

Solving Frustration-Free Spin Systems

N. de Beaudrap,¹ M. Ohliger,¹ T.J. Osborne,² and J. Eisert^{1,2}¹*Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany*²*Institute for Advanced Study Berlin, 14193 Berlin, Germany*

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We identify a large class of quantum many-body systems that can be solved exactly: natural frustration-free spin-1/2 nearest-neighbor Hamiltonians on arbitrary lattices. We show that the entire ground-state manifold of such models can be found exactly by a tensor network of isometries acting on a space locally isomorphic to the symmetric subspace. Thus, for this wide class of models, real-space renormalization can be made exact. Our findings also imply that every such frustration-free spin model satisfies an area law for the entanglement entropy of the ground state, establishing a novel large class of models for which an area law is known. Finally, we show that our approach gives rise to an ansatz class useful for the simulation of almost frustration-free models in a simple fashion, outperforming mean-field theory.

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Understanding the physics of quantum many-body systems is a central goal of modern physics, as they can exhibit exotic phenomena with no parallel in classical physics, including topological effects and quantum phase transitions at zero temperature. However, the very source of their rich physics also leads to a major roadblock in their study: The Hilbert space dimension of these systems scales exponentially with the number of particles. This means that brute-force numerical techniques fail even for systems of only a handful of particles.

A key insight in the study of local quantum many-body systems is that naturally occurring states occupy only a small subspace of the Hilbert space which, in principle, is available to them. Specifically, it has been realized that ground, thermal, and dynamically evolving states are only weakly entangled: The entanglement entropy satisfies what is referred to as an “area law” [1–3]. This insight is the basis of the density-matrix renormalization group approach and higher-dimensional analogues [4]. So successful are these methods in practice that one is tempted to boldly conjecture that all *physically* relevant systems will soon be tractable to one or another of the numerical tools we have at hand. Recent results give cause for caution, showing that general numerical methods cannot well approximate the physics of an *arbitrary* local quantum system, even in 1D; these include local glassy models where approximating the ground-state energy is NP-hard [5], suggesting that such systems would be intractable. However, these results do not give much reason for practical concern thus far, as at least in 1D they rely on rather baroque constructions (involving very large local dimensions).

In this work, we approach the issue of the complexity or “hardness” of finding ground states from the other direction: We establish a large class of models for which the task of finding the ground state is *easy*, in that the ground-state manifold can be described exactly and efficiently. This is the class of all natural frustration-free

spin-1/2 models with nearest-neighbor interaction on general lattices. (By the qualifier “natural,” we mean that all two-spin interaction terms have excited states which are entangled, which might be taken as implicit in the semantics of an “interaction term.”) Extending ideas of Ref. [6] on QUANTUM 2-SAT and going beyond 1D models as in Ref. [7], we find that the complete ground-state manifold of such Hamiltonians can be constructed by reduction to the symmetric subspace of a smaller system. In doing so, we find that the resulting ground-state manifold can be efficiently grasped in terms of tree-tensor networks. We discuss how this allows expectation values of local observables to be computed efficiently. What is more, the ground states satisfy an area law. Physically, we can view this work as describing a large class of models for which an instance of real-space renormalization provides an exact solution to the true genuine quantum many-body model. Finally, we see how this construction—a tree-tensor network with a symmetric subspace as an input—can serve as an ansatz class to simulate systems which are “close” to frustration-free models, outperforming mean-field approaches in a very simple fashion.

In our analysis, we allow for nearest-neighbor Hamiltonians on arbitrary lattices. This could be a cubic lattice of some dimension or, more generally, any graph, the vertex set of which we denote by V . On this lattice, the spin Hamiltonian H is represented as

$$H = \sum_{\{a,b\}} h_{a,b} \quad (1)$$

for terms $h_{a,b}$ acting on pairs of spins $\{a, b\} \subset V$. By rescaling, we may require that the ground energy of each term $h_{a,b}$ is zero. The ground-state manifold M of such a Hamiltonian may be degenerate: We identify the ground state ρ with the maximal mixture over M . (This is a pure state only if H is nondegenerate.) We describe properties of the ground state ρ and, more generally, the manifold M , given H as in Eq. (1). The Hamiltonian H is frustration-

free (or unfrustrated) if the ground-state vectors $|\Phi\rangle \in M$ correspond to ground states of individual coupling terms, that is, if $h_{a,b}|\Phi\rangle = 0$ holds for all $h_{a,b}$ and all $|\Phi\rangle \in M$; we say otherwise that H is frustrated.

We will call a spin Hamiltonian H natural if it contains no isolated subsystems, and each interaction term $h_{a,b}$ (considered as an operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$) has at least one entangled excited state (i.e., an entangled state orthogonal to the ground-state manifold of $h_{a,b}$). In what follows we will consider only such natural Hamiltonians.

Frustration-free spin Hamiltonians.—Our main results concern the class of frustration-free spin Hamiltonians H . We show that the ground-state manifold M of such a spin Hamiltonian on N spins has dimension at most $N + 1$. What is more, it is the image of a space of low Schmidt measure [8] under a tree-tensor network.

First, we describe the needed components of Ref. [6], in the language of frustration-free models. Consider a Hamiltonian H_U containing terms $h_{u,v}$ of rank 2 or 3. If H_U is frustration-free, the reduced state $\rho_{u,v}$ of any state vector $|\Phi\rangle \in \ker(H)$ is in the kernel of $h_{u,v}$; we may then consider a subspace $S_{u,v} \subset \mathcal{H}_u \otimes \mathcal{H}_v$ of dimension 2 which contains $\text{supp}(\rho_{u,v})$. By defining an isometry

$$R_{u:uv}: \mathcal{H}_2^{\otimes\{u\}} \rightarrow S_{u,v} \subset \mathcal{H}_2^{\otimes\{u,v\}}, \quad (2)$$

we can reduce to a Hamiltonian on fewer spins: We let

$$H'_U = R_{u:uv}^\dagger H_U R_{u:uv} = \sum_{\{a,b\}} R_{u:uv}^\dagger h_{a,b} R_{u:uv}. \quad (3)$$

Such a spin Hamiltonian H'_U is a sum of two-spin interactions (and possibly single-spin terms) of the form $h'_{a,b} = R_{u:uv}^\dagger h_{a,b} R_{u:uv}$. (If $h_{u,v}$ has rank 3, then $h'_{u,v}$ is a nonzero single-spin operator acting on u alone.) If H contains nonzero terms $h_{a,u}$ and $h_{a,v}$, we obtain two nonzero contributions $h'_{a,u} = R_{u:uv}^\dagger h_{a,u} R_{u:uv}$ and $h'_{a,v} = R_{u:uv}^\dagger h_{a,v} R_{u:uv}$ in the Hamiltonian H' , each of which act on $\{u, a\}$. The sum gives a combined term $\tilde{h}'_{a,u} = h'_{a,u} + h'_{a,v}$ in H'_U , possibly of higher rank than either $h'_{a,u}$ or $h'_{a,v}$ [9]. If the new Hamiltonian H'_U contains terms of rank 2 or 3, we may perform another such reduction, and so on. This reduction procedure has the following features:

a. Preservation of the kernel dimension.—By construction, we have $\ker(H_U) = R_{u:uv} \ker(H'_U)$. Thus, the kernels of H_U and H'_U have the same dimension. In particular, if H'_U has any terms of full rank acting on either one or two spins, then $\dim[\ker(H_U)] = 0$, in which case H_U is frustrated. If no full-rank terms are produced, each reduction leads to an operator acting on fewer spins, until we obtain a Hamiltonian having only terms of rank 1.

b. Arbitrariness of reduction order.—The dimension of the kernel is preserved by these reductions. We may perform such reductions until we obtain a Hamiltonian which either (i) contains only terms of rank 1 or (ii) contains a full-rank term. The latter cannot occur in the reduction of a frustration-free Hamiltonian; we discuss below the anal-

ysis for Hamiltonians having only rank-1 terms. Thus, we may choose any convenient reduction sequence.

The above features allow us to reduce to the special case of a Hamiltonian H'_U (acting on a system V') which has only interaction terms of rank 1. Each two-spin Hamiltonian term $h'_{a,b} = |\beta_{a,b}\rangle\langle\beta_{a,b}|$ may be regarded as imposing constraints on the corresponding two-spin marginals $\rho_{a,b}$ of states $|\Phi\rangle \in \ker(H)$: We aim to obtain additional constraints on pairs of spins $u, v \in V'$ by combining the known constraints. To this end, Ref. [6] shows that a state $|\Phi\rangle$ which is in the kernel of two functionals $\langle\beta_{a,b}|$ and $\langle\beta_{b,c}|$ is also in the kernel of

$$\langle\beta'_{a,c}| = (\langle\beta_{a,b}| \otimes \langle\beta_{b,c}|)(1 \otimes |\Psi^-\rangle \otimes 1) \quad (4)$$

acting on the spins $\{a, c\}$, where $|\Psi^-\rangle$ is the two-spin antisymmetric state vector. For each such “induced” constraint $\langle\beta'_{u,v}|$ on spins $\{u, v\}$, we may add the term $\tilde{h}_{u,v} = |\beta'_{u,v}\rangle\langle\beta'_{u,v}|$ to H'_U , resulting in a Hamiltonian \tilde{H}_U which has the same kernel as H'_U . (If H'_U contains a term $h'_{u,v} \neq \tilde{h}_{u,v}$, it can be subsumed into a term $\tilde{h}_{u,v}$ with rank at least 2, in which case we apply a reduction $R_{u:uv}$ as above.) One may induce further constraints from the terms of \tilde{H} , until we arrive at a “complete homogeneous” Hamiltonian H_c , having only terms of rank 1, for which the constraints $\langle\beta_{u,v}|$ are closed (up to scalars) under the constraint-induction procedure of Eq. (4).

Reference [6] shows that such a Hamiltonian H_c , acting on at least one spin and lacking single-spin operators [10], has a ground space containing product states. Thus, the above remarks essentially recap the following result.

Observation 1.—There is an efficient algorithm to determine whether a spin Hamiltonian is frustration-free.

We now extend the above results, to obtain a strong characterization of ground-state manifolds for natural frustration-free systems. We note the following three additional features of the isometric contraction scheme above:

c. Tree-tensor construction.—The complete network of isometric reductions T represents a tree-tensor network, a special case of the multiscale entanglement renormalization ansatz [11] which is related to real-space renormalization. Each isometry $R_{u:uv}$ has one free input tensor index and two free output indices, and the sequential nature of the reduction ensures that the network is directed and acyclic. Thus, any spin v introduced by an isometry $R_{u:uv}$ is a “daughter spin” of a unique parent u , leading to a treelike structure on the tensor network T . Note, however, that T has free input indices, corresponding to the roots of each tree: By construction, the ground space of H_U is the image $T|\Psi\rangle$ of states $|\Psi\rangle \in \ker(H_c)$.

d. Preservation of natural Hamiltonians.—Importantly, the isometric reductions above preserve the class of natural frustration-free spin Hamiltonians: That is, the mapping $h_{a,u} \mapsto R_{u:uv}^\dagger h_{a,u} R_{u:uv}$ does not decrease the rank of the interaction on $\{a, u\}$ and does not map the orthocomplement of the kernel to the space $|\phi\rangle \otimes \mathbb{C}^2$ for any $|\phi\rangle$.

e. Reduction to the symmetric subspace.—As a consequence of the previous feature, we may use the isometric reductions to map any natural frustration-free Hamiltonian to a complete homogeneous Hamiltonian H_c on a system V_c , in which the nonzero terms $h_{a,b} = |\beta_{a,b}\rangle\langle\beta_{a,b}|$ are supported on entangled states $|\beta_{a,b}\rangle$. We show that the kernel of such a Hamiltonian has small dimension and is spanned entirely by product states. For an arbitrary spin $a \in V_c$, we may let $L_a = \mathbb{1}$ and define a family of operators L_v satisfying

$$\langle\beta_{a,v}|\propto\langle\Psi^-|_{a,v}(\mathbb{1}_a\otimes L_v) \quad (5)$$

for spins $v \in V_c$ and operators $\langle\beta_{a,v}|$. One then finds that $C = \bigotimes_{v \in V_c} L_v$ is a linear isomorphism (not necessarily an isometry) from the subspace $\text{Sym}(\mathcal{H}_2^{\otimes V_c})$ of symmetric states to the ground space of H_c . (This isomorphism is also noted in Ref. [12], Sec. III A, for generic Hamiltonians with rank-1 interactions.) As $\text{Sym}(\mathcal{H}_2^{\otimes V_c})$ is spanned by uniform superpositions $|W_k\rangle$ of standard basis states having Hamming weight $0 \leq k \leq n_c = |V_c|$, we have $\dim[\text{Sym}(\mathcal{H}_2^{\otimes n_c})] = n_c + 1$. This subspace may also be spanned by product state vectors $|\alpha_0\rangle^{\otimes n_c}, \dots, |\alpha_{n_c}\rangle^{\otimes n_c}$ for any set of $n_c + 1$ pairwise independent state vectors $|\alpha_j\rangle \in \mathcal{H}_2$. Thus, any complete homogeneous (natural) Hamiltonian H_c has a ground space spanned by vectors

$$|\Psi_j\rangle = \bigotimes_{v \in V_c} (L_v|\alpha_j\rangle) = C|\alpha_j\rangle^{\otimes n_c}, \quad (6)$$

for some $|\alpha_j\rangle \in \mathcal{H}_2$ as above. Coupled with the tree-tensor structure of the isometric reductions, this characterization has the following consequences.

Observation 2.—For an unfrustrated spin Hamiltonian H_U , any constant k , and k -local operators A , $\langle A \rangle$ can be efficiently computed with respect to ground states of H .

Let H_c be a homogeneous Hamiltonian acting on n_c spins, obtained by isometric reduction of an unfrustrated Hamiltonian H_U . Consider a k -local operator \tilde{A} . As $\ker(H_c)$ is spanned by product vectors $|\Psi_0\rangle = C|\alpha_0\rangle^{\otimes n_c}, \dots, |\Psi_{n_c}\rangle = C|\alpha_{n_c}\rangle^{\otimes n_c}$ as in Eq. (6), we can efficiently compute the restriction of \tilde{A} to $\ker(H_c)$ by evaluating

$$W(\tilde{A}) = \sum_{j,k=0}^{n_c} |j\rangle\langle\Psi_j|\tilde{A}|\Psi_k\rangle\langle k| \quad (7)$$

followed by a suitable transformation. Specifically, consider the operator $B = W(\mathbb{1})$; we have $B = U\Delta U^\dagger$ for some U unitary and Δ positive and diagonal. We find

$$\Delta^{-1/2}U^\dagger \sum_{j=0}^{n_c} |j\rangle\langle\Psi_j| = \sum_{j=0}^{n_c} |j\rangle\langle\Phi_j|, \quad (8)$$

for some orthonormal basis $|\Phi_0\rangle, \dots, |\Phi_{n_c}\rangle$ of $\ker(H_c)$; thus, the restriction of \tilde{A} to $\ker(H_c)$ with respect to the basis of states $|\Phi_j\rangle$ may be computed as

$$\tilde{A} = \Delta^{-1/2}U^\dagger W(\tilde{A})U\Delta^{-1/2}. \quad (9)$$

[For \tilde{A} consisting of a single k -spin term, the inner products

of Eq. (7) are products of constant-dimensional inner products; for \tilde{A} a sum of multiple terms, we extend linearly.] Let $T: \ker(H_c) \rightarrow \ker(H_U)$ be the network of isometric reductions. Then, by considering operators $\tilde{A} = T^\dagger A T$, we may compute the restriction \tilde{A} of such operators A to the ground space of H_U . We may then efficiently compute expectation values by using such matrices.

Observation 3.—Ground states of frustration-free spin Hamiltonians H_U on lattices obey an entanglement area law.

For any contiguous subsystem A containing a spins, we may reduce the Hamiltonian $H_U^{(A)}$ acting internally on A —by a tree-tensor isometry T_A acting on A alone—to obtain a homogeneous Hamiltonian $H_c^{(A)}$, acting on at most a spins. The ground space of $H_c^{(A)}$ has dimension at most $a + 1$; as the ground space of $H_U^{(A)}$ is an isometric image of that of $H_c^{(A)}$, the same is true of $H_U^{(A)}$. As H_U is unfrustration, any ground state of H_U is also a ground state of $H_U^{(A)}$; it follows that the Schmidt measure [8] of $|\Psi\rangle$ with respect to the bipartition $V = A \cup (V \setminus A)$ is at most $\log(a + 1)$. For a spin lattice of any dimension, we obtain an area law for arbitrary subsystems by summing this logarithmic bound over the number of distinct connected components.

“Almost” frustration-free Hamiltonians.—We now leave the rigorous exact setting and turn to the observation that the above techniques can be used to grasp approximately frustration-free models. Observation 2, in particular, suggests a variational approach to estimating ground energies for Hamiltonians H for which

$$H = H_U + \lambda H_F \quad (10)$$

for some $\lambda \ll 1$, where H_U is frustration-free but the Hamiltonian H itself is frustrated. For such Hamiltonians H , if no phase transition is encountered, the eigenvalues and eigenstates may differ little from those of the unfrustrated Hamiltonian H_U (for related bounds on eigenvalues, see, e.g., Ref. [13]). If the lowest k eigenvectors (for some suitable $1 \leq k \leq n + 1$) have a sufficiently high overlap with the lowest k eigenvectors of H_U , we may approximately sample from the low-energy eigenvectors of H by restricting to the kernel of H_U , by using the efficient algorithm above. In particular, as this procedure is variational, estimates obtained in this way for the ground-state energy of H are guaranteed to be upper bounds.

We may consider improvements to this ansatz which retain more information about the “frustrating” component λH_F than in the tree-tensor renormalization procedure for H_U . To obtain better estimates—and to extend these techniques to the case where λ may be significantly large—we may consider partial reductions by tree-tensor networks, having many free input spins, and isometries depending on the terms of the perturbed Hamiltonian H (rather than those of H_U).

If the ground-state manifold of H_U is contained in a subspace \mathcal{K} which is spanned by product states and has

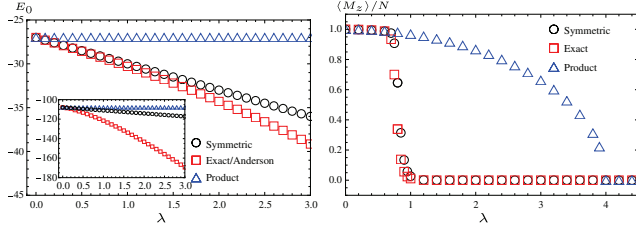


FIG. 1 (color online). Left: Ground-state energy for XXZ model on a trigonal lattice on a 3×3 torus, $h_{i,j} = -X_i X_j - Y_i Y_j - (1 - \lambda) Z_i Z_j$, by symmetric subspace estimate compared to product state ansatz and exact diagonalization. The inset shows the same model on a 6×6 torus where exact solution is not feasible and, therefore, is replaced by an Anderson lower bound. Right: Magnetization in z direction for Ising model in a transverse field on a 4×4 torus, $h_{i,j} = -Z_i Z_j$, $h_i = -\lambda X_i$, by symmetric subspace estimate compared to mean-field approximation (product state ansatz) and exact diagonalization.

“small” dimension (i.e., polynomial rather than exponential in the system size, as in the case of the symmetric subspace for ferromagnetic Ising or XXX models), we may indeed forgo isometric reductions entirely and estimate the ground energy of H by considering the restriction of H to \mathcal{K} by using the techniques described for Observation 2. In contrast to a full tree-tensor contraction, this has the advantage of yielding exact results for the frustration-free case $\lambda = 0$ while retaining more information about the frustrating component H_F . The resulting estimate for the ground-state energy will be a linear function of λ , whose value and first derivative with respect to λ agree with that of the exact ground energy at $\lambda = 0$. For small λ and modest system sizes, this may yield a good estimate of the ground-state energy of H ; see Fig. 1 [14].

To obtain estimates which account for spatially decaying correlations, we may perform a partial tree-tensor reduction with a small number of contraction layers and sample with respect to a subspace \mathcal{K} as described above. In each layer, we may fix a collection of (nonintersecting) adjacent site pairs $\{a, b\}$ to contract and for each such pair $\{a, b\}$ apply some isometric contraction as described in Eq. (3). However, rather than apply the reductions which would be suggested by the frustration-free Hamiltonian H_U , we may use isometries

$$Q_{a:ab} = |\psi_{a,b}^0\rangle\langle 0| + |\psi_{a,b}^1\rangle\langle 1|, \quad (11)$$

where $|\psi_{a,b}^0\rangle$ and $|\psi_{a,b}^1\rangle$ are the lowest energy eigenvectors of the interaction term of H on sites a and b . Given a tensor network T_1 consisting of a product of such two-site operators $Q_{a:ab}$, we may then consider the spin model given by $H' = T_1^\dagger H T_1$ and estimate the ground energy of H' with respect to a low-dimension subspace or another isometric contraction; this yields an upper bound on the ground energy of the original Hamiltonian H .

Summary.—In this work, we have introduced a class of spin models that can be completely solved: The entire

ground-state manifold can be explicitly given and parametrized by an entire symmetric subspace under a tensor network. This class of models is expected to provide a rich playground of exploring ideas on quantum lattice models, complementing work that exemplifies how computationally difficult it can be to approximate ground-state energies. The considered models can also be viewed as the parent Hamiltonian of the network, in a converse approach taken for tree-tensor networks in Ref. [15]. The models we consider obey area laws, establishing a class of models beyond free systems for which this holds. It is the hope that this work stimulates further research on models for which tensor networks arise not only as computational but as essentially analytical tools.

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