Fine-Grained Tensor Network Methods

Philipp Schmoll,¹ Saeed S. Jahromi,² Max Hörmann,³ Kai Phillip Schmidt,³ and Román Orús², ⁴, ⁵

¹Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany
²Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain
³Chair for Theoretical Physics I, FAU Erlangen-Nürnberg, Germany
⁴Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain
⁵Multiverse Computing, Pio Baroja 37, 20008 San Sebastián, Spain

We develop a strategy for tensor network algorithms that allows to deal very efficiently with lattices of high connectivity. The basic idea is to fine-grain the physical degrees of freedom, i.e., decompose them into more fundamental units which, after a suitable coarse-graining, provide the original ones. Thanks to this procedure, the original lattice with high connectivity is transformed by an isometry into a simpler structure, which is easier to simulate via usual tensor network methods. We prove the validity of our approach by numerically computing the ground-state properties of the ferromagnetic spin-1 transverse-field Ising model, as well as of the hard-core and soft-core Bose-Hubbard models on the triangular lattice. Our results are benchmarked against those obtained with other techniques, such as perturbative continuous unitary transformations and graph projected entangled pair states, showing excellent agreement and also improved performance in several regimes.

Introduction.- During the past decade there has been a rapid development of tensor network (TN) states and numerical methods [1–5] for simulating strongly correlated quantum many-body systems. These are mathematical objects which use the knowledge about the amount and structure of entanglement in quantum many-body states in order to reproduce the state accordingly. TN methods use such objects as ansätze to simulate quantum lattice systems in different regimes, and have been remarkably successful [6–14]. Inspiringly, TN states also show up in other disciplines, such as quantum gravity [15], artificial intelligence [16, 17] and even linguistics [18].

Despite being extremely versatile, TNs are not free from limitations, though. The most obvious one is the ability to capture the expected structure of entanglement in the TN ansatz, i.e., to incorporate the correct scaling of the entanglement entropy. The amount of entanglement is also a limitation itself, where one of the key parameters of the TN, the so-called bond dimension, may be just too large to simulate the system at hand when there is too much entanglement in the quantum state. In addition to these limitations, one also has to deal with geometric bottlenecks. For instance, the simulation of a triangular lattice with projected entangled pair states (PEPS) [1, 5, 19, 20] would naively imply tensors with six bond indices, if we were to use one tensor per lattice site. As such, handling tensors with so many indices quickly becomes computationally expensive for numerical simulations. The same problem also arises for higher-dimensional systems, where high-connectivity lattices are quite usual. This is a serious issue, since such large-connectivity lattices are usually linked to exotic phases of quantum matter such as topological quantum spin liquids [21–25].

Here we propose a physically motivated strategy to solve this problem, which on top is remarkably efficient and accurate. The idea is to break down the physical degrees of freedom into “smaller” pieces, i.e., to fine-grain the lattice. This can be done at the expense of introducing a set of fine-graining isometries. The key advantage is that the fine-grained lattice is easily amenable to TN methods. Unlike other proposals of TN methods for high-connectivity lattices [7, 10–13, 26, 27], our approach preserves the correct geometric structure of the system, thus being better-suited in terms of the entanglement structure. In what follows we explain the approach and use it to compute ground-state properties of the ferromagnetic spin-1 transverse-field Ising model, as well as of the hard-core and soft-core Bose-Hubbard models on the triangular lattice. We benchmark the results against those obtained with perturbative continuous unitary transformations (pCUTs) [28, 29] and graph projected entangled pair states (gPEPS) [13], showing excellent agreement and also improved performance in several regimes.

Method.- Our approach is based on a simple yet powerful idea: split the physical degrees of freedom into smaller, more fundamental entities which, when coarse-grained, reproduce the original physical ones. In other words, fine-grain the local Hilbert spaces at each site.

Before proceeding any further let us give a practical example. Imagine that we have a spin-1 particle. As is well known, this can always be understood as two spin-1/2 particles which are projected into their spin-1 subspace in the coupled basis. Mathematically, since for SU(2) irreps one has $1/2 \otimes 1/2 = 0 \oplus 1$, what we do is to project out the singlet part with spin 0 and keep the triplet with spin 1. In this way, we constructed a spin-1 out of two spins-1/2. But we can also consider the procedure the other way around: we fine-grain a spin-1 into two spins-1/2 by using the appropriate “inverse” projector, i.e. a fine-graining isometry, which in this particular case is the Clebsch-Gordan coefficient $(1/2, 1/2, m_1, m_2)_{1/2, 1/2, 1, m}$ with $m_{1,2} = \pm 1/2$ and $m = -1, 0, +1$, using the standard notation $(j_1, j_2, m_1, m_2 | j_1, j_2, 1, m)$. 
The idea above is generalized as follows: a physical degree of freedom described by a Hilbert space $\mathcal{H}_p$ can be understood as the coarse-grained space of some other fine-grained Hilbert spaces $\mathcal{H}^{[1]}_f$ and $\mathcal{H}^{[2]}_f$ via some isometry $W$, i.e.,

$$W : \mathcal{H}^{[1]}_f \otimes \mathcal{H}^{[2]}_f \rightarrow \mathcal{H}_p,$$

with $W = \sum_{f_1 f_2} W^i_{f_1 f_2} |f_1 \rangle \langle f_2|$. In TN language, the 3-index tensor $W^i_{f_1 f_2}$ coarse-grains the indices $f_1$ and $f_2$ into $i$. Seen in reverse, the physical index $i$ is fine-grained into indices $f_1$ and $f_2$ by the isometric tensor $W^i_{f_1 f_2}$. Since $W$ is an isometry, it implies that $W^\dagger W = I_p$, with $I_p$ the identity in the physical Hilbert space $\mathcal{H}_p$, see Fig. 1.a. Let us remark that we considered here the case of two fine-grained Hilbert spaces, but the idea can be easily generalized to having more than two. In fact, the whole isometry $W$ could even have a TN structure itself (as in, e.g., the multiscale entanglement renormalization ansatz (MERA) [30]), if required. Generically, the isometry can also be understood in the language of entanglement branching operators [31].

Next, we apply this fine-graining to the physical degrees of freedom of many-body systems with high-connectivity, which allows us to simplify the underlying lattice structure and therefore make them more amenable to TN simulation methods. Let us consider, without loss of generality, the case of a triangular lattice. As shown in Fig. 1.b-c, fine-graining every site maps the triangular lattice into a square lattice. The key point is to realize that, in such a scenario, operators on the triangular lattice are mapped to operators on the fine-grained square lattice via the isometry $W$, as shown in Fig. 1.c. For instance, for an one-site operator $O_p$ acting on one site of the physical lattice, one has

$$O_f = W O_p W^\dagger$$

with $O_f$ the corresponding operator on the fine-grained lattice. In the case of the triangular lattice that we are discussing, this maps a one-site operator $O_p$ on the triangular lattice to a two-site operator $O_f$ on the square lattice. In general, for a fine-graining isometry involving $n$ fine-grained Hilbert spaces, an $m$-body operator on the original lattice is mapped to an $(n \times m)$-body operator in the fine-grained one.

Our method can thus be summarized in three steps:

1. Find an isometry $W$ that reduces the connectivity of the lattice after fine-graining.
2. Use $W$ to map all operators involved in the TN algorithm to their fine-grained versions.
3. Run the TN algorithm on the fine-grained lattice using the fine-grained operators.

The mapping between lattices preserves locality inasmuch the isometry $W$ is local. This implies, for instance, that local expectation values in the original lattice may also be mostly local in the fine-grained one. Notice also that, at the level of TN optimization and calculation of local expectation values, one can fully operate in the fine-grained space only, see Fig. 1.c for an example.

A number of practical considerations are in order. First, the isometry $W$ is a new degree of freedom that enters the TN algorithm. It could be optimized following a MERA-like procedure, yet another option is to fix it to some reasonable choice and optimize over the tensors of the fine-grained TN. This choice is not unique and moreover it is also reasonable to think that some isometries may work better than others in practice depending on the symmetries of the system. Generally, an isometry that splits the physical Hilbert space symmetrically seems to be beneficial (e.g., a decomposition of $1 = 0 \otimes 1$ is valid but unbalanced). Second, interaction terms in the fine-grained Hamiltonian may become of slightly longer range. For instance, for a Hamiltonian with nearest-neighbour interactions on the triangular lattice, one gets interactions that span over four sites in the fine-grained square lattice. Third, and as we said above, more complicated isometries are also possible, even with an internal TN structure.

**Numerical results.**- In order to benchmark the validity of our approach we computed the ground-state properties of several models on the triangular lattice for a unit cell of $2 \times 2$ tensors. For this, we used fine-graining together
with the infinite-PEPS algorithm [32, 33] on the square lattice with a $2 \times 4$ unit cell and simple update, also for four-body interactions, and computed expectation values with Corner Transfer Matrix (CTM) techniques [7, 9, 33].

The first model that we considered is the spin-1 ferromagnetic quantum Ising model in a transverse field, described by the Hamiltonian [34]

$$H = -J \sum_{(i,j)} \sigma^i_{2} \sigma^j_{2} - h \sum_i \sigma^i_z,$$  \hspace{1cm} (3)

with $\sigma^i_{j}$ the $3 \times 3$ spin-one matrix at site $i$, $J > 0$ the ferromagnetic interaction strength, and $h$ the magnetic field. It realizes a polarized phase for small $J/h$ and a symmetry-broken ordered phase for large $J/h$ separated by a second-order phase transition in the 3D Ising universality class. The location of the critical point can be estimated precisely by the pCUT series of the one-particle gap in the polarized phase using Dlog Padé extrapolation which yields $(J/h)_c^{\text{pCUT}} = 0.1898(1)$ or equivalently in the inverse unit $(h/J)_c^{\text{pCUT}} = 5.269(3)$ [35].

For the fine-PEPS we choose to fine-grain each spin-1 into two spins-1/2 via an isometry that equals a Clebsch-Gordan coefficient, $W^{m_1, m_2}_{m_1, m_2} = (1/2, 1/2, 1/2, 1/2, 1, 1, m_1, m_2)$, in Fig. 2 we show the ground-state energy per site computed by fine-graining (fine-PEPS) with PEPS bond dimension $D = 3$, as well as using gPEPS with $D = 6$ and pCUT up to $O(12)$ in the high-field expansion in $J/h$. Remarkably, even for a small bond dimension $D = 3$, the agreement of fine-PEPS with pCUT for $J/h \leq (J/h)_c^{\text{pCUT}}$ within the polarized phase and with gPEPS for large $J/h$ inside the symmetry-broken ordered phase is almost perfect.

In Fig. 3 we also plot longitudinal and transverse magnetizations as computed by fine-PEPS and gPEPS, also in excellent agreement, and with an approximate quantum critical point of $(h/J)_c^{\text{fine-PEPS}} \approx 5.605$. Notice that the critical point obtained by the two tensor network methods deviates from the pCUT result $(h/J)_c^{\text{pCUT}}$. This is, however, due to the simple update, which does not make use of the full environment when updating the tensors. Simulations with the full environment would improve the accuracy close to criticality, shall this be required.

Furthermore, we simulated the Bose-Hubbard model on the triangular lattice, described by the Hamiltonian [36, 37]

$$H = -t \sum_{\langle i,j \rangle} (a^i_j + a^i_j \dagger h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i,$$  \hspace{1cm} (4)

with $a^i_j, a^i_j \dagger$ and $n_j = a^i_j a^i_j \dagger$ respectively being bosonic annihilation, creation and number operators at site $j$, $t$ the hopping strength, $U$ the on-site density-density interaction, and $\mu$ the chemical potential.

In the hard-core limit $U \to \infty$, where individual sites are either empty or occupied by one boson, this model realizes two exact gapped Mott phases with density zero and one as well as an intermediate gapless superfluid phase. The phase transitions at $\langle \mu/J \rangle_c = \pm 6$ between the Mott and superfluid phases can be determined exactly by first-order perturbation theory for the one-particle gap of the two Mott phases [35]. Technically, we fine-grain every hard-core boson into two hard-core bosons via an isometry with non-zero coefficients $W^0_{0,0} = 1, W^1_{1,0} = W^1_{0,1} = 1/\sqrt{2}$. Thus, if the physical site is occupied, then the hard-core boson can be on either of
the fine-grained sites. In Fig. 4 we show our numerical results for the particle density \( \rho = \langle a_j^\dagger a_j \rangle \) and the condensate fraction \( \rho_0 = |\langle a_j \rangle|^2 \) for fine-PEPS and gPEPS both up to \( D = 6 \) and with \( t = 1 \), showing excellent agreement in the superfluid and Mott-insulator phases.

Furthermore, we considered the soft-core case up to two bosons per lattice site so that the ground-state phase diagram consists of three Mott lobes with densities \( n \in \{0, 1, 2\} \) and superfluid phases. The empty \((n = 0)\) and completely filled \((n = 2)\) Mott states are again exact eigenstates of the system and the corresponding one-particle gap \( \Delta_{n=0} = -\mu - 6t \) (one-hole gap \( \Delta_{n=2} = -U + \mu - 12t \)) can be calculated exactly \([35]\). This is different for the Mott phase with \( n = 1 \) where the hopping term introduces quantum fluctuations. For the fine-PEPS we break down again each local site in terms of two hard-core bosons which, when both occupied, result in a double occupied physical site. For this we use an isometry with non-zero coefficients \( W_{0,0}^0 = 1, W_{1,0}^1 = W_{0,1}^1 = 1/\sqrt{2}, W_{1,1}^1 = 1 \). The particle density and condensate fraction for soft-core bosons is shown in Fig. 5, computed by fine-PEPS up to \( D = 5 \) and gPEPS up to \( D = 6 \) with \( t = 0.01 \) and \( U = 1 \), again showing an excellent agreement in all superfluid and Mott-insulating phases.

Conclusions. In this paper we have proposed an efficient approach to deal with lattices of high connectivity in TN methods, by using a fine-graining of the physical degrees of freedom. Under suitable conditions, this fine-graining simplifies the lattice and essentially keeps locality of interactions. After a fine-graining of operators, the approach allows us to apply usual TN methods on simpler lattices in a remarkably efficient way. We have explained in detail the example of the 2d triangular lattice, which in our approach can be simulated using standard 2d square-lattice PEPS algorithms. Our method has been benchmarked with numerical simulations of the ground state of the spin-1 ferromagnetic transverse-field Ising model as well as the hard-core and soft-core Bose-Hubbard models, all on the triangular lattice, with excellent accuracy when compared to other methods such as pCUT and gPEPS. We think that the approach in this paper will allow to overcome the computational cost associated to simulating lattices of high connectivity, such as the ones typically found for higher dimensional systems and frustrated quantum antiferromagnets. Moreover, the idea of fine-graining is of experimental relevance \([38]\) for facilitating the implementation and measurements of physical observables in optical lattices. We therefore believe that it will become an instrumental tool in the discovery of new exotic phases of quantum matter.

We acknowledge discussions with A. Haller, A. Kshetrimayum and M. Rizzi. We also acknowledge DFG funding through GZ OR 381/3-1 as well as GZ SCHM 2511/10-1.

References

[1] R. Orús, Annals of Physics 349, 117 (2014), arXiv:1306.2164 .
[2] R. Orús, Nature Reviews Physics 1, 538 (2019).
[3] S.-J. Ran, E. Tirrito, C. Peng, X. Chen, G. Su, and M. Lewenstein, (2017), 10.1016/j.jhrm.2011.11.009, arXiv:1708.09213 .
[4] J. Biamonte and V. Bergholm, (2017), arXiv:1708.00006 .
[5] F. Verstraete, V. Murg, and J. I. Cirac, Advances in Physics 57, 143 (2008), arXiv:0907.2796 .
[6] B. Bauer, P. Corboz, A. M. Läuchli, L. Messio, K. Penc,
M. Troyer, and F. Mila, Physical Review B - Condensed Matter and Materials Physics 85, 125116 (2012), arXiv:1112.1100v1.

[7] P. Corboz, J. Jordan, and G. Vidal, Physical Review B - Condensed Matter and Materials Physics 82, 245119 (2010), arXiv:1008.3937.

[8] P. Corboz, R. Orús, B. Bauer, and G. Vidal, Physical Review B - Condensed Matter and Materials Physics 81, 165104 (2010), arXiv:0912.0646.

[9] P. Corboz, T. M. Rice, and M. Troyer, Physical Review Letters 113, 046402 (2014), arXiv:1402.2859.

[10] P. Corboz and F. Mila, Physical Review Letters 112, 147203 (2014), arXiv:1401.3778v1.

[11] S. S. Jahromi and R. Orús, Physical Review B 98, 155108 (2018).

[12] S. S. Jahromi, R. Orús, M. Kargarian, and A. Langari, Physical Review B 97, 115161 (2018).

[13] S. S. Jahromi and R. Orús, Physical Review B 99, 195105 (2019).

[14] M. Sadrzadeh, R. Haghshenas, S. S. Jahromi, and A. Langari, Physical Review B 94, 214419 (2016).

[15] B. Swingle, Physical Review D - Particles, Gravitation and Cosmology 86 (2012), 10.1103/PhysRevD.86.065007, arXiv:0905.1317.

[16] E. M. Stoudenmire, Quantum Science and Technology 3 (2018), 10.1088/2058-9565/aaba1a, arXiv:1801.00315.

[17] W. Huggins, P. Patil, B. Mitchell, K. B. Whaley, and E. M. Stoudenmire, Quantum Science and Technology 4, 024001 (2019), arXiv:1803.11537.

[18] A. J. Gallego and R. Orús, (2017), arXiv:1708.01525.

[19] F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Physical Review Letters 96, 220601 (2006), arXiv:0601075 [quant-ph].

[20] R. Orús, European Physical Journal B 87, 280 (2014), arXiv:1407.6552.

[21] L. Savary and L. Balents, Reports on Progress in Physics 80, 016502 (2017).

[22] L. Balents, Nature 464, 199 (2010), arXiv:0904169 [cond-mat].

[23] S. Yan, D. A. Huse, and S. R. White, Science (New York, N.Y.) 332, 1173 (2011).

[24] S. S. Jahromi, M. Kargarian, S. F. Masoudi, and A. Langari, Physical Review B 94, 125145 (2016), arXiv:1608.00254.

[25] S. S. Jahromi and A. Langari, Journal of Physics A: Mathematical and Theoretical 50, 145305 (2017).

[26] P. Corboz, K. Penc, F. Mila, and A. M. Läuchli, Physical Review B - Condensed Matter and Materials Physics 86, 041106 (2012), arXiv:1204.6682.

[27] I. Niesen and P. Corboz, Physical Review B 97 (2018), 10.1103/PhysRevB.97.245146, arXiv:1805.00354.

[28] C. Knetter and G. S. Uhrig, European Physical Journal B 13, 209 (2000).

[29] C. Knetter, K. P. Schmidt, and G. S. Uhrig, Journal of Physics A: Mathematical and General 36, 7889 (2003).

[30] G. Vidal, Physical Review Letters 99 (2007), 10.1103/PhysRevLett.99.220405, arXiv:0512165 [cond-mat].

[31] K. Harada, Phys. Rev. B 97, 045124 (2018).

[32] H. N. Phien, J. A. Bengua, H. D. Tuan, P. Corboz, and R. Orús, Physical Review B - Condensed Matter and Materials Physics 92, 035142 (2015), arXiv:1503.05345.

[33] R. Orús and G. Vidal, Physical Review B - Condensed Matter and Materials Physics 80, 094403 (2009), arXiv:0905.3225.

[34] M. Powalski, K. Coester, R. Moessner, and K. P. Schmidt, Physical Review B - Condensed Matter and Materials Physics 87 (2013), 10.1103/PhysRevB.87.054404, arXiv:1212.0736.

[35] Philipp Schmoll, Saeed S. Jahromi, Max Hormann, Kai Philipp Schmidt and R. Orus, Supplementary Materials.

[36] A. Kshetrimayum, M. Rizzi, J. Eisert, and R. Orús, Physical Review Letters 122, 070502 (2019), arXiv:1809.08258.

[37] Y. C. Wang, W. Z. Zhang, H. Shao, and W. A. Guo, Chinese Physics B 22 (2013), 10.1088/1674-1056/22/9/096702, arXiv:1302.1376.

[38] M. Boll, T. A. Hilker, G. Salomon, A. Omran, J. Nespola, L. Pollet, I. Bloch, and C. Gross, Science 353, 1257 (2016).
This supplementary material contains details about the simple update for the triangular fine-grained iPEPS, the calculation of expectation values of local operators within the fine-grained iPEPS, the method of perturbative continuous unitary transformations, and exact considerations for the Mott phases of the Bose-Hubbard model.

I. SIMPLE UPDATE FOR THE TRIANGULAR FINE-GRAINED IPEPS

In the simple update of the fine-grained triangular lattice we use the standard infinite time-evolving block decimation (iTEBD) [1] procedure to determine the tensors that represent the ground state of the model. One step of the simple update includes all links in the triangular lattice, and the procedure is repeated with decreasing Trotter steps until convergence of the singular values is reached. Choosing an \( L_x \) times \( L_y \) unit cell on the triangular lattice we have to update \( 3L_xL_y \) links, which is done in the resulting \( L_x \) times \( 2L_y \) unit cell on the square lattice. Due to the splitting of the physical sites the update of every link now involves four iPEPS tensors instead of only two. In order to lower the computational cost we decompose the input tensors so that all virtual indices that are not affected by the update are separated [2, 3], and the simple update can be performed more efficiently on the reduced tensors. After the Suzuki-Trotter gate has been applied the resulting tensor is decomposed using a singular-value decomposition (SVD), which yields the updated singular values on the particular link as well as the tensors \( U \) used to restore tensors A and B on the left, and \( V^\dagger \) used to restore tensors C and D on the right. Notice that the singular values \( S_{AB} \) and \( S_{CD} \) between tensors A, B and tensors C, D respectively are updated too, even though their links are introduced artificially due to the splitting. Eventually this procedure is a simple update for the triangular lattice with extra steps to maintain the fine-grained structure, however we can exploit the fine-graining for the computation of expectation values in the next.
II. EXPECTATION VALUES OF LOCAL OPERATORS

Computing the ground state wave function using simple update as described above is not too expensive even for high-connectivity tensors. However computing expectation values becomes more difficult, also because of the geometric structure of the triangular lattice. It is convenient to resort to the square lattice for which one can define an effective environment easily. The environment tensors are computed in a directional CTM algorithm [4–6] for an arbitrary $L_x \times L_y$ unit cell, the iPEPS tensors are absorbed into all lattice directions iteratively until the environment is converged. The CTM tensors then represent the contraction of the infinite two-dimensional square lattice. For the computation of expectation values we can use the CTM tensors as an effective environment for the iPEPS tensors in the unit cell. Since we can directly compute expectation values in the fine-grained lattice the operator support will be doubled, e.g. a one-site operator on the triangular lattice will become a two-site operator in the square lattice, and so on. Computing the energy per link in the triangular lattice is then done by computing the expectation value of a four-site operator in the square lattice, which is obtained by fine-graining the physical indices of the regular two-site Hamiltonian. For a more efficient contraction of the resulting tensor networks in Fig. 2 we can decompose the four-body gate into two parts that act on both fine-grained sites.

![Figure 2](image)

FIG. 2: Computation of two-site observables like the Hamiltonian in the triangular lattice translates to evaluating four-site operators in the fine-grained square lattice. Here we show the expectation values for horizontal and one type of diagonal links, see also Fig. 1.

is computed similarly, just without the operators. For one-site operators like the particle density $\rho = \langle a^\dagger_j a_j \rangle$ we only use two two fine-grained sites and their respective environment tensors.

III. PERTURBATIVE CONTINUOUS UNITARY TRANSFORMATION

The high-order linked-cluster expansions are realized with the help of perturbative continuous unitary transformations (pCUTs) [7, 8]. In the following we describe its generic aspects and refer to the literature for further details.

One can always rewrite any Hamiltonian $\mathcal{H}$ exactly as

$$\mathcal{H} = \mathcal{H}_0 + \sum_j \lambda_j \mathcal{V}^{(j)},$$

(1)

where the $\lambda_j$ are the perturbative parameters and the unperturbed part $\mathcal{H}_0$ is diagonal in appropriate supersites. For the high-field expansion in the spin-1 transverse-field Ising model as well as for the density $n = 1$ Mott phase in the softcore Bose-Hubbard model we use single sites as supersites. In both cases one can express $\mathcal{H}_0$ in appropriate units as

$$\mathcal{H}_0 = E_0 + \mathcal{Q},$$

(2)

where $E_0$ denotes a constant and $\mathcal{Q}$ is a counting operator of local excitations. This decomposition of $\mathcal{H}_0$ is always possible, since the local spectra of the supersites is equidistant in all considered cases.

Supersites interact via the perturbation $\mathcal{V} = \sum_j \lambda_j \mathcal{V}^{(j)}$. In this work always pairs of nearest-neighbor supersites on the triangular lattice are linked by the perturbation. As a consequence of Eq. (2), one can rewrite Eq. (1) as

$$\mathcal{H} = \mathcal{H}_0 + \sum_{n=-N}^{N} \hat{T}_n,$$

(3)
so that $[Q, \hat{T}_n] = n\hat{T}_n$. Physically, the operator $\hat{T}_n \equiv \sum_j \lambda_j \hat{T}^{(j)}_n$ corresponds to all processes where the change of energy quanta with respect to $H_0$ is exactly $n$. The maximal (finite) change in energy quanta is called $\pm N$, which is always $N = 2$ in the models considered below.

In pCUTs, Hamiltonian (3) is mapped model-independently up to high orders in perturbation to an effective Hamiltonian $H_{\text{eff}}$ with $[H_{\text{eff}}, Q] = 0$. The general structure of $H_{\text{eff}}$ is then a weighted sum of operator products $\hat{T}_{n_1} \cdots \hat{T}_{n_k}$ in order $k$ perturbation theory. The block-diagonal $H_{\text{eff}}$ conserves the number of quasi-particles (qp). This represents a major simplification of the quantum many-body problem, since one can treat each quasi-particle block, corresponding only to a few-body problem, separately, e.g., the 0qp-block is given by a single matrix element which represents the ground-state energy in all considered cases.

The more demanding part in pCUTs is model-dependent and corresponds to a normal-ordering of $H_{\text{eff}}$ for which the explicit processes of $H_0$ and $V$ have to be specified. This can be either done via a full graph decomposition in linked graphs using the linked-cluster theorem and an appropriate embedding scheme afterwards [9] or by calculations on large enough finite clusters, which include all relevant virtual processes. Here we did a full graph decomposition and we concentrated on the 0qp and 1qp pCUT sector, which allows us to extract the ground-state energy per site $e_0$ and the elementary gap $\Delta$.

### A. Extrapolation

We perform standard DlogPadé extrapolations for the one-particle gap $\Delta$. We refer to the literature for a general review of this topic, as for example given in Ref. 10. Here we give specific information which is relevant for the particular extrapolation we performed in the main body of the manuscript.

Our series are all of the form

$$ F(\lambda) = \sum_{k \geq 0}^{k_{\text{max}}} c_k \lambda^k = c_0 + c_1 \lambda + c_2 \lambda^2 + \cdots c_{k_{\text{max}}} \lambda^{k_{\text{max}}}, \quad (4) $$

with $\lambda \in \mathbb{R}$ and $c_k \in \mathbb{R}$. If one has power-law behavior near a critical value $\lambda_c$, the true physical function $\tilde{F}(\lambda)$ close to $\lambda_c$ is given by

$$ \tilde{F}(\lambda) \approx \left(1 - \frac{\lambda}{\lambda_c}\right)^{-\theta} A(\lambda), \quad (5) $$

where $\theta$ is the associated critical exponent. If $A(\lambda)$ is analytic at $\lambda = \lambda_c$, we can write

$$ \tilde{F}(\lambda) \approx \left(1 - \frac{\lambda}{\lambda_c}\right)^{-\theta} A_{\lambda=\lambda_c} \left(1 + O\left(1 - \frac{\lambda}{\lambda_c}\right)\right). \quad (6) $$

Near the critical value $\lambda_c$, the logarithmic derivative is then given by

$$ \tilde{D}(\lambda) := \frac{d}{d\lambda} \ln \tilde{F}(\lambda) \approx \frac{\theta}{\lambda_c - \lambda} \left\{ 1 + O(\lambda - \lambda_c) \right\}. \quad (7) $$

In the case of power-law behavior, the logarithmic derivative $\tilde{D}(\lambda)$ is therefore expected to exhibit a single pole at $\lambda \equiv \lambda_c$

The latter is the reason why so-called DlogPadé extrapolation is often used to extract critical points $\lambda_c$ from high-order series expansions. DlogPadé extrapolants of $F(\lambda)$ are defined by

$$ dP[L/M]_F(\lambda) = \exp \left( \int_0^\lambda P[L/M]_D \, d\lambda' \right) \quad (8) $$

and represent physically grounded extrapolants in the case of a second-order phase transition. Here $P[L/M]_D$ denotes a standard Padé extrapolation of the logarithmic derivative

$$ P[L/M]_D := \frac{P_L(\lambda)}{Q_M(\lambda)} = \frac{p_0 + p_1 \lambda + \cdots + p_L \lambda^L}{q_0 + q_1 \lambda + \cdots + q_M \lambda^M}, \quad (9) $$
with $p_i \in \mathbb{R}$, $q_i \in \mathbb{R}$, and $q_0 = 1$. Additionally, $L$ and $M$ have to be chosen so that $L + M \leq k_{\text{max}} - 1$. Physical poles of $P[L/M]|_D(\lambda)$ then indicate critical values $\lambda_c$.

For our results we study the possible combinations of the order of the numerator and denominator polynomial $L$ and $M$. We sort them into the families $[n, n - 3], [n, n + 3], [n, n - 2], [n, n + 2], [n, n - 1], [n, n + 1]$, and $[n, n]$ and analyze their convergence.

### B. Series expansion Results for the Spin-1 Triangular transverse-field Ising model

The spin-1 ferromagnetic quantum Ising model in a transverse field on the triangular lattice is given by

$$
\mathcal{H} = -J \sum_{\langle i, j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^z,
$$

with $\sigma_i^z$ the $3 \times 3$ spin-one matrix at site $i$, $J > 0$ the ferromagnetic interaction strength, and $h$ the magnetic field.

We perform a high-field linked-cluster expansion using the pCUT method. Indeed, in the limiting case $J = 0$ the unperturbed system consists of isolated spin-ones and has an equidistant spectrum. In the following we set $h = 1$ which fixes the local energy quanta of a single spin one to unity. Indeed, the local energies of a single spin-one are then given by $\epsilon_m = m$ for the states $|1, m\rangle$ with $m \in \{\pm 1, 0\}$. The field term can be written as

$$
\mathcal{H}_0 = E_0 + \mathcal{Q},
$$

where $E_0 = -N$ with $N$ the number of sites is the bare ground-state energy where all spin-ones are in the $m = +1$ configuration and $\mathcal{Q} = \sum_i (\hat{n}_i^{m=0} + 2\hat{n}_i^{m=-1})$ is the counting operator of local energy quanta with $\hat{n}_i^{m=0}$ ($\hat{n}_i^{m=-1}$) the occupation number operator of $m = 0$ ($m = -1$) configurations on site $i$.

The Ising interaction links always nearest-neighbor sites on the triangular lattice and it changes the number of energy quanta (eigenvalues of $\mathcal{Q}$) by $\pm 2$ or $0$. As a consequence, the Ising perturbation can be expressed as

$$
\mathcal{V} = J \left( \hat{T}_- + \hat{T}_0 + \hat{T}_+ \right) .
$$

The pCUT method allows now to map, order by order in $J$, this Hamiltonian to an effective one which commutes with $\mathcal{Q}$ so that the number of quasi-particles (qp) is a conserved quantity.

We performed a full graph decomposition on the triangular lattice and we focused on the 0qp and 1qp sector. The 0qp block contains solely the ground-state energy per site $e_0$, which we determined up to order 12 in $J$ and reads

$$
e_0 = -1 - \frac{3}{2} J^2 - 3 J^3 - \frac{309}{16} J^4 - \frac{405}{4} J^5 - \frac{83649}{128} J^6 - \frac{1128897}{256} J^7 - \frac{390430787}{2048} J^8 - \frac{490430787}{2048} J^9 .
$$

(13)

The 1qp block represents a one-particle hopping Hamiltonian on the triangular lattice for a single excitation with $m = 0$. It can be diagonalized by a Fourier transformation which yields the one-particle dispersion $\omega(\kappa)$. The minimum of the dispersion corresponds to the one-parcle gap $\Delta$, which is located at $\kappa = 0$ for ferromagnetic interactions. We again reached order 12 in $J$ for this quantity. The series is given by

$$
\Delta = 1 - 6 J - 15 J^2 - \frac{147}{2} J^3 - \frac{3705}{8} J^4 - \frac{103203}{16} J^5 - \frac{397611}{32} J^6 - \frac{14037072288726122493}{7036874417764} J^7 - \frac{623020145561549967244959}{9161896774402989476221315} J^9 - \frac{72057594037927936}{1351079882211488} J^8 - \frac{432345564227567616}{5132573391520145132731581} J^9 - \frac{373843963970302121493464787}{4503599627370496} J^{10} - \frac{360287970818963968}{4503599627370496} J^{11} .
$$

(14)

We use Dlog Padé extrapolation to locate the quantum critical point $(J/h)_{pCUT}$ between the polarized and the ordered phase of the spin-1 transverse-field Ising model on the triangular lattice. The corresponding results are displayed in Fig. 3. In addition, we biased the extrapolation with the known critical exponent $\nu = 0.6299$ of the 3D Ising universality class [11] which yields $(J/h)_{pCUT, \text{bias}} = 0.1899$. Overall, this yields the estimate $(J/h)_{pCUT} = 0.1898(1)$ taking into account the biased value $(J/h)_{pCUT, \text{bias}}$ and the Dlog Padé extrapolations of the highest order.
FIG. 3: Critical point \( (J/h)^{p\text{CUT}} \) of the spin-1 transverse-field Ising model on the triangular lattice as a function of the perturbative order \( n \) from Dlog Padé extrapolation of the pCUT gap \( \Delta \). Connected symbols represent a family of Dlog Padé extrapolants \([L, M]\) with \( L - M \) fixed. This results in the estimate \( (J/h)^{p\text{CUT}} = 0.1898(1) \), where the uncertainty reflects the difference of the families in the highest orders as well as the value of the Dlog Padé extrapolation when biasing with the known critical exponent of the 3D Ising universality class (horizontal dashed cyan line).

IV. EXACT CALCULATIONS FOR THE MOTT PHASES OF THE BOSE-HUBBARD MODEL ON THE TRIANGULAR LATTICE

In the following we give some information on the exact analytical properties of the empty and completely filled Mott phases of the Bose-Hubbard model on the triangular lattice.

A. Hard-Core Bose-Hubbard model on the Triangular lattice

In the hardcore limit the local occupation numbers of the Bose-Hubbard model are restricted to zero and one. As a consequence, besides a superfluid phase, there are two Mott phases which are related exactly by particle-hole symmetry. For both Mott phases the ground state corresponds to exact product states which are given by \( |0^{n=0}\rangle \equiv |0\ldots 0\rangle \) \((|0^{n=1}\rangle \equiv |1\ldots 1\rangle\) with ground-state energy \( E_0^{n=0} = 0 \) \( (E_0^{n=1} = -\mu N) \) for density \( n = 0 \) \( (n = 1) \).

As a consequence, the elementary gap of both Mott phases can be calculated exactly, since it reduces to a nearest-neighbor hopping problem of a single particle (single hole) on the triangular lattice which can be diagonalized by Fourier transformation. Specifically, we define a single-particle state and a single-hole state on site \( i \) by

\[
|1p^{n=0},i\rangle \equiv |0\ldots 01,0\ldots 0\rangle \quad (15)
\]
\[
|1h^{n=1},i\rangle \equiv |1\ldots 10,1\ldots 1\rangle \quad . \quad (16)
\]

The kinetic term of the Bose-Hubbard model induces a nearest-neighbor hopping of the particle and the hole, respectively. The dispersion of both excitations is then given by

\[
\omega^{1p}(\vec{k}) = -\mu - 2t (\cos(k_1) + \cos(k_2) + \cos(k_1 - k_2)) \quad (17)
\]
\[
\omega^{1h}(\vec{k}) = +\mu - 2t (\cos(k_1) + \cos(k_2) + \cos(k_1 - k_2)) \quad , \quad (18)
\]

where \( \vec{k} = (k_1, k_2) \) denotes the two-dimensional wave-vector. The gaps are located at \( \vec{k} = 0 \) so that

\[
\Delta^{1p} = -\mu - 6t \quad (19)
\]
\[
\Delta^{1h} = +\mu - 6t \quad . \quad (20)
\]
These gaps close therefore exactly at $\mu/t = \pm 6$.

### B. Soft-Core Bose-Hubbard model on the Triangular lattice

In the soft-core limit the local occupation numbers of the Bose-Hubbard model are restricted to zero, one, and two. As a consequence, besides a superfluid phase, there are three Mott phases. For the empty and completely filled Mott phase the ground state corresponds again to exact product states which are given by $|0^{n=0}\rangle \equiv |0\ldots0\rangle$ ($|0^{n=2}\rangle \equiv |2\ldots2\rangle$) with ground-state energy $E_{0}^{n=0} = 0$ ($E_{0}^{n=2} = (U - 2\mu)N$) for density $n = 0$ ($n = 2$). As a consequence, the elementary gap of these two Mott phases can again be calculated exactly. Specifically, we define a single-particle state and a single-hole state on site $i$ by

$$
|1p^{n=0},i\rangle \equiv |0\ldots010\ldots0\rangle \quad (21)
$$

$$
|1h^{n=2},i\rangle \equiv |2\ldots212\ldots2\rangle . \quad (22)
$$

The dispersion of both excitations is then given by

$$
\omega^{1p}(\vec{k}) = -\mu - 2t(\cos(k_{1}) + \cos(k_{2}) + \cos(k_{1} - k_{2})) \quad (23)
$$

$$
\omega^{1h}(\vec{k}) = +\mu - 4t(\cos(k_{1}) + \cos(k_{2}) + \cos(k_{1} - k_{2})) - U , \quad (24)
$$

where $\vec{k} = (k_{1},k_{2})$ denotes the two-dimensional wave-vector. The gaps are located at $\vec{k} = 0$ so that

$$
\Delta^{1p} = -\mu - 6t \quad (25)
$$

$$
\Delta^{1h} = +\mu - 12t - U . \quad (26)
$$

[1] G. Vidal, *Physical Review Letters* **91**, 147902 (2003), arXiv:0301063 [quant-ph] .
[2] H. N. Phien, J. A. Bengua, H. D. Tuan, P. Corboz, and R. Orús, *Physical Review B - Condensed Matter and Materials Physics* **92**, 035142 (2015), arXiv:1503.05345 .
[3] S. S. Jahromi and R. Orús, *Physical Review B* **99**, 195105 (2019).
[4] R. Orús and G. Vidal, *Physical Review B - Condensed Matter and Materials Physics* **80**, 094403 (2009), arXiv:0905.3225 .
[5] P. Corboz, T. M. Rice, and M. Troyer, *Physical Review Letters* **113**, 046402 (2014), arXiv:1402.2859 .
[6] P. Corboz, J. Jordan, and G. Vidal, *Physical Review B - Condensed Matter and Materials Physics* **82**, 245119 (2010), arXiv:1008.3937 .
[7] C. Knetter and G. S. Uhrig, *European Physical Journal B* **13**, 209 (2000).
[8] C. Knetter, K. P. Schmidt, and G. S. Uhrig, *Journal of Physics A: Mathematical and General* **36**, 7889 (2003).
[9] K. Coester and K. P. Schmidt, *Phys. Rev. E* **92**, 022118 (2015).
[10] A. C. Guttmann, *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz, Vol. 13 (Academic Press, New York, 1989).
[11] F. Kos, D. Poland, D. Simmons-Duffin, and A. Vichi, *J. High Energy Phys.* **2016**, 36 (2016).