Quantum Hamiltonian Complexity

Sevag Gharibian* Yichen Huang† Zeph Landau*

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Abstract

We survey the growing field of Quantum Hamiltonian Complexity, which includes the study of Quantum Constraint Satisfaction. In particular, our aim is to provide a computer science-oriented introduction to the subject in order to help bridge the language barrier between computer scientists and physicists in the field. As such, we include the following in this paper: (1) The basic ideas, motivations, and history of the field, (2) a glossary of many-body physics terms explained in computer-science friendly language, (3) overviews of central ideas from many-body physics, such as Mean Field Theory and Tensor Networks, and (4) brief expositions of selected computer science-based results in the area. This paper is based largely on the discussions of the quantum reading group at UC Berkeley in Spring 2013.

> *"Computers are physical objects, and computations are physical processes. What computers can or cannot compute is determined by the laws of physics alone..."*
> — *David Deutsch*

1 Introduction

The Cook-Levin Theorem [Coo72, Lev73], which states that the SATISFIABILITY problem is NP-complete, is one of the cornerstones of modern computational complexity theory [AB09]. One of its implications is the following simple, yet powerful, statement: Computation is, in a well-defined sense, *local*. Yet, as David Deutsch's quote above perhaps foreshadows, this is not the end of the story, but rather its beginning. Indeed, just as classical bits can be governed by local constraints (as in, say, 3-SAT), the quantum world around us evolves according to local *quantum* constraints. The study of such quantum constraint systems underpins the emerging field of *quantum Hamiltonian complexity*.

More formally, a k-local quantum constraint satisfaction system acting on n qu*d*its is described by a *k-local Hamiltonian* $H \in \mathcal{H}\left(\mathbb{C}^d\right)^{\otimes n}$ (see Section 3 for Notation), where $H = \sum_i H_i$ for Hermitian operators $H_i \in \mathcal{H}\left(\mathbb{C}^d\right)^{\otimes k}$ which act non-trivially on subsets of k qudits. Often, one is interested in the smallest eigenvalue or *ground state energy* of H, along with its corresponding eigenvector or *ground state*. The physics intuition for this is as follows: Quantum systems in Nature typically evolve according to local Hamiltonians, and in particular, cooling such a system to "low temperature" allows the system to relax into its ground state. Thus, understanding the "solutions" (i.e. energies and eigenvectors) to quantum constraint satisfaction problems is central to understanding the structure and behavior of the physical world around us. It is important to note that solving for such quantities is computationally difficult, as we require an efficient algorithm to run in time polynomial in n, the number of qudits, as opposed to in d^n, which is the dimension of the space H acts on.

From a computer science perspective, determining ground state energies of local Hamiltonians is interesting for two reasons. First, it generalizes classical constraint satisfaction

*Simons Institute for Theoretical Computing and Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, CA 94720, USA

†Department of Physics, University of California, Berkeley, Berkeley, CA 94720, USA

as follows. Let ϕ denote an instance of 3-CSP with clauses c_i which are arbitrary Boolean functions on 3 bits. Then, corresponding to each clause c_i, we add a diagonal Hamiltonian constraint $H_i \in \mathcal{H}\left(\mathbb{C}^2\right)^{\otimes 3}$ which penalizes all non-satisfying assignments, i.e.

$$H_i = \sum_{\substack{x \in \{0,1\}^3 \\ \text{s.t. } c_i(x)=0}} |x\rangle\langle x|.$$

Then, a product state $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ representing a satisfying binary assignment will achieve energy 0 on $H = \sum_i H_i$, i.e.

$$\mathrm{Tr}(H|\psi\rangle\langle\psi|) = 0.$$

On the other hand, an unsatisfiable formula has energy at least 1; this is because all H_i simultaneously diagonalize in the computational basis, and thus without loss of generality, one can choose the ground state as a binary string. Second, just as SATISFIABILITY was the first known NP-complete problem [Coo72, Lev73], the LOCAL HAMILTONIAN problem was the first known QMA-complete problem (first presented by Kitaev at [Kit99], and later written up in [KSV02]), where Quantum Merlin-Arthur (QMA) is the quantum generalization of NP (more accurately, of Merlin-Arthur (MA)), and where LOCAL HAMILTONIAN is formally defined as follows:

Problem 1 (k-Local Hamiltonian (k-LH) [KSV02])**.** *Given as input a k-local Hamiltonian H acting on n qudits, specified as a collection of constraints $\{H_i\}_{i=1}^r \subseteq \mathcal{H}\left(\mathbb{C}^d\right)^{\otimes k}$ where $k, d \in \Theta(1)$, and threshold parameters $a, b \in \mathbb{R}$, such that $0 \leq a < b$ and $(b-a) \geq 1$, decide, with respect to the complexity measure $\langle H\rangle + \langle a\rangle + \langle b\rangle$:*

1. *If $\lambda_{\min}(H) \leq a$, output YES.*
2. *If $\lambda_{\min}(H) \geq b$, output NO.*

Here, $\langle A\rangle$ denotes the encoding length of object A in bits, and $\lambda_{\min}(A)$ denotes the smallest eigenvalue of A. Note that often k-LH is phrased with $(b-a) \geq 1/p(n)$ for some polynomial p; such an inverse polynomial gap can straightforwardly be boosted to the constant 1 above by defining H to have $p(n)$ many copies of each local term H_j [Wat09].

For completeness, we also define QMA formally (see Reference [Wat09] for further discussion).

Definition 2 (QMA)**.** *A promise problem $A = (A_{\text{yes}}, A_{\text{no}})$ is in QMA if and only if there exist polynomials p, q and a polynomial-time uniform family of quantum circuits $\{Q_n\}$, where Q_n takes as input a string $x \in \Sigma^*$ with $|x| = n$, a quantum proof $|y\rangle \in (\mathbb{C}^2)^{\otimes p(n)}$, and $q(n)$ ancilla qubits in state $|0\rangle^{\otimes q(n)}$, such that:*

- *(Completeness) If $x \in A_{\text{yes}}$, then there exists a proof $|y\rangle \in (\mathbb{C}^2)^{\otimes p(n)}$ such that Q_n accepts $(x, |y\rangle)$ with probability at least $2/3$.*
- *(Soundness) If $x \in A_{\text{no}}$, then for all proofs $|y\rangle \in (\mathbb{C}^2)^{\otimes p(n)}$, Q_n accepts $(x, |y\rangle)$ with probability at most $1/3$.*

Thus far, we have introduced the study of local Hamiltonians from a computer science perspective involving constraint systems. However, the initial motivation for this research stems from quantum many-body physics. In particular, the latter would more generally define quantum Hamiltonian complexity as the study of how difficult it is to simulate physical systems [Osb12]. In this view, k-LH can be phrased as a special case of the more general Simulation Problem [Osb12], which roughly asks the following: Given a description of a Hamiltonian H, an initial state ρ, an observable M, and a time $t \in \mathbb{C}$, estimate the expectation

$$\mathrm{Tr}\left[M \frac{(e^{iHt})^\dagger \rho e^{iHt}}{\mathrm{Tr}\left((e^{iHt})^\dagger \rho e^{iHt}\right)}\right]. \tag{1}$$

The local Hamiltonian problem is then recovered by choosing H as a local Hamiltonian, setting $M = H$, $\rho = I/\mathrm{Tr}(I)$, and considering $t = i\beta$ for $\beta \in \mathbb{R}$ and $\beta \to \infty$.

Organization of this paper. We begin in Section 2 with a brief survey of the history of the field of quantum Hamiltonian complexity from both computer science and physics

perspectives. Section 3 sets notation. In Section 4, we attempt to give computer science oriented explanations of common many-body physics terminology, as well as overviews of select important research directions and developments, such as Mean Field Theory, Tensor Networks (including Matrix Product States, Density Matrix Renormalization Group, and Multi-Scale Entanglement Renormalization Ansatz). Section 5 reviews select key computer science-based results in the area, including a new quantum information theoretic presentation of Bravyi's polynomial time algorithm [Bra06] for Quantum 2-SAT (Section 5.4).

This paper assumes background in quantum computing and information; the interested reader is referred to the standard text of Nielsen and Chuang [NC00] (see also [KSV02, KLM07] for alternate textbooks) or the thesis of Gharibian [Gha13] for a self-contained brief introduction. For a review of quantum complexity theory, see the survey of Watrous [Wat09]. For a physics-oriented introduction to Hamiltonian complexity, we refer the reader to the survey of Osborne [Osb12].

2 A brief history

Unsurprisingly, the history of quantum Hamiltonian complexity has its roots in both physics and computer science. In this section, we attempt to give a brief survey of both perspectives, beginning with the latter.

2.1 A computer science perspective

The general LH problem. In 1999, Alexei Kitaev presented [Kit99, KSV02] what is regarded as the quantum analogue of the Cook-Levin theorem, proving that k-LH is in QMA for $k \geq 1$ and QMA-hard for $k \geq 5$. His proof is based on a clever combination of the ideas behind the Cook-Levin theorem and early ideas for a quantum computer of Feynman [Fey85], and is surveyed in Section 5.1. The fact that 3-LH is also QMA-complete was shown subsequently by Kempe and Regev [KR03] (an alternate proof was later given by Nagaj and Mozes [NM07]). Kempe, Kitaev, and Regev then showed [KKR06] that 2-LH is QMA-complete; see Section 5.2 for an exposition of the proof. Note that 1-LH is in P, since one can simply optimize for each 1-local term independently.

From a physicist's perspective, however, the Hamiltonians involved in the QMA-hardness reductions above are arguably not "physical", i.e. occurring in Nature. To address this, Oliveira and Terhal next showed [OT08] that 2-LH with the Hamiltonians restricted to nearest-neighbor interactions on a 2D grid is still QMA-complete. Furthermore, in stark contrast to the classical case of MAX-2-CSP on the line (which is in P), Aharanov, Gottesman, Irani and Kempe [AGIK09] showed that 2-LH with nearest-neighbor interactions on the line is also QMA-complete if the local systems have dimension at least 12. The latter was improved to 11 [Nag08] and subsequently to 8 [HNN13]. Gottesman and Irani [GI09] obtained related results for translationally invariant 1D systems; see also Kay [Kay07] for results regarding the latter setting. Very recently, Cubitt and Montanaro gave [CM13] a quantum generalization of Schaeffer's Dichotomy Theorem [Sch78] for the setting of 2-LH on qubits, essentially completely classifying the complexity of LH based on which set of 2-qubit quantum constraints one incorporates in the constraint system. Their classification contains the following levels: Problems are either in P, NP-complete, TIM-complete, or QMA-complete, where TIM is defined [CM13] as the set of problems which are polynomial-time equivalent to solving the general Ising model with transverse magnetic fields.

Quantum SAT. To be precise, the LH problem does not generalize k-CSP, but rather (the decision version of) its optimization variant MAX-k-CSP. One can ask how the complexity of LH changes if we instead focus on a restricted version intended to generalize k-CSP. In this direction, in 2006 Bravyi [Bra06] defined Quantum k-SAT (k-QSAT), in which all local constraints are positive semidefinite, and the question is whether the ground state energy is zero (in this case, H is called *frustration-free*, in that the optimal assignment lies in the null space of every interaction term), or bounded away from zero (i.e. the Hamiltonian is *frustrated*). He showed that 2-QSAT is in P (see Section 5.4 for an exposition), and that k-QSAT is QMA_1-complete for $k \geq 4$, where QMA_1 is QMA with perfect completeness.

Recently, Gosset and Nagaj showed [GN13] that 3-QSAT is also QMA_1-complete.

Commuting LH. Unlike classical constraint satisfaction problems, quantum constraints do not necessarily pairwise commute. It is thus natural to ask how crucial this non-commuting property is to the QMA-completeness of LH. In this direction, Bravyi and Vyalyi showed [BV05] that commuting 2-LH on qudits is in NP. Aharonov and Eldar subsequently showed [AE11] that 3-LH Hamiltonian on *qubits* is in NP, as well as for qutrits on "nearly Euclidean" interaction graphs. Schuch showed that 4-LH on qubits arranged in a square lattice is in NP [Sch11b]. Finally, Aharonov and Eldar proved that approximating the ground state energy of commuting local Hamiltonians on good locally-expanding graphs within an additive error of $O(\epsilon)$ is in NP [AE13b, AE13a]. In terms of efficiently solvable variants of commuting LH, Yan and Bacon [YB12] showed that the special case in which all commuting terms are products of Pauli operators is in P.

Stoquastic LH. Another natural special case of LH is that of *stoquastic* local Hamiltonians, in which the local constraints have only non-positive off-diagonal matrix elements in the computational basis. In this setting, the Stoquastic k-SAT problem, defined as the stoquastic variant of Quantum k-SAT, was shown to be in Merlin-Arthur (MA) for $k \geq 1$ and MA-complete for $k \geq 6$ by Bravyi, Bessen, and Terhal [BBT06] and Bravyi and Terhal [BT09]. (Incidentally, this was the first non-trivial example of an MA-complete promise problem.) The problem Stoquastic LH-MIN, defined as k-LH with stoquastic Hamiltonians, was shown to be contained in AM [BDOT08] and complete for the class StoqMA [BBT06] for $k \geq 2$. Here, StoqMA is a variant of QMA in which the verifier is restricted to preparing qubits in the states $|0\rangle$ and $|+\rangle$, performing classical reversible gates, and measuring in the Hadamard (i.e. $|+\rangle, |-\rangle$) basis. Finally, Jordan, Gosset, and Love showed that computing the *largest* eigenvalue of a stoquastic local Hamiltonian is QMA-complete [JGL10].

Approximation algorithms for LH. Given the prevalence of heuristic algorithms for solving k-LH, a natural question is whether rigorous (classical) approximation algorithms for k-LH can be derived. Here, Bansal, Bravyi and Terhal showed [BBT09] that k-LH on bounded degree planar graphs, as well as on the unbounded degree star graph, could be approximated within $(1-\epsilon)$ relative error for any $\epsilon \in \Theta(1)$ in polynomial time, i.e. they gave a Polynomial Time Approximation Scheme (PTAS). Gharibian and Kempe next gave [GK11] a PTAS for approximating the best *product-state* solution for k-LH on dense interaction graphs, and showed that product state solutions yield a (d^{1-k})-approximation to the optimal solution for *arbitrary* (i.e. even non-dense) interaction graphs on d-dimensional systems. Based on numerical evidence, they conjectured [GB1] that for dense graphs, a quantum de Finetti theorem without symmetry holds, which can in turn be exploited to yield a PTAS for dense k-LH (as suggested by mean-field theory folklore). Indeed, Brandão and Harrow recently proved [BH13] this conjecture, along with other results: A PTAS for planar graphs (improving on Reference [BBT09]), and an efficient approximation algorithm for graphs of low threshold rank.

Hardness of approximation for LH. The PCP Theorem [AS98, ALM+98] is one of the crowning achievements of modern complexity theory. As such, a major open question in quantum Hamiltonian complexity is whether a *quantum* version of this theorem holds [AN02, Aar06]. Rigorously formulated in the work of Aharanov, Arad, Laundau and Vazirani [AALV09], the question has attracted much attention in the last decade. For example, Reference [AALV09] proved that a quantum analogue of Dinur's gap amplification step in her proof of the PCP theorem [Din07] can be shown in the quantum setting. For further details on the quantum PCP conjecture, we refer the reader to the recent survey dedicated to the topic by Aharonov, Arad, and Vidick [AAV13].

More generally, in terms of hardness of approximation for quantum complexity classes, Gharibian and Kempe [GK12] defined a quantum version of Σ_2^p (the second level of the Polynomial Time Hierarchy), and showed hardness of approximation for various local Hamiltonian-related problems such as Quantum Succinct Set Cover. Reference [GK12] also showed a hardness of approximation and completeness result for QCMA, which is defined as QMA with a *classical* prover [AN02]. (QCMA is also known by the name Merlin-Quantum-Arthur

(MQA) [Wat09].)

2.2 A physics perspective

We now briefly describe the history of quantum Hamiltonian complexity from a physics perspective. This section is by no means comprehensive; the reader is referred to the surveys of Verstraete, Murg, and Cirac [VMC08] and Osbore [Osb12], for example, or to their friendly neighborhood physicist for further details.

Classical Hamiltonians. Beginning with the case of classical Hamiltonians, an early and canonical [Osb12] example of computational hardness is Baharona's work [Bah82], which showed that finding a ground state and computing the magnetic partition function of an Ising spin glass in a nonuniform magnetic field are NP-hard tasks. Jerrum and Sinclair, on the other hand, showed [JS93] #P-completeness of computing the partition function of the ferromagnetic Ising model, and gave a Fully Polynomial Randomized Approximation Scheme (FPRAS) in the same paper. As mentioned above, however, the Ising model is classical in that all variables are assigned values in the set $\{+1, -1\}$; thus, the ground state has an efficient classical description.

Quantum Hamiltonians. In contrast, for *quantum* Hamiltonians, the last two decades have seen much effort towards classifying when a ground state can be described efficiently classically [VMC08]. One of the main instigators of this push was White's celebrated Density Matrix Renormalization Group[1] (DMRG) method [Whi92, Whi93], which is a heuristic algorithm performing remarkably well in practice for finding ground states of 1D quantum systems. It was later realized [ÖR95, RÖ97, VPC04, VMC08, WVS$^+$09] that DMRG can be viewed as a variational algorithm over the class of tensor network states known as Matrix Product States (MPS).

Appearing early on in the work of Affleck, Kennedy, Lieb and Tasaki [AKLT88], Matrix Product States have proven invaluable in the study of many-body quantum systems. For example, they were exploited by Vidal [Vid03, Vid04] to efficiently classically simulate "slightly entangled" quantum computations. Generalizations of MPS to higher dimensions, such as the Projected Entangled Pair States (PEPS) of Verstraete and Cirac [VC04, VWPGC06], and the Multiscale Entanglement Renormalization Ansatz (MERA) of Vidal [Vid07, Vid08], soon followed. Note that while MPS and MERA networks can be efficiently contracted, Schuch, Wolf, Verstraete and Cirac have shown that contracting a PEPS network is in general #P-complete [SWVC07].

Finally, Hastings showed [Has07] in 2007 that the ground state of gapped 1D Hamiltonians can be well approximated by an MPS; this helped explain the effectiveness of DMRG. However, the latter is a heuristic, and a rigorous proof that such an optimal MPS can be found in polynomial time required further work. In this direction, Aharanov, Arad, and Irani [AAI10] and Schuch and Cirac [SC10] showed that given a fixed bond dimension as input, the optimal MPS of that bond dimension can be found efficiently. Arad, Kitaev, Landau and Vazirani subsequently gave a subexponential time algorithm [AKLV13] for arbitrary bond dimension. Finally, Landau, Vazirani, and Vidick showed [LVV13] that the problem of finding an approximation to the ground state of a 1D gapped system is in BPP.

Area laws. A key problem in quantum many-body physics is understanding the entanglement structure of a ground state. Here, a specific question which has attracted much attention is the possible existence of area laws. Roughly, an *area law* says that for any subset S of particles chosen from an n-particle ground state, the amount of entanglement crossing the cut between S and its complement scales not with the size of S, but rather with the size of the *boundary* of the cut. In this direction, a breakthrough result was Hastings' proof [Has07] of an area law for gapped 1D systems. A combinatorial proof improving on Hasting's result for the frustration-free case was later given by Aharonov, Arad, Landau and Vazirani [AALV11], followed by a proof of Arad, Kitaev, Landau, and Vazirani's [AKLV13] which applies in frustrated settings as well. Whether a 2D area law holds remains a chal-

[1]Note: The word *Group* does not actually refer to a group in the usual mathematical sense here.

lenging open question. The reader is refered to the review of Eisert, Cramer, and Plenio for further details [ECP10].

3 Notation

Let $\mathcal{L}(\mathcal{X})$, $\mathcal{U}(\mathcal{X})$, and $\mathcal{H}(\mathcal{X})$ denote the sets of linear, unitary, and Hermitian operators acting on complex Euclidean space $\mathcal{X}$, respectively. The operators σ_x, σ_y, and σ_z denote the Pauli X, Y, and Z operators, respectively. We define vector $\overrightarrow{S}_i := (\sigma_i^x, \sigma_i^y, \sigma_i^z)$, and dot-product

$$\overrightarrow{S}_i \cdot \overrightarrow{S}_j := \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z,$$

where there is an implicit tensor product between (e.g.) σ_i^x and σ_j^x above.

4 Physics for computer scientists

In this section, we discuss various concepts developed by the physics community in the field of Quantum Hamiltonian Complexity. We begin in Section 4.1 by providing a glossary of selected common terms which appear in many-body physics literature. Section 4.2 discusses Mean Field Theory. In Sections 4.3, 4.4, 4.4.1, and 4.5, we review Tensor Networks and their special cases (e.g. MPS and MERA), as well the DMRG algorithm for MPS states.

4.1 Definitions of physics terms

The following is a glossary of commonly encountered physics terms in the condensed matter literature.

Basic terminology.

- *Singlet*: The singlet is the two-qubit Bell state

$$|\psi^-\rangle := \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

  Note that for two-qubit systems, the singlet projects onto the antisymmetric space, and $I - |\psi^-\rangle\langle\psi^-|$ projects onto the symmetric space.

- *Spin*: There are at least two notions of spin we are aware of. The first is the notion of a *spin-(k/2)* system for k a positive integer. Such a system corresponds to a qudit with dimension $d = k + 1$. The second is the notion of *directions along which to measure* spin; this refers to some set of observables $\{S_x, S_y, S_z\}$ for performing measurements along the axes for the three spatial dimensions our world works in.

  The relationship between these two concepts is as follows. The second concept can be thought of as giving a set of three orthonormal axes with respect to which we wish to perform a measurement, and the first concept tells us how large the magnitude of a measurement result can be. For example, upon measurement, a spin-(1/2) particle can yield outcomes $\pm 1/2$, whereas a spin-(3/2) particle can yield $\pm 1/2$ and $\pm 3/2$.

- *Hamiltonian model*: The specification of a particular Hamiltonian model is analogous to choosing a family of constraint types allowed in a classical CSP. For example, one might call the "3-SAT model" one in which all constraints are 3-local Boolean formulae in Conjunctive Normal Form (CNF). Note that Hamiltonian models can be either classical or quantum, such as the classical and quantum Ising models.

- *Interaction (hyper)graph*: The (hyper)graph illustrating which sets of particles are constrained by a common local Hamiltonian constraint. For 2-local Hamiltonians, this corresponds to a graph G, i.e. (i, j) is an edge in G if there exists a Hamiltonian constraint H_{ij} acting jointly on particles i and j.

- *To solve a model*: The meaning of this phrase depends largely on context. Typically, one is assumed to have a classical description of a local Hamiltonian H, and we wish to determine some property of the system described by H. For example, we may wish to

solve for the ground state energy of H, or determine when a phase transition occurs. *Solving the model* means calculating the value of whichever property of H you are interested in.

Commonly studied Hamiltonian models.

- *Classical Ising Model*: The classical local Hamiltonian

$$H(\boldsymbol{x}) = \sum_{\langle i,j \rangle} J_{ij} x_i x_j, \tag{2}$$

where $x_i \in \{+1, -1\}$, interactions J_{ij} are constants, and the notation $\langle i, j \rangle$ means we consider interactions on only nearest-neighbor pairs (i, j) (according to whichever underlying geometry we are interested in, such as a 1D chain or 2D lattice). We remark that physics literature often writes simply H instead of $H(\boldsymbol{x})$ for notational simplicity. An assignment $\boldsymbol{x}$ is called a *configuration*, and the objective function value $H(\boldsymbol{x})$ is called the *energy* of a configuration.

To illustrate the connection to classical complexity theory, note that setting all $J_{ij} = -1$ and searching for the maximum energy configuration of the Hamiltonian $|E|+H(\boldsymbol{x})$ is equivalent to the MAX CUT problem, where $|E|$ is the size of the edge set of the interaction graph.

Note that H can also be defined with an additional linear term, i.e.

$$H(\boldsymbol{x}) = \sum_{\langle i,j \rangle} J_{ij} x_i x_j + \mu \sum_i m_i x_i,$$

where m_j models the effect of an external magnetic field on site i, and μ is the magnetic moment.

- *Quantum Ising Model*: The quantum Ising Model is the 2-local Hamiltonian (see, e.g. [Pfe70, Sac11, Dzi05])

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

where J is the exchange constant, g is a dimensionless coupling constant, and recall σ^z and σ^x are the Pauli Z and X matrices, respectively. This model, also known as the transverse field Ising model, has recently found itself characterizing a new complexity class called TIM [CM13].

- *Heisenberg model*: The Heisenberg model is given by

$$H = -\sum_{\langle i,j \rangle} (J_x \sigma_i^x \sigma_j^x + J_y \sigma_i^y \sigma_j^y + J_z \sigma_i^z \sigma_j^z) + h \sum_i \sigma_i^z,$$

where J_x, J_y, and J_z are coupling constants, and h is the external magnetic field. Various special cases of this model can be considered, such as the XY model [LSM61],

$$H = J \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y,$$

the XXZ model (see, e.g. [YY66a, YY66b, Sac11]),

$$H = -\sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \lambda \sigma_i^z \sigma_j^z,$$

and the anti-ferromagnetic Heisenberg model (see below).

- *Anti-ferromagnetic Heisenberg model*: The anti-ferromagnetic Heisenberg model is given as follows. If we assume the underlying interaction graph is a cycle, i.e. a 1D chain with periodic boundary conditions, then in physics notation one often writes

$$H = \sum_i \overrightarrow{S}_i \cdot \overrightarrow{S}_{i+1}.$$

(Of course, in principle the underlying interaction graph can be any simple graph.) To intuitively understand what this 2-local constraint enforces for the spin-1/2 particle case, note that

$$I - (\sigma^x\sigma^x + \sigma^y\sigma^y + \sigma^z\sigma^z) \propto |\psi^-\rangle\langle\psi^-|,$$

where recall $|\psi^-\rangle$ is the singlet. Hence, the ground state of this 2-local constraint is the 1-dimensional anti-symmetric subspace, in which spins are aligned in a conflicting fashion, i.e. up-down or down-up.

We now discuss the known properties of this model. For spin-1/2 systems in 1D, the anti-ferromagnetic Heisenberg model is solvable exactly using the Bethe ansatz [Bet31]. Its spectrum is gapless, and the spin correlations (e.g., $\langle\sigma_i^z\sigma_j^z\rangle$) decay as a power law in $|i-j|$. For spin-1 systems in 1D, the model is already difficult to solve, and was historically expected to be gapless and exhibit power law decay. Surprisingly, in 1983, Haldane [Hal83a, Hal83b] predicted that the properties of the 1D spin-S Heisenberg model depend strongly on whether S is a half-odd-integer or an integer: For half-odd-integer S the model was predicted to be gapless and exhibit power law decay, while for integer S, it was believed to be gapped and exhibit exponential decay. The first of these, i.e. the absence of a non-zero energy gap for half-odd-integer S, was proven rigorously [AL86] by using an extension of the Lieb-Shultz-Mattis theorem [LSM61]. As for the second, evidence for the existence of the Haldane gap for $S = 1$ has been found both numerically and experimentally [BMA$^+$86, MBAH88, RVR$^+$87].

- *AKLT model*: As the 1D spin-1 Heisenberg model has proven difficult to solve, Affleck, Kennedy, Lieb, and Tassaki proposed and studied the similar so-called AKLT model in 1987 [AKLT87, AKLT88]. The AKLT model is artificial, and hence not believed to be experimentally realizable. However, it has the following desirable properties: (i) It looks superficially similar to the spin-1 Heisenberg model (ii) it can be solved exactly (iii) Haldane's argument (see *anti-ferromagnetic Heisenberg model*) can be rigorously verified for this model. The AKLT model is also a useful example for understanding matrix product states, symmetry protected topological order, etc...

  The 1D spin-1 AKLT Hamiltonian is defined as

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2.$$

  This model is best understood via the correspondence between a qutrit (spin-1) and the symmetric subspace of two qubits (spin-1/2):

$$|+\rangle \leftrightarrow |11\rangle, |0\rangle \leftrightarrow (|00\rangle + |11\rangle)/\sqrt{2}, |-\rangle \leftrightarrow |00\rangle.$$

  Then, the ground state of the AKLT model can be constructed in three steps: (1) Split the ith qutrit into two qubits labeled i_L and i_R, (2) i_R and $(i+1)_L$ form a singlet, and (3) symmetrize i_L and i_R. The ground state is called a "valence-bond state" as it is a tensor product of singlets in the qubit representation. We emphasize that the second term in the Hamiltonian of the AKLT model is intentionally added to ensure exact solvability, i.e. that step (2) is the optimal strategy to minimize the energy. (Omitting this second term yields the anti-ferromagnetic Heisenberg model.) The AKLT Hamiltonian has the following properties [AKLT87, AKLT88]:

  1. The model is gapped, since excitations break at least one singlet and cost non-vanishing energy.
  2. The ground state degeneracy depends on boundary conditions: The dimension of the ground state space is 1 for periodic boundary conditions, and 4 for open boundary conditions. This is because in the latter case we have two free qubits 1_L and n_R (n is the number of sites), while in the former case these two qubits form a singlet.
  3. Correlation functions decay exponentially as the "structure" of the ground states is short ranged.
  4. The ground state can be written exactly as a matrix product state of bond dimension 2 [Sch11a], as its Schmidt rank across any bipartite cut is 2.

Physical phenomena.

- *Ferromagnetic and anti-ferromagnetic order*: When a system demonstrates ferromagnetic order, it means the ground state has all spins aligned, e.g. all spin up. Anti-ferromagnetic order on a bipartite lattice means that the ground state has alternating up and down spins (i.e., neighbouring spins point in opposite directions). For example, $H = -\sum_i \sigma_i^z \sigma_{i+1}^z$ has ferromagnetic order (i.e. its ground states are the all zeroes and all ones states), whereas $-H$ has anti-ferromagnetic order. At an intuitive level, ferromagnetic order means that if we cool the system down to its ground state, then we observe some global magnetization effect taking place (since all spins point in the same direction).
- *Thermal equilibrium & Gibbs state*: When a classical system is in *thermal equilibrium*, the *Gibbs formalism* states that given the Hamiltonian H, the probability of observing a configuration $\boldsymbol{x}$ of the system is proportional to $\exp(-\beta H(\boldsymbol{x}))$, where the parameter β is the *inverse temperature*[2]. The distribution so induced on the configurations is called the *Gibbs distribution* or canonical ensemble. An important quantity associated with the *Gibbs distribution* is the *free energy per unit volume*. We first define the *partition function* Z, which is merely the normalization constant in the Gibbs distribution:
$$Z(\beta) := \sum_{\boldsymbol{x} \in \{-1,1\}^n} \exp(-\beta H(\boldsymbol{x})). \tag{3}$$
One can then define the *free energy per unit volume* as
$$F(\beta) := -\frac{1}{|V|} \log Z(\beta). \tag{4}$$
The reason for the negative sign is mostly historical; a version without the negative sign, called the *pressure*, is sometimes used [Sim93].
When a quantum system is in *thermal equilibrium*, the state of the system is described by the density matrix $\rho \propto \exp(-\beta T) = \exp(-H/T)$ for H some Hamiltonian, and T the temperature. This state is also known as the *Gibbs* or *thermal* state. The concepts of partition function and free energy can be defined analogously to the classical setting. Note here that zero-temperature makes sense, in that it is defined in terms of the limit $T \to 0$. Also, it should be noted that theoretical physicists typically think of all quantities as being dimensionless, meaning there are no specific units attached to T (such as Kelvin, Celsius, etc). For this reason, it doesn't make much sense to define "room temperature" as being, say, $T = 25$, as it depends on which temperature scale one chooses.
- *Quantum phase transitions and criticality*: Here we are given a Hamiltonian $H(\lambda)$ as a function of some tuning parameter λ. We say H has a quantum phase transition if its "ground state is not analytical". As a rough but intuitive example, if the dimension of the ground state space of $H(\lambda)$ is 2 for $\lambda < \lambda_c$ and 1 for $\lambda > \lambda_c$, respectively, then there is a quantum phase transition at $\lambda = \lambda_c$. We call $\lambda = \lambda_c$ a *critical point*, and $H(\lambda_c)$ a *critical system*. A critical system is usually associated with certain scale invariance. The physics at and near critical points is called *critical phenomena*.
For a more concrete example, consider the transverse field Ising model, defined as
$$H = -\sum_{i=-\infty}^{\infty} \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^x.$$
Here, taking the *thermodynamic limit* means that the number of spins goes to infinity (the indices above range from $-\infty$ to ∞). For this model, when $\lambda \to \infty$, the ground state is $|\to\to\to\to\to\cdots\rangle$, where $|\to\rangle$ is the 1-eigenvector of σ^x (i.e., $\sigma^x|\to\rangle = |\to\rangle$). When $\lambda = 0$, the ground state is degenerate, and is either all spins up or all spins down. More generally, when $\lambda < 1$, we have a 2-fold degenerate ground state, and when $\lambda > 1$, we have a unique ground state.

[2]We note here that when the Gibbs formalism is applied to actual physical systems (such as the motion of molecules in gases) with respect to the SI units, β is actually $\frac{1}{kT}$ where T is the temperature and k is the Boltzmann constant. For our purposes, we may work as if the units are rescaled so that $k = 1$.

4.2 Mean field theory

We now discuss mean field theory. Often in condensed matter theory, one wishes to compute some property of a given local Hamiltonian. In general, computing such properties can be complexity-theoretically hard, so one needs approximate or heuristic approaches for dealing with such hardness. One approach is *mean-field theory*, which approximates a Hamiltonian H by a similar but exactly solvable Hamiltonian H_{mf}. The mean-field Hamiltonian H_{mf} may contain some unknown coefficients to be determined. In general, there is no guarantee as to how well H_{mf} approximates the properties of H which are of interest; as such, mean-field models are heuristic approaches. Mean-field theory is arguably the most widely used approximation method in condensed matter physics.

We demonstrate the approach with a textbook example concerning the classical Ising model

$$H(\boldsymbol{x}) = -J \sum_{\langle i,j \rangle} x_i x_j$$

on a d-dimentional hypercubic lattice (see Equation (2)), where $\langle i, j \rangle$ denotes summation over nearest neighbors. Our goal is to "solve this model", which in this context means to determine the critical temperature T_c at which the system undergoes a phase transition. For $d = 1$ the model is easily solved by the transfer matrix method. For $d = 2$ the model was first solved by Onsager [Ons44]. Onsager's solution is mathematically involved, and from a modern point of view a technically simpler approach is fermionization. For $d \geq 3$ no exact solution is known. In the mean-field approximation we consider the mean-field Hamiltonian

$$H_{mf} = -\frac{J}{2} \sum_i x_i \left(\sum_{j \text{ neighbor of } i} \langle x_j \rangle \right) = -dJ\langle x \rangle \sum_i x_i.$$

We have set $\langle x_i \rangle = \langle x \rangle$ for all i as the magnetization is expected to be uniform. Note that we view $\langle x \rangle$ just as a parameter similar to J. The mean-field Hamiltonian H_{mf} is decoupled (non-interacting) and can be solved easily. We now compute the magnetization with respect to H_{mf}:

$$\langle x_i \rangle_{mf} = \frac{\sum_{x_i = \pm 1} x_i \exp(-\beta H_{mf})}{\sum_{x_i = \pm 1} \exp(-\beta H_{mf})} = \frac{\sum_{x_i = \pm 1} x_i \exp(\beta dJ \langle x \rangle)}{\sum_{x_i = \pm 1} \exp(\beta dJ \langle x \rangle)} = \tanh(\beta dJ \langle x \rangle).$$

We require the mean-field theory to be self-consistent:

$$\langle x_i \rangle_{mf} = \langle x \rangle \Rightarrow \langle x \rangle = \tanh(\beta dJ \langle x \rangle).$$

This equation has only one solution $\langle x \rangle = 0$ when $\beta dJ \leq 1$ and has three solutions $\langle x \rangle = 0, \pm m$ when $\beta dJ > 1$. One easily finds that the mean-field free energy $F_{mf} = -\ln Z_{mf}$ (Z_{mf} is the mean-field partition function) at $\langle x \rangle = \pm m$ is lower than that at $\langle x \rangle = 0$ in the regime that there are three solutions. Hence mean-field theory predicts spontaneous magnetization when $\beta dJ > 1$ or $T_c = dJ$.

A seemingly different but essentially equivalent approach is not to impose the self-consistency equation by hand. Instead, we minimize the mean-field free energy F_{mf} with respect to $\langle x \rangle$ (F_{mf} is a function of $\langle x \rangle$ because H_{mf} is a function of $\langle x \rangle$). One finds that the condition $\partial F_{mf} / \partial \langle x \rangle = 0$ is equivalent to the self-consistency equation. Indeed, the equivalence of these two mean-field approaches is a general result due to the Hellmann-Feynman theorem [Fey39]. We point motivated readers to standard physics textbooks (e.g., [Sac11]) for more examples of mean-field theory.

4.3 Tensor networks

Since arbitrary quantum states $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ may require $\Theta(\exp(n))$ bits to represent classically, physicists have derived clever ways of encoding certain classes of entangled quantum states in succinct forms. One such approach is via *tensor networks*. Such networks include as special cases (for example) Matrix Product States (MPS) [AKLT88, Vid03] and Projected Entangled Pair States (PEPS)[VWPGC06].

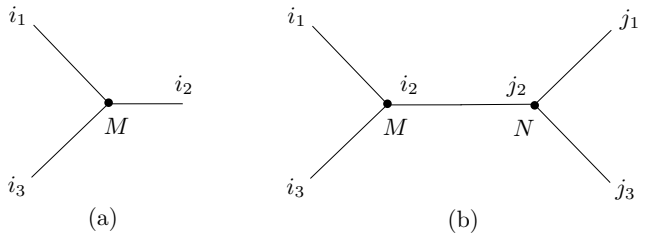

Figure 1: (a) A single tensor $M(i_1, i_2, i_3)$. (b) Two tensors $M(i_1, i_2, i_3)$ and $M(i_1, i_2, i_3)$ contracted on the edge (M, N).

Informally, to a computer programmer, a *tensor* $M(i_1, i_2, \ldots, i_k)$ is simply a k-dimensional array; one plugs in k indices, and out pops a complex number. Hence, in terms of linear algebra, a 1-dimensional tensor is a vector, and a 2-dimensional tensor is a matrix. Physicists often like to make this more confusing than it is by simplifying the notation and placing indices as super- or sub-scripts — for example, they might denote a 3D array $M(i_1, i_2, i_3)$ by $M_{i_3}^{i_1,i_2}$. To make it easier to work with tensors, however, there is a simple but extremely useful graph theoretical framework for depicting them. Figure 1(a) shows M, for example. Here, the vertex corresponds to the tensor M. Each edge corresponds to one of the input parameters to M.

Continuing our informal discussion, in Figure 1(b), an edge with two vertices as endpoints corresponds to the operation of *contracting* tensors on edges. Specifically, Figure 1(b) takes two 3D tensors M and N, and contracts them on their i_2 and j_2 inputs, respectively. The resulting mathematical object is a 4-dimensional tensor P defined as

$$P(i_1, i_3, j_1, j_3) = \sum_k M(i_1, k, i_3) N(j_1, k, j_3).$$

Note the resulting tensor in Figure 1 has four "legs" (i.e. edges with only one endpoint); this is because P takes in four inputs.

More formally, a k-dimensional tensor M (as defined above) is a map $M : [d_1] \times \cdots \times [d_k] \mapsto \mathbb{C}$, where each d_i is a natural number. (We remark that sometimes the dimension k of a tensor is referred to as its *rank*. Note that this notion of "rank" is *not* the same as the usual linear algebraic notion of rank for matrices.) For this reason, we can observe the following straightforward way to connect n-qubit states $|\psi\rangle$ and n-tensors. Let $|\psi\rangle = \sum_{i=1}^{2^n} \alpha_i |i\rangle$ for $\{|i\rangle\}_{i=1}^{2^n} \subseteq (\mathbb{C}^2)^{\otimes n}$ the computational basis. Then, for any $i \in [2^n]$, letting $i_1 \cdots i_n$ denote the binary expansion of i, we can define an n-tensor $M(i_1, \ldots, i_n)$ for $i_k \in \{0, 1\}$ which simply stores all 2^n amplitudes of $|\psi\rangle$, i.e. $M(i_1, \ldots, i_n) := \alpha_{i_1 \ldots i_n}$. In other words, we can write

$$|\psi\rangle = \sum_{i=1}^{2^n} M(i_1, \ldots, i_n) |i\rangle. \tag{5}$$

More generally, one can generalize this correspondence to represent n-qudit systems with local dimension d. Then, each index to M would take a value in $[d]$, and d is called the *bond dimension*.

Question 1. *In Figure 2, we depict five different tensor networks. For simplicity, we assume here that all input parameters to a tensor are from the set* $[d]$.

1. *For (a), what type of linear algebraic object does the figure correspond to?*
2. *Which operations on objects of the type in (a) do images (b) and (c) depict? What is the output of the tensors in (b) and (c)?*
3. *How many tensors is the network in (d) composed of? How many input parameters does each of these constituent tensor networks have (before contraction)? How many input parameters does the final, contracted tensor network have?*
4. *Image (d) corresponds to an m-dimensional tensor, which using the tensor-vector correspondence in Equation (5), can be thought of as representing an n-qubit vector $|\psi\rangle$ (whose amplitudes are computed using the specific contractions between tensors indicated by the network). With this picture in mind, what does (e) correspond to?*

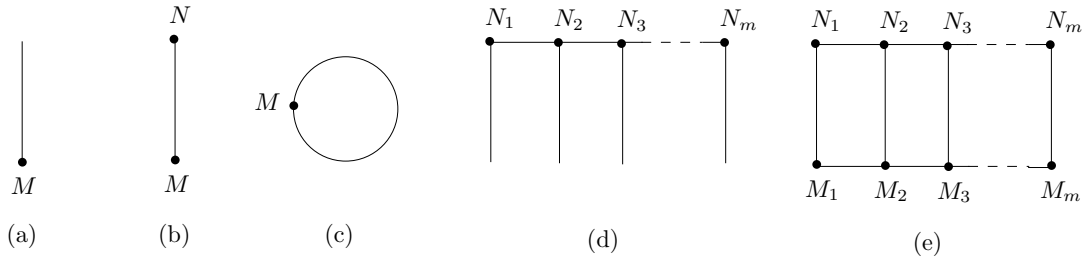

Figure 2: Five tensor networks, studied in Question 1.

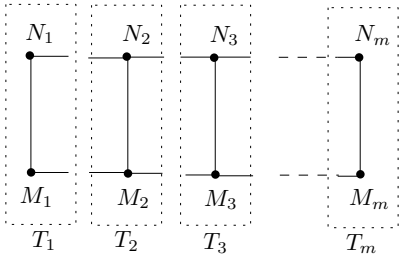

Figure 3: Demonstrating the linear map view of tensor networks.

5. *Image (e) combines* $2m$ *tensors into a network which takes no inputs and outputs a complex number* α*. Assuming the bond dimension* d *is a constant, given these* $2m$ *tensors, how can we compute* α *in time polynomial in* m*? Hint: Consider an iterative algorithm which in step* $i \in [m]$ *considers all tensors up to* N_i *and* M_i*.*

There is another view of tensors which also proves useful, in which a tensor is seen as a linear map. Let S denote the set of legs of a tensor M, and partition S into subsets S_1 and S_2. Then, by fixing inputs to all legs in S_1, we "collapse" M into a new tensor M' corresponding to some vector in $(\mathbb{C}^d)^{\otimes |S_2|}$. For example, consider again our tensor M in Figure 1(a), and let $S_1 = \{i_1\}$ and $S_2 = \{i_2, i_3\}$. Then, denote by M_k the tensor obtained by hardcoding $i_1 = k$, i.e. $M_k(i_2, i_3) := M(k, i_2, i_3)$. By Equation (5), M_k corresponds to some vector $|\psi_k\rangle \in (\mathbb{C}^2)^{\otimes |S_2|}$. In other words, we have just demonstrated a mapping which, given any computational basis state $|k\rangle \in \mathbb{C}^d$, outputs a vector $|\psi_k\rangle \in (\mathbb{C}^d)^{\otimes 2}$, i.e. we have a linear map $\Phi : \mathbb{C}^d \mapsto (\mathbb{C}^d)^{\otimes 2}$. Returning to our more general example with M, S, S_1 and S_2, this approach allows us to view a tensor M with legs in S as a linear map $M : (\mathbb{C}^d)^{\otimes |S_1|} \mapsto (\mathbb{C}^d)^{\otimes |S_2|}$.

To demonstrate the effectiveness of this linear map view of tensors, we revisit Question 1(5). This time, we break up this tensor into tensors T_i, as depicted in Figure 3. Then, we can think of T_1 as representing the conjugate transpose of a vector $|\psi\rangle \in (\mathbb{C}^d)^{\otimes 2}$. Next, T_i for $i \in \{2, \ldots, m-1\}$ can be thought of as linear maps from $(\mathbb{C}^d)^{\otimes 2}$ to $(\mathbb{C}^d)^{\otimes 2}$, where the two left legs are the inputs, and the two right legs are outputs. It follows that after contracting T_1 through T_{m-1}, the result is the conjugate transpose of some vector $|\psi\rangle \in (\mathbb{C}^d)^{\otimes 2}$. Since the last tensor T_m represents some $|\phi\rangle \in (\mathbb{C}^d)^{\otimes 2}$, performing the final contraction computes the inner product $\langle\psi|\phi\rangle$ outputting a scalar, as claimed in Question 1(5). Note that since the bond dimension d is considered a constant, this linear map view implies that the contraction of the entire network can clearly be performed in time polynomial in m.

4.4 Density Matrix Renormalization Group

Having introduced the concept of tensor networks in Section 4.3, we now discuss the Density Matrix Renormalization Group (DMRG) algorithm, which is nowadays generally considered the most powerful numerical method for studying one-dimensional quantum many-body systems. In many applications of DMRG, we are able to obtain the low-energy physics (such as, for example, the ground state energy, correlation functions, etc...) of a 1D quantum lattice model with extraordinary precision and moderate computational resources. Historically, White's invention of DMRG [Whi92, Whi93] in the early 1990's was stimulated by the fail-

ure of Wilson's numerical renormalization group [Wil75] for homogeneous systems. A subsequent milestone was achieved when it was realized [ÖR95, RÖ97, VPC04, VMC08, WVS+09] that DMRG is in fact a variational algorithm over a specific class of tensor networks known as Matrix Product States (MPS) (introduced in Section 4.4.1 below).

The purpose of this section is to outline at a high level how DMRG works from the MPS point of view. For further details, we refer the reader to the following review papers on the topic. Schollwöck [Sch11a] is a very detailed account of coding with MPS. The earlier paper of Schollwöck [Sch05] discusses DMRG mostly in its original formulation without explicit mention of MPS. Finally, Verstraete, Murg and Cirac [VMC08] and Cirac and Verstraete [CV09] focus on the role MPS plays in DMRG, as well as other variational classes of states, such as Tree Tensor States, Multiscale Entanglement Renormalization Ansatz (MERA) and Projected Entangled Pair States (PEPS).

4.4.1 Matrix Product States

Matrix Product States (MPS) are the simplest class of tensor network states, and as such, have received much attention. Consider a 1D quantum lattice system of local dimension d. We associate each site i with d matrices $A_i^{j=1,2,\ldots,d}$ of dimension $D \times D$, except at the boundaries, where $A_1^{j=1,2,\ldots,d}$ is of dimension $1 \times D$ and $A_n^{j=1,2,\ldots,d}$ is of dimension $D \times 1$ (where n is the total number of sites). Then an MPS is given by

$$|\psi\rangle = \sum_{j_1,\ldots,j_n=1}^{d} A_1^{j_1} A_2^{j_2} \ldots A_n^{j_n} |j_1, \ldots, j_n\rangle.$$

How can one interpret this expression for $|\psi\rangle$? First, note that for any $i \in \{2, \ldots, n-1\}$, we have $A_i^{j_i} : [d] \mapsto \mathcal{L}\left(\mathbb{C}^D \otimes \mathbb{C}^D\right)$. In other words, fixing an index j_i pops out a $D \times D$ complex matrix $A_i^{j_i}$. Similarly, $A_n^{j_i}$ ($A_1^{j_i}$) outputs a complex vector (conjugate transpose of a complex vector). It follows that for any string $j_1 \cdots j_n \in \{0,1\}^n$, the expression $A_1^{j_1} A_2^{j_2} \ldots A_n^{j_n}$ yields a complex number (since it is of the form $\langle v_1 | V_2 \cdots V_{n-1} | v_n \rangle$), i.e. it yields the *amplitude* corresponding to $\boldsymbol{j}$. Thus, the amplitudes are encoded as products of matrices, justifying the name *Matrix Product State*. Some additional terminology: The indices j_i are referred to as *physical* indices, as their dimension d is fixed by the physical system. The value D is called the *bond dimension*, which we discuss in more depth shortly. Graphically, an MPS is given by Figure 2(d), where the vertical lines denote physical indices, and the horizontal lines represent tensor contractions or matrix products.

With a bit of thought, one can see that *any* state $|\psi\rangle \in (\mathbb{C}^d)^{\otimes n}$ can be written as an MPS exactly if the bond dimension D is chosen large enough. Indeed, this can be achieved by setting D to be at least the maximum Schmidt rank of $|\psi\rangle$ across any bipartite cut. In general, however, such a value of D unfortunately grows exponentially with n, and thus large values of D are not computationally feasible. The strength of MPS is hence as follows: Any n-particle quantum states whose entanglement across bipartite cuts is "small" (i.e. of polynomial Schmidt rank in n) can be represented succinctly by an MPS.

Moreover, this niche filled by MPS turns out to be quite interesting, as condensed matter physicists are mainly interested in ground states which are highly *non*-generic. For example, recall that in 1D gapped systems, we have an area law [Has07, AKLV13, ECP10], implying that in the 1D setting the entanglement entropy across any bipartite cut is bounded by a constant independent of n. This, in turn, implies that ground states of 1D gapped systems can be well approximated by an MPS with constant bond dimension D. In gapless or critical systems the area law is slightly violated with a logarithmic factor $\sim \ln n$ [CC04, CC09], implying that MPS is still a fairly efficient parametrization.

Finally, a key property of MPS is that, given an MPS description of a quantum state, we can *efficiently* compute its physical properties, such as energy, expectation of order parameters, correlation functions, and entanglement entropy [Sch11a]. This is in sharp constrast to more complicated tensor networks such as Projected Entangled Pair States (PEPS), which are known to be #P-complete to contract [SWVC07].

4.4.2 Implementation of DMRG

Having introduced MPS, we now briefly review the idea behind DMRG from an MPS perspective. Specifically, given an in input Hamiltonian H, to compute the MPS that best approximates the ground state, our goal is to minimize the expectation $\langle\psi|H|\psi\rangle$ with respect to all MPS $|\psi\rangle$ with some fixed bond dimension D, i.e., with respect to $O(ndD^2)$ parameters. Unfortunately, in general this problem can be NP-hard even for frustration-free Hamiltonians [SCV08]. To cope with this, DMRG is thus a *heuristic* algorithm for finding local minima: There is no guarantee that the local minima we find are global minima, nor that the algorithm converges rapidly. However, perhaps surprisingly, DMRG works fairly well in practice.

At a high level, the DMRG algorithm proceeds as follows. We start with a random MPS denoted by $\{A_{i=1,2,\ldots,n}^{j=1,2,\ldots,d}\}$, and subsequently perform a sequence of local optimizations. A local optimization at site i_0 means minimizing $\langle\psi|H|\psi\rangle$ with respect to $A_{i_0}^{j=1,2,\ldots,d}$, while keeping all other matrices $A_{i\neq i_0}^{j=1,2,\ldots,d}$ fixed. Such local optimizations are performed in a number of "sweeps" until our solution $\{A_{i=1,2,\ldots,n}^{j=1,2,\ldots,d}\}$ converges. Here, a *sweep* consists of applying local optimizations in sequence starting at site 1 up to site n, and then backwards back to site 1. In other words, we apply the optimization locally in the following order of sites: $1, 2, \ldots, n-1, n, n-1, \ldots, 2, 1$.

4.5 Multi-Scale Entanglement Renormalization Ansatz

We now discuss a specific type of tensor network known as the Multi-Scale Entanglement Renormalization Ansatz (MERA) [Vid07, Vid08] (see Section 4.3 for a definition of tensor networks), which falls somewhere between MPS and PEPS. Like MPS and unlike PEPS, the expectation value of local observables for MERA states can be computed exactly efficiently. Like PEPS and unlike MPS, MERA can be used to well-approximate (certain) states in D-dimensional lattices for $D \geq 1$. It should be noted that, as with MPS and PEPS, there is not necessarily any guarantee as to how well MERA can approximate a particular state; rather, as with many ideas in physics, MERA is an intuitive idea which appears to work well for certain Hamiltonian models, such as the 1D quantum Ising model with transverse magnetic field on an infinite lattice [Vid07].

There are two equivalent ways to think about MERA. The first is to give an efficient (log-depth) quantum circuit which, given a MERA description of a state $|\psi\rangle$, prepares $|\psi\rangle$ from the state $|0\rangle^{\otimes n}$. The disadvantage of this view, however, is that it does not yield much intuition as to why MERA is structured the way it is. The second way to think about MERA is through a physics-motivated view in terms of DMRG; as this view provides the beautifully simple rationale behind MERA, we present it first.

The DMRG-motivated view. This viewpoint is presented in [Vid07], and proceeds as follows. To begin, the general idea behind Wilson's real-space renormalization group (RG) methods (see [WN92]) is to partition the sites of a given quantum system into *blocks*. One then simplifies the description of this space by truncating part of the Hilbert space corresponding to each block; this process is known as *coarse-graining*. The entire coarse-graining procedure is repeated iteratively on the new lower dimensional systems produced, until one obtains a polynomial-size (approximate) description (in the number of sites, n) of the desired system.

The key insight of White [Whi92, Whi93] was to realize that for 1D systems, the "correct" choice of truncation procedure on a block B of sites is to simply discard the Hilbert space corresponding to the "small" eigenvalues of ρ_B, where ρ_B is the reduced state on B of the initial n-site state $|\psi\rangle$. Here, the value of "small" depends on the approximation precision desired in the resulting tensor network representation. Intuitively, such an approximation works well if B in $|\psi\rangle$ is not highly entangled with the remaining sites. When this condition does not hold, however, DMRG seems to be in a bind. The idea of MERA is hence to precede each truncation step by a *disentangling* step, i.e. by a local unitary which attempts to reduce the amount of entanglement along the boundary of B between B and the remaining sites before the truncation is carried out.

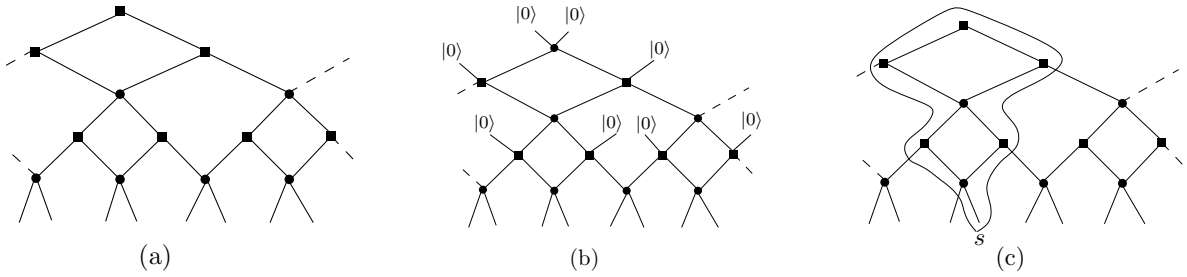

Figure 4: A MERA network on 8 sites. The circle vertices represent "disentangling" unitaries. The square vertices represent isometries. (a) The tensor network view. (b) The quantum circuit view. (c) The causal cone of the site labeled s.

More formally, MERA is defined on a D-dimensional lattice L as follows [Vid07]. For simplicity, we restrict our attention to the case of $D = 1$ on spin-$(1/2)$ systems with periodic boundary conditions, but the ideas here extend to $D \geq 1$ on higher dimensional systems. Let L correspond to Hilbert space $V_L \equiv \bigotimes_{s \in L} V_s$, where $s \in L$ denote the lattice sites with respective finite-dimensional Hilbert spaces V_s. Consider now a block $B \subset L$ of neighboring sites, whose Hilbert space we denote as $V_B \equiv \bigotimes_{s \in B} V_s$. For simplicity, let us assume B consists of two sites s_1 and s_2, with neighboring sites s_0 and s_3 immediately to the left and right, respectively. The disentangling step is performed by carefully choosing unitaries $U_{01}, U_{23} \in \mathcal{U}\left(\mathbb{C}^4\right)$ (the specific choice of U_{01}, U_{23} depends on the input state $|\psi\rangle$), and applying U_{ij} to consecutive sites i and j. The *truncation* step follows next by applying isometry $V_{12} : \mathcal{L}\left(\mathbb{C}^4\right) \mapsto \mathcal{L}\left(\mathbb{C}^2\right)$ to sites 1 and 2, where $\mathbb{C}^2$ is the truncated space we wish to keep and where $V_{12} V_{12}^\dagger = I$. By applying this procedure to neighboring disjoint pairs of spins, we obtain a new spin chain with $n/2$ sites (assuming n is even in this example). The entire procedure is now repeated on these $n/2$ coarse-grained sites. After $O(\log n)$ iterations, we end up with a single site. The tensor network is then obtained by writing down tensors corresponding to the linear maps of each U_{ij} and V_{ij}, and connecting these tensors according to the geometry underlying the process outlined above. The resulting tensor network has a tree-like structure, with a single vertex at the top, and n legs at the bottom corresponding to each of the n original sites. It is depicted in Figure 4(a).

Note that if we assume the bond dimension for each isometric tensor V_{ij} is d, then the MERA representation requires $O(nd^4)$ bits of storage; this is because there are $2n-1$ tensors in the network, and each tensor stores at most $O(d^4)$ complex numbers.

The quantum circuit view. In a sense, we have cheated the reader, because the DMRG view already prescribes the method for the quantum circuit view of MERA. Specifically, imagine we reverse the coarse-graining procedure described above, i.e. instead of working our way from the n sites of $|\psi\rangle$ up to a single site, we go in the opposite direction. Then, intuitively, the DMRG view yields a quantum circuit which, starting from the state $|0\rangle^{\otimes n}$, prepares (an approximation to) the desired state $|\psi\rangle$ via a sequence of the same isometries and unitaries prescribed by the tensor network. This view is depicted in Figure 4(b).

Computing with MERA. A succinct representation of a quantum system would not necessarily be useful without the ability to compute *properties* of the system from this succinct format. A strength of MERA is that, indeed, expectation values of local observables against $|\psi\rangle$ can be efficiently computed. This follows simply because given a MERA network M representing $|\psi\rangle$, the reduced state of $|\psi\rangle$ on $\Theta(1)$ sites can be computed in time $O(\log n)$ (assuming the dimension D of our lattice is considered a constant). To see this, we partition the tensors in our MERA network in terms of horizontal layers or *time slices* from top to bottom. Specifically, in Figure 4(b), time slice 0 is before the top unitary is run, slice 1 immediately after the top unitary is run and before the following pair of isometries are run, and so forth until slice 5, which is immediately after the four bottom-most unitaries are run. Then, in each layer, the causal cone C_s for any site s can be shown to have at most *constant*

width (more generally, at most $4 \cdot 3^{D-1}$ width [Vid08]). Here, the *causal cone* of C_s is the set of vertices and edges in the network which influence the leg of the network corresponding to site s; see Figure 4(c). The *width* of C_s in a time slice is the number of edges in C_s in that slice. Thus, by viewing the MERA network in terms of the quantum circuit view, we see that the reduced state on site s is given by a quantum circuit with $O(\log n)$ gates. Moreover, at any point in the computation, this circuit needs to keep track of the state of only $\Theta(1)$ qubits. Such a circuit can be straightforwardly simulated classically in $O(\log n)$ time via brute force (i.e. multiply the unitaries in the circuit and trace out qubits which are no longer needed), yielding the claim.

5 Reviews of selected results

Having discussed a number of Hamiltonian complexity concepts originating from the physics literature in Section 4, this section next discusses a selected number of central computer science-based results in the area. Section 5.1 reviews Kitaev's original proof that 5-local Hamiltonian is QMA-complete. Section 5.2 discusses the ensuing proof by Kitaev, Kempe and Regev using perturbation theory-based gadgets that 2-local Hamiltonian is QMA-complete. In Section 5.3, we review Bravyi and Vyalyi's Structure Lemma and its use in proving that the 2-local commuting Hamiltonian problem is in NP, and thus unlikely to be QMA-hard. Finally, Section 5.4 gives a quantum information theoretic interpretation of Bravyi's polynomial time algorithm for Quantum 2-SAT.

5.1 5-local Hamiltonian is QMA-complete

One of the cornerstones of classical computational complexity theory is the Cook-Levin theorem, which states that classical constraint satisfaction is NP-complete. The quantum version of this theorem is due to Kitaev, who showed that the 5-local Hamiltonian problem is QMA-complete [KSV02]. In this section, we review Kitaev's proof. For a more in-depth treatment, we refer the reader to the detailed surveys of Aharonov and Naveh [AN02] and Gharibian [Gha13].

We begin by showing that k-local Hamiltonian for any $k \in \Theta(1)$ is in QMA.

Local Hamiltonian is in QMA

Theorem 3. *(Kitaev [KSV02]) For any constant $k \geq 1$,* k-LH $\in$ QMA.

Proof sketch. The basic idea is that whenever we have a YES instance of k-LH, the quantum proof sent to the verifier is essentially the ground state of the local Hamiltonian H in question. The verifier then runs a simple "local" version of phase estimation to roughly determine the energy penalty incurred by the given proof.

To begin, suppose we have an instance (H, a, b) of k-LH with k-local Hamiltonian $H = \sum_{j=1}^{r} H_j \in \mathcal{L}((\mathbb{C}^2)^{\otimes n})$. We construct an efficient quantum verification circuit V as follows. First, the quantum proof is $|\psi\rangle \in \mathbb{C}^r \otimes (\mathbb{C}^2)^{\otimes n} \otimes \mathbb{C}^2$, s.t.

$$|\psi\rangle = \left(\frac{1}{\sqrt{r}} \sum_{j=1}^{r} |j\rangle \right) \otimes |\eta\rangle \otimes |0\rangle, \tag{6}$$

for $\{|j\rangle\}_{j=1}^{r}$ an orthonormal basis for $\mathbb{C}^r$, and $|\eta\rangle$ an eigenvector corresponding to some eigenvalue λ of H. We call the first register of $|\psi\rangle$ the *index* register, the second the *proof* register, and the last the *answer* register. The circuit V is defined as $V := \sum_{j=1}^{r} |j\rangle\langle j| \otimes W_j$, where W_j is defined as follows. For our Hamiltonian $H = \sum_{j=1}^{r} H_j$, suppose H_j has spectral decomposition $H_j = \sum_s \lambda_s |\lambda_s\rangle\langle\lambda_s|$. Then, define W_j acting on the proof and answer registers with action

$$W_j \left(|\lambda_s\rangle \otimes |0\rangle \right) = |\lambda_s\rangle \otimes \left(\sqrt{\lambda_s}|0\rangle + \sqrt{1-\lambda_s}|1\rangle \right). \tag{7}$$

Question 2. *Show that if we apply V to the proof $|\psi\rangle$ and measure the answer register in the computational basis, the probability of obtaining outcome 1 is $1 - \frac{1}{r}\langle\eta|H|\eta\rangle$. Conclude that since the thresholds a and b are inverse polynomially separated,* k-LH $\in$ QMA.

Hint 1. *Observe that since we may assume the index register is implicitly measured at the end of the verification, V above can be thought of as using the index register to choose an index $j \in [r]$ uniformly at random, followed by applying W_j to the proof register. As a result, the probability of outputting* 1 *can be expressed as*

$$\Pr(\textit{output 1}) = \sum_{j=1}^{r} \frac{1}{r} \Pr(\textit{output 1} \mid W_j \textit{ is applied}). \tag{8}$$

Hint 2. *When considering the action of any W_j on $|\eta\rangle$, rewrite $|\eta\rangle$ in the eigenbasis of H_j as $|\eta\rangle = \sum_s \alpha_s |\lambda_s\rangle$ (the values of the coefficients α_s will not matter).*

5-Local Hamiltonian is QMA-hard

To show that 5-local Hamiltonian is QMA-hard, Kitaev gives a quantum adaptation of the Cook-Levin theorem [KSV02]. Specifically, he shows a polynomial-time many-one or Karp reduction from an arbitrary problem in QMA to 5-LH, which we now discuss.

Let P be a promise problem in QMA, and let $V = V_L V_{L-1} \dots V_1$ be a verification circuit for P composed of unitaries V_k. Without loss of generality, we may assume each V_k acts on pairs of qubits, and that $V \in \mathcal{U}((\mathbb{C}^2)^{\otimes m} \otimes (\mathbb{C}^2)^{\otimes N-m})$, where the m-qubit register contains the proof V verifies, and the remaining qubits are ancilla qubits. Using V, our goal is to define a 5-local Hamiltonian H that has a small eigenvalue if and only if there exists a proof $|\psi\rangle \in (\mathbb{C}^2)^{\otimes m}$ causing V to accept with high probability.

We let H act on $(\mathbb{C}^2)^{\otimes m} \otimes (\mathbb{C}^2)^{\otimes N-m} \otimes \mathbb{C}^{L+1}$, which is simply the initial space V acts on, tensored with an $(L+1)$-dimensional *counter* or *clock* register. We label the three registers H acts on as p for proof, a for ancilla, and c for clock, respectively. We now define H itself:

$$H := H_{\text{in}} + H_{\text{prop}} + H_{\text{out}}, \tag{9}$$

with the terms H_{in}, H_{prop}, and H_{out} defined as follows. Let

$$H_{\text{in}} := I_p \otimes (I_a - |0\dots0\rangle\langle 0\dots0|_a) \otimes |0\rangle\langle 0|_c \tag{10}$$

$$H_{\text{out}} := \left(|0\rangle\langle 0| \otimes I_{(\mathbb{C}^2)^{\otimes m-1}}\right)_p \otimes I_a \otimes |L\rangle\langle L|_c \tag{11}$$

$$H_{\text{prop}} := \sum_{j=1}^{L} H_j, \quad \text{where}$$

$$H_j := -\frac{1}{2} V_j \otimes |j\rangle\langle j-1|_c - \frac{1}{2} V_j^\dagger \otimes |j-1\rangle\langle j|_c + \tag{12}$$

$$\frac{1}{2} I \otimes (|j\rangle\langle j| + |j-1\rangle\langle j-1|)_c. \tag{13}$$

Question 3. *Suppose that for any YES-instance of promise problem P, V accepts a valid proof $|\psi\rangle$ with* certainty*. Verify that the following state $|\eta\rangle$, known as the* history state*, lies in the null space of H. Why do you think $|\eta\rangle$ is called the history state?*

$$|\eta\rangle := \frac{1}{\sqrt{L+1}} \sum_{j=0}^{L} \left(V_j \dots V_1 |\psi\rangle_p \otimes |0\rangle_a^{\otimes N-m}\right) \otimes |j\rangle_c. \tag{14}$$

In order to ease the analysis of H's smallest eigenvalue, it turns out to be extremely helpful to apply the following change-of-basis operator to H:

$$W = \sum_{j=0}^{L} V_j \dots V_1 \otimes |j\rangle\langle j|_c. \tag{15}$$

Question 4. *Show that:*

1. $|\hat{\eta}\rangle := W|\eta\rangle = |\psi\rangle_p \otimes |0\rangle_a^{\otimes N-m} \otimes |\gamma\rangle_c$, *where we define* $|\gamma\rangle := \frac{1}{\sqrt{L+1}} \sum_{j=0}^{L} |j\rangle$.
2. $\hat{H}_{\text{in}} := W^\dagger H_{\text{in}} W = H_{\text{in}}$,
3. $\hat{H}_{\text{out}} := W^\dagger H_{\text{out}} W = (V^\dagger \otimes I_c) H_{\text{out}} (V \otimes I_c)$,

4. $\hat{H}_j := W^\dagger H_j W = I_{p,a} \otimes \frac{1}{2}(|j-1\rangle\langle j-1| - |j-1\rangle\langle j| - |j\rangle\langle j-1| + |j\rangle\langle j|)_c$*, and hence*

$$\hat{H}_{\text{prop}} = I_p \otimes I_a \otimes \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & \dots \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 & \dots \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \dots \\ 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \dots \\ 0 & 0 & 0 & -\frac{1}{2} & \ddots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} =: I_p \otimes I_a \otimes E_c, \tag{16}$$

where we have let E *denote a tridiagonal matrix acting on the clock register.*

Henceforth, when we refer to H, H_{in}, H_{out}, H_{prop}, H_j, and $|\eta\rangle$, we implicitly mean $\hat{H}$, $\hat{H}_{\text{in}}$, $\hat{H}_{\text{out}}$, $\hat{H}_{\text{prop}}$, $\hat{H}_j$, and $|\hat{\eta}\rangle$, respectively.

The YES case: H has a small eigenvalue

Question 5. *Suppose that given proof* $|\psi\rangle$*,* V *accepts with probability at least* $1-\epsilon$ *for* $\epsilon \geq 0$*. Show that*

$$\langle\eta|H|\eta\rangle \leq \frac{1}{L+1}\epsilon. \tag{17}$$

Conclude that if there exists a proof $|\psi\rangle$ *accepted with "high" probability by* V*, then* H *has a "small" eigenvalue.*

The NO case: H has no small eigenvalues

If there is no proof $|\psi\rangle$ accepted by V with high probability, then we wish to show that H has no small eigenvalues. To do so, write $H = A_1 + A_2$ for $A_1 := H_{\text{in}} + H_{\text{out}}$ and $A_2 := H_{\text{prop}}$. If A_1 and A_2 were to commute, then analyzing the smallest eigenvalues of A_1 and A_2 independently would yield a lower bound on the smallest eigenvalue of H. Unfortunately, A_1 and A_2 do not commute; hence, if we wish to use information about the spectra of A_1 and A_2 to lower bounds H's eigenvalues, we will need a stronger technical tool, given below.

Lemma 1 (Kitaev [KSV02], Geometric Lemma, Lemma 14.4)**.** *Let* $A_1, A_2 \succeq 0$*, such that the minimum* non-zero *eigenvalue of both operators is lower bounded by* v*. Assume that the null spaces* $\mathcal{L}_1$ *and* $\mathcal{L}_2$ *of* A_1 *and* A_2*, respectively, have trivial intersection, i.e.* $\mathcal{L}_1 \cap \mathcal{L}_2 = \{\mathbf{0}\}$*. Then*

$$A_1 + A_2 \succeq 2v \sin^2 \frac{\alpha(\mathcal{L}_1, \mathcal{L}_2)}{2} I \ , \tag{18}$$

where the angle $\alpha(\mathcal{X}, \mathcal{Y})$ *between* $\mathcal{X}$ *and* $\mathcal{Y}$ *is defined over vectors* $|x\rangle$ *and* $|y\rangle$ *as*

$$\cos\left[\angle(\mathcal{X}, \mathcal{Y})\right] := \max_{\substack{|x\rangle \in \mathcal{X}, |y\rangle \in \mathcal{Y} \\ \| |x\rangle \| = \| |y\rangle \| = 1}} |\langle x|y\rangle| \, .$$

Question 6. *For complex Euclidean spaces* $\mathcal{X}$ *and* $\mathcal{Y}$*, is the statement* $\mathcal{X} \cap \mathcal{Y} = \{\mathbf{0}\}$ *equivalent to* $\mathcal{X}$ *and* $\mathcal{Y}$ *being orthogonal spaces?*

We use Kitaev's Geometric Lemma with $A_1 = H_{\text{in}} + H_{\text{out}}$ and $A_2 = H_{\text{prop}}$ to lower bound the smallest eigenvalue of H in the NO case.

Question 7. *For* $A_1 = H_{\text{in}} + H_{\text{out}}$ *and* $A_2 = H_{\text{prop}}$*, what non-zero value of* v *can we use for the Geometric Lemma?*

Hint 3. *For* A_1*, recall that commuting operators simultaneously diagonalize.*

Hint 4. *For* A_2*, the eigenvalues are given by* $\lambda_k = 1 - \cos[\pi k/(L+1)]$ *for* $0 \leq k \leq L$*. Use this to show that the smallest* positive *eigenvalue of* A_2 *is at least* $1 - \cos(\pi/(L+1)) \geq c/L^2$*.*

Question 8. *In order to compute $\alpha(\mathcal{L}_1, \mathcal{L}_2)$, convince yourself first that*

$$\begin{aligned}\mathcal{L}_1 &= \left[((\mathbb{C}^2)^{\otimes m})_p \otimes |0\rangle_a^{\otimes N-m} \otimes |0\rangle_c\right] \oplus \\ &\quad \left[((\mathbb{C}^2)^{\otimes N})_{p,a} \otimes \mathrm{span}(|1\rangle, \ldots |L-1\rangle)_c\right] \oplus \\ &\quad \left[V^\dagger(|1\rangle \otimes (\mathbb{C}^2)^{\otimes N-1})_{p,a} \otimes |L\rangle_c\right], \qquad (19) \\ \mathcal{L}_2 &= ((\mathbb{C}^2)^{\otimes N})_{p,a} \otimes |\gamma\rangle_c, \qquad (20)\end{aligned}$$

To compute $\sin^2 \frac{\alpha(\mathcal{L}_1,\mathcal{L}_2)}{2}$ for the Geometric Lemma, we now upper bound

$$\cos^2 \alpha(\mathcal{L}_1, \mathcal{L}_2) \leq 1 - \frac{1-\sqrt{\epsilon}}{L+1}.$$

Question 9. *Show that* $\cos^2 \alpha(\mathcal{L}_1, \mathcal{L}_2) = \max_{\substack{|y\rangle \in \mathcal{L}_2 \\ \| |y\rangle \| = 1}} \langle y|\Pi_{\mathcal{L}_1}|y\rangle$.

Observe from Equation (19) that $\mathcal{L}_1$ is a direct sum of three spaces, and hence the projector onto $\mathcal{L}_1$ can be written as the sum of three respective projectors $\Pi_1 + \Pi_2 + \Pi_3$.

Question 10. *Observe by Equation (20) that for any $|y\rangle \in \mathcal{L}_2$, $|y\rangle = |\zeta\rangle_{p,a} \otimes |\gamma\rangle_c$ for some $|\zeta\rangle \in (\mathbb{C}^2)^{\otimes m} \otimes (\mathbb{C}^2)^{\otimes N-m}$.*

1. *Show that $\langle y|\Pi_1|y\rangle = \frac{L-1}{L+1}$.*
2. *One can show that*

$$\langle y|\Pi_2 + \Pi_3|y\rangle \leq \cos^2 \varphi(\mathcal{K}_1, \mathcal{K}_2),$$

where $\mathcal{K}_1 = (\mathbb{C}^2)^{\otimes m} \otimes |0\rangle^{\otimes N-m}$ and $\mathcal{K}_2 = V^\dagger|1\rangle \otimes (\mathbb{C}^2)^{\otimes N-1}$. Use the fact that in the NO case, any proof is accepted by V with probability at most ϵ to conclude that

$$\langle y|\Pi_2 + \Pi_3|y\rangle \leq \frac{1}{L+1}(1 + \sqrt{\epsilon}).$$

Combining the results of the question above, we have that $\cos^2 \alpha(\mathcal{L}_1, \mathcal{L}_2) \leq 1 - ((1-\sqrt{\epsilon})/(L+1))$. Using the identities $\sin^2 x + \cos^2 x = 1$ and $\sin(2x) = 2 \sin x \cos x$, this yields

$$\sin^2 \frac{\alpha(\mathcal{L}_1, \mathcal{L}_2)}{2} \geq \frac{1}{4} \sin^2 \alpha(\mathcal{L}_1, \mathcal{L}_2) \geq \frac{1-\sqrt{\epsilon}}{4(L+1)}.$$

We conclude that in the NO case, the minimum eigenvalue of H scales as $\Omega((1-\sqrt{\epsilon})/L^3)$.

Question 11. *Recall that in the YES case, the smallest eigenvalue of H is upper bounded by $\epsilon/(L+1)$. Why do the eigenvalue bounds we have obtained in the YES and NO cases thus suffice to show that* 5-LH *is QMA-hard?*

Making H 5-local

We are almost done! The only remaining issue is that we would like H to be 5-local, but a binary representation of the $(L+1)$-dimensional clock register is unfortunately $\log(n)$-local. To alleviate this [KSV02], we switch to a *unary* representation of time. In other words, we now let H act on $(\mathbb{C}^2)^{\otimes m} \otimes (\mathbb{C}^2)^{\otimes N-m} \otimes (\mathbb{C}^2)^{\otimes L}$, where the counter register is now given in *unary*, i.e. $|j\rangle \in \mathbb{C}^{L+1}$ is represented as

$$|\underbrace{1, \ldots, 1}_{j}, 0, \ldots, 0\rangle. \qquad (21)$$

The operator basis $|i\rangle\langle j|$ for $\mathcal{L}(\mathbb{C}^{L+1})$ translates easily to this new representation (omitted here; see Reference [KSV02]). To enforce the clock register to indeed always be a valid representation of some time j in unary, we add a new fourth penalty term to H which acts only on the clock register, namely

$$H_{\mathrm{stab}} := I_{p,a} \otimes \sum_{j=1}^{L-1} |0\rangle\langle 0|_j \otimes |1\rangle\langle 1|_{j+1}. \qquad (22)$$

Hence, the new H is given by $H = H_{\mathrm{in}} + H_{\mathrm{prop}} + H_{\mathrm{out}} + H_{\mathrm{stab}}$. By using the fact that both $H_{\mathrm{in}} + H_{\mathrm{prop}} + H_{\mathrm{out}}$ and H_{stab} act invariantly on the original space the old H used to act on, it is a fairly straightforward exercise to verify that the analysis obtained above goes through for this new definition of H as well [KSV02]. We conclude that 5-LH is QMA-hard.

5.2 2-local Hamiltonian is QMA-complete

In [KSV02], Kitaev showed that the 5-local Hamiltonian problem is QMA-complete. In this section, we review Kitaev, Kempe, and Regev's perturbation theory proof that even 2-local Hamiltonian is QMA-hard [KKR06]. Note that Reference [KKR06] also provides an alternative "simpler" proof based on elementary linear algebra and the so-called *Projection Lemma* in the same paper; however, as the Projection Lemma can be derived via perturbation theory, and since Reference [KKR06]'s idea of using perturbation theory gadgets has since proven useful elsewhere in Hamiltonian complexity (e.g. [OT08]), we focus on the latter proof technique. Besides, perturbation theory is a standard tool in a physicist's toolbox, and our goal in this survey is to better understand what goes on in physicists' minds!

The proof that 2-local Hamiltonian is QMA-complete is quite complicated. To aid in its assimilation, we therefore begin with a high-level overview of how the pieces of the proof fit together.

Overview of the proof. To prove that 2-LH is QMA-hard, the approach is to show a Karp or mapping reduction from an arbitrary instance of 3-LH to 2-LH. To achieve this, given a 3-local Hamiltonian H acting on n qubits, we map it to a 2-local Hamiltonian $\widetilde{H}$ as follows.

- (Step 1: Rewrite H by isolating 3-local terms) Rewrite H in a form which resembles $Y - 6B_1B_2B_3$, where $B_1B_2B_3$ is shorthand for $B_1 \otimes B_2 \otimes B_3$, the B_i are one-local and positive semidefinite, and Y is a 2-local Hamiltonian.
- (Step 2: Construct $\widetilde{H}$) Define $\widetilde{H} = Q + P(Y, B_1, B_2, B_3)$, where P is an operator with small norm and which depends on Y, B_1, B_2, B_3, and where Q has large spectral gap and depends only on the spectral gap of H. We refer to P as the *perturbation* and $\widetilde{H}$ as the *perturbed Hamiltonian*.

This outlines the reduction itself. It now remains to outline the proof of correctness, i.e. to show that the 2-local Hamiltonian $\widetilde{H}$ reproduces the low energy spectrum of the input 3-local Hamiltonian H. In order to facilitate understanding, we present the analysis in a backwards fashion compared to the presentation in [KKR06].

- (Step 3: Define an effective Hamiltonian H_{eff}) We first define an *effective* 3-local Hamiltonian H_{eff} whose low-energy spectrum is (by inspection) identical to that of H. We will see next that $\widetilde{H}$ has been cleverly chosen to simulate H_{eff} with only 2-local interactions.
- (Step 4: Define the self-energy, $\Sigma_-(z)$) A standard tool in perturbation theory is an operator-valued function known as the *self-energy*, denoted $\Sigma_-(z)$, for $z \in \mathbb{C}$. In this step, we show that for an appropriate choice of z, we have $\| H_{\text{eff}} - \Sigma_-(z) \|_\infty \leq \epsilon$ for some small $\epsilon > 0$. Intuitively, this relationship will hold because H_{eff} is simply a truncated version of the series expansion of $\Sigma_-(z)$.
- (Step 5: Relate the low energy spectrum of $\Sigma_-(z)$ to that of $\widetilde{H}$) This step is where the actual perturbation theory analysis comes in. The outcome of this step will be that, assuming $\| H_{\text{eff}} - \Sigma_-(z) \|_\infty \leq \epsilon$, the jth smallest eigenvalue of H_{eff} is ϵ-close to the jth smallest eigenvalue of $\widetilde{H}$.

To recap, once we define the 2-local Hamiltonian $\widetilde{H}$, the spectral analysis we perform follows the chain of relationships:

$$H \approx H_{\text{eff}} \approx \Sigma_-(z) \approx \widetilde{H},$$

where here $\approx$ roughly indicates that the two operators in question share a similar ground space. We now discuss each of these steps in further detail.

5.2.1 Step 1: Rewrite H by isolating 3-local terms

Question 12. *Convince yourself that H can be rewritten, up to rescaling by a constant, in the form*

$$H \propto Y - 6 \sum_{i=1}^{M} B_{i1} \otimes B_{i2} \otimes B_{i3}, \tag{23}$$

where each B_{ij} is a one-local positive semidefinite operator and Y is a 2-local Hamiltonian whose operator norm is upper bounded by an inverse polynomial in n.

Hint 5. *Rewrite each local term of H in the local Pauli operator basis, i.e. as a linear combination of terms of the form $\sigma_1 \otimes \sigma_2 \otimes \sigma_3$ for $\sigma_i \in \{I, \sigma^x, \sigma^y, \sigma^z\}$. Then, for each such term involving Pauli operators, try to add 1-local multiples of the identity in order to obtain positive semidefinite terms $B_{i1} \otimes B_{i2} \otimes B_{i3}$. You will then have to subtract off certain terms to make up for this addition; these subtracted terms will form Y. Think about why Y must indeed be 2-local.*

5.2.2 Step 2: Construct $\widetilde{H}$

Using the decomposition of H in Equation (23), we can now construct our desired 2-local Hamiltonian, $\widetilde{H}$. As done in [KKR06], for simplicity, we assume that $M = 1$ in Equation (23), i.e. that $H = Y - 6B_1B_2B_3$. The extension to arbitrary M follows similarly [KKR06].

To construct $\widetilde{H}$, suppose $H \in \mathcal{L}((\mathbb{C}^2)^{\otimes n})$. Then, we introduce three auxilliary qubits and define $\widetilde{H} \in \mathcal{L}((\mathbb{C}^2)^{\otimes n} \otimes (\mathbb{C}^2)^{\otimes 3})$ as follows [KKR06].

$$\widetilde{H} := Q + P, \tag{24}$$

$$Q := -\frac{1}{4\delta^3} I \otimes (\sigma_1^z\sigma_2^z + \sigma_1^z\sigma_3^z + \sigma_2^z\sigma_3^z - 3I), \tag{25}$$

$$P := (Y + \frac{1}{\delta}(B_1^2 + B_2^2 + B_3^2)) \otimes I - \frac{1}{\delta^2}(B_1 \otimes \sigma_1^x + B_2 \otimes \sigma_2^x + B_3 \otimes \sigma_3^x), \tag{26}$$

where $\delta > 0$ is some small constant, and σ_j^i denotes the ith Pauli operator applied to qubit j. Notice that the "unperturbed" Hamiltonian Q contains no information about H itself, whereas the term that *does* contain the information about H, P, is thought of as the "perturbation". The reason for this is that Q is thought of as a *penalty term* with a large spectral gap (compared to $\| P \|_\infty$), so that intuitively, the ground space of $\widetilde{H}$ will be forced to be a subspace of the ground space of Q (since Q will enforce a large penalty on any vector not in this space).

Question 13. *Show that Q has eigenvalues 0 and $1/\delta^3$. Conclude that for "small" constant δ, Q has a "large" constant-sized spectral gap.*

Question 14. *Show that associated with the null space of Q is the space*

$$L_- = (\mathbb{C}^2)^{\otimes n} \otimes \mathit{Span}\left(|000\rangle, |111\rangle\right).$$

For simplicity, we henceforth define $C := \mathit{Span}\left(|000\rangle, |111\rangle\right)$. Conclude that we can think of C as a logical *qubit, and that we can define logical Pauli operators σ_C^i acting on C.*

5.2.3 Step 3: Define an effective Hamiltonian H_{eff}

Question 15. *Show that the effective Hamiltonian*

$$H_{\text{eff}} := Y \otimes I_C - 6B_1B_2B_3 \otimes \sigma_C^x \tag{27}$$

has the same ground state energy as $H = Y - 6B_1B_2B_3$. Conclude that it suffices to show that the ground state energy of H_{eff} approximates that of $\widetilde{H}$.

5.2.4 Step 4: Define the self-energy $\Sigma_-(z)$

Let $\delta > 0$ be a small constant. In this section, we define an operator-valued function $\Sigma_-(z)$, known as the self-energy, and show that for certain values of z, we have $\| H_{\text{eff}} - \Sigma_-(z) \|_\infty \in O(\delta)$. At a high-level, the claim follows by using the series expansion of $\Sigma_-(z)$ to observe that for appropriate z, one has $\Sigma_-(z) = H_{\text{eff}} + O(\delta)$.

Definition of $\Sigma_-(z)$. To begin, suppose $\widetilde{H} = Q + P$ acts on Hilbert space $\mathcal{H}$, for Q the unperturbed Hamiltonian and P the perturbation. Let $\lambda_* \in \mathbb{R}$ be some cutoff value. Then, let $\mathcal{L}_-$ ($\mathcal{L}_+$) denote the span of Q's eigenvectors with eigenvalue strictly less than λ_* (at least λ_*), and let Π_- (Π_+) denote the projector onto $\mathcal{L}_-$ ($\mathcal{L}_+$). For notational convenience, for any operator A, we define

$$\begin{aligned} A_+ &:= \Pi_+ A \Pi_+ \\ A_{+-} &:= \Pi_+ A \Pi_- \\ A_{-+} &:= \Pi_- A \Pi_+ \\ A_- &:= \Pi_- A \Pi_-. \end{aligned}$$

To define the self-energy operator $\Sigma_-(z)$, we now require the notion of the *resolvent* of an operator A, defined $R(z, A) := (zI - A)^{-1}$. Then, the self-energy is defined $\Sigma_-(z) := zI_- - R_-^{-1}(z, \widetilde{H})$. In this section, we use the fact [KKR06] that $\Sigma_-(z)$ has a simple and useful series expansion, given by

$$\Sigma_-(z) = Q_- + P_- + P_{-+} R_+ P_{+-} + P_{-+} R_+ P_{++} R_+ P_{+-} + P_{-+} R_+ P_+ R_+ P_+ R_+ P_{+-} + \cdots \quad (28)$$

$\Sigma_-(z)$ is close to H_{eff}. For our specific definition of $\widetilde{H}$, to show that $\Sigma_-(z)$ is close to H_{eff}, we simply show that H_{eff} is the series expansion of $\Sigma_-(z)$ up to the third order. Define $\Delta := 1/\delta^3$, and consider Equation (28).

Question 16. *We now compute the expression for $\Sigma_-(z)$ for $\widetilde{H}$. Recall that our goal is to show that the low order terms of $\Sigma_-(z)$ are precisely our desired effective Hamiltonian, H_{eff}.*

1. *Show that the zeroth order term of $\Sigma_-(z)$ is zero, i.e. $Q_- = 0$.*
2. *Show that $R_+ = (z - \Delta)^{-1} I_{\mathcal{L}_+}$.*
3. *Use parts 1 and 2 above to conclude that in our case,*

$$\Sigma_-(z) = P_- + \frac{1}{z - \Delta} P_{-+} P_{+-} + \frac{1}{(z - \Delta)^2} P_{-+} P_{++} P_{+-} + \frac{1}{(z - \Delta)^3} P_{-+} P_+ P_+ P_{+-} + \cdots \quad (29)$$

4. *Show that*

$$P_{-+} = -\frac{1}{\delta^2} \quad (\quad B_1 \otimes |000\rangle\langle 100| + B_2 \otimes |000\rangle\langle 010| + B_3 \otimes |000\rangle\langle 001| + \quad (30)$$

$$B_1 \otimes |111\rangle\langle 011| + B_2 \otimes |111\rangle\langle 101| + B_3 \otimes |111\rangle\langle 110|). \quad (31)$$

   Derive similar expressions for P_{+-}, P_-, and P_+.

5. *For ease of notation, define $X := (Y + \frac{1}{\delta}(B_1^2 + B_2^2 + B_3^2))$, and let I_C denote the projector onto space C from Question 14. Show that*

$$P_- = X \otimes I_C, \quad (32)$$

$$P_{-+} P_{+-} = \frac{1}{\delta^4}(B_1^2 + B_2^2 + B_3^2) \otimes I_C, \quad (33)$$

$$P_{-+} P_{++} P_{+-} = \frac{1}{\delta^4}(B_1 X B_1 + B_2 X B_2 + B_3 X B_3) \otimes I_C - \frac{6}{\delta^6} B_1 B_2 B_3 \otimes \sigma_C^x. \quad (34)$$

6. *By setting $z \ll \Delta$ a constant, show that $(z - \Delta)^{-1} = -\delta^3 + O(\delta^6)$.*
7. *Finally, using all parts above, show that, as desired,*

$$\Sigma_-(z) = Y \otimes I_C - 6 B_1 B_2 B_3 \otimes \sigma_C^x + O(\delta) = H_{\text{eff}} + O(\delta). \quad (35)$$

   Conclude that $\| H_{\text{eff}} - \Sigma_-(z) \|_\infty \in O(\delta)$.

5.2.5 Step 5: Relate the low energy spectrum of $\Sigma_-(z)$ to that of $\widetilde{H}$

In this section, we plug in Theorem 3 of [KKR06], which allows us to conclude that the small eigenvalues of $\Sigma_-(z)$ are close to the small eigenvalues of $\widetilde{H}$.

Theorem 4. *(Kitaev, Kempe, Regev [KKR06], Theorem 3) Let λ_* be the cutoff on the spectrum of Q, as before. Assume the eigenvalues of Q lie in the range $(-\infty, \lambda_* + \alpha/2] \cup [\lambda_* + \alpha/2, \infty)$ for some $\alpha \in \mathbb{R}$, and that $\| P \|_\infty < \alpha/2$. Fix arbitrary $\epsilon > 0$. Then, if there exists operator H_{eff} whose eigenvalues lie in the range $[c, d]$ for some $c < d < \lambda_* - \epsilon$, and such that $\| \Sigma_-(z) - H_{\text{eff}} \|_\infty \leq \epsilon$ for all $z \in [c - \epsilon, d + \epsilon]$, then the jth eigenvalue of $\widetilde{\Pi}_- \widetilde{H} \widetilde{\Pi}_-$ is ϵ-close to the jth eigenvalue of H_{eff}. Here, we assume eigenvalues are ordered for each operator in non-decreasing order, and we define $\widetilde{\Pi}_-$ as the projector onto the span of the eigenvectors of $\widetilde{H}$ of eigenvalue strictly less than λ_*.*

Question 17. *Apply Theorem 4 with $c = -\| H_{\text{eff}} \|_\infty$, $d = \| H_{\text{eff}} \|_\infty$, $\lambda_* = \Delta/2$ to complete the proof of correctness for the reduction.*

5.3 Commuting k-local Hamiltonians and the Structure Lemma

A natural case of the k-local Hamiltonian problem whose complexity remains open (for arbitrary k and local dimension d) is that of *commuting* local Hamiltonians, i.e. where the local constraints pairwise commute. This class of Hamiltonians is particularly interesting, in that it intuitively seems "closer" to the classical world of constraint satisfaction (in which all constraints are diagonal in the computational basis and hence commute), and yet such Hamiltonians are neverthess rich enough to give rise to highly entangled ground states, such as the Toric code Hamiltonian [Kit03]. The main complexity theoretic question in this area is to characterize the complexity of the problem for various values of k and d: Is it in NP? QCMA (i.e. QMA with a classical prover)? Or could it be QMA-complete?

To date, it is known that the commuting cases of 2-local Hamiltonian for $d \geq 2$ [BV05], 3-local Hamiltonian with $d = 2$ (as well as $d = 3$ with a "nearly Euclidean" interaction graph) [AE11], and 4-local Hamiltonian with $d = 2$ on a square lattice are in NP [Sch11b]. At the heart of these results is Bravyi and Vyalyi's *Structure Lemma* [BV05], which is a powerful tool for dissecting the structure of commuting local Hamiltonians. The primary focus of this section is to prove and discuss this lemma.

We remark that often the commuting k-LH problem is phrased with each local term being an orthogonal projection; this is without loss of generality, as since all terms simultaneously diagonalize, the ground state lies completely in some eigenspace of each constraint.

5.3.1 Statement of the Structure Lemma

Intuitively, the Structure Lemma says the following. Suppose we have two Hermitian operators $A \in \mathcal{H}(\mathcal{X} \otimes \mathcal{Y})$ and $B \in \mathcal{H}(\mathcal{Y} \otimes \mathcal{Z})$ for complex Euclidean spaces $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$, such that A and B commute. Then, the space $\mathcal{Y}$ can be sliced up in such a way, that if we focus on just one slice $\mathcal{Y}_i$ of the space (which is claimed by the NP prover to contain the ground state), then in this subspace A and B are completed *decoupled*. Specifically, the lemma says we can write $\mathcal{Y} = \bigoplus_i \mathcal{Y}_i$, such that if we restrict A and B to any one space $\mathcal{Y}_i$, the resulting operators can be seen to act on disjoint parts of the space $\mathcal{Y}_i$, hence eliminating their overlap. We now state the lemma more formally.

Lemma 2 (Structure Lemma [BV05])**.** *Suppose $A \in \mathcal{H}(\mathcal{X} \otimes \mathcal{Y})$ and $B \in \mathcal{H}(\mathcal{Y} \otimes \mathcal{Z})$ for complex Euclidean spaces $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$, and such that $[A, B] = 0$. Then, one can write $\mathcal{Y} = \bigoplus_i \mathcal{Y}_i$, such that for any i, the following two properties hold:*

1. *A and B act invariantly on $\mathcal{Y}_i$, and*
2. *$\mathcal{Y}_i = \mathcal{Y}_{i1} \otimes \mathcal{Y}_{i2}$ for some Hilbert spaces $\mathcal{Y}_{i1}$ and $\mathcal{Y}_{i2}$, such that $A|_{\mathcal{Y}_{i1}} \in \mathcal{H}(\mathcal{X} \otimes \mathcal{Y}_{i1})$ and $B|_{\mathcal{Y}_{i2}} \in \mathcal{H}(\mathcal{Y}_{i2} \otimes \mathcal{Z})$.*

The strength of the Structure Lemma in proofs placing variants of commuting Hamiltonian in NP is as follows. First, note that by property 1 above, when looking for the joint ground state $|\psi\rangle$ of A and B, we can safely restrict our attention to one appropriately chosen slice i. But which slice i does $|\psi\rangle$ live in? This is not obvious *a priori*; hence, we ask the

NP prover to send us the correct choice of i. Then, by restricting A and B to space $\mathcal{Y}_i$, by property 2 above the resulting Hamiltonians are decoupled. We can hence now easily diagonalize this system and determine the ground state energy, thus confirming whether it is indeed zero or bounded away from zero. Applying this idea repeatedly allows one to place the commuting 2-local Hamilltonian problem in NP.

5.3.2 Proof of the Structure Lemma

In this section, we prove the Structure Lemma. The proof cleverly uses basic C^* algebraic techniques. We remark that readers unfamiliar with C^* algebras should not be put off; the Structure Lemma is a powerful tool worth understanding, and to be clear, once the terminology barrier of the C^* formalism is overcome, the underlying proof is rather intuitive and simple. For this reason, we begin by defining the basic terminology required for the proof.

Algebra: Let A be a vector space over $\mathbb{C}$. Then A is an algebra if it is endowed with a bilinear operation $\cdot : A \times A \mapsto A$. In our setting, A will be some subset of linear operators taking $\mathbb{C}^k$ to itself, and $\cdot$ is simply matrix multiplication.

C* Algebra: To get a C^* algebra, we start with a Banach algebra A over $\mathbb{C}$, and add a $*$-operation which has the following properties:

1. For all $x \in A$, $x = (x^*)^* = x^{**}$.
2. For all $x, y \in A$, $(xy)^* = y^* x^*$ and $(x+y)^* = x^* + y^*$.
3. For all $c \in \mathbb{C}$ and $x \in A$, $(cx)^* = \overline{c} x^*$.
4. For all $x \in A$, $\| xx^* \| = \| x \|^2$.

In our setting, the $*$-operation is simply the conjugate transpose of a matrix.

Commutant: Let $S \subseteq \mathcal{L}\left(\mathbb{C}^k\right)$. Then, the commutant of S is defined as

$$S' := \left\{ x \in \mathcal{L}\left(\mathbb{C}^k\right) : xs = sx \text{ for all } s \in S \right\}.$$

A few facts about commutants come in handy: S' is a C^* algebra, $S \subseteq S^{''}$ (known as the closure of S), and $S^{'''} = S'$. Further, the following holds.

Lemma 3. *Let $A, B \subseteq \mathcal{L}\left(\mathbb{C}^k\right)$, and suppose for all $a \in A$ and $b \in B$, we have $ab = ba$. Then, for all $a \in A^{''}$ and $b \in B^{''}$, we have $ab = ba$.*

Proof. Observe that $B \subseteq A^{'}$. Thus, the elements in $A^{''}$ pair-wise commute with all elements of B, as well as those in $A^{'} \backslash B$. This implies $A^{''} \subseteq B^{'}$. But the elements of $B^{''}$ pairwise commute with those of $B^{'}$, which in turn implies they commute with the elements of $A^{''}$. □

Center: The center of algebra A is the set of all elements in A which commute with everyone else in A, i.e. $C(A) := A \cap A'$ (recall A' is the commutant of A). A *trivial* center is one which satisfies $C(A) = \{cI \mid c \in \mathbb{C}\}$.

A simple application of the definition of the center yields some very useful well-known properties for all $x \in A$, as stated in the following lemma.

Lemma 4. *Let A be a C^* algebra such that $A \subseteq \mathcal{L}(\mathcal{X})$ for complex Euclidean space $\mathcal{X}$. Suppose there exists $M \in C(A)$ with diagonalization $M = \sum_i \lambda_i \Pi_i$, where $\lambda \in \mathbb{R}$ and Π_i are (not necessarily one-dimensional) orthogonal projections. Then, any $N \in A$ has a block diagonal structure with respect to basis $\{\Pi_i\}$, i.e. can be written*

$$N = \bigoplus_i N_i$$

where N_i is an operator acting on the space Π_i projects onto.

Proof. We claim that it is true that for all i, $\Pi_i \in C(A)$; assuming this is true, the statement of the lemma holds simply because any $N \in A$ must now commute with each Π_i. To thus see that $\Pi_i \in C(A)$, note that if $M \in C(A)$, then for any polynomial p, $p(M) \in C(A)$. Then, defining for all j a polynomial p_j such that $p_j(\lambda_i) = \delta_{ij}$ completes the proof. □

Corollary 5. *If C^* algebra $A \subseteq \mathcal{L}(\mathcal{X})$ has a non-trivial center, then there exists a direct sum decomposition $\mathcal{X} = \bigoplus_i \mathcal{X}_i$ such that any $M \in A$ acts invariantly on each subspace $\mathcal{X}_i$.*

Proof of Structure Lemma. We can now proceed with the proof of the Structure Lemma (Lemma 2). As in the statement of the claim, let $A \in \mathcal{H}(\mathcal{X} \otimes \mathcal{Y})$ and $B \in \mathcal{H}(\mathcal{Y} \otimes \mathcal{Z})$ such that $[A, B] = 0$. For an appropriate choice of operators $\{A_{ij}\}, \{B_{kl}\} \subseteq \mathcal{L}(\mathcal{Y})$, one can write

$$A = \sum_{ij} |i\rangle\langle j|_{\mathcal{X}} \otimes (A_{ij})_{\mathcal{Y}} \otimes I_{\mathcal{Z}} \tag{36}$$

$$B = \sum_{kl} I_{\mathcal{X}} \otimes (B_{kl})_{\mathcal{Y}} \otimes |k\rangle\langle l|_{\mathcal{Z}}. \tag{37}$$

Question 18. *Use Equations (36) and (37) and the fact that $[A, B] = 0$ to conclude that for all i, j, k, l, we have $[A_{ij}, B_{kl}] = 0$.*

Consider now algebras $\widetilde{A}$ and $\widetilde{B}$ generated by $\{A_{ij}\}$ and $\{B_{kl}\}$, respectively, i.e. $\widetilde{A} = \{A_{ij}\}''$ and $\widetilde{B} = \{B_{kl}\}''$, whose elements pairwise commute by Lemma 3. Focusing first on $\widetilde{A}$, assume that $\widetilde{A}$ has non-trivial center. We reduce this case to one with trivial center, which can then be solved directly. Specifically, by Corollary 5, we can first decompose $\mathcal{Y} = \bigoplus_i \mathcal{Y}_i$ such that $\widetilde{A}$ acts invariantly on each $\mathcal{Y}_i$. In order to decouple A and B, recall that our goal is to split $\mathcal{Y}_i = \mathcal{Y}_{i1} \otimes \mathcal{Y}_{i2}$ such that A and B act non-trivially only on $\mathcal{Y}_{i1}$ and $\mathcal{Y}_{i2}$, respectively. To this end, let $\widetilde{A}_i$ denote $\widetilde{A}$ restricted to space $\mathcal{Y}_i$, and assume without loss of generality that the subalgebra $\widetilde{A}_i$ has trivial center (otherwise, we can decompose the space further). We now apply the following lemma.

Lemma 5 ([KLV00, BV05])**.** *Let $A \subseteq \mathcal{L}(\mathcal{Y})$ be a C^* algebra with trivial center. Then one can decompose $\mathcal{Y} = \mathcal{Y}_1 \otimes \mathcal{Y}_2$ such that $A = \mathcal{L}(\mathcal{Y}_1) \otimes I_{\mathcal{Y}_2}$.*

We hence obtain a decomposition $\mathcal{Y}_i = \mathcal{Y}_{i1} \otimes \mathcal{Y}_{i2}$ such that $\widetilde{A}_i$ acts non-trivially only on $\mathcal{Y}_{i1}$. In sum, we have thus far shown the following.

Observation 6. *The algebra $\widetilde{A}$ is precisely the set of all operators $W \in \mathcal{L}(\mathcal{Y})$ which can be written as $W = \bigoplus_i (W_i)_{\mathcal{Y}_i} = \bigoplus_i (W_i)_{\mathcal{Y}_{i1}} \otimes I_{\mathcal{Y}_{i2}}$.*

We now use Observation 6 to uncover the structure of $\widetilde{B}$.

Question 19. *For any $V \in \widetilde{B}$ and $\mathcal{Y}_i$ in the decomposition of $\mathcal{Y}$ above, show that V acts invariantly on $\mathcal{Y}_i$. Conclude that V can also be written as a direct sum over spaces $\mathcal{Y}_i$, i.e. that $V = \bigoplus_i (V_i)_{\mathcal{Y}_i}$. (Hint: Use the fact that all operators in $\widetilde{A}$ and $\widetilde{B}$ pairwise commute, and Observation 6.)*

Having answered Question 19, we can now let $\widetilde{B}_i$ denote $\widetilde{B}$ restricted to space $\mathcal{Y}_i$. The answer to the following question completes the proof.

Question 20. *Prove that any $V \in \widetilde{B}_i$ has the form $V = I_{\mathcal{Y}_{i1}} \otimes (V_i)_{\mathcal{Y}_{i2}}$. (Hint: Use the fact that all operators in $\widetilde{A}$ and $\widetilde{B}$ pairwise commute, and Observation 6.)*

5.4 Quantum 2-SAT is in P

In this section, we discuss Bravyi's polynomial time algorithm [Bra06] for the Quantum 2-SAT problem. To begin, recall that in k-SATISFIABILITY (k-SAT), one is given as input a set of k-local constraints $\{\Pi_i\}$ acting on subsets of k binary variables out of a total of n variables $x_1, \ldots, x_n$. Each clause has the form

$$\Pi_i = x_{i,1} \vee \cdots \vee x_{i,k},$$

where each $x_{i,j}$ is a *literal* corresponding to either a variable or its negation. The question is whether there exists an assignment to the variables $x_1, \ldots, x_n$ such that all Π_i evaluate to 1.

The study of k-SAT has a long and rich history, which we shall not attempt to survey here. However, as is well-known, SAT is historically the first problem to be proven NP-complete [Coo72, Lev73]. Further, its restricted version k-SAT remains NP-complete for

$k \geq 3$ [Kar72], but is polynomial-time solvable for $k = 2$ [Kro67, EIS76, APT79]. This raises the natural question: Can one define an appropriate quantum generalization of k-SAT, and could this generalization also lie in P when $k = 2$?

In 2006, Bravyi answered both these questions in the affirmative [Bra06]. Here, we define Quantum k-SAT as follows.

Definition 7 (Quantum 2-SAT (2-QSAT) [Bra06])**.** *Given a set of 2-local orthogonal projections $\{\Pi_{ij} \mid 1 \leq i, j, \leq n\}$ acting on n qubits, does there exist a satisfying quantum assignment, i.e. does there exist a state $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ such that $\Pi_{ij}|\psi\rangle = 0$ for all $1 \leq i, j, \leq n$?*

Note that unlike in SAT, which would correspond to rank 1 projections Π_{ij}, here the projections are allowed to be arbitrary rank. Thus, Bravyi's definition is more accurately a generalization of 2-CSP, where arbitrary Boolean 2-local constraints are allowed.

5.4.1 The algorithm

We now discuss Bravyi's algorithm for 2-QSAT. We remark that Bravyi's original exposition involved heavy use of tensors, which are perhaps not a typical tool in the computer scientist's toolkit. In contrast, we give a different description of the algorithm in terms of *local filters* [Gis96] from entanglement theory, which, in our opinion, is arguably more accessible to the quantum computing community.

To begin, Bravyi's algorithm consists of three subroutines (defined subsequently), and can be described at a high level as follows.

1. While there exists a constraint Π_{ij} of rank at least 2, run *rankReduction*(Π_{ij}). If the call fails, reject.
2. Run *generateConstraints*. If the call succeeds, return to Step 1.
3. Accept and return the output of *solveSaturatedSystem*.

Roughly, *rankReduction* outputs a 2-QSAT instance (on a possibly smaller number of qubits) in which all constraints are rank 1. Once all constraints are rank 1, *generateConstraints* attempts to add "new" constraints which are already implicit in the present constraint system in an attempt to "saturate" the system. If the call succeeds, we return to Step 1 to try to once again simplify the system. If, on the other hand, *generateConstraints* fails, then we have arrived at a "saturated" system of constraints [Bra06]. At this point, we conclude the system is satisfiable; indeed, *solveSaturatedSystem* outputs a satisfying assignment. We now discuss each of these three procedures briefly in greater detail.

rankReduction(Π_{ij})**.** Given a constraint Π_{ij} of rank at least 2, act as follows:

- If $\text{rank}(\Pi_{ij}) = 4$, return *fail*, as no assignment could satisfy this clause.
- If $\text{rank}(\Pi_{ij}) = 3$, the assignment to qubits i and j is forced to be $I - \Pi_{ij}$. Set this as their assignment and remove them from the system, updating any 2-local clauses acting on i or j as necessary.
- If $\text{rank}(\Pi_{ij}) = 2$, qubits i and j are allowed to live in a 2-dimensional subspace. Hence, combine i and j into a single merged qubit via an appropriate isometry. Update clauses acting on i or j as necessary.

generateConstraints. This subroutine examines all triples of qubits $\{a, b, c\}$ on which there exist clauses $\Pi_{ab} = |\phi\rangle\langle\phi|_{ab}$ and $\Pi_{bc} = |\phi\rangle\langle\phi|_{bc}$, and attempts to generate a new clause Π_{ac}.

To motivate the idea [Bra06], suppose $|\phi\rangle_{ab} = |\phi\rangle_{bc} = |\psi^-\rangle$, for $|\psi^-\rangle = |01\rangle - |10\rangle$ the singlet (we omit normalization for simplicity). Then, since for two qubits $I - |\psi^-\rangle\langle\psi^-|$ projects onto the symmetric space, it follows that any assignment $|\psi\rangle$ must live in the symmetric space on qubits $\{a, b\}$ and $\{b, c\}$, and hence also on $\{a, c\}$. Thus, we can safely add the new (implicit) constraint $\Pi_{ac} = |\phi\rangle\langle\phi|_{ac}$.

Now, what if (say) $|\phi\rangle_{ab}$ is not the singlet? Here, we use the fact that any pure state on two qubits can be produced from the singlet via a *local filter* [Gis96]. Specifically, there exist linear operators $A, C \in \mathcal{L}\left(\mathbb{C}^2\right)$ such that

$$|\phi\rangle_{ab} = A_a \otimes I_b |\psi^-\rangle_{ab} \qquad \text{and} \qquad |\phi\rangle_{bc} = I_b \otimes C_c |\psi^-\rangle_{bc}. \tag{38}$$

Note that while local filters were originally introduced to *increase* the entanglement of a previously entangled state [Gis96] (in which case the filter must be invertible, as otherwise one can create entanglement via a local operation from a product state), in this setting, we are *reducing* entanglement using a filter; thus, A and C in general will not be invertible. The following is our analogue of Lemma 1 in Reference [Bra06].

Lemma 6. *For $|\phi\rangle_{ab}$ and $|\phi\rangle_{bc}$ as in Equation (38), suppose $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ satisfies $\langle\psi|\phi_{ab}\rangle = \langle\psi|\phi_{bc}\rangle = 0$. Then, the constraint $|\phi\rangle_{ac} = A_a \otimes C_c|\psi^-\rangle$ on $\{a, c\}$ satisfies $\langle\psi|\phi_{ac}\rangle = 0$.*

Proof. Suppose for assignment $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ that

$$\langle\psi|\phi_{ab}\rangle = \langle\psi|A_a \otimes I_b|\psi^-\rangle_{ab} = 0.$$

This implies that $A_a^\dagger \otimes I_b|\psi\rangle$ lives in the symmetric subspace on qubits a and b. An analogous argument implies that $I_b \otimes C_c^\dagger|\psi\rangle$ lives in the symmetric subspace on b and c. It follows that $A_a^\dagger \otimes C_c^\dagger|\psi\rangle$ lives in the symmetric subspace of both $\{a, b\}$ and $\{b, c\}$, and hence also of $\{a, c\}$. Thus, $\langle\psi|\phi_{ac}\rangle = \langle\psi|A_a \otimes C_c|\psi^-\rangle = 0$, as desired. □

Remark. For the reader interested in comparing Lemma 6 above directly with Lemma 1 of Reference [Bra06], the correspondence is given by $A = \phi\epsilon^\dagger$ and $C = \theta^T\epsilon$. This is easily seen by using the vec mapping [Wat08] (where roughly, vec "reshuffles" matrices into vectors) and its property that $A \otimes B\,\mathrm{vec}(X) = \mathrm{vec}(AXB^T)$.

In sum, *generateConstraints* applies Lemma 6 on triples of qubits until it generates a new clause on some pair of qubits $\{a, c\}$ which is linearly independent from existing clauses on $\{a, c\}$. If no such clause is found, the subroutine returns *fail*.

solveSaturatedSystem. A *saturated* system of constraints is one in which (1) all constraints are rank 1, and (2) for any triple of qubits $\{a, b, c\}$, Lemma 6 fails to produce a new linearly independent constraint on $\{a, c\}$. We now give our analogue of Lemma 2 of Reference [Bra06].

Lemma 7. *For any saturated system of constraints $\{\Pi_{ij}\}$, there exists an efficiently computable product state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$ with $|\psi_i\rangle \in \mathbb{C}^2$ such that $\Pi_{ij}|\psi\rangle = 0$ for all i, j.*

In order to prove Lemma 7, we first require the following.

Lemma 8. *Let $E := iY$ for Pauli operator Y. Then, for any $A \in \mathcal{L}\left(\mathbb{C}^2\right)$,*

$$A \otimes I|\psi^-\rangle = I \otimes E^\dagger A^T E|\psi^-\rangle.$$

Proof. Let $|\phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. Then,

$$A \otimes I|\psi^-\rangle = (I \otimes E^\dagger)(A \otimes E)|\psi^-\rangle = (I \otimes E^\dagger)(I \otimes A^T)|\phi^+\rangle = I \otimes E^\dagger A^T E|\psi^-\rangle,$$

where the first equality follows since $E^\dagger E = I$, the second since $I \otimes E|\psi^-\rangle = |\phi^+\rangle$ and $A \otimes I|\phi^+\rangle = I \otimes A^T|\phi^+\rangle$, and the third again since $I \otimes E|\psi^-\rangle = |\phi^+\rangle$. □

Proof of Lemma 7. We give a simple deterministic polynomial time algorithm which outputs $|\psi\rangle$. Pick an arbitrary qubit, q_1, and set its assignment to $|0\rangle$, i.e. set $|\psi_1\rangle = |0\rangle$. Now consider the neighbor set of q_1, denoted $N(q_1)$. For any $q_i \in N(q_1)$, suppose the forbidden space is spanned by $|\phi_{1,i}\rangle$. Then, observing that $|\phi_i\rangle := \langle\psi_1|\phi_{1,i}\rangle \in \mathbb{C}^2$ and that $\langle v|E\overline{|v\rangle} = 0$ for any $|v\rangle \in \mathbb{C}^2$ and where $\overline{|v\rangle}$ denotes the entry-wise complex conjugate of $|v\rangle$, it follows that $\langle\phi_{1,i}|(|\psi_1\rangle \otimes E\overline{|\phi_i\rangle}) = 0$. Thus, setting $|\psi_i\rangle = E\overline{|\phi_i\rangle}$ satisfies all clauses between q_1 and its neighbors. Moreover, by Lemma 6, we immediately have that any clause between distinct qubits $q_i, q_j \in N(q_1)$ is also satisfied by this assignment.

Let S denote the set of qubits whose shortest path from q_1 is precisely 2 in the interaction graph, i.e. $S = N(N(q_1))\backslash(N(q_1) \cup \{q_1\})$. If we can now show that for all $q_i \in N(q_1)$ and $q_j \in S$, the clause $|\phi_{i,j}\rangle$ is satisfied by the current assignment regardless of the assignment on q_j, then note that the proof is complete, as we can simply iterate the argument above by discarding all clauses which act on qubits in $\{q_1 \cup N(q_1)\}$ and choosing a new starting vertex $q_j \in S$.

Thus, we now prove that for all $q_i \in N(q_1)$ and $q_j \in S$, $\langle \phi_{i,j} | \psi_i \rangle = 0$. Let the clauses on $(1,i)$ and (i,j) be given by

$$|\phi_{1,i}\rangle = A_1 \otimes I_i |\psi^-\rangle \qquad \text{and} \qquad |\phi_{i,j}\rangle = I_i \otimes C_j |\psi^-\rangle.$$

Then, analogous to Reference [Bra06], the key observation is that since $(1,j)$ is not an edge, then by Lemma 6, we must have $A \otimes C |\psi^-\rangle = 0$. This, along with Lemma 8, together imply:

$$\begin{aligned}
\langle \phi_{i,j} | \psi_i \rangle &= (\langle \psi^- | I_i \otimes C_j^\dagger)((\overline{\langle \psi_1 |} \otimes E_i)\overline{|\phi_{1,i}\rangle}) \\
&= (\langle \psi^- | I_i \otimes C_j^\dagger)((\overline{\langle \psi_1 |} \otimes E_i)(\overline{A}_1 \otimes I_i |\psi^-\rangle)) \\
&= (\langle \psi^- | I_i \otimes C_j^\dagger)((\overline{\langle \psi_1 |} \otimes E_i)(I_1 \otimes E_i^\dagger A_i^\dagger E_i |\psi^-\rangle)) \\
&= (\langle \psi^- | A_i^\dagger \otimes C_j^\dagger)(\overline{\langle \psi_1 |} \otimes E_i)|\psi^-\rangle \\
&= 0.
\end{aligned}$$

□

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