ \beta_L = \pm}} \sum_{\substack{\alpha = \pm \\ \beta = \pm}} \sum_{\substack{\alpha_R = \pm \\ \beta_R = \pm}} \left(|\Phi_{\alpha_L}^{[1, \dots, k-1]} \rangle \langle \Phi_{\beta_L}^{[1, \dots, k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L, \beta_L} O_k^{\alpha_L \alpha, \beta_L \beta} \Lambda_{k,k+1}^{\alpha, \beta} \left[\frac{\partial O_{k+1}^{\alpha \alpha_R, \beta \beta_R}}{\partial \theta_{k+1}} \right] \Lambda_{k+1,k+2}^{\alpha_R, \beta_R} \left(|\Phi_{\alpha_R}^{[k+2, \dots, N]} \rangle \langle \Phi_{\beta_R}^{[k+2, \dots, N]} | \right)
\end{aligned} \tag{151}$$

leading to the metric elements

$$\begin{aligned}
g(\theta_k, \theta_{k+1}) &= -\frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \cos\left(\theta_{k+\frac{3}{2}}\right)}{2} \\
g(\theta_k, \phi_{k+1}) &= -\frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \sin\theta_{k+1}}{2} \\
g(\phi_k, \theta_{k+1}) &= -\frac{\sin\theta_k \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \cos\left(\theta_{k+\frac{3}{2}}\right)}{2} \\
g(\phi_k, \phi_{k+1}) &= \frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \cos\theta_k \sin^2\left(\theta_{k+\frac{1}{2}}\right) \cos\theta_{k+1} \cos\left(\theta_{k+\frac{3}{2}}\right) + \sin\theta_k \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \sin\theta_{k+1}}{2}
\end{aligned} \tag{152}$$

3. *Metric coefficients between the angles associated to the two sites (k) and ($k+r$) with $r > 1$*

Here the appropriate common decomposition involves the interval ket of Eq. 62

$$\begin{aligned}
V_{\theta_k} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_1=\pm \\ \beta_1=\pm}} \sum_{\substack{\alpha_2=\pm \\ \beta_2=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} \left[\frac{\partial O_k^{\alpha_L\alpha_1,\beta_L\beta_1}}{\partial \theta_k} \right] \Lambda_{k,k+1}^{\alpha_1,\beta_1} \\
&\quad \left(|I_{\alpha_1,\alpha_2}^{[k+1,\dots,k+r-1]} \rangle \langle I_{\beta_1,\beta_2}^{[k+1,\dots,k+r-1]} | \right) \Lambda_{k+r-1,k+r}^{\alpha_2,\beta_2} O_{k+r}^{\alpha_2\alpha_R,\beta_2\beta_R} \Lambda_{k+r,k+r+1}^{\alpha_R,\beta_R} \left(|\Phi_{\alpha_R}^{[k+r+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1,\dots,N]} | \right)
\end{aligned} \tag{153}$$

$$\begin{aligned}
V_{\theta_{k+r}} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_1=\pm \\ \beta_1=\pm}} \sum_{\substack{\alpha_2=\pm \\ \beta_2=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} O_k^{\alpha_L\alpha_1,\beta_L\beta_1} \Lambda_{k,k+1}^{\alpha_1,\beta_1} \\
&\quad \left(|I_{\alpha_1,\alpha_2}^{[k+1,\dots,k+r-1]} \rangle \langle I_{\beta_1,\beta_2}^{[k+1,\dots,k+r-1]} | \right) \Lambda_{k+r-1,k+r}^{\alpha_2,\beta_2} \left[\frac{\partial O_{k+r}^{\alpha_2\alpha_R,\beta_2\beta_R}}{\partial \theta_{k+r}} \right] \Lambda_{k+r,k+r+1}^{\alpha_R,\beta_R} \left(|\Phi_{\alpha_R}^{[k+r+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1,\dots,N]} | \right)
\end{aligned} \tag{154}$$

Using the scalar products of the interval ket (Eq 63), one obtains that the metric coefficients involve the overlap $\omega_{k+1,k+r-1}$ of Eq. 64, that contains all the bond variables of the interval and that corresponds to the factor that governs the decay of correlations as explained in the previous section (Eq. 113 and Eq. 114)

$$\begin{aligned}
g(\theta_k, \theta_{k+r}) &= \frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \sin\left(\phi_{k+\frac{1}{2}}\right) \right] \omega_{k+1,k+r-1} \left[\sin\left(\theta_{k+r-\frac{1}{2}}\right) \sin\left(\phi_{k+r+\frac{1}{2}}\right) \right] \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{2} \\
g(\theta_k, \phi_{k+r}) &= -\frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \sin\left(\phi_{k+\frac{1}{2}}\right) \right] \omega_{k+1,k+r-1} \left[\sin\left(\theta_{k+r-\frac{1}{2}}\right) \cos\left(\phi_{k+r+\frac{1}{2}}\right) \right] \sin\theta_{k+r}}{2} \\
g(\phi_k, \theta_{k+r}) &= -\frac{\sin\theta_k \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \omega_{k+1,k+r-1} \left[\sin\left(\theta_{k+r-\frac{1}{2}}\right) \sin\left(\phi_{k+r+\frac{1}{2}}\right) \right] \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{2} \\
g(\phi_k, \phi_{k+r}) &= \frac{\sin\theta_k \left[\sin\left(\theta_{k+\frac{1}{2}}\right) \cos\left(\phi_{k+\frac{1}{2}}\right) \right] \omega_{k+1,k+r-1} \left[\sin\left(\theta_{k+r-\frac{1}{2}}\right) \cos\left(\phi_{k+r+\frac{1}{2}}\right) \right] \sin\theta_{k+r}}{2}
\end{aligned} \tag{155}$$

H. Metric coefficients between bond angles and sites angles

1. Metric coefficients between the angles of the site k and the angles of the bond $(k, k+1)$

Here the appropriate common decomposition reads

$$\begin{aligned}
V_{\theta_k} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} \left[\frac{\partial O_k^{\alpha_L\alpha_R,\beta_L\beta_R}}{\partial \theta_k} \right] \Lambda_{k,k+1}^{\alpha_R,\beta_R} \left(|\Phi_{\alpha_R}^{[k+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+1,\dots,N]} | \right) \\
V_{\theta_{k+\frac{1}{2}}} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} O_k^{\alpha_L\alpha_R,\beta_L\beta_R} \left[\frac{\partial \Lambda_{k,k+1}^{\alpha_R,\beta_R}}{\partial \theta_{k+\frac{1}{2}}} \right] \left(|\Phi_{\alpha_R}^{[k+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+1,\dots,N]} | \right)
\end{aligned}$$

Using Eq. 144 and 145 one obtains

$$\begin{aligned}
g(\theta_k, \theta_{k+\frac{1}{2}}) &= 0 \\
g(\theta_k, \phi_{k+\frac{1}{2}}) &= 0 \\
g(\phi_k, \theta_{k+\frac{1}{2}}) &= 0 \\
g(\phi_k, \phi_{k+\frac{1}{2}}) &= \frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \cos(\theta_k) \sin^2\left(\theta_{k+\frac{1}{2}}\right)}{2}
\end{aligned} \tag{156}$$

Similarly, the metric elements between the bond $(k, k+1)$ and the site $(k+1)$ read

$$\begin{aligned}
g(\theta_{k+\frac{1}{2}}, \theta_{k+1}) &= 0 \\
g(\phi_{k+\frac{1}{2}}, \theta_{k+1}) &= 0 \\
g(\theta_{k+\frac{1}{2}}, \phi_{k+1}) &= 0 \\
g(\phi_{k+\frac{1}{2}}, \phi_{k+1}) &= \frac{\sin^2\left(\theta_{k+\frac{1}{2}}\right) \cos(\theta_{k+1}) \cos\left(\theta_{k+\frac{3}{2}}\right)}{2}
\end{aligned} \tag{157}$$

2. Metric between the angles of the site k and the angles of the bond $(k+r, k+r+1)$ with $r > 1$

Here the appropriate common decomposition involves the interval ket of Eq. 62

$$\begin{aligned}
V_{\theta_k} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} \\
&\quad \left[\frac{\partial O_k^{\alpha_L\alpha,\beta_L\beta}}{\partial \theta_k} \right] \Lambda_{k,k+1}^{\alpha,\beta} \left(|I_{\alpha,\alpha_R}^{[k+1,\dots,k+r]} \rangle \langle I_{\beta,\beta_R}^{[k+1,\dots,k+r]} | \right) \Lambda_{k+r,k+r+1}^{\alpha_R,\beta_R} \left(|\Phi_{\alpha_R}^{[k+r+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1,\dots,N]} | \right) \\
V_{\theta_{k+r+\frac{1}{2}}} &= \sum_{\substack{\alpha_L=\pm \\ \beta_L=\pm}} \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \sum_{\substack{\alpha_R=\pm \\ \beta_R=\pm}} \left(|\Phi_{\alpha_L}^{[1,\dots,k-1]} \rangle \langle \Phi_{\beta_L}^{[1,\dots,k-1]} | \right) \Lambda_{k-1,k}^{\alpha_L,\beta_L} \\
&\quad O_k^{\alpha_L\alpha,\beta_L\beta} \Lambda_{k,k+1}^{\alpha,\beta} \left(|I_{\alpha,\alpha_R}^{[k+1,\dots,k+r]} \rangle \langle I_{\beta,\beta_R}^{[k+1,\dots,k+r]} | \right) \left[\frac{\partial \Lambda_{k+r,k+r+1}^{\alpha_R,\beta_R}}{\partial \theta_{k+r+\frac{1}{2}}} \right] \left(|\Phi_{\alpha_R}^{[k+r+1,\dots,N]} \rangle \langle \Phi_{\beta_R}^{[k+r+1,\dots,N]} | \right)
\end{aligned} \tag{158}$$

Using Eq 63, one obtains that the following metric elements vanish as a consequence of Eq. 135

$$\begin{aligned}
g(\theta_k, \theta_{k+r+\frac{1}{2}}) &= 0 \\
g(\theta_k, \phi_{k+r+\frac{1}{2}}) &= 0 \\
g(\phi_k, \theta_{k+r+\frac{1}{2}}) &= 0 \\
g(\phi_k, \phi_{k+r+\frac{1}{2}}) &= 0
\end{aligned} \tag{159}$$

I. Summary of the metric coefficients for each variable

Let us summarize the properties of this metric from the point of view of each variable :

- (i) the bond angle $\theta_{k+\frac{1}{2}}$ is orthogonal to all the other angles.
- (ii) the bond angle $\phi_{k+\frac{1}{2}}$ has non-vanishing off-diagonal metric coefficients with ϕ_k and ϕ_{k+1} only.
- (iii) the site angle θ_k has non-vanishing off-diagonal metric coefficients with all the other site angles (θ_{k+r}, ϕ_{k+r}) with $r \neq 0$, where the decay with the distance is governed by the overlap $\omega_{k+1, k+r-1}$ of Eq. 64.
- (iv) the site angle ϕ_k has non-vanishing off-diagonal metric coefficients with the two bond angles ($\phi_{k-\frac{1}{2}}, \phi_{k+\frac{1}{2}}$), and with all the other site variables (θ_{k+r}, ϕ_{k+r}) with $r \neq 0$, where the decay with the distance is again governed by the overlap $\omega_{k+1, k+r-1}$ of Eq. 64.

The in-depth analysis of all the properties of this metric clearly goes beyond the scope of the present work and is left for the future studies.

VIII. GENERALIZATION OF THE SIMPLEST MPS TO ANY STRUCTURE WITHOUT LOOPS

Since Matrix-Product-States for chains can be directly generalized to any tree-like structure without loops [60], it is interesting to describe in this section how the MPS of Eq. 24 can be extended to such tree-like structures without loops.

A. Parametrization of the ket on an arbitrary tree-like structure without loops

For each bond b that cuts the tree-like structure into two independent parts A and B , the Schmidt decomposition across this bond b keeps its meaning, and one can thus still introduce the two angles θ_b and ϕ_b to parametrize the two complex Schmidt values as in Eq 15

$$\begin{aligned}\lambda_b^+ &\equiv \cos\left(\frac{\theta_b}{2}\right) \\ \lambda_b^- &\equiv \sin\left(\frac{\theta_b}{2}\right) e^{i\phi_b}\end{aligned}\tag{160}$$

For each site k , one can still introduce the two Bloch angles θ_k and ϕ_k that parametrize the new appropriate local basis $|\tau_k^z = \pm\rangle$. With respect to the one-dimensional chain, the novelty is that each site k is connected to a certain number $c_k \geq 1$ of bonds that will be labelled by $b_1^{[k]}, \dots, b_{c_k}^{[k]}$. The leaves of the tree correspond to the sites k connected to a single link $c_k = 1$. The direct generalization of the MPS of Eq. 24 reads

$$|\psi\rangle = \left[\prod_b \left(\sum_{\alpha_b = \pm} \lambda_b^{\alpha_b} \right) \right] \left[\prod_k |\tau_k^z = \prod_{j=1}^{c_k} \alpha_{b_j^{[k]}}\rangle \right]\tag{161}$$

The corresponding MPO generalization of the density matrix of Eq. 28 reads

$$\rho = |\psi\rangle \langle\psi| = \left[\prod_b \left(\sum_{\substack{\alpha_b = \pm \\ \beta_b = \pm}} \Lambda_b^{\alpha_b, \beta_b} \right) \right] \left[\prod_k O_k^{\prod_{j=1}^{c_k} \alpha_{b_j^{[k]}}, \prod_{j=1}^{c_k} \beta_{b_j^{[k]}}} \right]\tag{162}$$

and involves a number of parameters given by

$$P_{N, N_b}^{Tree} = 2N + 2N_b\tag{163}$$

in terms of the number N of spins and the number N_b of bonds.

B. Reduced density matrix ρ_k of the site k alone

Around the site k , the c_k outgoing bonds labelled by $b_{j=1, \dots, c_k}^{[k]}$ corresponds to independent branches of the tree, and are thus associated to two orthonormal Schmidt eigenvectors $|\Phi_{\pm}^{b_j^{[k]}}\rangle$, so the MPS of Eq. 161 can be rewritten as

$$|\psi\rangle = \sum_{\alpha_1=\pm} \sum_{\alpha_2=\pm} \dots \sum_{\alpha_{c_k}=\pm} \left[\prod_{j=1}^{c_k} \lambda_{b_j^{[k]}}^{\alpha_j} |\Phi_{\alpha_j}^{b_j^{[k]}}\rangle \right] |\tau_k^z = \prod_{j=1}^{c_k} \alpha_j\rangle \quad (164)$$

with the corresponding full density matrix

$$\rho = |\psi\rangle \langle \psi| = \sum_{\substack{\alpha_1=\pm \\ \beta_1=\pm}} \sum_{\substack{\alpha_2=\pm \\ \beta_2=\pm}} \dots \sum_{\substack{\alpha_{c_k}=\pm \\ \beta_{c_k}=\pm}} \left[\prod_{j=1}^{c_k} \Lambda_{b_j^{[k]}}^{\alpha_j, \beta_j} \left(|\Phi_{\alpha_j}^{b_j^{[k]}}\rangle \langle \Phi_{\beta_j}^{b_j^{[k]}}| \right) \right] O_k^{\prod_{j=1}^{c_k} \alpha_j, \prod_{j=1}^{c_k} \beta_j} \quad (165)$$

The trace over the c_k outgoing branches imposes $\beta_j = \alpha_j$ for $j = 1, \dots, c_k$, so the reduced density matrix of the site k alone reads using the explicit expressions of Eq. 31 and Eq. 35

$$\begin{aligned} \rho_k &= \sum_{\alpha_1=\pm} \sum_{\alpha_2=\pm} \dots \sum_{\alpha_{c_k}=\pm} \left[\prod_{j=1}^{c_k} \Lambda_{b_j^{[k]}}^{\alpha_j, \alpha_j} \right] O_k^{\prod_{j=1}^{c_k} \alpha_j, \prod_{j=1}^{c_k} \alpha_j} \\ &= \frac{1}{2^{1+c_k}} \sum_{\alpha_1=\pm} \sum_{\alpha_2=\pm} \dots \sum_{\alpha_{c_k}=\pm} \left[\prod_{j=1}^{c_k} \left(1 + \alpha_j \cos(\theta_{b_j^{[k]}}) \right) \right] \left(1 + \left(\prod_{j=1}^{c_k} \alpha_j \right) \tau_k^z \right) \\ &= \frac{1}{2} + \frac{\tau_k^z}{2} \prod_{j=1}^{c_k} \cos(\theta_{b_j^{[k]}}) \end{aligned} \quad (166)$$

So the two ket $|\tau_k^z = \pm\rangle$ are still the two eigenvectors of the reduced density matrix ρ_k , and the corresponding eigenvalues

$$p_k^{\pm} = \frac{1}{2} \left[1 \pm \prod_{j=1}^{c_k} \cos(\theta_{b_j^{[k]}}) \right] \quad (167)$$

now involves the c_k angles $\theta_{b_{j=1, \dots, c_k}^{[k]}}$ of the c_k bonds connected to the site k , instead of the two angles of Eq. 51 for the chain.

C. Reduced density matrix ρ_{k_L, k_R} of two neighboring sites (k_L, k_R) connected by the bond b

Let us now focus on two neighboring sites (k_L, k_R) connected by the bond b : the site k_L is connected to $(c_{k_L} - 1)$ other bonds that will be relabeled by $\theta_{b_{j_L=1, \dots, (c_{k_L}-1)}^{[k_L]}}$, and the site k_R is connected to $(c_{k_R} - 1)$ other bonds that will be relabeled by $\theta_{b_{j_R=1, \dots, (c_{k_R}-1)}^{[k_R]}}$. All these out-going branches are independent, so the appropriate decomposition of the ket of Eq. 161 reads

$$|\psi\rangle = \sum_{\alpha=\pm} \left[\prod_{j_L=1}^{c_{k_L}-1} \sum_{\alpha_{j_L}^L=\pm} \lambda_{b_{j_L}^{[k_L]}}^{\alpha_{j_L}^L} |\Phi_{\alpha_{j_L}^L}^{b_{j_L}^{[k_L]}}\rangle \right] \left[\prod_{j_R=1}^{c_{k_R}-1} \sum_{\alpha_{j_R}^R=\pm} \lambda_{b_{j_R}^{[k_R]}}^{\alpha_{j_R}^R} |\Phi_{\alpha_{j_R}^R}^{b_{j_R}^{[k_R]}}\rangle \right] |\tau_{k_L}^z = \alpha \prod_{j_L=1}^{c_{k_L}-1} \alpha_{j_L}^L \rangle \lambda_b^\alpha |\tau_{k_R}^z = \alpha \prod_{j_R=1}^{c_{k_R}-1} \alpha_{j_R}^R \rangle \quad (168)$$

with the corresponding full density matrix

$$\rho = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} \left[\prod_{j_L=1}^{c_{k_L}-1} \sum_{\substack{\alpha_{j_L}^L \\ \beta_{j_L}^L}} \Lambda_{b_{j_L}^{[k_L]}}^{\alpha_{j_L}^L, \beta_{j_L}^L} \left(|\Phi_{\alpha_{j_L}^L}^{b_{j_L}^{[k_L]}}\rangle \langle \Phi_{\beta_{j_L}^L}^{b_{j_L}^{[k_L]}}| \right) \right] \left[\prod_{j_R=1}^{c_{k_R}-1} \sum_{\substack{\alpha_{j_R}^R \\ \beta_{j_R}^R}} \Lambda_{b_{j_R}^{[k_R]}}^{\alpha_{j_R}^R, \beta_{j_R}^R} \left(|\Phi_{\alpha_{j_R}^R}^{b_{j_R}^{[k_R]}}\rangle \langle \Phi_{\beta_{j_R}^R}^{b_{j_R}^{[k_R]}}| \right) \right] \\ \alpha \prod_{j_L=1}^{c_{k_L}-1} \alpha_{j_L}^L, \beta \prod_{j_L=1}^{c_{k_L}-1} \beta_{j_L}^L \quad \alpha \prod_{j_R=1}^{c_{k_R}-1} \alpha_{j_R}^R, \beta \prod_{j_R=1}^{c_{k_R}-1} \beta_{j_R}^R \\ O_{k_L}^{\alpha, \beta} \Lambda_b^{\alpha, \beta} O_{k_R}^{\alpha, \beta} \quad (169)$$

The trace over the $(c_{k_L} - 1) + (c_{k_R} - 1)$ outgoing branches imposes $\beta_{j_L}^L = \beta_{j_L}^L$ for $j_L = 1, \dots, c_{k_L} - 1$ and $\beta_{j_R}^R = \beta_{j_R}^R$ for $j_R = 1, \dots, c_{k_R} - 1$ so the reduced density matrix of the two neighboring sites (k_L, k_R) reads

$$\rho_{k_L, k_R} = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} W_{[k_L]}^{\alpha, \beta} \Lambda_b^{\alpha, \beta} W_{k_R}^{\alpha, \beta} \\ = \sum_{\substack{\alpha=\pm \\ \beta=\pm}} W_{[k_L]}^{\alpha, \beta} \left[\delta_{\alpha, \beta} \left(\frac{1 + \alpha \cos \theta_b}{2} \right) + \delta_{\alpha, -\beta} \left(\frac{\sin \theta_b [\cos \phi_b - i \alpha \cos \phi_b]}{2} \right) \right] W_{k_R}^{\alpha, \beta} \quad (170)$$

in terms of the two modified operators that are the analog of Eqs 78 79 80

$$W_{[k_L]}^{\alpha, \beta} = \left[\prod_{j_L=1}^{c_{k_L}-1} \sum_{\alpha_{j_L}^L = \pm} \Lambda_{b_{j_L}^{[k_L]}}^{\alpha_{j_L}^L, \alpha_{j_L}^L} \right] O_{k_L}^{\alpha} \prod_{j_L=1}^{c_{k_L}-1} \alpha_{j_L}^L, \beta \prod_{j_L=1}^{c_{k_L}-1} \alpha_{j_L}^L = \frac{\delta_{\alpha, \beta}}{2} \left(1 + \alpha \tau_{k_L}^z \mathcal{C}_{out}^{[k_L]} \right) + \frac{\delta_{\alpha, -\beta}}{2} \left(\tau_{k_L}^x + i \alpha \tau_{k_L}^y \mathcal{C}_{out}^{[k_L]} \right) \\ W_{k_R}^{\alpha, \beta} = \left[\prod_{j_R=1}^{c_{k_R}-1} \sum_{\alpha_{j_R}^R = \pm} \Lambda_{b_{j_R}^{[k_R]}}^{\alpha_{j_R}^R, \alpha_{j_R}^R} \right] O_{k_R}^{\alpha} \prod_{j_R=1}^{c_{k_R}-1} \alpha_{j_R}^R, \beta \prod_{j_R=1}^{c_{k_R}-1} \alpha_{j_R}^R = \frac{\delta_{\alpha, \beta}}{2} \left(1 + \alpha \tau_{k_R}^z \mathcal{C}_{out}^{[k_R]} \right) + \frac{\delta_{\alpha, -\beta}}{2} \left(\tau_{k_R}^x + i \alpha \tau_{k_R}^y \mathcal{C}_{out}^{[k_R]} \right) \quad (171)$$

where the two coefficients involve all the angles of the outgoing links

$$\mathcal{C}_{out}^{[k_L]} \equiv \prod_{j_L=1}^{c_{k_L}-1} \cos \left(\theta_{b_{j_L}^{[k_L]}} \right) \\ \mathcal{C}_{out}^{[k_R]} = \prod_{j_R=1}^{c_{k_R}-1} \cos \left(\theta_{b_{j_R}^{[k_R]}} \right) \quad (172)$$

The final result

$$\rho_{k_L, k_R} = \frac{1}{8} \sum_{\alpha=\pm 1} (1 + \alpha \cos \theta_b) \left(1 + \alpha \tau_{k_L}^z \mathcal{C}_{out}^{[k_L]} \right) \left(1 + \alpha \tau_{k_R}^z \mathcal{C}_{out}^{[k_R]} \right) \\ + \frac{\sin \theta_b}{8} \sum_{\alpha=\pm 1} (\cos \phi_b - i \alpha \cos \phi_b) \left(\tau_{k_L}^x + i \alpha \tau_{k_L}^y \mathcal{C}_{out}^{[k_L]} \right) \left(\tau_{k_R}^x + i \alpha \tau_{k_R}^y \mathcal{C}_{out}^{[k_R]} \right) \\ = \frac{1}{4} + \cos \theta_b \left[\frac{\tau_{k_L}^z \mathcal{C}_{out}^{[k_L]} + \tau_{k_R}^z \mathcal{C}_{out}^{[k_R]}}{4} \right] + \frac{\tau_{k_L}^z \tau_{k_R}^z \mathcal{C}_{out}^{[k_L]} \mathcal{C}_{out}^{[k_R]}}{4} \\ + \sin \theta_b \cos \phi_b \left[\frac{\tau_{k_L}^x \tau_{k_R}^x - \tau_{k_L}^y \tau_{k_R}^y \mathcal{C}_{out}^{[k_L]} \mathcal{C}_{out}^{[k_R]}}{4} \right] + \sin \theta_b \sin \phi_b \left[\frac{\tau_{k_L}^x \tau_{k_R}^y \mathcal{C}_{out}^{[k_R]} + \tau_{k_L}^y \tau_{k_R}^x \mathcal{C}_{out}^{[k_L]}}{4} \right] \quad (173)$$

is thus a direct generalization of the corresponding result of Eq. 94 concerning the chain.

D. Discussion

The reduced density matrices for a single site (Eq. 167) and for two neighboring sites (Eq. 173) can be then used to compute the energy of Hamiltonians containing only one-body and two-body terms in order to optimize the MPS parameters as described in section V. Here we have chosen to remain very general with an arbitrary tree-like structure without loops, but to analyze the more global properties of the MPS, one should specify the specific global geometry of the tree structure one is interested in, so this is left for future studies.

IX. GENERALIZATION OF THE SIMPLEST MPS TO A PERIODIC RING OF N SPINS

In the main text we have focused on the case of an open chain, but since Matrix-Product-States are also much used in the presence of periodic boundary conditions, it is interesting to discuss the changes that are needed for a ring of N spins.

A. MPS ket on the ring with its normalization

On a ring, the cut of a single bond does not give two independent parts, so the bond variables $\lambda_{k,k+1}^{\alpha=\pm}$ unfortunately lose their direct interpretation in terms of the Schmidt decomposition, but one can nevertheless adapt the MPS ket of the open chain (Eq 24) by adding on the bond $(N, N+1) = (N, 1)$ that join the two boundaries the following variables as in Eq. 23

$$\begin{aligned}\lambda_{N,1}^+ &\equiv \cos\left(\frac{\theta_{N+\frac{1}{2}}}{2}\right) \\ \lambda_{N,1}^- &\equiv \sin\left(\frac{\theta_{N+\frac{1}{2}}}{2}\right) e^{i\phi_{N+\frac{1}{2}}}\end{aligned}\quad (174)$$

and by adding some normalization K_N that will be computed below

$$|\psi^{Ring}\rangle = \frac{1}{K_N} \sum_{\alpha_1=\pm} \dots \sum_{\alpha_{N-1}=\pm} \sum_{\alpha_N=\pm} \left[\prod_{k=1}^N \lambda_{k,k+1}^{\alpha_k} \right] \left[\prod_{k=1}^N |\tau_k^z = \alpha_{k-1}\alpha_k\rangle \right] \quad (175)$$

This can be rewritten in terms of the interval ket of Eq. 62 as

$$|\psi^{Ring}\rangle = \frac{1}{K_N} \sum_{\alpha=\pm} \lambda_{N,1}^{\alpha} |I_{\alpha,\alpha}^{[1,\dots,N]}\rangle \quad (176)$$

so the normalization can be computed with the scalar product of Eq 63

$$\begin{aligned}1 = \langle \psi^{Ring} | \psi^{Ring} \rangle &= \frac{1}{K_N^2} \sum_{\alpha=\pm} \sum_{\beta=\pm} \lambda_{N,1}^{\alpha} \overline{\lambda_{N,1}^{\beta}} \langle I_{\beta,\beta}^{[1,\dots,N]} | I_{\alpha,\alpha}^{[1,\dots,N]} \rangle = \frac{1}{K_N^2} \sum_{\alpha=\pm} \sum_{\beta=\pm} \Lambda_{N,1}^{\alpha,\beta} [\delta_{\alpha,\beta} + \delta_{\alpha,-\beta} \omega_{1,N}] \\ &= \frac{1}{K_N^2} \sum_{\alpha=\pm} \left[\Lambda_{N,1}^{\alpha,\alpha} + \Lambda_{N,1}^{\alpha,-\alpha} \omega_{1,N} \right] = \frac{1 + \omega_N^{Ring}}{K_N^2}\end{aligned}\quad (177)$$

where ω_N^{Ring} is the generalization of Eq 64 for the total ring and thus involves the $(2N)$ bond angles of the whole ring

$$\omega_N^{Ring} \equiv \omega_{1,N+1} \equiv \prod_{n=1}^N \left[\sin\left(\theta_{n+\frac{1}{2}}\right) \cos\left(\phi_{n+\frac{1}{2}}\right) \right] \quad (178)$$

The normalization factor K_N thus reads

$$K_N = \sqrt{1 + \omega_N^{Ring}} \quad (179)$$

B. Reduced density matrix ρ_k for the site k alone

In order to focus on the spin k , the appropriate decomposition of Eq. 175 involves the interval ket $|I_{\alpha_R, \alpha_L}^{[k+1, \dots, N+k-1]}\rangle$ of the Ring without the site k (instead of Eq. 47 for the open chain)

$$|\psi\rangle = \frac{1}{K_N} \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \lambda_{k-1, k}^{\alpha_L} |\tau_k^z = \alpha_L \alpha_R\rangle \lambda_{k, k+1}^{\alpha_R} |I_{\alpha_R, \alpha_L}^{[k+1, \dots, N+k-1]}\rangle \quad (180)$$

with the corresponding full density matrix (instead of Eq. 48 for the open chain)

$$\rho = |\psi\rangle \langle \psi| = \frac{1}{K_N^2} \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \sum_{\beta_L = \pm} \sum_{\beta_R = \pm} \Lambda_{k-1, k}^{\alpha_L, \beta_L} (|\tau_k^z = \alpha_L \alpha_R\rangle \langle \tau_k^z = \beta_L \beta_R|) \Lambda_{k, k+1}^{\alpha_R, \beta_R} \left(|I_{\alpha_R, \alpha_L}^{[k+1, \dots, N+k-1]}\rangle \langle I_{\beta_R, \beta_L}^{[k+1, \dots, N+k-1]}| \right) \quad (181)$$

The trace over the other $(N-1)$ sites $(k+1, \dots, N+k-1)$ can be computed using Eq. 63

$$\begin{aligned} \rho_k &= \text{Tr}_{\{k+1, \dots, N+k-1\}}(\rho) = \frac{1}{K_N^2} \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \sum_{\beta_L = \pm} \sum_{\beta_R = \pm} \Lambda_{k-1, k}^{\alpha_L, \beta_L} O_k^{\alpha_L \alpha_R, \beta_L \beta_R} \Lambda_{k, k+1}^{\alpha_R, \beta_R} \langle I_{\beta_R, \beta_L}^{[k+1, \dots, N+k-1]} | I_{\alpha_R, \alpha_L}^{[k+1, \dots, N+k-1]} \rangle \\ &= \frac{1}{K_N^2} \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \sum_{\beta_L = \pm} \sum_{\beta_R = \pm} \Lambda_{k-1, k}^{\alpha_L, \beta_L} O_k^{\alpha_L \alpha_R, \beta_L \beta_R} \Lambda_{k, k+1}^{\alpha_R, \beta_R} \delta_{\beta_L \beta_R, \alpha_L \alpha_R} [\delta_{\alpha_L, \beta_L} + \delta_{\alpha_L, -\beta_L} \omega_{k+1, N+k-1}] \end{aligned} \quad (182)$$

The explicit expressions of Eq. 31 and of Eq. 35 lead to the final result

$$\rho_k = \frac{1}{2} + \frac{\tau_k^z}{2} \left(\frac{\cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+\frac{1}{2}}\right) - \omega_N^{Ring} \tan\left(\phi_{k-\frac{1}{2}}\right) \tan\left(\phi_{k+\frac{1}{2}}\right)}{1 + \omega_N^{Ring}} \right) \quad (183)$$

So the two ket $|\tau_k^z = \pm\rangle$ are still the two eigenvectors of the reduced density matrix ρ_k as for the open chain (Eq 50), even if the corresponding eigenvalues have changed with respect to Eq. 51, and have lost their locality since ω_N^{Ring} contains the bond angles of the whole ring.

C. Reduced density matrix $\rho_{k, k+1}$ of two consecutive sites

If one wishes to focus on the two consecutive spins k and $(k+1)$, the appropriate decomposition of Eq. 175 reads

$$|\psi\rangle = \frac{1}{K_N} \sum_{\alpha_L = \pm} \sum_{\alpha = \pm} \sum_{\alpha_R = \pm} \lambda_{k-1, k}^{\alpha_L} |\tau_k^z = \alpha_L \alpha\rangle \lambda_{k, k+1}^{\alpha} |\tau_{k+1}^z = \alpha \alpha_R\rangle \lambda_{k+1, k+2}^{\alpha_R} |I_{\alpha_R, \alpha_L}^{[k+2, \dots, N+k-1]}\rangle \quad (184)$$

with the corresponding full density matrix (instead of Eq. 48 for the open chain)

$$\begin{aligned} \rho &= \frac{1}{K_N^2} \sum_{\alpha_L = \pm} \sum_{\alpha_R = \pm} \sum_{\alpha = \pm} \sum_{\beta_L = \pm} \sum_{\beta_R = \pm} \sum_{\beta = \pm} \Lambda_{k-1, k}^{\alpha_L, \beta_L} O_k^{\alpha_L \alpha, \beta_L \beta} \Lambda_{k, k+1}^{\alpha, \beta} O_{k+1}^{\alpha \alpha_R, \beta \beta_R} \Lambda_{k+1, k+2}^{\alpha_R, \beta_R} \left(|I_{\alpha_R, \alpha_L}^{[k+2, \dots, N+k-1]}\rangle \langle I_{\beta_R, \beta_L}^{[k+2, \dots, N+k-1]}| \right) \end{aligned} \quad (185)$$

The trace over the other $(N-2)$ sites $(k+2, \dots, N+k-1)$ yields using Eq. 63, Eq. 31 and Eq. 35

$$\begin{aligned}
\rho_{k,k+1} &= \text{Tr}_{\{k+2,\dots,N+k-1\}}(\rho) = \frac{1}{K_N^2} \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} \sum_{\alpha=\pm} \sum_{\beta_L=\pm} \sum_{\beta_R=\pm} \sum_{\beta=\pm} \\
&\Lambda_{k-1,k}^{\alpha_L,\beta_L} O_k^{\alpha_L\alpha,\beta_L\beta} \Lambda_{k,k+1}^{\alpha,\beta} O_{k+1}^{\alpha\alpha_R,\beta\beta_R} \Lambda_{k+1,k+2}^{\alpha_R,\beta_R} \delta_{\beta_L\beta_R,\alpha_L\alpha_R} [\delta_{\alpha_L,\beta_L} + \delta_{\alpha_L,-\beta_L} \omega_{k+2,N+k-1}] \\
&= \frac{1}{4} + \frac{\tau_k^z}{4} \left(\frac{\cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{1}{2}}) - \omega_N^{Ring} \tan(\phi_{k-\frac{1}{2}}) \tan(\phi_{k+\frac{1}{2}})}{1 + \omega_N^{Ring}} \right) \\
&+ \frac{\tau_{k+1}^z}{4} \left(\frac{\cos(\theta_{k+\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) - \omega_N^{Ring} \tan(\phi_{k+\frac{1}{2}}) \tan(\phi_{k+\frac{3}{2}})}{1 + \omega_N^{Ring}} \right) \\
&+ \frac{\tau_k^z \tau_{k+1}^z}{4} \left(\frac{\cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) - \omega_N^{Ring} \tan(\phi_{k-\frac{1}{2}}) \tan(\phi_{k+\frac{3}{2}})}{1 + \omega_N^{Ring}} \right) \\
&+ \frac{\tau_k^x \tau_{k+1}^x}{4} \left(\frac{\sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}}) + \frac{\omega_N^{Ring}}{\sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}})}}{1 + \omega_N^{Ring}} \right) \\
&- \frac{\tau_k^y \tau_{k+1}^y}{4} \left(\frac{\cos(\theta_{k-\frac{1}{2}}) \cos(\theta_{k+\frac{3}{2}}) \sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}}) - \frac{\omega_N^{Ring} \tan(\phi_{k-\frac{1}{2}}) \tan(\phi_{k+\frac{3}{2}})}{\sin(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}})}}{1 + \omega_N^{Ring}} \right) \\
&+ \frac{\tau_k^x \tau_{k+1}^y}{4} \left(\frac{\cos(\theta_{k+\frac{3}{2}}) \sin(\theta_{k+\frac{1}{2}}) \sin(\phi_{k+\frac{1}{2}}) + \frac{\omega_N^{Ring} \tan(\phi_{k+\frac{3}{2}})}{\tan(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}})}}{1 + \omega_N^{Ring}} \right) \\
&+ \frac{\tau_k^y \tau_{k+1}^x}{4} \left(\frac{\cos(\theta_{k-\frac{1}{2}}) \sin(\theta_{k+\frac{1}{2}}) \sin(\phi_{k+\frac{1}{2}}) + \frac{\omega_N^{Ring} \tan(\phi_{k-\frac{1}{2}})}{\tan(\theta_{k+\frac{1}{2}}) \cos(\phi_{k+\frac{1}{2}})}}{1 + \omega_N^{Ring}} \right)
\end{aligned} \tag{186}$$

So again the same eight Pauli operators appear as for the open chain (Eq. 94) even the coefficients are more complicated.

X. CONCLUSION

In this paper, we have focused on the simplest inhomogeneous Matrix-Product-State for an open chain of N quantum spins that involves two angles per site and two angles per bond with a very clear physical meaning : the two angles associated to the site k are the two Bloch angles that parametrize the two orthonormal eigenvectors of the reduced density matrix ρ_k of the spin k alone, while the two angles associated to the bond $(k, k+1)$ parametrize the entanglement properties of the Schmidt decomposition across the bond $(k, k+1)$ within the gauge fixing described in section II. We have then described how this simple structure allows to compute explicitly many observables, including (i) the reduced density matrix $\rho_{k,k+1}$ of two consecutive sites needed to evaluate the energy of two-body Hamiltonians (ii) the reduced density matrix $\rho_{k,k+r}$ of two sites at distance r needed to evaluate the spin-spin correlations at distance r (iii) the Riemann metric of the MPS manifold as parametrized by these $(4N-2)$ angles. Finally, we have discussed the generalization to any tree-like structure without loops and to the chain with periodic boundary conditions.

Our main conclusion is thus that besides the outstanding achievements obtained by the Tensor Networks algorithms over the years, it is interesting to consider simple Tensor Networks of small dimension to compute explicitly their properties. In the future, we hope to use the present framework to construct toy models of Many-Body-Localization where all the eigenstates are Matrix-Product-States [61], to generalize the present approach to other entanglement

architectures like MERA in order to describe critical states of disordered spin chains [62], and to use the tangent space geometry to analyse dynamical problems [62].

Appendix A: Diagonal form of the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of $(r+1)$ consecutive sites in the bulk

Many properties of the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of $(r+1)$ consecutive sites in the bulk have already been discussed in section IV in the text. In this Appendix, we analyze its spectral decomposition. But first it is instructive to analyze how the Left part $[1, \dots, k-1]$ and the Right part $[k+r+1, \dots, N]$ are entangled.

1. Diagonalization of the reduced density matrix $\rho_{[1,\dots,k-1],[k+r+1,\dots,N]}$ of the Left and Right parts together

The reduced density matrix $\rho_{[1,\dots,k-1],[k+r+1,\dots,N]}$ of the Left and Right parts together can be computed from the full density matrix of Eq. 72 by taking the trace over the interval spins $(k, \dots, k+r)$ that involve the scalar products of Eq. 63

$$\text{Tr}_{\{k,\dots,k+r\}} \left(\left(|I_{\alpha_L, \alpha_R}^{[k,\dots,k+r]}\rangle \langle I_{\beta_L, \beta_R}^{[k,\dots,k+r]}| \right) \right) = \langle I_{\beta_L, \beta_R}^{[k,\dots,k+r]} | I_{\alpha_L, \alpha_R}^{[k,\dots,k+r]} \rangle = \delta_{\beta_L \beta_R, \alpha_L \alpha_R} [\delta_{\alpha_L, \beta_L} + \omega_{k,k+r} \delta_{\alpha_L, -\beta_L}] \quad (\text{A1})$$

and one obtains the following form in terms of the two Schmidt eigenvectors $|\Phi_{\pm}^{[1,\dots,k]}\rangle$ of the Left part alone and in terms of the two Schmidt eigenvectors $|\Phi_{\pm}^{[k+1,\dots,N]}\rangle$ of the Right part alone

$$\begin{aligned} \rho_{[1,\dots,k-1],[k+r+1,\dots,N]} &\equiv \text{Tr}_{\{k,\dots,k+r\}} (\rho) \\ &= \sum_{\alpha_L=\pm} \sum_{\alpha_R=\pm} \sum_{\beta_L=\pm} \sum_{\beta_R=\pm} \rho_{L,R}^{(\alpha_L, \alpha_R), (\beta_L, \beta_R)} \left(|\Phi_{\alpha_L}^{[1,\dots,k]}\rangle \otimes |\Phi_{\alpha_R}^{[k+1,\dots,N]}\rangle \right) \left(\langle \Phi_{\beta_L}^{[1,\dots,k]} | \otimes \langle \Phi_{\beta_R}^{[k+1,\dots,N]} | \right) \end{aligned}$$

where the matrix elements in this basis of the Schmidt eigenvectors can be computed using Eq. 31

$$\begin{aligned} \rho_{L,R}^{(\alpha_L, \alpha_R), (\beta_L, \beta_R)} &= \delta_{\beta_L \beta_R, \alpha_L \alpha_R} [\delta_{\alpha_L, \beta_L} + \omega_{k,k+r} \delta_{\alpha_L, -\beta_L}] \Lambda_{k-1,k}^{\alpha_L, \beta_L} \Lambda_{k+r,k+r+1}^{\alpha_R, \beta_R} \\ &= \delta_{\beta_L \beta_R, \alpha_L \alpha_R} [\delta_{\alpha_L, \beta_L} + \omega_{k,k+r} \delta_{\alpha_L, -\beta_L}] \left[\delta_{\alpha_L, \beta_L} \left(\frac{1 + \alpha_L \cos(\theta_{k-\frac{1}{2}})}{2} \right) + \delta_{\alpha_L, -\beta_L} \left(\frac{\sin(\theta_{k-\frac{1}{2}})}{2} e^{-i\alpha_L \phi_{k-\frac{1}{2}}} \right) \right] \\ &\quad \left[\delta_{\alpha_R, \beta_R} \left(\frac{1 + \alpha_R \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) + \delta_{\alpha_R, -\beta_R} \left(\frac{\sin(\theta_{k+r+\frac{1}{2}})}{2} e^{-i\alpha_R \phi_{k+r+\frac{1}{2}}} \right) \right] \\ &= \delta_{\alpha_L, \beta_L} \delta_{\alpha_R, \beta_R} \left(\frac{1 + \alpha_L \cos(\theta_{k-\frac{1}{2}})}{2} \right) \left(\frac{1 + \alpha_R \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) \\ &\quad + \delta_{\alpha_L, -\beta_L} \delta_{\alpha_R, -\beta_R} \omega_{k,k+r} \left(\frac{\sin(\theta_{k-\frac{1}{2}})}{2} e^{-i\alpha_L \phi_{k-\frac{1}{2}}} \right) \left(\frac{\sin(\theta_{k+r+\frac{1}{2}})}{2} e^{-i\alpha_R \phi_{k+r+\frac{1}{2}}} \right) \end{aligned} \quad (\text{A2})$$

This 4×4 matrix is thus block-diagonal in the basis $(++, --, +-, -+)$

$$\rho_{L,R} = \begin{pmatrix} D^{++} & \Omega_F & 0 & 0 \\ \overline{\Omega}_F & D^{--} & 0 & 0 \\ 0 & 0 & D^{+-} & \Omega_A \\ 0 & 0 & \overline{\Omega}_A & D^{-+} \end{pmatrix} \quad (\text{A3})$$

with the four diagonal elements

$$D^{(\alpha_L, \alpha_R)} \equiv \rho_{L,R}^{(\alpha_L, \alpha_R), (\alpha_L, \alpha_R)} = \left(\frac{1 + \alpha_L \cos(\theta_{k-\frac{1}{2}})}{2} \right) \left(\frac{1 + \alpha_R \cos(\theta_{k+r+\frac{1}{2}})}{2} \right) \quad (\text{A4})$$

and the two off-diagonal elements

$$\begin{aligned}\Omega_F &\equiv \rho_{L,R}^{(+,+),(-,-)} = \frac{\omega_{k,k+r}}{4} \sin\left(\theta_{k-\frac{1}{2}}\right) \sin\left(\theta_{k+r+\frac{1}{2}}\right) e^{-i\phi_{k-\frac{1}{2}} - i\phi_{k+r+\frac{1}{2}}} \\ \Omega_A &\equiv \rho_{L,R}^{(+,-),(-,+)} = \frac{\omega_{k,k+r}}{4} \sin\left(\theta_{k-\frac{1}{2}}\right) \sin\left(\theta_{k+r+\frac{1}{2}}\right) e^{-i\phi_{k-\frac{1}{2}} + i\phi_{k+r+\frac{1}{2}}}\end{aligned}$$

with their complex conjugates $\overline{\Omega_F}$ and $\overline{\Omega_A}$. The overlap $\omega_{k,k+r}$ of Eq. 64 appears in all the off-diagonal elements and will thus govern the magnitude of the entanglement between the Left part and the Right part separated by the distance r , in agreement with the fact that the overlap $\omega_{k,k+r}$ also governs the correlations between the two spins r and $k+r$ as described in section VI.

The traces of the two blocks of the matrix of Eq. A3 read respectively

$$\begin{aligned}\mathcal{T}_F &\equiv D^{(++)} + D^{(--)} = \left(\frac{1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{2} \right) \\ \mathcal{T}_A &\equiv D^{(+-)} + D^{(-+)} = \left(\frac{1 - \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{2} \right)\end{aligned}\quad (\text{A5})$$

while they have the same determinant

$$\mathcal{D} \equiv D^{(++)}D^{(--)} - |\Omega_F|^2 = D^{(+-)}D^{(-+)} - |\Omega_A|^2 = \frac{(1 - \omega_{k,k+r}^2) \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)}{16}\quad (\text{A6})$$

so their eigenvalues read respectively

$$\begin{aligned}p_{\pm}^F &= \frac{\mathcal{T}_F \pm \sqrt{\mathcal{T}_F^2 - 4\mathcal{D}}}{2} \\ &= \frac{1 + \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right) \pm \sqrt{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) + \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)}}{4} \\ p_{\pm}^A &= \frac{\mathcal{T}_A \pm \sqrt{\mathcal{T}_A^2 - 4\mathcal{D}}}{2} \\ &= \frac{1 - \cos\left(\theta_{k-\frac{1}{2}}\right) \cos\left(\theta_{k+r+\frac{1}{2}}\right) \pm \sqrt{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) - \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)}}{4}\end{aligned}\quad (\text{A7})$$

The corresponding eigenvectors read

$$\begin{aligned}|\Phi_{LR}^{F+}\rangle &= \cos\left(\frac{\theta_F}{2}\right) |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle + \sin\left(\frac{\theta_F}{2}\right) e^{i\phi_F} |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle \\ |\Phi_{LR}^{F-}\rangle &= \sin\left(\frac{\theta_F}{2}\right) |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle - \cos\left(\frac{\theta_F}{2}\right) e^{i\phi_F} |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle \\ |\Phi_{LR}^{A+}\rangle &= \cos\left(\frac{\theta_A}{2}\right) |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle + \sin\left(\frac{\theta_A}{2}\right) e^{i\phi_A} |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle \\ |\Phi_{LR}^{A-}\rangle &= \sin\left(\frac{\theta_A}{2}\right) |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle - \cos\left(\frac{\theta_A}{2}\right) e^{i\phi_A} |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle\end{aligned}\quad (\text{A8})$$

in terms of the angles

$$\begin{aligned}
\phi_F &\equiv \phi_{k-\frac{1}{2}} + \phi_{k+r+\frac{1}{2}} \\
\phi_A &\equiv \phi_{k-\frac{1}{2}} - \phi_{k+r+\frac{1}{2}} \\
\cos(\theta_F) &\equiv \frac{\cos\left(\theta_{k-\frac{1}{2}}\right) + \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) + \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)} \\
\sin(\theta_F) &\equiv \frac{\omega_{k,k+r} \sin\left(\theta_{k-\frac{1}{2}}\right) \sin\left(\theta_{k+r+\frac{1}{2}}\right)}{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) + \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)} \\
\cos(\theta_A) &\equiv \frac{\cos\left(\theta_{k-\frac{1}{2}}\right) - \cos\left(\theta_{k+r+\frac{1}{2}}\right)}{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) - \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)} \\
\sin(\theta_A) &\equiv \frac{\omega_{k,k+r} \sin\left(\theta_{k-\frac{1}{2}}\right) \sin\left(\theta_{k+r+\frac{1}{2}}\right)}{\left[\cos\left(\theta_{k-\frac{1}{2}}\right) - \cos\left(\theta_{k+r+\frac{1}{2}}\right)\right]^2 + \omega_{k,k+r}^2 \sin^2\left(\theta_{k-\frac{1}{2}}\right) \sin^2\left(\theta_{k+r+\frac{1}{2}}\right)} \tag{A9}
\end{aligned}$$

2. Diagonal form of the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of the Interval $[k, \dots, k+r]$

The diagonal form of $\rho_{k,k+1,\dots,k+r}$ can be directly obtained from the eigenvectors found in Eq A8 with the inversion formula

$$\begin{aligned}
|\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle &= \cos\left(\frac{\theta_F}{2}\right) |\Phi_{LR}^{F+}\rangle + \sin\left(\frac{\theta_F}{2}\right) |\Phi_{LR}^{F-}\rangle \\
|\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle &= e^{-i\phi_F} \left[\sin\left(\frac{\theta_F}{2}\right) |\Phi_{LR}^{F+}\rangle - \cos\left(\frac{\theta_F}{2}\right) |\Phi_{LR}^{F-}\rangle \right] \\
|\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle &= \cos\left(\frac{\theta_A}{2}\right) |\Phi_{LR}^{A+}\rangle + \sin\left(\frac{\theta_A}{2}\right) |\Phi_{LR}^{A-}\rangle \\
|\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle &= e^{-i\phi_A} \left[\sin\left(\frac{\theta_A}{2}\right) |\Phi_{LR}^{A+}\rangle - \cos\left(\frac{\theta_A}{2}\right) |\Phi_{LR}^{A-}\rangle \right] \tag{A10}
\end{aligned}$$

that can be plugged into the initial full ket of Eq. 61 to obtain the Schmidt decomposition between the interval and the exterior (Left and Right together) in the two sectors

$$\begin{aligned}
|\psi^F\rangle &\equiv |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle \lambda_{k-1,k}^+ \lambda_{k+r,k+r+1}^+ |I_{+,+}^{[k,\dots,k+r]}\rangle + |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle \lambda_{k-1,k}^- \lambda_{k+r,k+r+1}^- |I_{-,-}^{[k,\dots,k+r]}\rangle \\
&= \sqrt{p_F^+} |\Phi_{LR}^{F+}\rangle |I_F^+\rangle + \sqrt{p_F^-} |\Phi_{LR}^{F-}\rangle |I_F^-\rangle \\
|\psi^A\rangle &\equiv |\Phi_+^{[1,\dots,k-1]}\rangle |\Phi_-^{[k+r+1,\dots,N]}\rangle \lambda_{k-1,k}^+ \lambda_{k+r,k+r+1}^- |I_{+,+}^{[k,\dots,k+r]}\rangle + |\Phi_-^{[1,\dots,k-1]}\rangle |\Phi_+^{[k+r+1,\dots,N]}\rangle \lambda_{k-1,k}^- \lambda_{k+r,k+r+1}^+ |I_{+,-}^{[k,\dots,k+r]}\rangle \\
&= e^{i\phi_R} \left[\sqrt{p_A^+} |\Phi_{LR}^{A+}\rangle |I_A^+\rangle + \sqrt{p_A^-} |\Phi_{LR}^{A-}\rangle |I_A^-\rangle \right] \tag{A11}
\end{aligned}$$

where the four orthonormal ket concerning the interval $[k, \dots, k+r]$

$$\begin{aligned}
|I_F^+\rangle &= \frac{1}{\sqrt{p_F^+}} \left[\cos\left(\frac{\theta_F}{2}\right) \cos\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \cos\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{+,+}^{[k,\dots,k+r]}\rangle + \sin\left(\frac{\theta_F}{2}\right) \sin\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{-,-}^{[k,\dots,k+r]}\rangle \right] \\
|I_F^-\rangle &= \frac{1}{\sqrt{p_F^-}} \left[\sin\left(\frac{\theta_F}{2}\right) \cos\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \cos\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{+,+}^{[k,\dots,k+r]}\rangle - \cos\left(\frac{\theta_F}{2}\right) \sin\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{-,-}^{[k,\dots,k+r]}\rangle \right] \\
|I_A^+\rangle &= \frac{1}{\sqrt{p_A^+}} \left[\cos\left(\frac{\theta_A}{2}\right) \cos\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{+,-}^{[k,\dots,k+r]}\rangle + \sin\left(\frac{\theta_A}{2}\right) \sin\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \cos\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{-,+}^{[k,\dots,k+r]}\rangle \right] \\
|I_A^-\rangle &= \frac{1}{\sqrt{p_A^-}} \left[\sin\left(\frac{\theta_A}{2}\right) \cos\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \sin\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{+,-}^{[k,\dots,k+r]}\rangle - \cos\left(\frac{\theta_A}{2}\right) \sin\left(\frac{\theta_{k-\frac{1}{2}}}{2}\right) \cos\left(\frac{\theta_{k+r+\frac{1}{2}}}{2}\right) |I_{-,+}^{[k,\dots,k+r]}\rangle \right]
\end{aligned}$$

are the four eigenvectors of the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ of the interval $[k, \dots, k+r]$, associated to the four eigenvalues $(p_F^+, p_F^-, p_A^+, p_A^-)$

$$\rho_{k,\dots,k+r} = p_F^+ |I_F^+\rangle \langle I_F^+| + p_F^- |I_F^-\rangle \langle I_F^-| + p_A^+ |I_A^+\rangle \langle I_A^+| + p_A^- |I_A^-\rangle \langle I_A^-| \quad (\text{A12})$$

3. Application to the construction of Parent Hamiltonians that have the MPS as exact ground-state

Since the reduced density matrix $\rho_{k,k+1,\dots,k+r}$ is of dimension $2^{r+1} \times 2^{r+1}$, and has only four non-trivial eigenvalues as discussed above, this means that there are $n_0(r) = (2^{r+1} - 4)$ vanishing eigenvalues. For $r = 1$ corresponding to an interval $[k, k+1]$ of two sites, there are no vanishing eigenvalue ($n_0(r=1) = 0$), but for $r = 2$ corresponding to an interval $[k, k+1, k+2]$ of three sites, there are already $n_0(r=2) = 4$ vanishing eigenvalues. One may then introduce the projector on the support of $\rho_{k,k+1,k+2}$ of Eq. A12

$$\mathcal{P}_{k,k+1,k+2} \equiv |I_F^+\rangle \langle I_F^+| + |I_F^-\rangle \langle I_F^-| + |I_A^+\rangle \langle I_A^+| + |I_A^-\rangle \langle I_A^-| \quad (\text{A13})$$

in order to construct the following Parent Hamiltonians [1, 15] with arbitrary positive couplings $J_k > 0$

$$H^{\text{Parent}} = \sum_k J_k (1 - \mathcal{P}_{k,k+1,k+2}) \quad (\text{A14})$$

The energy of the MPS is zero by construction and the MPS is thus an exact ground state of these local Hamiltonians with three-body interactions.

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- [1] D. Perez-Garcia, F. Verstraete, M. M. Wolf and J. I. Cirac, *Quantum Inf. Comput.* 7, 401 (2007).
 - [2] F. Verstraete, V. Murg, J.I. Cirac, *Advances in Physics* 57 (2), 143 (2008).
 - [3] J. I. Cirac, F. Verstraete, *J. Phys. A: Math. Theor.* 42, 504004 (2009).
 - [4] G. Vidal, "Entanglement Renormalization: an introduction", chapter of the book "Understanding Quantum Phase Transitions", edited by Lincoln D. Carr (Taylor and Francis, Boca Raton, 2010)
 - [5] U. Schollwöck, *Annals of Physics* 326, 96 (2011)
 - [6] G. Evenbly, PhD thesis "Foundations and Applications of Entanglement Renormalization", arXiv:1109.5424.
 - [7] G. Evenbly and G. Vidal, chapter 4 in the book "Strongly Correlated Systems. Numerical Methods", edited by A. Avella and F. Mancini (Springer Series in Solid-State Sciences, Vol. 176 (2013)).
 - [8] M. Hauru, Master Thesis "Multiscale Entanglement Renormalisation Ansatz" (2013).
 - [9] R. Orus, *Annals of Physics* 349, 117 (2014).
 - [10] R. Orus, *Eur. Phys. J. B* 87, 280 (2014).
 - [11] R. Orus, *Nature Reviews Physics* 1, 538 (2019)
 - [12] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, *Entanglement in many-body systems* *Rev. Mod. Phys.* 80, 517 (2008).
 - [13] R. Horodecki, P. Horodecki, M. Horodecki and K. Horodecki, *Rev. Mod. Phys.* 81, 865 (2009).
 - [14] P. Calabrese, J. Cardy and B. Doyon (Eds. of the special issue) *Entanglement entropy in extended quantum systems*, *J. Phys. A* 42 500301 (2009).
 - [15] B. Zeng, X. Chen, D.L. Zhou, X.G. Wen "Quantum Information Meets Quantum Matter : From Quantum Entanglement to Topological Phase in Many-Body Systems", arXiv:1508.02595.

- [16] N. Laflorencie, Phys. Rep. 643, 1 (2016).
- [17] G. De Chiara and A. Sanpera, Report on Prog. Phys. 81 074002 (2018).
- [18] M. B. Hastings, JSTAT, P08024 (2007).
- [19] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003)
- [20] S. R. White, Phys. Rev. Lett. 69, 2863 (1992)
- [21] S. R. White, Phys. Rev. B 48, 10345 (1992).
- [22] U. Schollwoeck, Rev. Mod. Phys. 77, 259 (2005).
- [23] D. Pekker and B.K. Clark, Phys. Rev. B 95, 035116 (2017).
- [24] X. Yu, D. Pekker and B.K. Clark, Phys. Rev. Lett. 118, 017201 (2017)
- [25] M. Friesdorf, A.H. Werner, W. Brown, V. B. Scholz and J. Eisert, Phys. Rev. Lett. 114, 170505 (2015).
- [26] A. Chandran, J. Carrasquilla, I.H. Kim, D.A. Abanin and G. Vidal, Phys. Rev. B 92, 024201 (2015).
- [27] V. Khemani, F. Pollmann and S. L. Sondhi, Phys. Rev. Lett. 116, 247204 (2016).
- [28] T. Devakul, V. Khemani, F. Pollmann, D. Huse and S. Sondhi, Philosophical Transactions of the Royal Society of London A, 375, 2108 (2017)
- [29] C. Zhang, F. Pollmann, S. L. Sondhi, R. Moessner, Annalen der Physik 529.7 (2017)
- [30] J.M. Stephan, S. Furukawa, G. Misguich and V. Pasquier, Phys. Rev. B 80, 184421 (2009).
- [31] J.M. Stephan, G. Misguich and V. Pasquier, Phys. Rev. B 82, 125455 (2010).
- [32] J.M. Stephan, G. Misguich and V. Pasquier, Phys. Rev. B 84, 195128 (2011).
- [33] M.P. Zaletel, J.H. Bardarson and J.E. Moore, Phys. Rev. Lett. 107, 020402 (2011).
- [34] Y.Y. Atas and E. Bogomolny, Phys. Rev. E 86, 021104 (2012).
- [35] H.W. Lau and P. Grassberger, Phys. Rev. E 87,022128 (2013).
- [36] Y.Y. Atas and E. Bogomolny, Phil. Trans. R. Soc. A 372, 20120520 (2014).
- [37] D.J. Luitz, F. Alet and N. Laflorencie, Phys. Rev. Lett. 112, 057203 (2014).
- [38] D.J. Luitz, F. Alet and N. Laflorencie, Phys. Rev. B 89, 165106 (2014).
- [39] D.J. Luitz, F. Alet and N. Laflorencie, J. Stat. Mech. P08007 (2014).
- [40] D.J. Luitz, X. Plat, N. Laflorencie and F. Alet, Phys. Rev. B 90, 125105 (2014).
- [41] J.M. Stephan, Phys. Rev. B 90, 045424 (2014).
- [42] F.C. Alcaraz and M.A. Rajabpour, Phys. Rev. B 90, 075132 (2014).
- [43] F.C. Alcaraz and M.A. Rajabpour, Phys. Rev. B 91, 155122 (2015).
- [44] C. Monthus, J. Stat. Mech. P04007 (2015).
- [45] M. Brockmann and J.M. Stephan, J. Phys. A: Math. Theor. 50, 354001 (2017).
- [46] C. Monthus, J. Phys. A: Math. Theor. 51 095301 (2018).
- [47] D. J. Luitz, N. Laflorencie and F. Alet, Phys. Rev. B 91, 081103 (2015)
- [48] N. Macé, N. Laflorencie and F. Alet, SciPost Phys. 6, 050 (2019)
- [49] N. Macé, F. Alet and N. Laflorencie, arXiv:1812.10283
- [50] D. J. Luitz, I. M. Khaymovich and Y. Bar Lev, arXiv:1909.06380
- [51] I. Bengtsson and K. Zyczkowski, " Geometry of Quantum States: An Introduction to Quantum Entanglement ", Cambridge University Press (2006)
- [52] J. Haegeman, M. Marien, T. J. Osborne and F. Verstraete, J. Math. Phys. 55, 021902 (2014)
- [53] L. Vanderstraeten, J. Haegeman and F. Verstraete, SciPost Phys. Lect. Notes 7 (2019).
- [54] J. Haegeman, J. I. Cirac, Tobias J. Osborne, I. Pizorn, H. Verschelde, F. Verstraete, Phys. Rev. Lett. 107, 070601 (2011)
- [55] A. Milsted, J. Haegeman, T. J. Osborne, F. Verstraete, Phys. Rev. B 88, 155116 (2013)
- [56] J. Haegeman, T. J. Osborne and F. Verstraete, Phys. Rev. B 88, 075133 (2013)
- [57] J. Haegeman, C. Lubich, I. Oseledets, B. Vandereycken and F. Verstraete, Phys. Rev. B 94, 165116 (2016)
- [58] S. Paeckel, T. Khler, A. Swoboda, S. R. Manmana, U. Schollwoeck, C. Hubig, arXiv:1901.05824
- [59] D. Bauernfeind and M. Aichhorn, arXiv:1908.03090
- [60] Y. Shi, L. Duan and G. Vidal, Phys. Rev. A 74, 022320 (2006)
- [61] C. Monthus, arXiv:1910.12500
- [62] C. Monthus, in preparation.