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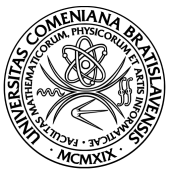

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Local Hamiltonians and their Ground States: Computation, Proofs & Entanglement

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Abstract

Quantum Hamiltonian Complexity is a field on the boundary of Condensed matter physics and Theoretical computer science. Condensed matter physics provides and motivates the relevant models and Computational complexity theory and Quantum information processing bring us powerful tools and new vantage points to study them. Bringing these together, our goal is to study, understand, and classify both the difficulty of computing and the structure of global properties of physical systems described by models with local interactions. The central topics are local Hamiltonians, their ground states, and their properties — for example determining the ground state energy as in the local Hamiltonian problem. In this thesis, we study where the intrinsic complexity of local Hamiltonians and their ground states comes from. We then explore its limitations, as a slight change of parameters can possibly make a simple looking system difficult to deal with computationally. We focus on the properties of these difficult instances, types of quantum (ground) states that can serve as proofs, and scaling of entanglement in ground states.

First, focusing on the QMA-complete instances (believed to be intractable even for quantum computers) of the local Hamiltonian problem, we improve its precision parameter. Studying the hard constructions further, we provide an efficient way to achieve a higher overlap with the desired states for QMA-complete constructions as well as for the dynamic Feynman-like Hamiltonian Computer.

Second, exploring what one can verify from classical and quantum witness states, we find a way how to shorten long classical witnesses for the quantum, naturally QCMA-complete Ground state connectivity problem, provided we have two copies of quantum witnesses. The price we pay is a polynomial decrease in the completeness-soundness gap. This result is inspired by shorter unentangled proofs for classical NP-complete problems.

Third, we study what is the possible amount of entanglement for ground states of translationally invariant spin chains with low local qudit dimension. Exploring the relationship between the spectral gap and entanglement entropy and spin chain parameters, we find that our exactly solvable Pair-flip model achieves a power law area law violation for a qutrit (spin-1) chain with an inverse polynomial gap. We build our construction on formal languages and intriguing combinatorial structures.

Keywords: computational complexity, quantum computation, Hamiltonian complexity, local Hamiltonians, ground state complexity

Abstrakt

Zložitosť Kvantových Hamiltoniánov je výskumná oblasť na hraniciach fyziky tuhých látok a teoretickej informatiky. Fyzika tuhých látok nám dodáva a motivuje podstatné modely, zatiaľ čo teória výpočtovej zložitosti a spracovanie kvantovej informácie prinášajú silné nástroje a nové pohľady na ich štúdium. Spájajúc ich, naším cieľom je skúmať, porozumieť, a klasifikovať zložitosť výpočtov a štruktúr globálnych vlastností fyzikálnych systémov popísaných modelmi s lokálnymi interakciami. Centrálnymi témami sú lokálne Hamiltoniány a vlastnosti ich základ-ných stavov, napríklad určenie základnej energie vo výpočtovej úlohe nazvanej Lokálny Hamiltonián. V tejto práci študujeme, odkiaľ sa berie prirodzená zložitosť lokálnych Hamiltoniánov a ich základných stavov. Skúmame limity tejto zložitosti, keďže aj malá zmena parametrov môže zmeniť jednoducho vyzerajúci systém na taký, ktorý je ťažko výpočtovo zvládnuteľný. Zameriavame sa na vlastnosti týchto ťažkých prípadov, typy kvantových (základných) stavov, ktoré môžu slúžiť ako dôkazy, a nakoniec škálovanie previazania v základných stavoch.

Najprv sa zameriame na QMA-úplné prípady (výpočtovo pravdepodobne nezvládnuteľné aj pre kvantové počítače) varianty úlohy Lokálny Hamiltonián a vylepšíme jej parameter presnosti. Ďalším štúdiom výpočtovo ťažkých QMA-úplných konštrukcií ponúkneme efektívny spôsob zvýšenia prekryvu s cieľovými stavmi, ako aj pre dynamickú verziu s kvantovým počítaním s Hamiltoniánmi podobnými tomu Feynmanovmu.

Druhá skupina výsledkov vychádza zo skúmania, čo sa dá overiť pomocou klasických a kvantových stavov – dôkazov. Nájdeme spôsob, akým skrátiť dlhé klasické dôkazy pre kvantovú, prirodzene QCMA-úplnú úlohu Prepojenia priestoru základných stavov (Ground state connectivity), pomocou dvoch nepreviazaných kópií kvantových dôkazov. Cena, ktorú za to zaplatíme je polynomiálne zmenšenie medzery medzi úplnosťou a bezpečnosťou úlohy. Tento výsledok je inšpirova-ný krátkymi nepreviazanými kvantovými dôkazmi pre klasické NP-úplné úlohy.

Nakoniec študujeme, koľko previazania je možné nájsť v základných stavoch translačne invariantných spinových reťazcov s malou lokálnou dimenziou. Skúmajúc vzťah medzi spektrálnou medzerou, entropiou previazania a parametrami spinových reťazcov, ukážeme, že náš presne riešiteľný Pair-flip model preukazuje mocninové narušenie zákona plochy pre reťazec qutritov (spin-1) s inverzne polynomiálnym škálovaním medzery v spektre. Naša konštrukcia je založená na formálnych jazykoch a zaujímavých kombinatoriálnych štruktúrach.

Kľúčové slová: výpočtová zložitosť, kvantové počítanie, zložitosť Hamiltoniánov, lokálne Hamiltoniány, zložitosť základných stavov

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Introduction & Goals

The advent of the digital information age brought along not only enormous progress in what we can calculate and simulate, but also deep questions about computational complexity. What computational tasks are treatable with our limited computing ability? If we can't manage them ourselves, is there possibly a way to at least verify the correctness of received data or proofs? How do these computational problems relate to the real, physical world? How does adding quantum mechanics into the range of questions, but also possible computation treatments change the situation? Nature is quantum, and so is information [8] — and its processing should be too. Already Feynman envisioned the importance of quantum computing for simulations of quantum mechanical systems [19] in the following words:

> "Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." — R.P. Feynman

Without this, we are too often severely limited by the exponential scaling requirements of dealing with systems with ever-increasing size. There has been remarkable progress [51] in methods of quantum simulation since Lloyd's proof [35]. Still, even quantum

computation [40, 1] has its limits in calculating the properties of physical systems. In this work, we study these limits and powers, focusing on local Hamiltonians and their ground states. We will showcase their potential for computation, as well as the complexity of their properties.

The goal of the thesis (as stated in the assignment) is: "... to better understand and characterize where this complexity comes from, and what its limits are – when a change of parameters can turn simple problems about ground state preparation into difficult ones, the possibilities of using this complexity in proof systems, and to investigate the complexity of correlations and entanglement in ground states of simple spin systems, especially frustration-free ones."

We fulfill these aims by analyzing a set of local Hamiltonian constructions, working out and understanding the rich structure of their ground (and low-energy) states as well as the intricacies of unitary evolution with these Hamiltonians.

1 Local Hamiltonians and their Ground States

Quantum Hamiltonian complexity [20, 42, 51] is an intriguing field drawing from both many-body physics and theoretical computer science. Many-body physics provides models, while computational complexity theory and quantum information processing provide tools to study them. The main questions of quantum Hamiltonian complexity are:

How difficult is to compute the properties of quantum many body systems? Can we compute them efficiently now, or only if we had a suitable quantum computer, or are there some fundamental limitations? How "complex" can the ground state or low-energy states be? How do simulations of these physical systems scale with their system size?

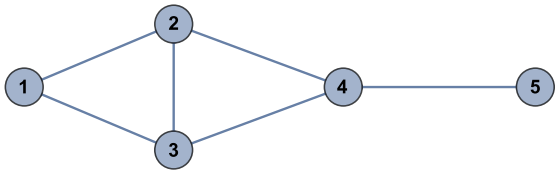
Condensed matter physics studies emergent properties of matter in its condensed phase, when the number of constituents is immense and the interactions between them are substantial, such as in the solid or liquid phases. They can possibly be described by huge systems of coupled differential equations coming from their microscopic properties. To study their properties, they are usually simplified by *models* derived from microscopic properties or phenomenologically, based on experimental observations. They typically have a finite range, but sometimes also interactions decaying over long distances. The primary purpose of these models is derivation or calculation of *global out of local properties* of their constituents and the interactions between them.

In quantum physics, we describe such systems by Hamiltonians. The Hamiltonian is the energy operator of the system and by a postulate of quantum mechanics specifies an infinitesimal time evolution via the Schrödinger equation. To study a system and its properties, the *eigenstates (eigenvectors)* of the Hamiltonians and their *energies*

(eigenvalues) are particularly interesting. The quantum nature: "states as superpositions, unitary dynamics, entanglement and correlations" of such systems are manifested at zero (or close to zero) temperature. Low energy states are interesting from the viewpoint of optimization while they can also exhibit unexpected properties like topological order, quantum Hall effect, superconductivity, superfluidity, and so on.

In this work we consider time independent spin Hamiltonians with local interactions. Local for us basically means few-body, and when the particles sit on a lattice, it also means geometrically local. A few simple examples are [47]: quantum Ising or Heisenberg models in a transverse field used to study magnetic properties of matter. A more complicated example is the Hubbard model, for studying metallic and non-metallic properties of matter. In general, the models are sums of local interacting terms $H = \sum_j H_j$, where each H_j is a Hermitian term acting nontrivially on at most a constant k number of sites (qudits), and we call them *k-local Hamiltonians* [30].

There is an interesting connection between local Hamiltonians and canonical problems from computer science. To give an example, consider a *classical* antiferromagnetic spin Hamiltonian on the following interaction graph:



Thanks to the antiferromagnetic interaction, the states with low energy tend to have interacting spins oriented in opposite directions. In general, the question about the ground state and its energy is in fact identical to the question about what is the best configuration of spins satisfying the most local constraints given by the interactions, i.e. optimizing a *global* property over *local* constraints. In the given example we cannot satisfy all the constraints at the same time, since it contains a cycle of length 3, where at least one of the constraints will always be unsatisfied; altogether, we can satisfy at most all but one constraint. This type of frustration and dificulties in deciding what is the best way to go can be found between some canonical problems from complexity theory such as satisfiability, constraint satisfaction, or MAX-SAT. There, we also ask whether one can fulfill a set of local constraints (or in its optimization variant: what is the maximum number of them we can fulfill). In general, we do not know an efficient algorithm for those problems, and the best what one can do so far (up to some heuristics) is to try all possible configurations. However, we do not have a mathematical proof that an exhaustive search is necessary.

On the other hand, such problems in computational complexity share the following property. Someone *(the prover)* could claim that the ground state energy is below some threshold and he knows the ground state. He could demonstrate this to us by giving us the ground state. In this example, it would be the best configuration of spins, and

we would simply plug this *witness* into the Hamiltonian and easily *verify* the energy. Furthermore, some of these problems share the intrinsic difficulty of all such problems. The situation gets even more exciting if one considers quantum Hamiltonians and a quantum setting, where we have problems that can be verified in this way on a quantum computer, given a quantum or a classical witness, tightly related to the structure of ground states.

In complexity theory [46], we usually simplify the questions to *decision problems* — yes/no questions (or *promise problems* with some promise on both yes and no answers). The quintessential problem of quantum Hamiltonian complexity is to consider a k-local Hamiltonian and attempt to determine its ground state energy:

(The k-local Hamiltonian (LH) problem [30], k-LH) Given a k-local Hamiltonian H over n qudits (system size) and parameters a, b, such that *the promise gap*: $b - a$ is at least an inverse polynomial in n. Decide which is the case:

"yes" there exists a state $|\psi\rangle$, with a "low" energy $\langle\psi|H|\psi\rangle \leq a$, or

"no" all possible states have a "high" expected energy $\langle\psi|H|\psi\rangle \geq b$.

Complexity theory then asks how do the *resources* — the number of (easy to implement) steps of an algorithm solving a problem *scale asymptotically with the size* of its input in the *worse-case* scenario. Complexity theory classifies problems into *complexity classes* that coarse-grain the asymptotic properties and studies relationships between these classes. The most important for quantum Hamiltonian complexity are the classes of "efficiently" solvable problems and of problems whose solutions we can at least "efficiently verify". Let us begin with the former ones:

P **— efficiently solvable on a classical computer** — the number of steps scales polynomially with the input size. For example, determining whether a 2-local Hamiltonian with qubits is frustration-free (there exists a ground state that is a common ground state of each of the local terms) [10], or finding a ground state of a gapped quantum Hamiltonian on a line [33].

BQP **— efficiently solvable on a quantum computer.** Other problems would be easy for universal quantum computers — the number of steps or gates scale polynomially. For some of them, we do not know an efficient classical algorithm, such as a simulation of a quantum system evolved by a Hamiltonian [35, 19].

Next, we have the classes of problems, whose solutions can be at least efficiently verified:

NP **— when the "yes" answer can be efficiently verified on a classical computer.** For some properties, we do not know an efficient algorithm, neither a classical nor a quantum one. Is it so that only we did not succeed in finding one, or is there a fundamental difficulty in them? For some problems, if someone gives us *a proof or a witness*

of the "yes" answer, we can at least verify it in a polynomial time (efficiently). We call the class of such problems NP. Moreover, some of those problems were proven to be *the hardest* within this class and we call them NP-complete. Any problem in this complexity class can be efficiently *reduced* (in polynomial time) to them. They come from many areas (e.g. optimization or condensed-matter physics). For such problems we do not know an efficient algorithm; we do not have a proof that one day someone will not find one. Still, these problems are widely believed to be "intractable". They include tasks such as calculating the partition function or the ground state energy of a 3D Ising spin glass [6], used to study properties of magnetic alloys with impurities. Furthermore, we call a problem NP-hard whenever it is at least as hard as the hardest problem within NP; an NP-hard problem does not have to belong to this complexity class.

Building on the NP complexity class, hardness, completeness, and polynomial time reductions, let us look at their quantum analogs.

QMA, QCMA — when the "yes" answer can be efficiently verified on a quantum computer. Other problems have an efficient quantum verifier (using a quantum computation), for either a quantum or a classical proof, QMA and QCMA, respectively. Examples of QMA-complete problems (the hardest within this complexity class) are: the 2D local Hamiltonian problem with qubits [41] or 1D LH with qudits of dimension $d \geq 8$ [25]. An example of a QCMA-complete problem is the local Hamiltonian problem with low-complexity (efficiently preparable) low-energy states [50]. Another is the ground state connectivity problem [21] (even with a Hamiltonian having commuting terms [22]) about the possibilities of ground space traversal, which we describe in Section 3.

As usual in complexity theory, we do not have a proof showing those complexity classes are separated or equal (such results are quite rare); the trivial containments are[1] $\mathsf{P} \subseteq \mathsf{NP} \subseteq \mathsf{PSPACE}$ and $\mathsf{P} \subseteq \mathsf{BQP} \subseteq \mathsf{QCMA} \subseteq \mathsf{QMA} \subseteq \mathsf{PSPACE}$. Moreover, the question $\mathsf{P} \stackrel{?}{=} \mathsf{NP}$ is a deep unanswered question of theoretical computer science [2], related to the existence of efficient cooling procedures for reaching the global energy minimum in physical systems.

The structure of the ground states is important for the complexity of local Hamiltonians. By a simple counting argument, there are way more quantum states then local Hamiltonians. *We can thus ask: Do ground states lay in some "physical corner" of the whole Hilbert space, possibly with some special structure? Can they be prepared efficiently?* We mentioned that the k-LH problem with low-complexity low-energy states is QCMA-complete. The related question to the structure of states is the $\mathsf{QCMA} \stackrel{?}{=} \mathsf{QMA}$ open question — are quantum witnesses more powerful then classical ones? Moreover, in 1D, the structure of ground states and the amount of entanglement (measured as entanglement entropy) greatly varies with the complexity of the local Hamiltonian problem. The basic gapped systems provably obey an *area law* [27] limiting the amount of

[1] PSPACE contains problems solved on a classical computer using polynomial amount of memory.

entanglement entropy scaling with the boundary of the cut region, and are solvable in P [33], However, without this restriction on the gap, we quickly see behavior ranging from NP-complete [45] to QMA-complete [25] ones. We showcase the range of complexity in the problems we consider in this thesis.

2 Clock constructions in Kitaev's Hamiltonian and Feynman's computer

Kitaev's QMA-hardness circuit-to-Hamiltonian construction for the 5-local Hamiltonian problem [30] reduces any QMA verifier (a quantum circuit checking if a witness is acceptable) to a problem in physics (determine the ground state energy for a system). This proof established the inherent difficulty of the 5-LH problem, i.e. any problem in QMA complexity class can be efficiently (in polynomial time) reduced to it (a quantum analogue of the Cook-Levin theorem [46]). In the "yes" case, the whole progress of an accepting verification $|\varphi_0\rangle, U_1|\varphi_0\rangle, U_2U_1|\varphi_0\rangle, \ldots, U_N\cdots U_1|\varphi_0\rangle$ is encoded in the ground state of the constructed Hamiltonian called the *history state*. It is the uniform superposition of its steps labeled by ticks of a clock (in the 5-local construction realized by a domain wall progression):

$$|\Psi_{\text{history}}\rangle = \frac{1}{\sqrt{N+1}} \sum_{t=0}^{N} |t\rangle_{\text{clock}} \otimes (U_t U_{t-1} \ldots U_1 |\varphi_0\rangle)_{\text{data}}.$$

Notice that we cannot simply design a local Hamiltonian that would give a high energy penalty to an improper sequence of progression given by a list of its states, since each local term in a Hamiltonian "sees" only a constant cut of the whole state and is not directly sensitive to "global correlations"[2][4, 5]. We call such an encoding *static* — a computation is "statically" stored in the ground state.

This construction was inspired [30] by Feynman's Hamiltonian computer [19] performing a quantum computation (a unitary evolution) by a time independent Hamiltonian. Feynman [19] realized that finding a Hamiltonian implementing a composition of elementary quantum gates $U_N \ldots U_1$ on a system at some particular time T appears to be difficult (i.e. finding H such that $U_N \ldots U_1 = e^{iHT}$ for possibly noncommuting $U_1, \ldots, U_N$). However, adding a *clock* system with a program step counter can solve this issue — combining a Hamiltonian acting on the *data* together with a *clock* register.

For instance, Feynman suggested to use a *pointer* particle (a cursor), like an electron moving between $N+1$ holes on a line, indicating time progression from 0 to N. If a site t is occupied by the electron and it then moves to the position $t+1$, the U_{t+1} gate is

[2]To see this consider two states $1/\sqrt{2}(|0\ldots0\rangle \pm |1\ldots1\rangle)$ one can be obtained from the other by application of Pauli Z gate on one of its qubits, however they have the same reduced density matrices on all but one qubits [4].

applied on the data subsystem. At the beginning, the data subsystem is initialized with the input state $|\varphi\rangle$ and there is a single clock cursor at position 0. If we let the system evolve for a sufficiently long time and measure the clock subsystem at position N, which happens with an average probability $\Theta(N^{-1})$, the data subsystem collapses to the state $U_N \dots U_1|\varphi\rangle$, the desired final state of the computation. Moreover, the computation can be implemented locally by Feynman's Hamiltonian. We call such constructions *dynamic* — a computation is "dynamically" performed by the unitary evolution generated by the (time-independent) Hamiltonian.

The details of how the clock is implemented is a crucial component of both circuit-to-Hamiltonian constructions and Feynman's Hamiltonian computer. Here, we present a collection of our results about clock constructions, tied together by quantum walk techniques. *In particular, we are interested in precision requirements for the local Hamiltonian problem and the overlap with states that contain the finished computation in the data register (or the success rate of finding the computation done for the dynamic construction).* We improve the analysis of precision requirements — the promise gap — for Kitaev's circuit-to-Hamiltonian construction. Second, we increase the number of clock states for which the computation is done. There, the construction does not involve the data register and simply "idles the engine". We do this in a surprisingly spatially efficient way with a tunable success rate for both static and dynamic constructions. First, we present an *idling chain* suitable for static construction with a logarithmic number of idling qubits and then a *multi-cog clock* approach, a less effective (but still with a sublinear number of qubits) usable for the dynamic construction. Finally, we showed how to use the pulse clock variant (from Feynman's Hamiltonian for the dynamic version) in the static construction and improve bounds on its spectral gap. This section is based on our article [12].

2.1 A new promise gap bound for Kitaev's QMA-complete local Hamiltonian

We prove that it is QMA-hard to determine whether the 3-local Hamiltonian problem has a ground state with energy below E_{yes}, or all its eigenstates have energy above E_{no}, already for $E_{\text{no}} - E_{\text{yes}} = O(N^{-2})$. This is an improvement from $O(N^{-3})$ of [30, 38]. Furthermore, this improvement applies also for 4-local frustration-free case of [10]. We achieve this result by carefully analyzing the soundness part of Kitaev's QMA-hardness circuit-to-Hamiltonian construction for the 5-local Hamiltonian problem.

First we build a toolbox by analyzing continuous time quantum walks with tunable end-point self-loops. Relying on Jordan's lemma, we characterize the dynamics of the terms in Kitaev's Hamiltonian. This lemma says that we can look at them in 1D and 2D invariant subspaces. There, the relevant actions reduce to a quantum walk with one end self-loop, or (in 2D) two walks on a line connected by a perturbation, see Fig. 1. A similar result was obtained simultaneously, using a different technique, by Bausch and Crosson [7].

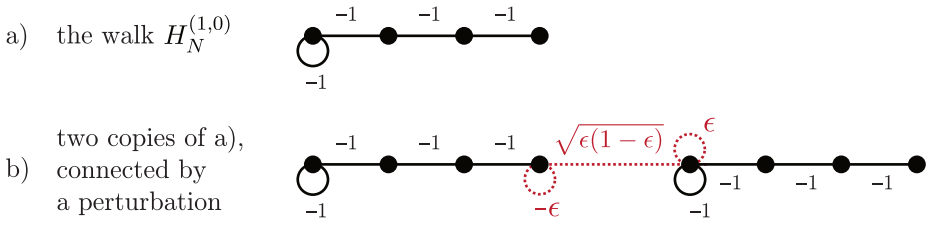


Fig. 1: The special cases of walks with endpoint projectors appearing in the proof of the promise gap lower bound a) in 1D invariant subspaces, and b) in the 2D invariant subspaces.

2.2 Doing nothing (efficiently) can improve a computation

Could one increase the overlap of the ground state with the finished computation for Kitaev's Hamiltonian (i.e. in the history state) or achieve a high success probability for finding the computation done for Feynman's Hamiltonian computer? A straightforward approach to achieve this is to extend the quantum circuit with N gates to $N + A$ gates, choosing to "do nothing" with the data for A steps at the end of the computation. The fraction of states with the computation done would then be $\frac{1+A}{N+1+A}$.

We found two ways how to achieve a tunable (high) success rate much more efficiently, in terms of the number of required extra clock qubits. 1) *The Idling chain* — suitable for the static (complexity theory) constructions, with only logarithmic (in original clock qubit number) extra idling qubits; 2) *The Multicog Clock construction* — suitable for dynamic constructions (i.e. actually building a computer), using square root extra qubits.

The Idling chain This construction extends the original unary clock in Kitaev's Hamiltonian (a progression of states with a single domain wall). For 4 clock steps, the domain wall progression would read: $|10000\rangle, |11000\rangle, |11100\rangle, |11110\rangle$. We start with the unary clock of length N, and introduce C *extra* unary clock qubits. Below these, we add another row of C *idling* qubits that are active only if the clock part reached them and then they can be both 0 or 1, i.e.

$$\begin{array}{c|ccccc} 1\cdots 1 & 1 & \cdots & 1 & 0\cdots 0 \\ \hline & 0/1 & \cdots & 0/1 & 0\cdots 0 \end{array} . \tag{1}$$

This creates a huge number, exponential in C, of idling states connected by possible clock progressions, illustrated in Fig. 2. The construction is designed such that the ground state of the Hamiltonian is the uniform superposition of all the "legal" clock states described above. The spectral gap of this Hamiltonian is asymptotically lower-bounded by N^{-2} for a polylogarithmic idling part C, so it does not destroy the gap

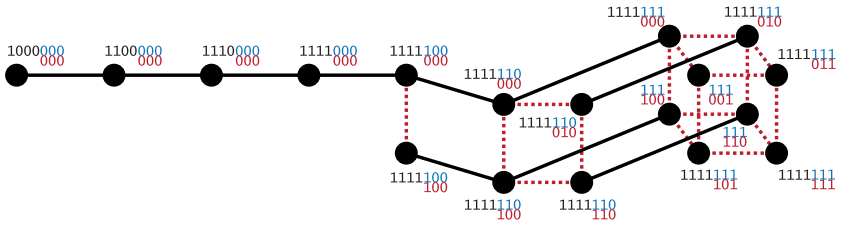


Fig. 2: An illustration of the possible progression of our Idling chain construction for an $N = 4$ computing domain-wall clock and a $C = 3$ idling part. The original computing clock connected to the data register has N unary bits (black). The idling part contains extra C unary bits (blue) and C idling bits (red). Each line corresponds to a projector onto the antisymmetric combination of the clock states (vertices) coming from the local terms of the Idling chain Hamiltonian. The graph is a line (the original clock), connected to the idling part: a line connected to a square, to a cube, and so on.

scaling of the original Hamiltonian without idling. Most importantly, it achieves our goal: the overlap of the ground state with the finished computation (idling part) can be made arbitrarily high.

It is not easy to prove that a dynamical version of this construction (with hopping, instead of projector terms) would perform well for a Feynman-like Hamiltonian computer. We even have some unfavorable numerical results for $C = \log N$ idling qubits. Therefore, we provide another construction for building a computer.

The Multi-cog clock This construction builds on multiple synchronized cog wheels with cyclic progression, see Fig. 3. For two wheels, it requires a square root extra idling qutrits (it can also be implemented with qubits) and behaves just like a quantum walk on a line with a known behavior [29]

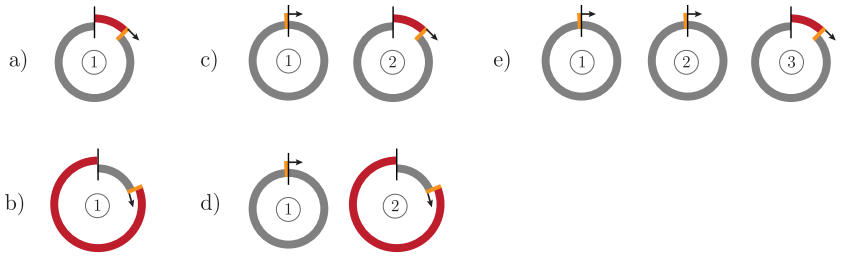


Fig. 3: A multi-cog clock construction is made from several synchronized wheels. It is a generalization of the domain-wall clock on a cyclic structure with multiple levels that can progress once the previous level revolutions are completed.

3 Shorter Unentangled Proofs and QCMA

It is natural to ask whether local Hamiltonians can have highly complex ground states, which cannot be efficiently prepared or even approximated. This is directly related to the open question $\mathsf{QCMA} \stackrel{?}{=} \mathsf{QMA}$ from complexity theory, i.e. whether quantum witnesses are more powerful than classical ones. One way to answer that they have the same power would be, if indeed all ground states of local Hamiltonians were efficiently preparable on a quantum computer and the classical description of the circuit (the recipe) would be the witness. On the other hand, even if $\mathsf{QCMA} = \mathsf{QMA}$, there still can be some local Hamiltonians without any efficiently preparable/approximable ground state.

This is why we ask: What can we verify and what can we store/read from n qubits compared to n classical bits? Do qubits behave more like classical bits or can we exploit their exponential nature? The Holevo bound tells us that we cannot faithfully transmit more than n bits of classical information using n qubits. Nevertheless, this tells us about the amount of information we can communicate or store/retrieve, but what can we verify from quantum states? Notice that in this case we want to obtain a single bit of information. Moreover, we want to ask this not only for general states, but states specifically related to local Hamiltonians (the ground states).

We can take another step and explore what is possible to verify if we have not one but *two copies of a quantum witness*. $\mathsf{QMA}(2)$ is a complexity class similar to QMA only with *two unentangled witnesses*. Thanks to the product test [26], it can be seen as having two copies of a witness available for verification. It turns out that the promise of unentanglement between the two copies of the proof (witness) gives the verifier quite a bit of power — he can check consistency between the proofs, and extract extra information from them. Surprisingly, we have seen $\mathsf{QMA}(2)$ protocols substantially shortening witnesses for classical, NP-complete problems [3, 9]. Whereas a similar shortening without unentanglement would imply a subexponential quantum algorithm for satisfiability of propositional formulas — the SAT problem (with spectacular consequences).

We build on these ideas (quantum witnesses for classical problems) and present the first $\mathsf{QMA}(2)$ protocol with *shorter unentangled proofs for a truly quantum problem.* For our protocol, we look at a naturally QCMA-complete problem: *Ground state connectivity* (GSCON) introduced by Gharibian and Sikora [21]. This problem asks a question about the ground (or low-energy) space structure of local Hamiltonians — whether two low energy states can be connected by a series of local transformations while not hitting an energy "barrier", illustrated in Fig. 4. We consider the frustration free variant and show that it is possible to shorten its proof to two unentangled proofs of length $O(n \log n)$ (notice that a standard QCMA proof is a sequence of local unitaries, with length polynomial in n) while lowering the promise gap to a small inverse polynomial in n, where n is the system size. We can observe two main shortcomings of our protocol: a) the shortening is significant only if the original QCMA proof is long and b) the promise gap becomes very small. Notice that there is not known amplification of

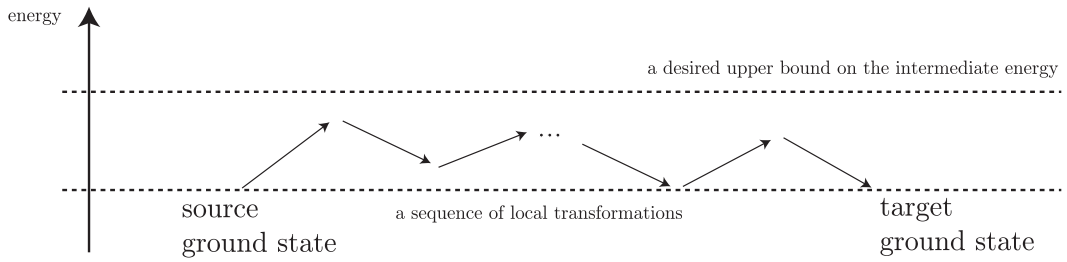


Fig. 4: An illustration of a ground state connectivity traversal.

the promise gap reusing witnesses [26, 39]. Our protocol should thus serve as a proof of principle and hopefully serve as an inspiration for other unentangled protocols for quantum problems or to further explore what is possible to prove with two copies of a quantum witness. This section is based on our article [14]. We sketch the ideas of our protocol.

3.1 Shorter unentangled proofs for FF-GSCON

Let us first state the QCMA-complete variant of the frustration free ground state connectivity problem (FF-GSCON) [21].

(FF-GSCON) Given a positive semidefinite frustration-free local Hamiltonian H over n qubits (system size) and two zero energy frustration-free ground states: source $|\psi\rangle$ and target $|\phi\rangle$ (represented succinctly via polynomial size quantum circuits) as well as two parameters m polynomial in the system size n and η inverse polynomial in n. Decide whether

"yes" there exists a frustration free traversal between $|\psi\rangle$ and $|\phi\rangle$, i.e. there is a sequence of 2-qubit unitary gates $U_1, \ldots, U_m$ (we consider them to come from some universal gate set of at most $\mathsf{poly}(n)$ size), such that: $U_m \cdots U_1|\psi\rangle \approx |\phi\rangle$ and each intermediate state $|\psi_j\rangle = U_j \cdots U_1|\psi\rangle$ is a ground state of H, or

"no" for all such sequences $U_j \cdots U_1|\psi\rangle$ has expected energy at least η.

The "natural" classical witness for the "yes" answer is the traversal $U_1, \ldots, U_m$, for which the verifier can check the required conditions in polynomial-time on a quantum computer. Observe, that this witness has the size $m\times$ the description of gates, which is asymptotically polynomial in n.

We design a $\mathsf{QMA}(2)$ protocol shortening this classical witness to 2 unentangled quantum witnesses. The length of the quantum witnesses is $O(n \log n)$ compared to the

classical $O(\mathsf{poly}(n))$. Our protocol is inspired by the ideas of Blier and Tapp [9] and their protocol with short unentangled proofs and an inverse polynomial promise gap for graph 3-coloring.

In our $\mathsf{QMA}(2)$ protocol the verifier asks the prover for two copies of witnesses (i.e. 4 unenetangled witnesses; then we utilize the Product test [26] to lower it to 2), together encoding a cycle of local transformations from $|\psi\rangle$ to $|\phi\rangle$ and back to $|\psi\rangle$ illustrated in Fig. 5:

$$|U\rangle = \frac{1}{\sqrt{2m}} \sum_{j=1}^{2m} |j\rangle|u_j\rangle \quad \text{and} \quad |S\rangle = \frac{1}{\sqrt{2m}} \sum_{j=1}^{2m} |j\rangle|\psi_j\rangle. \tag{2}$$

There $|U\rangle$ encodes the sequence of unitaries (as *label* and *gate* registers — the string u_j encodes the gate U_j) and $|S\rangle$ encodes the sequence of low-energy states of the traversal (as *label* and *data*).

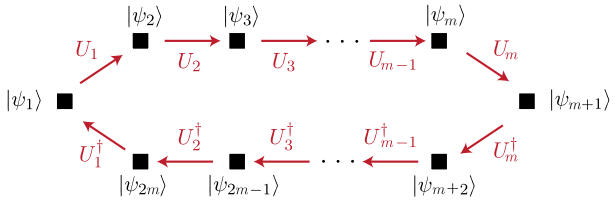


Fig. 5: A cycle of states $|\psi_1\rangle$, ..., $|\psi_{m+1}\rangle$, ..., $|\psi_{2m}\rangle$, connected via the unitaries $U_1, \ldots, U_m, U_m^\dagger, \ldots, U_1^\dagger$.

Observe that both states $|U\rangle$ and $|S\rangle$ can be given as $O(n \log n)$ qubits, where $O(\log n)$ is for the label and n for either a traversed state, or an encoding of a gate. The cyclic sequence of low-energy states should start with the initial state $|1\rangle|\psi_1\rangle = |1\rangle|\psi\rangle$ and contain $|m+1\rangle|\psi_{m+1}\rangle = |m+1\rangle|\phi'\rangle$ in the middle, where $|\phi'\rangle$ is close to the target state $|\phi'\rangle \approx |\phi\rangle$. Furthermore, this sequence should obey $U_j|\psi_j\rangle = |\psi_{j+1}\rangle$ and $U_{2m}|\psi_{2m}\rangle = |\psi_1\rangle$ at the end, for all U_j from the sequence of unitaries.

We come up with 8 specific tests for the verifier to probabilistically run on. The tests are designed to give him a reasonable assurance that the state $|U\rangle$ contains a nearly uniform superposition of the sequence of labeled, computational-basis encoded unitaries, applying these unitaries to the state $|S\rangle$ doesn't change it, the sequence of states in $|S\rangle$ contains each term $|j\rangle|\psi_j\rangle$ with a significant amplitude, the initial and final states $|\psi_1\rangle$ and $|\psi_{m+1}\rangle$ are what we asked for, and that the energy of each state $|\psi_j\rangle$ is low enough.

We prove that, if the answer is "yes" the prover can persuade the verifier about that with high enough probability, while in the opposite case the verifier has at least a tiny chance to detect a cheating prover. There remains an inverse polynomial promise gap between these acceptance probabilities — the difference.

4 Very Entangled Spin Chains

How entangled can ground states of "simple" local Hamiltonians be? We focus now on translationally invariant spin chains with low qudit dimension $d = 2, 3, 4, \ldots$. Such systems might be too restricted to be universal for computation, or even for encoding a hard problem from the QMA class into its ground state energy. However, they can still exhibit a surprising amount of correlations and entanglement, in violation of the area law. We will investigate, how one can achieve this with the lowest possible qudit dimension, and the highest possible spectral gap.

There is an interesting interplay between the gap and the entanglement entropy for spin chains. 1D gapped systems provably obey an area law [27] and thus have only constant entanglement entropy. This property makes them tractable on classical computers [33], or with heuristics like DMRG [49]. On the other hand, systems with a very small, inverse exponential, gap can have lots of entanglement in their ground states and manifest an entanglement *volume law* — the entropy scales with the volume of the cut region [34, 52].

We will focus on systems where the gap closes with the system size, but slowly, as an inverse polynomial, going slightly beyond the area law regime. Such systems remind us of critical systems. For those, in 1D, one would expect logarithmic correction to the entropy area law, as we have seen in the critical Ising, Heisenberg, or generally (1+1)D CFT [32, 34, 17] models. On the other hand, we know of two models designed specifically in order to exhibit volume law entanglement entropy in the ground state, while having an inverse polynomial gap [28, 24]. However they both have large qudit dimension (21 and 9) and are not naturally translationally invariant.

Thus, we ask: Can one achieve a similar behavior in models that involve low dimensional qudits, translationally invariant interactions and a unique ground state? Surprisingly, there are spin chains with an inverse polynomial gap, low qudit dimension, and $\sqrt{N}$ entanglement entropy — exponentially more then the logarithmic correction. Movassagh and Shor [37] showed the colored Motzkin spin chain (extending our colorless case [11]) with the half chain entanglement entropy of its unique ground state exhibits a power law violation of the area law. It is a translationally invariant (in a bulk) spin chain with boundary conditions, local particle dimension $d = 5$, and an inverse polynomial gap. Later, Salberger and Korepin [44, 16] found out that the colored Fredkin spin chain achieves similar properties with local particle dimension $d = 4$ having next-nearest-neighbor interaction.

In our search for such spin chains we choose to study a restricted class of "rewriting" Hamiltonians. Their ground states (and overall structure) have beautiful connections to formal languages and string rewriting rules. These multidisciplinary motivations bring forth success in our quest: we find the desired entropy scaling described in systems above, already in qutrit spin chains. We design the new Pair-flip (PF) model, a family of

spin chains with nearest neighbor, frustration-free translationally invariant interaction and an inverse polynomial spectral gap. Already for qutrits, it has a $\sqrt{N}$ entanglement entropy scaling for one of its ground states. Based on partial analytical and numerical results, we conjecture that this particular ground state can be made unique by adding a small translationally-invariant perturbation, while retaining the entropy scaling. This section is based on our preprint article [13] (about the PF model) and some additional unpublished results.

Let us set the stage. A *rewriting Hamiltonian* is a Hamiltonian on a line described by a family of rewriting rules of the form $A \leftrightarrow B$, where A and B are substrings of the same constant length (they will correspond to the interaction locality). Such a rule connects two words $\alpha A\beta$ and $\alpha B\beta$, where α, β are substrings. We identify qudit basis states with letters and associate a translationally invariant Hamiltonian (rewriting interaction[3]) term with this rule $1/2(|A\rangle - |B\rangle)(\langle A| - \langle B|)$, acting trivially on the rest of the chain. This interaction splits the whole Hilbert space into invariant subspaces of states connected by rewriting interactions. The terms energetically prefer uniform superpositions of the states $|\alpha A\beta\rangle$ and $|\alpha B\beta\rangle$. Thus, these Hamiltonians have ground states that are uniform superpositions of computational basis states connected by their rewriting rules, one in each invariant subspace. As a last step, we look at using additional translationally invariant penalizing terms to split the ground state degeneracy. For our model, we choose those to be projectors onto local (e.g. 2-qudit) computational basis states.

4.1 The pair-flip model

Our pair-flip model (PF) Hamiltonian is based on a very simple type of rewriting rule: $AA \leftrightarrow BB$ for any two distinct letters A and B. Let us write down the Hamiltonian first and explore the rich structure these rules can create. The PF model Hamiltonian reads $H_{\text{PF}} = H^{\text{PF}}_{\text{flip}} + \delta H^{\text{PF}}_{\text{cost}}$. The rewriting rules translate into:

$$H^{\text{PF}}_{\text{flip}} = \frac{1}{2}\sum_{i=1}^{N-1}\sum_{t=1}^{d}\sum_{t'\neq t}(|t't'\rangle - |tt\rangle)(\langle t't'| - \langle tt|)_{i,i+1}, \tag{3}$$

while the additional cost term favoring neighbors of the same type (pair counting) is:

$$H^{\text{PF}}_{\text{cost}} = -\sum_{i=1}^{N-1}\sum_{t=1}^{d}|tt\rangle\langle tt|_{i,i+1}, \tag{4}$$

where d is the number of distinct letters and thus local qudit dimension.

What structure can the pair flip rewriting rules create? The rules can indirectly facilitate "movement" of letters (particles): the letter 1 in the word 122 can "move"

[3]We could seen this type of interactions in QMA-hardness constructions [30] and also [28].

two positions to the right by the sequence of pair-flip transitions $122 \leftrightarrow 111 \leftrightarrow 221$. This allows to spread a pair $\ldots AA \ldots$ apart into strings such as $\ldots A \ldots A \ldots$ and create rich nested bracket-like structures similar to Motzkin and Fredkin spin chains. The ground states of the Motzkin and the Fredkin Hamiltonians can be understood as a uniform superposition of well-bracketed (in the colored case with different bracket species) words with and without spaces, respectively. Here is an example of a colorless Motzkin spin chain ground state (L, R are opening and closing brackets, respectively) on a 4-spin chain:

$$|\mathsf{M}_4\rangle = 1/\sqrt{9}(|0000\rangle + |00LR\rangle + |0L0R\rangle + |0LR0\rangle + |L00R\rangle + |L0R0\rangle + |LR00\rangle + |LRLR\rangle + |LLRR\rangle).$$

In the Motzkin and the Fredkin spin chains ground states, the matched particles (brackets) have a dedicated opening/closing part. In contrast to that, nesting in the pair-flip model is created by the alternating of colors. Intuitively, since the nesting comes from alternating of colors, on the base level (no nesting yet) we have d choices to increase the nesting, and on all other levels $d-1$ of them — those will have a similar structure as $d-1$ colored well-bracketed words without spaces (Dyck paths). We illustrate this on examples in Fig. 6. The rewriting term of the PF model $H^{\text{PF}}_{\text{flip}}$ (3) splits the Hilbert space

Fig. 6: Examples of fully reducible (balanced) colored words with depicted pairing for a) Motzkin b) Fredkin c) PF models.

into invariant subspaces of words that can be rewritten into each other. We characterize those by an *irreducible string* that can be obtained by subsequent removal of neighboring pairs (until there is no pair left). Furthermore, we call the invariant subspace with the empty irreducible string *fully reducible* and its ground state the *PF state*. We conjecture that the PF state (with some small perturbation) can be make unique by adding the pair counting cost term, while its high-entanglement properties remain unchanged. Let us look at the properties of our PF model.

Qubit PF model. Interestingly, the qubit PF model is in fact the Heisenberg XXX model in disguise (with the cost term XXZ model in a paramagnetic phase near the (isotropic) ferromagnetic point). Much is already known about this model, its spectral gap $\Theta(N^{-2})$, and entropy $\Theta(\log N)$ [48, 31, 43]. Here, we understand analytically what the pair-counting term does, as it splits the ground state degeneracy with $\delta = \mathsf{poly}^{-1}(N)$.

The Entanglement Entropy. We use the combinatorial properties of PF words and their relation to Fredkin model words. Relying on tools from analytical combinatorics,

we bound both from above and from below the Schmidt coefficients of a half chain cut by those of Fredkin model ground state. We thus obtain $\Theta(\sqrt{N})$ asymptotic scaling for the $d \geq 3$ PF model. Furthermore, this scaling is present also for any significant two-part cut (with the smaller part) and also for a middle-part cut-out.

An inverse-polynomial gap. We prove an inverse polynomial spectral gap of the PF model without perturbation for all of its invariant subspaces. We build on our proof for colorless Motzkin spin chain [11] as well as related results [37, 36].

A unique ground state. Without the cost term, the PF model has a degenerate ground state — one for each irreducible string of length k. Analytically (for constant-k) and numerically (for high k growing with n), we show that the former ground state from the fully-reducible subspace gets a larger energy shift. We conjecture that the cost term with $\delta = N^{-3}$ (or smaller) selects a unique ground state, while the asymptotic entropy scaling remains intact. This is demonstrated by our numerical investigation, illustrated in Fig. 7.

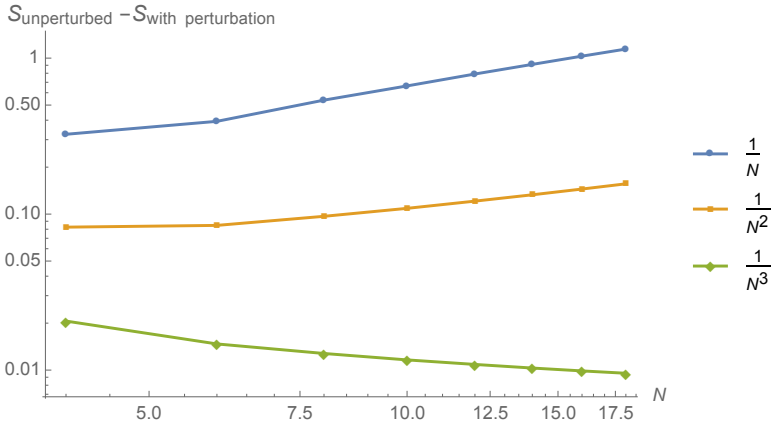


Fig. 7: Differences between the half cut entanglement entropy of unperturbed and perturbed qutrit PF model ground state, displayed for various δ-intensities.

Violation of the cluster decomposition property. Similarly to the colored Motzkin and Fredkin spin chains [16] the qutrit (and higher) PF state has a nonvanishing connected correlation function in the thermodynamic limit ($N \to \infty$) and thus violates the cluster decomposition property. We observed its robustness numerically in the presence of the pair counting perturbation term splitting the ground state degeneracy.

4.2 1D rewriting Hamiltonians with qubits

As an additional result, we also analyze all 1D (nearest-neighbor interactions) rewriting Hamiltonians with qubits. We performed our analysis of the entanglement entropy by

an interesting connection between the matrix product state representation and finite automata, exactly specifying regular languages [15]. We found out that most of the ground states of rewriting Hamiltonians with qubits satisfy an area law. However, there are two of them with logarithmic entanglement entropy (for a particular choice of ground states): our qubit PF model $00 \leftrightarrow 11$, and the rule $01 \leftrightarrow 10$, which is in fact the Heisenberg XXX model.

5 Conclusion

In this thesis we set out to study the power and limits of quantum computation. Our main area of investigation were local Hamiltonians and their ground states. We focused on exploring various parameters that can make computational tasks (e.g. determining the ground state energy or preparing the ground state or finding its properties) much more difficult, and understanding this computational complexity. Our motivation was to discover interesting phenomena that appear already in simple spin systems, and to test their behavior with respect to the relevant parameters. For example, increasing the locality of interaction from 2 to 3 [10, 23], increasing the local spin dimension from 2 to 3 [11], allowing for nonlinear geometry [23], varying the scaling of the promise gap for decision problems in both directions [4, 18], etc., already results in very interesting emerging properties. Using tools from computational complexity, Hamiltonian complexity, Markov chains, graph theory and analytic combinatorics, we addressed the following three different interconnected topics about local Hamiltonians and their ground states:

1. Improving the parameters of QMA-hardness and universality constructions with ground-/eigen- states that encode a quantum computation.

2. The surprising power of quantum proofs thanks to unentanglement.

3. Large entanglement in ground states of low qudit ($d \geq 3$), translationally Hamiltonians in 1D, beyond the area law regime.

The work has appeared in two published papers [12, 14] and one unpublished, but already 5-times cited preprint [13]. We believe our results not only tie some loose ends and open questions about known constructions, but bring a collection of new ideas, models and open questions that will serve as a basis for ongoing research and quest for better understanding of the surprising complexity of the ground states of quantum many-body systems.

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The work in this paper was presented at the following conferences: preliminary ideas were presented as a poster at QIP 2016 (Banff, Canada) and as a contributed talk at 4th Work Meeting on Quantum Optics & Information 2016 (Pécs, Hungary). The pair-flip model was presented as a contributed talk at YQIS 2018 (Vienna, Austria), as a poster at TENSOR 2018 (Dresden, Germany), and together with additional results and focusing on combinatorial techniques as a contributed talk at CEQIP 2019 (Skalice, Slovakia), and as a poster at YQIS 2019 (Sopot, Poland), where it won the best poster award.

Other publications (not part of this thesis)

1. S. Bravyi, L. Caha, R. Movassagh, D. Nagaj, P. Shor, *Criticality without frustration for quantum spin-1 chains* Phys. Rev. Lett. 109, 207202 (2012). [citations: 51 (WoK, Scopus)]

This work from the time of our undergraduate diploma thesis was the initial motivation for, and gave us the basic set of tools for the work in Section 4.