

Research plan: Thermal and ground states of local Hamiltonians

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(Dated: September 1, 2015)

Information theory, multiparticle correlations, and quantum entanglement are closely connected. In this context, we plan to investigate the so called irreducible correlations and sets of thermal and ground states of local Hamiltonians, with which one can classify the complexity of quantum states, and to some extent, their entanglement properties. Then, the adiabatic connectivity of the resulting ground state spaces will be explored: Given two ground states, can they be connected by a continuous path of ground states whose corresponding Hamiltonian is always of local structure? Finally, we aim to characterise the set of states accessible by time evolution of local Hamiltonians, important for preparing quantum states using single-shot unitaries.

I. STATE OF GENERAL RESEARCH

Investigating correlations between quantum particles is a long-standing endeavour. Starting with the famous Einstein-Podolsky-Rosen paper, quantum states resulting in distributions that cannot be separated into parts are coined with the term entanglement. While the characterisation of entanglement properties of only two particles is well established, characterising quantum systems consisting of a higher number of parties presents an ongoing challenge. In this research plan, we use an approach originating in information geometry to characterise the complexity or the irreducible correlations of quantum states. The resulting families of states are thermal states of local Hamiltonians (also called Gibbs states) and include ground states in the limit of “low” temperature.

Traditionally, the focus in solid state physics has been on solving physical models for their ground states, alongside with interesting bulk properties such as the onset of phase transitions. We will take a somewhat inverse approach here, and characterise which states generally can be thermal or ground states of physically reasonable Hamiltonians.

In order to describe our research plan, we will first explain the exponential families \mathcal{Q}_k consisting of thermal and ground states of k -local Hamiltonians, the irreducible correlations C_k , and the connections between these two concepts. Then, we will motivate our planned investigations into the adiabatic connectivity of \mathcal{Q}_k and its subsets, relevant for understanding the topology of these sets as well as the limits of adiabatic quantum computing.

A. Thermal and ground states of local Hamiltonians

A thermal or Gibbs state can be written as

$$\tau = \frac{e^{-\beta H}}{\text{tr } e^{-\beta H}}. \quad (1)$$

This can also be seen as a way of parametrising any density matrix, the so called exponential description of quantum states. Then, the corresponding Hamiltonian H is not necessarily a physical one. However, this parametrisation is quite natural to consider, as quantum states quickly thermalise when in contact with the environment. That is, they tend towards thermal states allowing a description as in (1), where the Hamiltonian is also physically relevant. Cooling down a quantum system to a temperature low enough relaxes it into its ground state. In specifying the corresponding Hamiltonian one implicitly describes the ground state, albeit in a non-trivial fashion.

Many physically relevant models have Hamiltonians containing a restricted set of possible interaction terms. As an example, the Hamiltonian of the Ising model describing ferromagnetic solid state systems has, apart from the magnetic field term, nearest neighbour interactions. The Hamiltonian is said to be 2-local, as each interaction term acts on at most two spin sites at once. In general, a Hamiltonian whose interaction terms act on at most k particles non-trivially is said to be k -local or k -body. It can be written as $H_k = \sum_j I_k^j$, where $\text{weight}(I_k^j) \leq k$. Here, $\text{weight}(\cdot)$ counts the number of terms not equal to the identity in the tensor product expansion.

Additionally, a geometrical layout of the particles is often considered, such as in the case of the Ising model, where only adjacent sites interact. As another example, ions in a trap affected by Coulomb forces interact almost exclusively with their neighbours, and are typically arranged in a linear fashion. The resulting Hamiltonian is not only 2-local, but its interaction structure is further restricted by the geometry of the physical system under consideration.

The sets of states we explore are the exponential families of many-qubit thermal states of k -local Hamiltonians [1]

$$\mathcal{Q}_k = \left\{ \tau_k \mid \tau_k = \frac{e^{-\beta H_k}}{\text{tr } e^{-\beta H_k}} \right\}. \quad (2)$$

Ground states are included in the limit of $\beta \rightarrow \infty$. The exponential family \mathcal{Q}_1 consists of product states, and the separable or non-entangled states form its convex hull

$$\left\{ \sum_i p_i \rho_i^{(1)} \otimes \rho_i^{(2)} \otimes \cdots \otimes \rho_i^{(n)} \mid \sum_i p_i = 1, p_i \geq 0 \right\}. \quad (3)$$

Apart from the whole quantum state space \mathcal{Q}_n , the sets \mathcal{Q}_k are generally non-convex. Therefore, one frequently considers the convex hull $\text{conv}(\mathcal{Q}_k)$. This especially in connection with witnesses, which represent hyperplanes cutting through the state space. The hierarchy of quantum exponential families is formed by $\mathcal{Q}_1 \in \mathcal{Q}_2 \in \cdots \in \mathcal{Q}_n$, and was first elucidated in Ref. [1] and Ref. [2] for quantum states and classical probability distributions respectively. As an alternative description, \mathcal{Q}_k contains the states having a maximum von Neumann entropy under the constraints of given k -party reduced density matrices [3], assuming the latter to be consistent. These states therefore can be seen as being least biased while fulfilling the local constraints, according to the Jaynes principle of maximum entropy [4]. We will make use of both characterisations later.

To motivate these sets further, thermal states of local Hamiltonians are related to a problem in Hamiltonian complexity: Do typical states allow a succinct description? A n qubit system generally requires 2^n variables for its unique description, rather than only of order n as for classical systems. Are there classes of quantum states allowing a polynomial description, too? This is the case for thermal states of k -local Hamiltonians, as their parametrisation requires less parameters if $k < n$. As most naturally occurring Hamiltonians have a local structure, we are led to conclude that most thermalised quantum systems typically have a less complex description as might have been possible, considering the size of the Hilbert space alone. This is indeed generally true, as almost all pure states are determined by the reduced density matrices of a fraction of less than 2/3 of all parties, given a large number of parties [5]. There exist other succinct descriptions of quantum states and we mention two connections: Ground states of gapped local Hamiltonians are close to generalised matrix product states [6], and matrix product states can often be reconstructed by local measurements [7].

Further, certain states which are of interest for quantum computation have been shown not to be ground states of naturally occurring 2-local Hamiltonians. These include Greenberger-Horne-Zeilinger and graph states. This is quite unfortunate, as certain graph states such as cluster states are known to be universal resources for quantum information processing by measurement based quantum computing [8]. Conversely, if a state of interest happens to be a ground state of a local Hamiltonian, it might be easily prepared by engineering the required Hamiltonian and cooling down the system. Engineering higher order interactions between individual qubits can be experimentally challenging, and it is therefore of interest to know what part of state space is accessible given reasonable interaction structures.

B. Information Projection

The irreducible k -party correlation is based on the information contained in the k -party reduced density matrices, which is not already contained in the $(k-1)$ -party reduced states [9]. If higher order irreducible k -party correlations are absent, properties such as entanglement arise from locally available information, and can be acquired by local measurements, too [10]. However, irreducible correlations are strictly speaking not an entanglement measure, but can be seen as a measure of complexity that leads to a generalisation of notions such as full separability and relative entropy of entanglement.

In order to introduce the concept of irreducible correlations, we first define the information projection, representing a “best approximation” of a given state. The information projection $\tilde{\rho}_k$ of the state ρ onto the exponential family \mathcal{Q}_k is defined as the nearest state in \mathcal{Q}_k in terms of the quantum relative entropy $S(\rho||\sigma) = \text{tr}[\rho \log \rho] - \text{tr}[\rho \log \sigma]$,

$$\tilde{\rho}_k = \underset{\sigma \in \mathcal{Q}_k}{\text{argmin}} S(\rho||\sigma). \quad (4)$$

The state $\tilde{\rho}_k$ is said to have at most k -party irreducible correlations present. As an equivalent formulation, the information projection $\tilde{\rho}_k$ can also be defined by having a maximum von Neumann entropy $S(\sigma) = -\text{tr} \sigma \log \sigma$ of all states with the same k -party marginals as ρ ,

$$\tilde{\rho}_k = \underset{\sigma \in \mathcal{M}_k(\rho)}{\text{argmax}} S(\sigma). \quad (5)$$

Above, $\mathcal{M}_k(\rho)$ denotes the set of states with the same k -party reduced density matrices as ρ . As a third characterisation, the state is in the unique intersection $\tilde{\rho}_k = \mathcal{Q}_k \cap \mathcal{M}_k$.

With this, one defines the distance to \mathcal{Q}_k

$$D_k(\rho) = \min_{\sigma \in \mathcal{Q}_k} S(\rho||\sigma). \quad (6)$$

If $D_k(\rho)$ is sufficiently small, the state ρ is well approximated by $\tilde{\rho}_k$, in the sense of statistical inference. The irreducible correlations are defined by $C_k(\rho) = D_k(\rho) - D_{k-1}(\rho)$, and can be seen as a complexity measure of a quantum system.

The concept of irreducible correlations has first been introduced in the classical setting, where the Kullback-Leibler divergence was used as the classical equivalent of the relative entropy. Amongst other applications, it has been applied to statistical inference in biology, neuronal networks, and machine learning [2, 11, 12]. In the quantum setting, irreducible correlations have been used to characterise topological order [13] as well as quantum phase transitions [14]. Also, relationships with secret sharing have been shown [15].

There exist numerical programs to compute the classical information projection [11], and first algorithms have already been developed for the quantum case [16, 17]. However, the field lacks an algorithm that is sufficiently fast and robust, a task which we will take up in the second research line.

C. Adiabatic connectivity

Adiabatic quantum computation has been shown to be equivalent to standard quantum computation [18]. In adiabatic quantum computation, a controllable Hamiltonian is changed slowly with respect to the energy gap, keeping the system in its ground state. The state changes from the ground state of an easily engineered initial Hamiltonian H_i to its target ground state, which is usually the solution of a computationally interesting problem encoded in the target Hamiltonian H_t . While the initial and final ground state can be connected by a path, it is not clear if the path lies within a restricted set of ground states, such that the corresponding instantaneous Hamiltonian is always of local structure [19]. This leads to the notion of adiabatic connectivity: Two ground states $|\psi_0\rangle$ and $|\psi_1\rangle$ are adiabatically connected in \mathcal{Q}_k , if there exists a smoothly varying k -local Hamiltonian $H(s)$ having $|\psi_0\rangle$ as a ground state of $H(0)$ and $|\psi_1\rangle$ as ground state of $H(1)$ [20]. This is especially important for experiments, where higher order interactions are extremely challenging to implement. The final Hamiltonian can be seen as an instance of a 2-local quantum constraint satisfaction problem, which has shown to be QMA hard [21]. However, this does not prevent us from describing these sets for a small number of qubits or by witnesses, as the former statement concerns the scaling of the problem only.

D. State of own research

1. Characterising thermal and ground states of local Hamiltonians

Our preliminary work was motivated by a result from Linden, Popescu, and Wootters: Almost all pure states of three qubits are completely determined by their 2-party reduced density matrices [9]. That is, almost all states of three qubits, including those which are mixed, lie in the convex hull of \mathcal{Q}_2 . Our motivation was to generalise this statement. As a result, we showed that a similar statement is not valid for states of five or more qubits: There exist many pure states which are not determined by their 2-party reduced density matrices. While a similar result was known in the limit of a large number of qubits [5], we also provided a witness and a semi-definite program to detect states outside of $\text{conv}(\mathcal{Q}_2)$ [22].

Witnesses are standard tools for describing convex sets, and are regularly used to prove that certain sets of states have specific entanglement properties [23]. It is an observable \mathcal{W} that can detect some but not necessarily all states lying outside of a given convex set. Such a witness is typically constructed by calculating the maximum overlap between a state $|\psi\rangle$ (believed to be outside of C) and states in the set $\sigma \in C$

$$\alpha = \max_{\sigma \in C} \text{tr} [|\psi\rangle\langle\psi| \sigma]. \quad (7)$$

One then writes the projector based witness $\mathcal{W} = \alpha\mathbb{1} - |\psi\rangle\langle\psi|$, with the property that if $\text{tr}[\mathcal{W}\rho] < 0 \implies \rho \notin C$.

Having constructed a witness by computing the maximum overlap between ring cluster states and states in \mathcal{Q}_2 , we showed that a non-zero volume of states are outside of \mathcal{Q}_2 , and therefore not completely determined by their 2-party reduced density matrices and the principle of maximum entropy. As mentioned, a witness can generally not detect all states with a given property. In order to obtain quantitative results on the fraction of pure states outside of \mathcal{Q}_2 , we formulated a semi-definite program. Semi-definite programs are a type of convex problems and are efficiently solvable [24]. Both commercial as well as open source solvers are readily available, making the implementation, once the program is formulated, fairly straightforward. Further, the theory of semi-definite programs allows an optimality certification for solutions found, which makes it a numerically robust method. As a result, we obtained the fraction of pure five qubit states lying outside of \mathcal{Q}_2 , which is at roughly 30%.

As for the case of four qubits, we have strong numerical evidence pointing to a similar statement as in the case of three qubits. Almost all pure states seem to be in the exponential family \mathcal{Q}_2 . We suspect that certain states are not included, such as the four qubit $|\chi\rangle$ state, that maximises certain bipartite entanglement properties [23].

2. Maximum entropy production and Hopf bifurcations in evolutionary game theory

As a side project in complex systems, we have been working on stochastic systems in evolutionary game theory. There, the measure of entropy production in the context of stochastic thermodynamics seems to accompany Hopf bifurcations occurring in the system. We are investigating this in asymmetric oscillatory games such as rock-paper-scissor and the battle of sexes. There, we found a new lower bound for the entropy production which is less susceptible to nearly vanishing transition rates that have been obtained by numerical simulations [25].

E. First research line: Characterising ground states of local Hamiltonians and their adiabatic connectivity

Previously, we have developed a witness and formulated a semi-definite program to determine the membership to \mathcal{Q}_2 . Now, we will as a first task investigate subsets of \mathcal{Q}_2 , which arise from Hamiltonians with physically more natural geometries, such as found in solid state systems or in ion trap experiments. The interaction structure of the Hamiltonian is further restricted, and the possible thermal and ground state space can be smaller. Commonly found interaction structures are one dimensional lattices such as linear or periodic spin chains, as well as two dimensional lattices with square or hexagonal layout including toroidal lattices. We aim to characterise these subsets with both analytical and numerical methods.

First, we will consider small systems consisting of up to three to four qubits, and aim to find analytical witnesses to determine which quantum states cannot be ground states of 2-local Hamiltonians having certain restricted interaction structures. For larger systems, we will also develop a witness and formulate a semi-definite program to determine the membership to the ground state space of a given interaction structure. The code for this will be made public, such as on github.

Following this, open questions about the adiabatic connectivity of these state spaces will be explored: Does there exist a path from and to each ground state in these sets while maintaining a non-vanishing gap, such that no degeneracy occurs? Similar questions have been addressed with a path consisting of a Hamiltonian obtained by linear interpolation [26]. Paths which are not “straight” have also been considered, and often led to success in finding adiabatic connections where the common linear interpolation in Hamiltonian space has failed [27]. In this research plan, we consider the more general case of the existence of any path whose gap is non-vanishing, and aim to either prove or disprove topological connectivity. To tackle this question, we first focus on understanding the adiabatic connectivity of the aforementioned subsets of \mathcal{Q}_2 for a small number of qubits by both analytical methods and numerical hints. Once the adiabatic connectivity of these simpler interaction structures is sufficiently understood, we will have enough new knowledge to explore and determine the adiabatic connectivity of the larger set \mathcal{Q}_2 .

Milestones for the first research line:

M 1.1 Formulate a witness and a semi-definite program to determine the membership to sets of thermal and ground states of Hamiltonians having a restricted interaction structure.

M 1.2 Determine the adiabatic connectivity of \mathcal{Q}_2 and its subsets.

F. Second research line: Irreducible many-body correlations and unitaries of local Hamiltonians

As a second research line, we intend to compute the irreducible correlations for different classes of states in order to classify their complexity. Further, we aim to characterise the dynamics under local Hamiltonians, that is, delineate the state space accessible by unitary time evolution under k -local Hamiltonians.

Graph states are shown to be outside of \mathcal{Q}_2 [28], and we will examine a generalisation of this class of states, the so called hypergraph states [29]. Ref. [30] obtained analytical expressions for the irreducible correlations of graph states, and we want to obtain results for hypergraph states in a similar fashion. Both arise from a stabiliser formalism, but the elements of the stabiliser of hypergraph states are of non-product form, making their treatment more involved. Graph states are useful for measurement based quantum computation, and hypergraph states seem to promise similar applications. Their classification therefore is of interest, as it would be of advantage if they could be prepared or approximated by simply cooling down a physically realistic system.

As for a different class, we want to examine Gaussian states, whose Wigner functions are Gaussian shaped. They constitute an important class for experiments performed with light, and are notably easy to prepare and control.

They include coherent and squeezed states, and admit a succinct description as they are characterised by their first and second moments [31]. As a first application of exponential families to continuous variable quantum systems, we intend to characterise translationally invariant chains of harmonic oscillators, in order to complement entanglement studies performed in Ref. [32].

We will then compare the analytical results of the irreducible correlations to a novel algorithm. It was outlined in Ref. [17], but has not yet been implemented as it was not the main subject of this previous work. Taking advantage of the different definitions for the information projection, one can maximise the von Neumann entropy given k -party reduced density matrices acting as local constraints. The problem then becomes an instance of convex optimisation, which is a well studied subject and admits efficient solvers [33].

As a second focus of this research line, we are interested in single-shot unitary time evolution under local Hamiltonians. Thermal states can be seen as time evolution with an imaginary time, and vice versa. The dynamics under unitaries is of interest in digital quantum simulations, where many-body Hamiltonians have been simulated by applying sequences of 2-body interactions in a stroboscopic manner [34]. Our focus is on unitary accessibility: Given a fixed pure product state $\rho_p = \rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_n$, what other states are accessible by unitaries of 2-local Hamiltonians $U = \exp(-itH_2)$? The set we aim to characterise consists of

$$\{\rho \mid \rho = e^{-itH_2} \rho_p e^{itH_2}, H_2 \text{ is 2-local, } \rho_p \text{ is a fixed pure product state}\}. \quad (8)$$

By parameter counting, the full state space can clearly not be reached, and the question is: Which states are inaccessible? To begin investigating this problem, we first focus on hypergraph states. They have a similar definition as graph states, except that hyperedges generally connect more than only two vertices. Given a hypergraph (V, E) with vertices V and connected by hyperedges E , a hypergraph state can be defined by applying commuting controlled phase gates U_e to a product state [8]

$$|H\rangle = \prod_{e \in E} U_e |+\rangle^{\otimes |V|}. \quad (9)$$

In the case of all hyperedges connecting two vertices only, we obtain graph states. Thus they can be reached by unitaries of 2-local Hamiltonians, as all U_e act on two spin sites only and commute. For k being the largest number of vertices connected by any hyperedge, a hypergraph state is by definition accessible by the unitary $\prod_{e \in E} U_e$, whose Hamiltonian is k -local. It is however not clear if also k' -local Hamiltonians could be used with $k' < k$. If hypergraph states turn out to be inaccessible, one can construct a witness by calculating the maximum overlap

$$\alpha = \max_{H_2 \text{ is 2-local}} \text{tr} [|H\rangle\langle H| e^{-itH_2} \rho_p e^{itH_2}] \quad (10)$$

or a bound thereof. As last resort, we would compute the overlap numerically. Ideally, we would also find the fraction of inaccessible pure states, as done in our previous work for the case of five qubits and the set \mathcal{Q}_2 .

Milestones for the second research line:

M 2.1: Compute the irreducible correlations of hypergraph and Gaussian states. Implement the novel algorithm, taking advantage of the convex structure of the problem.

M 2.2: Give examples of states not accessible by unitaries of 2-local Hamiltonians. Provide a witness, and determine the fraction of inaccessible pure states.

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II. SCHEDULE OF THE PROJECT

The research will focus on the following:

Month 1-6 Focus on milestone M 1.1: Finding a witness and understanding the ground state space of 2-local Hamiltonians with restricted interaction structures for small quantum systems. Also, a semi-definite program will be implemented to determine the membership to these sets numerically.

Month 7-12 Focus on milestones M 1.2, M 2.1: Understanding the adiabatic connectivity of subsets of \mathcal{Q}_2 having typical interaction structures. Computing the irreducible correlation for hypergraph and Gaussian states, together with implementing the novel algorithm.

Month 13-18 Focus on milestones M 1.2, M 2.2: Understanding the adiabatic connectivity of \mathcal{Q}_2 . Characterising the state space accessible by unitaries of 2-local Hamiltonians.

III. PROSPECTS AND IMPACT

This project leads to a better understanding of the ground and thermal state space of local Hamiltonians. The results will contribute to the ongoing effort in studying multi-particle quantum correlations and entanglement, as well as provide tangible results for statistical inference in the quantum case. As we provide concrete tools for researchers to determine the membership to \mathcal{Q}_2 and its subsets, it might lead to new and exciting experiments, showing that a prepared state is not in $\text{conv}(\mathcal{Q}_2)$ and that 3-party interactions have been engineered. The results on adiabatic connectivity are of both theoretical and applied interest. It will determine the topological connectedness of the ground state space of 2-local Hamiltonians as well as identify new limits to adiabatic quantum computing. Lastly, unitary accessibility is of strong experimental interest, as it characterises the possible dynamics under a by nature restricted time evolution.

IV. REASON FOR THE CHOICE OF THE RESEARCH INSTITUTION

The University of Siegen is home to Professor Gühne's research group on theoretical quantum optics. The group focuses on entanglement and quantum information theory, as well as on foundations of quantum mechanics. I have spent the last year in his group working on witnesses for $\text{conv}(\mathcal{Q}_2)$ and on complex systems. Professor Gühne and members of the group published on exponential families and irreducible correlations, and my work is in continuation of an earlier project on this subject. He also is an expert on entanglement detection and characterisation. As my research concerns multiparticle correlations and leads to a generalisation of entanglement, working under his supervision is ideal, together with the productive environment in the group. Additionally, Professor Gühne has significant experience in supervising PhD students. For all these reasons, I believe that his research group at the University of Siegen provides the best place to carry out my research plan.

V. RELEVANCE FOR PERSONAL CAREER DEVELOPMENT

This Doc.Mobility scholarship would enable me to follow my own research interests, and to acquire the necessary knowledge and tools to pursue a research career. With it, I intend to continue and finish my Ph.D. at the University of Siegen by the end of this project. I aim to keep working on the (information) geometry of quantum states, ideally in a group active in this field, such as those of Professor K. Życzkowski (Kraków), Dr. M. Kleinmann (Bilbao), Prof I. Bengtsson (Stockholm), Dr. M. Huber (Barcelona), Dr. R. Kostecki (Waterloo) or Prof. R. Renner (Zürich). In the long term, I aim to return to Switzerland for family reasons and to work in groups such the ones in Basel, Geneva, or Zürich, all of which are strong in research on quantum information and computing.

VI. PLANNED PUBLICATIONS

In the first research line, we plan to publish the following:

1. Concerning small quantum systems, we aim to publish a paper with analytical witnesses delineating the convex hull of the ground state space of 2-local Hamiltonians with given interaction structure, together with results on its adiabatic connectivity. For larger systems, we aim to include a witness for lattices. The computer code to determine the membership to \mathcal{Q}_2 and its subsets will be made public, such that also other researchers can use this tool.
2. We aim at publishing results on the adiabatic connectivity of \mathcal{Q}_2 and its subsets. We will gain knowledge from small systems together with numerical hints to tackle the adiabatic connectivity of \mathcal{Q}_2 , which is by nature a more speculative project. This will allow a second publication, and will ideally include a proof or disproof of the adiabatic connectivity of \mathcal{Q}_2 .

In the second research line, we plan to publish the following:

1. Analytical results on the irreducible correlations of hypergraph and Gaussian states. This publication will be supported by numerical results obtained from the novel algorithm, whose code will be made public.
2. Results on the state space unitarily accessible by 2-local Hamiltonians, together with counterexamples, possibly obtained from hypergraph states.