Benchmarking global $SU(2)$ symmetry in 2d tensor network algorithms

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We implement and benchmark tensor network algorithms with $SU(2)$ symmetry for systems in two spatial dimensions and in the thermodynamic limit. Specifically, we implement $SU(2)$-invariant versions of the infinite Projected Entangled Pair States (iPEPS) and infinite Projected Entangled Simplex States (iPESS) methods. Our implementation of $SU(2)$ symmetry follows the formalism based on fusion trees from [P. Schmoll, S. Singh, M. Rizzi, R. Orús, arXiv:1809.08180]. In order to assess the utility of implementing $SU(2)$ symmetry the algorithms are benchmarked for three models with different local spin: the spin-1 bilinear-biquadratic model on the square lattice, and the Kagome Heisenberg antiferromagnets (KHAF) for spin-1/2 and spin-2. We observe that the implementation of $SU(2)$ symmetry provides better energies in general than non-symmetric simulations, with smooth scalings with respect to the number of parameters in the ansatz, and with the actual improvement depending on the specifics of the model. In particular, for the spin-2 KHAF model, our $SU(2)$ simulations are compatible with a quantum spin liquid ground state.

Introduction.- Tensor networks [1] (TN) are mathematical objects tailored to describe highly-correlated structures in an efficient way. In condensed matter physics they have been used to describe the structure of relevant quantum many-body wave functions, such as low-energy states of quantum matter. Recently, TNs have also found applications in other fields of science, such as machine learning [2] and quantum gravity [3].

The success of TN methods has been particularly impressive for one-dimensional (1d) systems, mostly thanks to the Density Matrix Renormalization Group (DMRG) [4] and related methods. On top of that, many applications of TN methods have also been developed to tackle strongly correlated systems in two spatial dimensions (2d), with increasing success. Those systems are generally difficult to simulate, and moreover, they pose some of the most important challenges in condensed matter physics. Archetypical examples are the determination of the ground state properties of the 2d Hubbard model, as well as of the spin-1/2 Kagome Heisenberg antiferromagnet (KHAF). Determining the properties of such low-energy states (superconductivity, topological order...) is a great numerical challenge. In this context, Projected Entangled Pair States (PEPS) [5] were proposed as a TN to tackle such problems. In the thermodynamic limit, the infinite-PEPS (iPEPS) algorithm [6] has been applied with success. Moreover, infinite Projected Entangled Simplex States (iPESS) [7] have also been applied with success to deal with several problems in the Kagome lattice [8].

An important technical problem in tensor networks, especially in 2d algorithms like iPEPS and iPESS, is how to deal with global non-abelian symmetries, $SU(2)$ being a common example. Many important 2d systems have $SU(2)$-invariant Hamiltonians, and their ground state is sometimes expected to preserve this symmetry. As an example, numerical simulations of the spin-1/2 KHAF seem to indicate [9] that its ground state is a quantum spin liquid and therefore an $SU(2)$ singlet. One would therefore expect, a priori, that the study of such a ground state with a TN algorithm would benefit from the explicit preservation of $SU(2)$ symmetry. While this has been done already using an $SU(2)$-invariant implementation of DMRG [10], the generalization to true 2d TN algorithms such as iPEPS and iPESS has proven to be a great technical challenge, and has been achieved only in very few and specific cases [11]. Moreover, the benefits of the implementation of $SU(2)$ symmetry in 2d TN algorithms are by far not obvious, since the number of variational parameters in the TN is much more constrained by the symmetry in 2d compared to, e.g., 1d Matrix Product State (MPS) simulations.

In this paper we implement $SU(2)$ symmetry in iPEPS and iPESS algorithms using the formalism from Ref. [12], which is based on fusion trees. We benchmark our implementation by computing ground state properties of three 2d models: the spin-1 bilinear-biquadratic model on the square lattice, and the spin-1/2 and spin-2 KHAF. We observe that the implementation of $SU(2)$ in the 2d simulations in general allows to produce lower energies than the ones obtained using non-symmetric TN algorithms. However, since $SU(2)$-invariant tensors are highly constrained, we find that the actual improvement depends a lot on the specifics of the model. In particular, for the spin-2 KHAF model, the $SU(2)$ simulations produce a ground state structure compatible with that of a quantum spin liquid to the best of our computational power.

Methods.- As discussed above, we implemented $SU(2)$-invariant versions of iPEPS and iPESS algorithms. The details of both iPEPS and iPESS have already been discussed extensively in the literature and will not be explained here. We refer the interested reader to Ref. [6] for details about iPEPS, and to Ref. [7] about iPESS. Let us just mention that, in this paper, we stick to the so-called simple update [14], which provides an efficient
tensor update for an imaginary-time evolution algorithm, also when combined with SU(2) symmetry. The accuracy of our calculations could always be improved by more precise tensor optimization schemes [6, 15, 16], but at the cost of extra computational expense. Expectation values in all cases are approximated using well-known Corner Transfer Matrix (CTM) techniques [17], which can also be easily adapted to deal with SU(2).

Concerning SU(2) itself, we decide to work here with the implementation from Ref. [12], based on fusion trees. In this implementation, a generic TN is decomposed into a degeneracy and a structural part, the structural part being only dependent on symmetries. In our implementation this structural part is codified in terms of the degeneracy tensors and a network of fusion trees. We focus first on the spin-1 bilinear-biquadratic model on the square lattice. Its Hamiltonian is given by

$$H = \sum_{\langle i,j \rangle} \left( \cos(\theta) \left( S_i \cdot S_j \right) + \sin(\theta) \left( S_i \cdot S_j \right)^2 \right),$$

where $\langle i,j \rangle$ are nearest-neighbour interactions, $S_i$ is the vector of spin-1 matrices, and $\theta$ tunes the relative coupling strength of the bilinear and biquadratic terms. The phase diagram of this model has already been computed previously with iPEPS, both without symmetries but also including $U(1)$ symmetry [18]. Here, we tune the coupling parameter to $\theta = 0.21\pi$, for which the ground state is believed to be in an SU(2)-symmetric Haldane phase corresponding to coupled spin-1 chains [18]. Thus, this point is a paradigmatic non-trivial benchmark for a 2d SU(2)-invariant iPEPS and iPESS. We choose to work with the simple update, a $2 \times 2$ unit cell, and Trotter steps of the imaginary-time evolution down to $10^{-4}$.

The ground state energy of the system is shown in Fig. 2(a) as a function of $1/D_{\text{eff}}$, in Fig. 2(b) as a function of $1/N$, and in Fig. 2(c) as a function of the discarded weight $\delta$, with the lines denoting the extrapolation to infinite bond dimension for SU(2) and $U(1)$ simulations. (d) Ground state energy per link in the unit cell. The structure is compatible with vertical Haldane chains coupled in the horizontal direction. The differences in the fourth relevant digit between the upper and lower horizontal link energies is due to truncation effects. $U(1)$ results in (a) are from Ref.[18] (replotted with permission).
include results obtained by using a CTM environment to compute expectation values, as well as using a mean-field (MF) environment estimation. This last option does not provide variational energies, but allows us to see the overall tendency for large bond dimension (for which the calculations using SU(2)-CTM algorithms are computationally costly). We see that the extrapolation $1/N \to 0$ is better behaved than the one for $1/D_{\text{eff}} \to 0$, and is actually comparable for SU(2) to the extrapolation in the discarded weight. In this last extrapolation one can also clearly see that the non-symmetric simulation is far from converged. Our extrapolated data for the ground state energy $e_0$ is $e_0(1/D_{\text{eff}} \to 0) = 0.309 \pm 0.003$, $e_0(1/N \to 0) = 0.311 \pm 0.004$, and $e_0(\delta \to 0) = 0.310 \pm 0.002$.

We notice from our plots that the simulations without symmetry yield the lowest ground state energy for small bond dimensions and the data points with SU(2) symmetry are considerably higher than those with lower or no symmetry. We take this as a first indication that the SU(2)-symmetric ansatz in 2d may sometimes be too restrictive, which is especially true for small bond dimension. However, for large bond dimension the situation is the opposite, and the SU(2) simulation produces lower energies. It is interesting, though, that the SU(2) numbers computed by CTM (which are variational, since the CTM bond dimension is converged [17]) tend to be always slightly above those obtained with an $U(1)$-symmetric ansatz, which we take as an indication that the SU(2)-invariant ansatz may actually be too constrained, and/or that more accurate tensor update schemes are needed. For the record, the obtained extrapolated energy with $U(1)$ symmetry in Fig. 2(a) is $e_0(1/D_{\text{eff}} \to 0) = 0.307 \pm 0.001$, and therefore very close to the SU(2) number. Finally, in order to understand better the nature of the SU(2)-invariant ground state that we obtain, we also plot its energy on each link of the iPEPS unit cell in Fig. 2(d). The observed structure with different energies in $x$- and $y$-directions is compatible with vertical coupled Haldane 1d chains, in accordance with the results from Ref. [18]. This difference in bond energies is also compatible with having half-integer spin representations on the vertical bonds, and integer ones on the horizontal bonds leading to different effective bond dimensions. Let us stress, for completeness, that there is some room for algorithmic improvement: one could for instance use more sophisticated tensor updates and/or CTM truncation schemes, as well as other unit cells.

These findings point towards an interesting fact: SU(2) symmetry in 2d, even if generically useful, can be highly restrictive in some cases. The variational space is highly constrained, and in some situations this could be too limited to find a good approximation to the ground state with “simple” tensor updates. In order to get an idea of the effect of the symmetry on the size of the variational space we evaluated the ratio between remaining variational parameters in the SU(2)-iPEPS and the number of variational parameters in the corresponding unconstrained TN for different bond dimensions. This is shown in Fig. 3, alongside with the same information for an SU(2)-symmetric infinite MPS simulation of a critical spin-1/2 ladder system [13]. The comparison between both cases allows us to understand better the effect of dimensionality in the reduction of variational parameters in a SU(2)-invariant TN ansatz. What we conclude from the plot is that the SU(2)-invariant ansatz becomes very restrictive with the bond dimension, as expected, but at a much faster rate in 2d than in 1d. In other words, SU(2) in 2d restricts the variational space faster than in 1d. A priori, this could be good news, since the number of pa-
The next model that we considered was the spin-1/2 KHAF. The Hamiltonian is given by

\[ H = \sum_{\langle i,j \rangle} S_i \cdot S_j, \tag{2} \]

where \( \langle i,j \rangle \) denotes nearest-neighbour interactions between sites of the Kagome lattice, and \( S_i \) is the spin-1/2 (vector) operator at site \( i \). The Kagome lattice exhibits corner-sharing triangles resulting in huge quantum fluctuations around the ground state due to strong geometric frustration, with many states very close in energy and competing to be the true ground state. This makes the simulation of the model very challenging. For the sake of this study, our goal here is not to provide better ground-state numbers than those obtained by other simulations \cite{9}, but rather to benchmark the utility of \( SU(2) \) symmetry for injectivity of the target state. For the non-symmetric 3-PESS, the non-symmetric 6-PESS and the \( SU(2) \)-invariant 6-PESS respectively.

We computed the ground state energy of the model for a 3-site and a 6-site unit cell without symmetry, and for a 6-site unit cell with \( SU(2) \) symmetry. The results are shown in Fig. 4. The symmetric results are compatible with those obtained without symmetries, with an algebraic convergence of the ground state energy as a function of \( 1/D_{\text{eff}} \) (see Fig. 4(a)), in turn reinforcing the observation that the ground state is a quantum spin liquid and therefore \( SU(2) \)-invariant. However, one can see again that the limit of infinite bond dimension is better achieved by the \( SU(2) \)-invariant simulations as a function of \( 1/N \) (see Fig. 4(b)), with extrapolated values \( e_0(1/D_{\text{eff}} \to 0) = -0.435 \pm 0.004 \) and \( e_0(1/N \to 0) = -0.435 \pm 0.002 \). Let us mention that for all the iPESS simulations that we performed, the extrapolation in the discarded weight was not possible because the discarded weight was always too small. The spin-spin correlators for each link of the unit cell are shown in Fig. 4(c-e), for the non-symmetric 3-PESS, the non-symmetric 6-PESS and the \( SU(2) \)-invariant 6-PESS respectively. While the 3-site unit cell produces a state that seems compatible with a quantum spin liquid, the 6-site unit cells seem to produce valence-bond crystal structures with strong and weak links, thus breaking invariance under translations and lattice rotations. We observe, in any case, that the valence bond crystal tends to melt when we increase the bond dimension of the iPESS ansatz, both for the non-symmetric and the \( SU(2) \)-invariant simulations, thus slowly recovering translation invariance (see Fig. 5 for plots of the correlator skewness as \( D_{\text{eff}} \) increases). Interestingly, we also observe in the figure that the non-symmetric simulations tend to melt faster than the \( SU(2) \)-symmetric ones. The observed pattern of local correlations for the non-symmetric 6-site iPESS in Fig. 4(d) is expected, since TN simulations tend to trade symmetry for injectivity of the target state. For the symmetric 6-site iPESS the correlators are even more skewed presumably due to non-uniform effective bond dimensions caused by the mixture of integer and half-
integer representations. This effect is expected to vanish in the limit of large bond dimensions, and also explains the slower melting in Fig. 5.

Finally, we computed the ground state energy of the spin-2 KHAF for a 3-site unit cell without and with SU(2) symmetry. Unlike in the spin-1/2 case, the fact that we have spin 2 in the physical indices allows us to use the 3-site unit cell (this, in fact, is true for all integer-spin Heisenberg models on the Kagome lattice). The results are shown in Fig. 6. This time, due to the large dimension of the physical spin at every site, we cannot reach values of $D_{\text{sym}}$ as large as for the spin-1/2 case. However, the effective bond dimension is larger for the spin-2 KHAF, as shown in Table I. We see in Figs. 6(a,b) that the SU(2)-invariant simulations can handle larger $D_{\text{eff}}$ and produce lower variational energy than the non-symmetric simulations. Moreover, both in the non-symmetric and symmetric cases we observe in Figs. 6(c,d) a structure of spin-spin correlators in the unit cell that seems compatible with that of a quantum spin liquid, which is also compatible with the algebraic behaviour of the ground state energy with $D_{\text{eff}}$ in Fig. 6(a). The energies are, however, difficult to extrapolate to infinite bond dimension, and hence we cannot be sure whether this is the true nature of the ground state. But we can claim that, to the best of our calculations, here the SU(2)-invariant iPESS with a 3-site unit cell produces the best variational energy for the ground state, which seems compatible with a quantum spin liquid. Moreover, we computed the expectation value of the chiral correlators $S_j \cdot (S_j \times S_k)$ on all triangles, and obtained exactly 0 everywhere, in turn also compatible with the structure of a non-chiral quantum spin liquid.

**Conclusions.** In Table I we make a comparison of the computed ground state energies for the maximum achievable bond dimensions, for the three models considered here, and for non-symmetric and SU(2)-symmetric simulations. The improvement due to SU(2) seems to depend on the gap: large for the spin-1 model (Haldane phase, large gap), and small for the spin-1/2 KHAF (quantum spin liquid, tiny gap). For the spin-2 model, the SU(2) simulations point towards a quantum spin liquid as a plausible ground state. From the results that we presented here, we can conclude that implementing SU(2) symmetry in 2d TN algorithms usually produces better energies than non-symmetric simulations, but the actual performance strongly depends on the specifics of the model and in particular on the gap of the phase being targeted. We expect that the full potential of symmetries in 2d TN methods will unfold once larger bond dimensions become accessible, in turn allowing to include many SU(2) quantum numbers.

**Acknowledgments.** We acknowledge Andreas Haller, Saeed Jahromi, Matteo Rizzi, and Sukhinder Singh for insightful discussions. We also acknowledge DFG funding through project GZ OR 381/3-1, as well as the MAINZ Graduate School of Excellence.

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**Table I:** Ground state energies obtained for the maximum achievable bond dimension for the bilinear-biquadratic (BLBQ) and KHAF models that we considered. We show $(D, e_0)$ for non-symmetric simulations and $(D_{\text{sym}}, D_{\text{eff}}, e_0)$ for SU(2)-invariant ones, with $D$ the non-symmetric bond dimension, $D_{\text{sym}}$ the symmetric bond dimension and $D_{\text{eff}}$ the effective bond dimension when using SU(2) averaged for all bonds, which can be integer or fractional.

| Model     | No symmetry | SU(2) |
|-----------|-------------|-------|
| $s = 1$ BLBQ | (7, 0.3188) | (6, 19.5, 0.3108) |
| $s = 1/2$ KHAF | (10, -0.4348) | (7, 17.75, -0.4349) |
| $s = 2$ KHAF | (10, -4.7975) | (5, 19, -4.8227) |

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