Gaussian augmented Tensor Networks for universal quantum simulations

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Introduction: Adaptation of the stabilizer tensor network formalism developed in [1] for Gaussian operations instead of stabilizer ones.

Ansatz mixing a basis of orbitals to an MPS:

$$|\psi\rangle = \sum_{i=1}^{2^L} \nu_i d_{\vec{b}_i} |\psi_{\rm G}\rangle, \tag{1}$$

Gaussian states: Majorana operators and fermionic operators are related as:

$$\gamma_{2j-1} = c_j^\dagger + c_j, \;\; \gamma_{2j} = -i(c_j^\dagger + c_j), \tag{2}$$

Covariance matrix:

$$\Gamma_{ab} = \frac{i}{2} \mathrm{Tr}\left(\rho[\gamma_a, \gamma_b]\right) \tag{3}$$

Diagonalizing the matrix Γ corresponds to a rotation of the majorana modes by a $2L \times 2L$ matrix R, which we dub the *stabilized basis* and denoted in the following by a single tilda on the operators:

$$\tilde{\gamma}_j = \sum_{k=1}^{2L} R_{jk} \gamma_k \tag{4}$$

The state can be simply written using the majorana modes or the corresponding orbitals if it is pure:

$$\begin{aligned} |\psi_{\rm G}\rangle &= \prod_{j=1}^{L} \left(\tilde{c}_j^\dagger\right)^{n_j} |0\rangle, \\ \rho_{\rm G} &= \frac{1}{2^L} \prod_{j=1}^{2L} \left(\mathbb{1} + i\lambda_j \tilde{\gamma}_{2j-1}\tilde{\gamma}_{2j}\right) \end{aligned} \tag{5}$$

This is valid in a given basis, where $n_j = \langle c_j^\dagger c_j \rangle = (1+\lambda_j)/2$ are the occupations of orbital j, and are known from the diagonalization of the covariance matrix. STABILIZERS

We also have a set of *destabilizers* formed by the set of odd majorana modes:

$$d_i = \prod_{j=1}^{L} \tilde{\gamma}_{2j-1}^{\vec{b}_i(j)}, \tag{6}$$

in which $\vec{b}_i$ is a vector into which the binary representation of i is encoded, such that $\vec{b}_i(j) \in \{0, 1\}$ tells if the occupation of the orbital j in the state to which the product of *destabilizers* is applied will change. The set of state generated by the combination of the Gaussian state and the destabilizers form an orthonormal basis of Gaussian states for the Hilbert space of dimension 2^L, since there are 2^L combination of the destabilizers, $d_j|\psi_{\rm G}\rangle$ is also a Gaussian state and $\langle\psi_{\rm G}|d_i d_j|\psi_{\rm G}\rangle = \delta_{ij}$. In the *stabilized basis*, each odd majorana mode corresponds to a physical legs of the MPS .

When a Gaussian operation is applied on the state, we only obtain a basis which is defined as a linear combination of the *stabilized* modes:

$$\tilde{\tilde{\gamma}}_j = \sum_{k=1}^{2L} R_{jk} \tilde{\gamma}_k, \tag{7}$$

which we call the *instantaneous* basis and is identified with operators with double tildas. In this basis, the set of stabilizers The basis of instantaneous natural orbitals can always be reconstructed through the rotated majoranas:

$$\tilde{\tilde{c}}_j = \frac{1}{2}\left(\tilde{\tilde{\gamma}}_{2j-1} + i\,\tilde{\tilde{\gamma}}_{2j}\right), \tag{8}$$

which form a set of *stabilizers* that allows with the corresponding natural occupations to fully determine a Gaussian state.

Algorithm: Equipped with the GaMPS representation of the state that allows to span the entire Hilbert space, we present below how to apply a quantum circuit to the GaMPS.

- **Gaussian operations**: Applying a Gaussian unitary $U_{\rm G}$ to the state is equivalent to update the basis of orbitals as $\tilde{\gamma}_j = \sum_{k=1}^{2L} G_{jk}\gamma_k$, as illustrated in Fig. 1. After each Gaussian operation, we update the orbital frame by successively multiplying the corresponding orthogonal transformations, thereby keeping track of the basis at all times. We dub this basis the instantaneous orbital basis, which defines the space spanned by physical legs in the associated MPS. Each stabilizer and destabilizer becomes non-local superposition of all orbitals.

- **Non-Gaussian operations**: The set of odd Majoranas (our *destabilizers*) together with the even ones forms a complete operator basis, allowing any operator to be expressed as $U = \sum_i \phi_i s_{u_i} d_{v_i}$. However, the local basis being a superposition of all orbitals, decomposing a gate that is local in a basis different from the stabilized basis (such as the instantaneous one) becomes an all-to-all operation. However, if the gate is k-local in some basis, it is possible to build a circuit that extract these k orbitals and makes them the local degrees of freedom of k legs of the MPS. This sequence of operations is depicted in Fig. 1, where σ is the non-local circuit that is applied to the MPS to make the non-Gaussian gate local. For a 2-local gate, this circuit together with the non-Gaussian gate produce at most an amount $\log(L)$ of entropy.

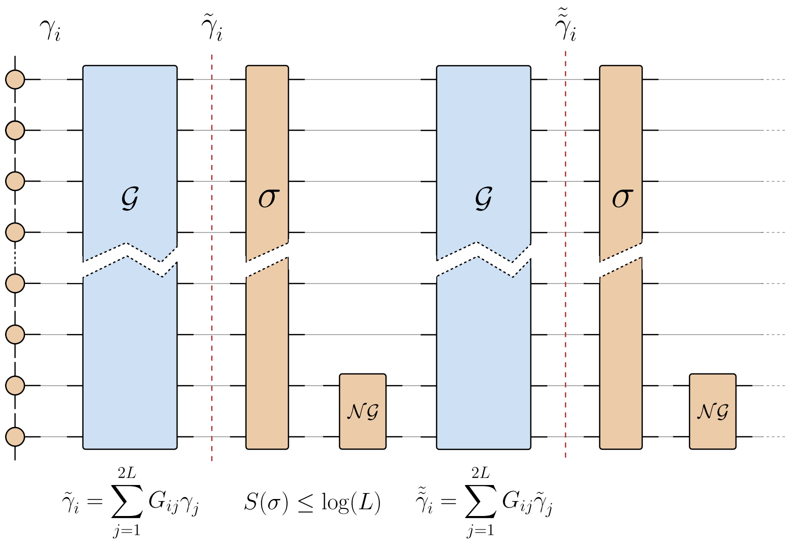

FIG. 1. Sketch.

- **Expectation values**: Expectation values are evaluated by decomposing the observable in the instantaneous orbital basis, $\langle\psi|\hat{O}|\psi\rangle = \sum_{k=1}^{L^r} a_k \langle\nu|\hat{O}_k|\nu\rangle$, where a_k denotes the weight associated with the operator $\hat{O}_k$ and r is the number of fermionic modes encoded in the observable. For instance, a density operator n_α can be expanded as $n_\alpha = \sum_{ij} R^*_{i\alpha} R_{\alpha j} \hat{\tilde{c}}^\dagger_i \hat{\tilde{c}}_j$, so that $a_{ij} = R^*_{i\alpha} R_{\alpha j}$.

I. CONCLUSION AND OUTLOOK

[1] S. Masot-Llima and A. Garcia-Saez, Stabilizer tensor networks: Universal quantum simulator on a basis of stabilizer states, Physical Review Letters **133** (2024).

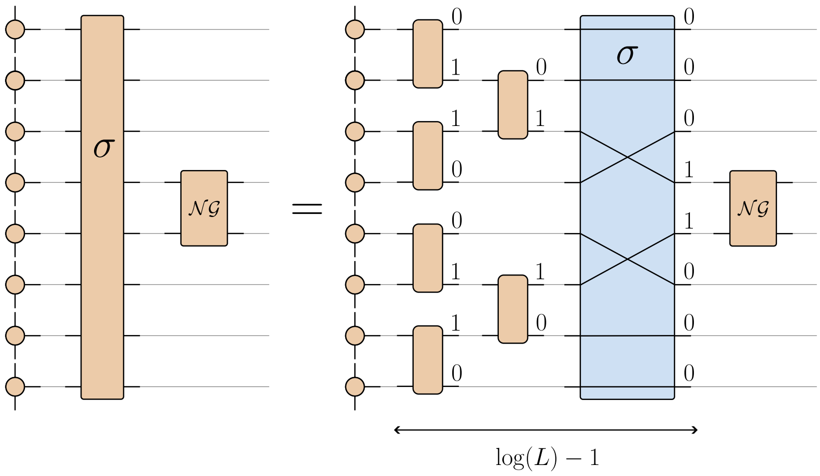

FIG. 2. Sketch of the permutation circuit required for applying a local gate.