Aspects of Topology and Measurement in Quantum Lattice Systems

Thesis by
Adam Artymowicz

In Partial Fulfillment of the Requirements for the
Degree of
Doctor of Philosophy

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California

2025
Defended May 15, 2025

Adam Artymowicz
ORCID: 0000-0002-5461-3991

ACKNOWLEDGEMENTS

I would like to thank my advisor Anton Kapustin for his patient mentorship throughout my PhD, and for being a constant source of inspiration. His physical intuition and mathematical style were instrumental in shaping me as a student.

I am grateful also to my collaborators Nikita Sopenko, Bowen Yang, Samuel Scalet, Omar Fawzi, and Hamza Fawzi for our lively discussions and for their tireless work in our collaborations.

Finally, to my friends and family who supported me over the years: thank you, I couldn't have done it without you.

ABSTRACT

In the first part of this thesis, topological invariants of gapped phases on the lattice are studied. These include the Berry curvature, Thouless pump, the Hall conductance, and their higher-dimensional analogs. These invariants are proven to obstruct the promotion of a global symmetry to a gauge symmetry. Two of these invariants, the 1d higher Berry curvature and the 2d higher Thouless pump, are studied in detail. First, it is shown that they are related by a relation involving flux insertion, which can be interpreted physically as identifying the higher Thouless pump invariant with the excess Berry curvature of a fluxon. Second, it is proven that these two invariants take on quantized values in an invertible state.

In the second part of this thesis, an algorithm is presented for learning Hamiltonian parameters from local expectation values of its Gibbs state via a local free-energy variational principle. The algorithm is benchmarked on the problem of black-box learning of a nearest-neighbour Hamiltonian in a 100-qubit spin chain, giving evidence of favourable scaling with system size. The theoretical analysis is then extended to incorporate measurement noise, as well as equipping the algorithm with certified a posteriori lower and upper error bounds on the inferred parameters. For commuting Hamiltonians, a priori convergence guarantees are also established.

PUBLISHED CONTENT AND CONTRIBUTIONS

[Art24] Adam Artymowicz. "Efficient Hamiltonian learning from Gibbs states". In: *arXiv e-prints*, arXiv:2403.18061 (Mar. 2024), arXiv:2403.18061. DOI: 10.48550/arXiv.2403.18061. arXiv: 2403.18061 [quant-ph].

[AKS24] Adam Artymowicz, Anton Kapustin, and Nikita Sopenko. "Quantization of the Higher Berry Curvature and the Higher Thouless Pump". In: *Communications in Mathematical Physics* 405.8 (July 2024). ISSN: 1432-0916. DOI: 10.1007/s00220-024-05026-2. URL: http://dx.doi.org/10.1007/s00220-024-05026-2.
All authors contributed equally.

[AKY24] Adam Artymowicz, Anton Kapustin, and Bowen Yang. "A mathematical theory of topological invariants of quantum spin systems". In: *arXiv e-prints*, arXiv:2410.19287 (Oct. 2024), arXiv:2410.19287. DOI: 10.48550/arXiv.2410.19287. arXiv: 2410.19287 [math-ph].
All authors contributed equally.

[Art+24] Adam Artymowicz et al. "Certified algorithms for quantum Hamiltonian learning via energy-entropy inequalities". In: *arXiv e-prints*, arXiv:2410.23284 (Oct. 2024), arXiv:2410.23284. DOI: 10.48550/arXiv.2410.23284. arXiv: 2410.23284 [quant-ph].
All authors contributed equally.

TABLE OF CONTENTS

Chapter 1

INTRODUCTION

1.1 Background for Chapters 2 and 3: topological invariants

Phases of matter

Consider a physical system parametrized by a set of variables. In practice one often considers thermodynamic variables such as pressure and temperature, but they may in principle be any parameters whatsoever, macroscopic or otherwise. At certain points in the parameter space it may happen that some property of the system ceases to be a continuous function of the parameter. At these points the system is said to undergo a phase transition. Two points in the parameter space will be said to be in the same phase of matter if there is a path between them that does not pass through any phase transition.

As an example, consider the phase diagram of water. At a pressure of 1 atmosphere, the system undergoes a phase transition at 100° C between a liquid and a gas. However, this does not mean that liquid water and water vapor belong to different phases of matter. Indeed, one can construct a path between these two that does not pass through any phase transition, by going around the critical point. Thus, liquid water and water vapor form one phase of matter.

On the other hand, ice forms a distinct phase of matter from the liquid/gas phase. This remains true no matter what extra parameters are added to the system, so long as we don't explicitly break spatial symmetry. This surprisingly strong result is a result of Landau theory, one of the cornerstones of modern statistical physics. One begins by looking at the symmetries present in the two phases: the liquid/gas phase is homogeneous and isotropic, while the solid phase is not, because the ice crystal lattice breaks translation and rotation symmetry. This is the phenomenon of spontaneous symmetry breaking, and Landau theory shows it must be accompanied by a phase transition. Thus, there is no path in any admissible parameter space from liquid water to ice that does not cross a phase transition.

The Landau approach of studying the phase diagram of a physical system using symmetries alone has been tremendously successful in modern physics.

However, one may ask if it gives a complete classification. Are there distinct phases of matter which cannot be told apart by their pattern of symmetry-breaking?

Topological phases

In the second half of the 20th century it became apparent that phases of matter beyond the Landau paradigm do indeed exist. It began with the study of the quantum Hall effect, where free electrons confined to a 2d plane are subjected to a strong magnetic field perpendicular to the plane. In such systems, an applied electric field V_x produces a transverse current J_y. The associated conductance $\sigma_{xy} := J_y/V_x$ is called the Hall conductance, and classical electrodynamics predicts that the Hall conductance is directly proportional to the applied magnetic field. However, experiments [KDP80] show that under suitable conditions the Hall conductance is in fact quantized: it takes on a discrete set of values $\sigma_{xy} = \nu e^2/h$ where $\nu = 1, 2, \ldots$. It was soon recognized that materials with distinct values of ν are in distinct phases of matter, and that these phases cannot be distinguished by their pattern of symmetry breaking.

The integer quantum Hall phases have several important features:

1. They are zero-temperature phenomena.
2. They involve no spontaneous symmetry breaking.
3. They have no local bulk excitations at low energies.

At a first pass, these may be taken as the defining criteria of a topological phase[1].

Field-theoretic description of topological phases

It is believed that topological phases are described in the IR limit by topological quantum field theories or TQFTs. For instance, the integer quantum Hall phase is captured by a theory with no dynamical fields but whose response to a background $U(1)$ gauge field is given by a Chern-Simons Lagrangian [Wen07]. A number of the properties of integer quantum Hall phases can be read off

[1] While it is accepted that these criteria are necessary, it is common to include additional physical assumptions, e.g. that ψ is a *spin liquid* as in [Wen07]. In this thesis, such additional assumptions will not play a role and it will only be important that topological phases satisfy the criteria 1 - 3 above.

from this Lagrangian, including quantization of Hall conductance, and the presence of chiral edge modes.

Despite the success of TQFT in describing the phenomenology of the quantum Hall effect and other topological phases, on a theoretical level it leaves much to be desired. One problem is that it doesn't give a microscopic explanation of the emergence of these properties. Another difficulty is that TQFTs are hard to classify beyond 2+1 dimensions. Perhaps the most serious problem is that it is not known in general whether all topological phases are described by TQFTs.

Microscopic description of topological phases via lattice models

In order to address these questions one must move beyond field theory, and study microscopic models of topological phases. Quantum lattice systems in infinite volume are the microscopic models of choice in this thesis. One begins by specifying a lattice system with an onsite[2] action of a symmetry group G (which can be the trivial group in the case that we do not wish to impose any symmetry). The objects of study are local Hamiltonians H , which we require to be G-invariant. The requirements 1 - 3 are expressed in the lattice formalism as follows:

1. Zero temperature $\leftrightarrow$ We are interested in the groundstate ψ of H.
2. No spontaneous symmetry breaking $\leftrightarrow$ ψ is invariant under all relevant symmetries.
3. No local low-energy excitations in the bulk $\leftrightarrow$ ψ is gapped.

Zero-temperature phase transitions occur when the gap closes, so two Hamiltonians are in the same phase if one can be smoothly deformed to the other such that each intermediate Hamiltonian is gapped. A key fact is that two gapped Hamiltonians are in the same phase if and only if their groundstates are related by a *locally-generated automorphism* or LGA. This implies that one may study topological phases of matter in terms of the state ψ alone, without reference to a particular parent Hamiltonian H. This fact has the physical interpretation that topological phases are patterns of entanglement in a state

[2] One can also include non-onsite symmetries such as lattice translations, but we do not consider this in the present work.

ψ, since it is known that LGAs cannot change the long-distance entanglement structure of the state.

Topological invariants

To study topological phases of states on the lattice, one looks for invariants: functions of the state which take on a single value within a phase of matter. An example is the Hall conductance, which labels the distinct integer quantum Hall phases. By the discussion above, any function which can be defined for gapped states and remains unchanged under the action of an LGA is an invariant of the topological phase, i.e. a *topological invariant*.

The first two Chapters of this thesis concern a family of such invariants which can be explicitly constructed in the lattice setting. These invariants generalize the Hall conductance in that they correspond to topological terms in the effective action for background gauge fields. Like the Hall conductance, they can be defined in terms of response functions, and can be related to properties of gapless edge excitations.

In Chapter 2, we focus on two particular invariants: the higher Berry curvature and the higher Thouless pump. We prove that they satisfy two properties that are expected from field theory. First, they take on quantized values for an appropriate class of states. Second, a physical process involving flux insertion relates the higher Thouless pump to the Berry curvature. In Chapter 3, we consider the general class of invariants to which the previous invariants belong. We show that they can be interpreted in terms of a lattice version of the t'Hooft anomaly, which again confirms, in the context of lattice models, an expectation from field theory.

1.2 Background for Chapters 4 and 5: Hamiltonian learning from Gibbs states

The second half of this thesis concerns systems in thermal equilibrium at finite temperature. Specifically, we will be concerned with the problem of *Hamiltonian learning*: let H be an unknown Hamiltonian on a lattice of n qubits, i.e. $H = \sum_{i=1}^{m} \lambda_i E_i$ where $E_1, \ldots, E_m$ is a suitable set of local Hermitian operators and $\lambda_1 \ldots \lambda_m \in \mathbb{R}$ is a set of unknown coefficients. The problem is to estimate the coefficients $\lambda_1, \ldots, \lambda_m$ using projective measurements on a Gibbs state of H. More precisely, we have:

Problem (Hamiltonian learning)**.** *Given access to N independent copies of $\rho = e^{-\beta H} / \operatorname{Tr}\big(e^{-\beta H}\big)$, estimate $\lambda_1, \ldots, \lambda_m$ to accuracy better than ε with probability greater than 0.99, for a given $\varepsilon > 0$.*

There are three important complexity measures to characterize the complexity of a given Hamiltonian learning algorithm as a function of the system size n and the parameters ε and δ. The *sample complexity* is the number N of copies of ρ required, and the *classical* (resp. *quantum*) *computational complexity* is the number of classical (resp. quantum) operations required. In order to be practically useful, one requires all three complexities to be polynomial in n and ε^{-1}.

In Chapter 4 we introduce an algorithm for the Hamiltonian learning problem. It is based on a set of correlation inequalities known as the *energy-entropy balance* or *EEB* inequalities. We give numerical evidence that the complexity is polynomial in n and ε^{-1}, with modest constants, so that the algorithm scales well enough for near-term applications.

In Chapter 5 we equip the above algorithm with rigorous *a posteriori* bounds on the coefficients $\lambda_1, \ldots, \lambda_m$. Furthermore, for commuting Hamiltonians, we prove *a priori* convergence, establishing rigorously that for this class of Hamiltonians the algorithm has polynomial complexity.

Chapter 2

QUANTIZATION OF THE HIGHER BERRY CURVATURE AND THE HIGHER THOULESS PUMP

The following Chapter is published as

[AKS24] Adam Artymowicz, Anton Kapustin, and Nikita Sopenko. "Quantization of the Higher Berry Curvature and the Higher Thouless Pump". In: *Communications in Mathematical Physics* 405.8 (July 2024). ISSN: 1432-0916. DOI: 10.1007/s00220-024-05026-2. URL: http://dx.doi.org/10.1007/s00220-024-05026-2.

2.1 Introduction

A smooth family of gapped Hamiltonians on a finite-dimensional Hilbert space defines a smooth vector bundle on the parameter space: the bundle of ground states [Sim83]. Its Chern classes are topological invariants of the family taking values in the integral cohomology of the parameter space. Their de Rham representatives are closed differential forms which are polynomials in the curvature of the celebrated Berry connection [Ber84]. The simplest of them is the trace of the Berry curvature divided by 2π, which is a closed 2-form with integral periods. It is the de Rham representative of the first Chern class of the bundle of ground states.

It is of considerable interest to generalize the Berry connection and the associated topological invariants to families of gapped infinite-volume systems in d spatial dimensions. From the field theory viewpoint, such topological invariants should describe topological terms in the effective action for $(d+1)$-dimensional σ-model obtained by integrating out the gapped degrees of freedom. If a continuous symmetry G is present for all values of the parameters, these terms may also depend on the gauge field for G. Such topological terms are known as (equivariant) Wess-Zumino-Witten terms (see [DF99] for a brief review), and the Berry connection can be viewed as a special case corresponding to $d = 0$ and trivial symmetry group. Non-trivial Wess-Zumino-Witten terms signal the presence of gapless loci in the parameter space [HKT20]. They also probe the topology of the space of gapped systems and thus can be used to test the Kitaev conjecture which posits that spaces of "invertible" gapped systems in all dimensions fit into a loop spectrum in the sense of homotopy theory [Kit].

Recent works [KS20b; KS20c; KS22] constructed some topological invariants of smooth families of infinite-volume gapped lattice systems. They showed how to assign a de Rham class $[\omega^{(d+2)}] \in H^{d+2}(M, \mathbb{R})$ to a smooth family of lattice systems on $\mathbb{R}^d$ parameterized by M. Since for $d = 0$ this class reduces to the cohomology class of the curvature of the Berry connection, the generalization to $d > 0$ is called the higher Berry class. By the usual Chern-Weil theory, the cohomology class of the Berry curvature is an obstruction for the existence of a global trivialization of the bundle of ground states. Similarly, the higher Berry class is an obstruction for the existence of a smooth family of automorphisms which maps the family of ground states to a constant family [KS22]. For G-equivariant families, where G is a compact connected Lie group, there is an equivariant refinement of higher Berry classes taking values in the equivariant cohomology $H^{d+2}_G(M, \mathbb{R})$ [KS22]. The higher Berry classes, as well as the equivariant higher Berry classes for $G = U(1)$, are reviewed in Section 2.2 below.

By analogy with the $d = 0$ case, one may ask if higher Berry classes are "quantized", or more precisely, if they can be refined to integral cohomology classes. A simple argument shows that this is not possible for arbitrary families of gapped systems. Let $d = 2$, $M = \{pt\}$ and $G = U(1)$. In this case the higher Berry class takes values in $H^4_{U(1)}(pt, \mathbb{R}) \simeq \mathbb{R}$ and is proportional to the Hall conductance [KS22]. It is well known that the Hall conductance of 2d gapped systems is not quantized, in general [Lau83]. Nevertheless, it can be shown to be quantized for short-range entangled systems, or more generally, for systems in an invertible phase [HM14; BBR24; Bac+19; KS20a]. One might hope that for such systems all higher Berry classes can be refined to integral cohomology classes. The only other case where this was shown to be true is $d = 1$, G a compact topological group, and $M = S^1$ (with G acting trivially on S^1), where the equivariant higher Berry class measures the net charge pumped across a section of a 1d system under a periodic variation of parameters [BBR24; Bac+22; KS20a]. This quantity is known as the Thouless pump [Tho83].[1]

[1] Quantization of the Thouless pump holds for arbitrary gapped 1d families. This is not

In this paper, we show how to construct integral refinements of higher Berry classes in two other interesting situations. The first one (Theorem 2.4.1) is $d = 1$, G trivial, M arbitrary. In this case the higher Berry class takes values in $H^3(M, \mathbb{R})$ and we show how to refine it to a class in $H^3(M, \mathbb{Z})$ for families of invertible 1d systems. At least for $M = S^3$, the integrality of the higher Berry class is very natural since it measures the flow of ordinary Berry curvature in a cyclic process [Wen+23]. The second case (Theorem 2.5.2) is $d = 2$, $G = U(1)$, M arbitrary with a trivial $U(1)$ action. In this case the equivariant higher Berry class takes values in $H^4_{U(1)}(M, \mathbb{R}) = H^4(M, \mathbb{R}) \oplus H^2(M, \mathbb{R}) \oplus H^0(M, \mathbb{R})$, where the three components correspond to the non-equivariant higher Berry class, the 2d generalization of the Thouless pump, and the Hall conductance, respectively. We show that for invertible 2d systems the $H^2(M, \mathbb{R})$ component can be refined to a class in $H^2(M, \mathbb{Z})$.

Our proof of Theorem 2.5.2 is based on a new physical interpretation of the 2d Thouless pump as the Berry curvature of a fluxon[2]. Given any $U(1)$-invariant state, one can obtain a new $U(1)$-invariant state by inserting a 2π flux. We will always choose the gauge transformation producing the flux insertion to be concentrated on a line in physical space terminating at the flux insertion point, which we will call the Dirac string. Given a family ψ_M of gapped $U(1)$-invariant systems (with a fixed $U(1)$ action) parameterized by M, one may form a new family ψ_{fluxon} over M by performing a flux insertion on each state in the family ψ_M. Since ψ_M and ψ_{fluxon} are families of 2d states, their (ordinary) Berry curvatures are divergent, but because the flux insertion is a point-like object, the *excess* Berry curvature of ψ_{fluxon} should be a well-defined 2-form on M. We obtain an expression for it as follows. Performing the flux insertion continuously, we have a family ψ of states on $M \times I$, $I = [0, 2\pi]$, which restricts to ψ_M and ψ_{fluxon} on $\partial(M \times I) = M \sqcup M$ (see Figure 2.2 in Section 2.5). Let D be a large disc in physical space containing the point where the flux insertion occurs. If $\nu \in \Omega^3(M \times I)$ is a 3-form which measures the current of ordinary Berry curvature flowing into the disc D then the excess Berry curvature of ψ_{fluxon} is given by the fiber integral $\int_I \nu \in H^2(M, \mathbb{R})$. Since we are taking a fiber integral of ν, we are only interested in its vertical component[3], which we

surprising, since all gapped 1d systems are believed to be short-range entangled.

[2]This should be compared to Laughlin's interpretation of the Hall conductance as the charge of a fluxon — see [Lau81] for the original argument and [KS20a] for a version Laughlin's argument in the formalism used in this work.

[3]The space of vertical forms on $M \times I$ is the quotient of $\Omega^\bullet(M \times I)$ by those ω for which

will call ν_{vert}. This component contains contributions only from the point at which the Dirac string intersects the boundary of D, and is thus $O(1)$ in the size of D. By contrast, the other components of ν will contain contributions from the whole boundary of D.

In this work, we perform the flux insertion "at infinity". This involves moving the flux insertion point off to infinity so that the Dirac string goes along the y-axis without terminating (see Figure 2.1 in Section 2.5). ψ is now a family of states on $M \times S^1$ such that for $x \in M$ and $\theta \in S^1$, $\psi_{(x,\theta)}$ equals $(\psi_M)_x$ with a θ-domain wall inserted on the y-axis, and ν measures the Berry curvature pumped along the domain wall. As discussed in [Wen+23], the pumping of Berry curvature is given by the higher Berry form $\omega^{(3)}$, and so $\nu = \omega^{(3)}$. Only the vertical component ν_{vert} of this form is well-defined, and in Section 2.5 we extract this component and show that it equals $\mu \wedge d\theta$, where $\mu \in \Omega^2(M)$ is a representative of the 2d Thouless pump invariant. In Section 2.5 we show that if the states in question are invertible then the proof of ordinary 1d Berry curvature quantization can be adapted to show that ν_{vert}, and thus the 2d Thouless invariant, is quantized.

Note that the relation $\nu_{vert} = \mu \wedge d\theta$ holds regardless of whether the family of systems in question is in an invertible phase or not. In particular, for topologically ordered 2d systems it may happen that the excess Berry curvature associated with a flux insertion has periods which are fractions of 2π. This is similar to how the charge of a flux insertion can be a fraction if the system is topologically ordered [Lau83].

A construction of the integral refinement of the higher Berry class for 1d systems was announced in [KS22]. A similar integral invariant was also introduced in the thesis [D23], but the connection to the higher Berry curvature was not proven there. We were informed by Y. Ogata about a different approach to the integral higher Berry class for continuous families of 1d and 2d spin systems [OK]. While this paper was in preparation, there appeared two papers which discuss the integral higher Berry class in the context of Matrix Product States [OTS23; OR23].

$\iota_X \omega = 0$ for $X = \frac{\partial}{\partial\theta}$.

2.2 Framework

A recent work [KS22] by the last two authors (TODO: go through and remove such references) introduced a framework for studying smoothly varying families of ground states of infinite-volume quantum statistical mechanical systems, and showed how this framework produces certain cohomological invariants, the (equivariant) higher Berry invariants. Since these are the subject of this paper, we begin by recalling this machinery. The reader is referred to [KS22] for all proofs.

Observables and derivations

We will be working with quantum lattice systems on the lattice $\mathbb{Z}^d$ for $d > 0$ (we will only need $d = 1, 2$ in what follows)[4]. We endow the lattice $\mathbb{Z}^d$ with the L^∞ metric[5] which we denote $d(\cdot,\cdot)$, and for a site j and an integer r we denote by $B_j(r)$ the ball of radius r around j. For a subset $\Lambda \subset \mathbb{Z}^d$ we define $\Lambda(r) := \{j \in \mathbb{Z}^d : d(j,\Lambda) \leq r\}$.

Fix $D > 0$ and associate to each site $j \in \mathbb{Z}^d$ the C*-algebra $\mathscr{A}_j := \mathcal{B}(\mathbb{C}^D)$ of linear operators on $\mathbb{C}^D$. To any finite subset X of $\mathbb{Z}^d$ we associate the algebra $\mathscr{A}_X := \bigotimes_{j\in X} \mathscr{A}_j$. For $X \subset X'$ we have the norm-preserving inclusion $\mathscr{A}_X \subset \mathscr{A}_{X'}$ taking $A \mapsto A \otimes \mathbf{1}$ and the union of the resulting net $\mathscr{A}_\ell = \cup_X \mathscr{A}_X$ is the **algebra of local observables**. It is a normed $*$-algebra which can be completed to form the C^*-algebra $\mathscr{A} := \overline{\mathscr{A}_\ell}^{\|\cdot\|}$ which we call the **algebra of quasilocal observables**. For an infinite subset $X \subset \mathbb{Z}^d$ we write $\mathscr{A}_X$ for the norm closure of $\cup \mathscr{A}_{Y\subset X}$, where Y ranges over all finite subsets of X.

We denote by $\overline{\mathrm{tr}}(A)$ the state which is defined on local observables $A \in \mathscr{A}_X$ by $\frac{1}{D^{|X|}}\overline{\mathrm{tr}}(A)$, where $|X|$ denotes the cardinality of X. We also have, for any (possibly infinite) subset $X \subset \mathbb{Z}^d$ the conditional expectation $\overline{\mathrm{tr}}_X$ onto $\mathscr{A}_{X^c}$, which is defined by the condition $\overline{\mathrm{tr}}_X(A \otimes B) := \overline{\mathrm{tr}}(A)B$ whenever $A \in \mathscr{A}_Y$ and $B \in \mathscr{A}_Z$ with $Y \subset X$ and $Z \subset X^c$.

Given two algebras of quasilocal observables $\mathscr{A}$ and $\mathscr{A}'$ with on-site dimensions D and D' we define $\mathscr{A} \otimes \mathscr{A}'$ to be the norm closure of $\otimes_j(\mathscr{A}_j \otimes \mathscr{A}'_j)$. It is also a quasilocal algebra, with on-site dimension DD'. Physically, it corresponds

[4] All results can be easily generalized to lattice systems whose sites are an arbitrary Delone subset of $\mathbb{R}^d$.

[5] This is done purely for convenience. In [KS22] Euclidean metric is used, but since each of the two metrics on $\mathbb{R}^d$ is upper-bounded by a multiple of the other, all the results in [KS22] remain true for the L^∞ metric.

to the “stacking” of two lattice systems described by algebras $\mathscr{A}$ and $\mathscr{A}'$.

In what follows we will rarely refer to the quasilocal algebra. Instead, we will mostly work with a subalgebra of $\mathscr{A}$ obtained by imposing a stricter notion of locality. For each $j \in \mathbb{Z}^d$ and $\alpha \in \mathbb{Z}_{\geq 0}$ we may define a seminorm on $\mathscr{A}_\ell$ by

$$\|A\|_{j,\alpha} := \|A\| + \sup_r (1+r)^\alpha \inf_{B \in \mathscr{A}_{B_j(r)}} \|A - B\|. \tag{2.1}$$

Fixing any $j \in \mathbb{Z}^d$ and allowing $\alpha \in \mathbb{Z}_{\geq 0}$ to vary we obtain a family of seminorms. The completion $\mathscr{A}_{al} := \overline{\mathscr{A}}^{\|\cdot\|_{j,\cdot}}$ with respect to this family of seminorms, which we term the **algebra of almost-local observables**, is a Fréchet space. The seminorms $\|\cdot\|_{j,\alpha}$ and $\|\cdot\|_{k,\alpha}$ are equivalent for any $j, k \in \mathbb{Z}^d$ so the resulting space and its topology do not depend on the choice of j.

For any $f : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ we say a quasilocal observable $A \in \mathscr{A}$ is f-confined at a site $j \in \mathbb{Z}^d$ if $\inf_{B \in \mathscr{A}_{B_j(r)}} \|A - B\| \leq f(r)$ for all $r \in \mathbb{Z}_{\geq 0}$. A function $f : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ has **superpolynomial decay** if $f(r) r^\alpha \to 0$ for all $\alpha \in \mathbb{Z}_{\geq 0}$, and $\mathscr{A}_{al}$ can alternatively be characterized as the set of quasilocal observables that are f-confined on a site j for some function f with superpolynomial decay.

In the most common approach to lattice systems in infinite volume, time-evolution is implemented by a strongly-continuous one-parameter family of automorphisms of $\mathscr{A}$. The generator of these automorphisms is a densely-defined derivation of $\mathscr{A}$. The appearance of densely-defined derivations is unavoidable because $\mathscr{A}$ has no nonzero globally defined outer derivations [Sak67], and the generator of time-evolution is typically outer. From this perspective the subalgebra $\mathscr{A}_{al}$ acts as a minimal domain of definition for physically relevant derivations[6]. In contrast to $\mathscr{A}$, the algebra $\mathscr{A}_{al}$ has many interesting globally-defined outer derivations, some of which we describe here. Below, all derivations are taken to satisfy $D(A^*) = D(A)^*$.

We call a **brick** in $\mathbb{Z}^d$ any subset of the form $X = \mathbb{Z}^d \cap \prod_{k=1}^d [a_i, b_i]$ for some $a_i, b_i \in \mathbb{Z}$ with $-\infty < a_i < b_i < \infty$. Let F be a derivation of $\mathscr{A}_{al}$. Given a brick X, $\overline{\mathrm{tr}}_{X^c} \circ \mathsf{F}|_{\mathscr{A}_X}$ is a derivation of $\mathscr{A}_X$ which is necessarily equal to conjugation by a unique traceless skew-adjoint element of $\mathscr{A}_X$ which we call F_X. Each $\mathscr{A}_X$ has an inner product given by $(A, B) := \overline{\mathrm{tr}}(A^* B)$, and we define F^X as the projection of F_X onto the orthogonal complement of $\bigoplus_Y \mathscr{A}_Y$, where Y ranges

[6] An analogy can be made with $C^\infty(\mathbb{R})$, which embeds into larger function spaces like $C(\mathbb{R})$ (the C* algebra of continuous functions on $\mathbb{R}$) as the minimal domain of definition for all differential operators.

over all bricks strictly contained in X. This way we have $\mathsf{F}_X = \sum_{Y \subset X} \mathsf{F}^Y$, and the **brick decomposition** of F is the formal sum

$$\mathsf{F} = \sum_X \mathsf{F}^X \tag{2.2}$$

with X ranging over all bricks in $\mathbb{Z}^d$. Using brick decompositions one can define a family of seminorms, indexed by $\alpha \in \mathbb{Z}_{\geq 0}$, on the space of derivations:

$$\|\mathsf{F}\|_\alpha := \sup_X (1 + \operatorname{diam}(X))^\alpha \|\mathsf{F}^X\|, \tag{2.3}$$

and we call a derivation **uniformly almost-local** (UAL) if $\|\mathsf{F}\|_\alpha < \infty$ for all $\alpha \in \mathbb{Z}_{\geq 0}$. We denote the space of UAL derivations by $\mathfrak{D}_{al}$ — it is a Fréchet space with respect to the locally convex topology generated by these seminorms. Furthermore, for any $\mathsf{F} \in \mathfrak{D}_{al}$ and any $A \in \mathscr{A}_{al}$, the sum $\mathsf{F}(A) = \sum_X \mathsf{F}^X(A)$ is absolutely convergent in the Fréchet topology on $\mathscr{A}_{al}$, and in particular in the uniform topology. It follows that $\overline{\operatorname{tr}}(\mathsf{F}(A)) = 0$ for any $\mathsf{F} \in \mathfrak{D}_{al}$ and any $A \in \mathscr{A}_{al}$.

The space of UAL derivations admits a certain kind of resolution by (higher) currents which we now describe. For $n > 0$ we define an **n-chain** f to be a collection $\mathsf{f}_{j_1,\ldots,j_n}$ of almost-local observables indexed by $(\mathbb{Z}^d)^n$ that are

i) Traceless:

$$\overline{\operatorname{tr}}(\mathsf{f}_{j_1,\ldots,j_n}) = 0 \tag{2.4}$$

ii) Skew-adjoint:

$$\mathsf{f}^*_{j_1,\ldots,j_n} = -\mathsf{f}_{j_1,\ldots,j_n} \tag{2.5}$$

iii) Skew-symmetric:

$$\mathsf{f}_{j_1,\ldots,j_n} = (-1)^{|\sigma|} \mathsf{f}_{j_{\sigma(1)},\ldots,j_{\sigma(n)}} \tag{2.6}$$

for any permutation σ of $\{1, \ldots, n\}$,

iv) Uniformly localized: for any $\alpha \in \mathbb{Z}_{\geq 0}$ we have

$$\sup_{j_1,\ldots,j_n \in \mathbb{Z}^d} \sup_{1 \leq i \leq n} \|\mathsf{f}_{j_1,\ldots,j_n}\|_{j_i,\alpha} < \infty. \tag{2.7}$$

Remark 2.2.1. *Our grading convention is shifted by* 1 *compared to Ref. [KS22].*

For $n > 0$ we define C^{-n} as the Fréchet space of n-chains with seminorms given by (2.7) for all $\alpha \geq 0$. We extend this $n = 0$ by letting $C^0 = \mathfrak{D}_{al}$. These form a (non-positively graded) cochain complex with the differential $\partial : C^{-n-1} \to C^{-n}$ is defined for $n > 0$ by

$$(\partial \mathsf{f})_{j_1,\dots,j_n} = \sum_{j_0 \in \mathbb{Z}^d} \mathsf{f}_{j_0,\dots,j_n}. \tag{2.8}$$

For $n = 0$ it is defined by

$$\partial \mathsf{f}(A) = \sum_{j \in \mathbb{Z}^d} [\mathsf{f}_j, A], \tag{2.9}$$

for any $A \in \mathscr{A}_{al}$. What's more, there is a graded Lie bracket $C^{-m} \times C^{-n} \to C^{-m-n}$ which is defined for $m, n > 0$ as

$$\{\mathsf{f}, \mathsf{g}\}_{j_1,\dots,j_{m+n}} := \sum_{\sigma} \frac{\operatorname{sgn}(\sigma)}{m!n!} [\mathsf{f}_{j_{\sigma(1)},\dots,j_{\sigma(m)}}, \mathsf{g}_{j_{\sigma(m+1)},\dots,j_{\sigma(m+n)}}], \tag{2.10}$$

where the sum is taken over all permutations on $m + n$ symbols. For $m = 0$ and $n > 0$ we let

$$\{\mathsf{F}, \mathsf{f}\}_{j_1,\dots,j_n} = [\mathsf{F}, \mathsf{f}_{j_1,\dots,j_n}], \tag{2.11}$$

while for $m = n = 0$ we let $\{\mathsf{F}, \mathsf{G}\} = [\mathsf{F}, \mathsf{G}]$. The differential ∂ and the graded bracket $\{\cdot, \cdot\}$ make $C^\bullet = \oplus_{n=0}^{\infty} C^{-n}$ into a (non-positively graded) dg-Lie algebra.

We conclude this section with a description of the class of automorphisms of $\mathscr{A}_{al}$ obtained by integrating paths of UAL derivations. Let $\mathsf{F} : \mathbb{R} \to \mathfrak{D}_{al}$ be a smooth path of derivations, denoted $t \mapsto \mathsf{F}_t$. By Prop. E.1 of [KS22], for every $A \in \mathscr{A}_{al}$ there is a unique smooth path $t \mapsto A_t \in \mathscr{A}_{al}$ of observables satisfying $A_0 = A$ and $\frac{dA_t}{dt} = \mathsf{F}_t(A_t)$. For each $t \in \mathbb{R}$ this gives a map $A \mapsto A_t$ which is a $*$-automorphism of $\mathscr{A}_{al}$ that extends to a $*$-automorphism of $\mathscr{A}$. We denote it

$$\tau \exp\left(\int_0^t \mathsf{F}_t dt\right). \tag{2.12}$$

We call automorphisms obtained in this way **locally generated automorphisms** or LGAs for short. These have an action on $\mathfrak{D}_{al}$ by conjugation which we write as

$$\alpha(\mathsf{F}) := \alpha \circ \mathsf{F} \circ \alpha^{-1}. \tag{2.13}$$

This action can be promoted to an action on the entire complex $C^\bullet$ which commutes with the differential by allowing an LGA to act on an n-chain elementwise: $\alpha(\mathsf{f})_{j_1,\dots,j_n} := \alpha(\mathsf{f}_{j_1,\dots,j_n})$.

States

If ψ is a state on $\mathscr{A}$ and α is an LGA, we write $\psi^\alpha := \psi \circ \alpha$. The fixed points of this action will play an important role in what follows. We say α preserves ψ if $\psi^\alpha = \psi$. A derivation $\mathsf{F} \in \mathfrak{D}_{al}$ is said to preserve ψ if $\psi(\mathsf{F}(A)) = 0$ for all $A \in \mathscr{A}_{al}$. An observable $A \in \mathscr{A}_{al}$ is said to preserve ψ if $\psi(\mathsf{F}(A)) = 0$ for all $\mathsf{F} \in \mathfrak{D}_{al}$. We write $\mathfrak{D}_{al}^\psi$ and $\mathscr{A}_{al}^\psi$ for the derivations and observables that preserve ψ; these are closed subspaces of $\mathfrak{D}_{al}$ and $\mathscr{A}_{al}$ in their respective Fréchet topologies. Unitary elements of $\mathscr{A}_{al}^\psi$ satisfy the following properties:

Lemma 2.2.1. *If $V \in U(\mathscr{A}_{al})$ preserves ψ then $\psi(V) \in U(1)$, and $\psi(VA) = \psi(V)\psi(A)$ for any $A \in \mathscr{A}_{al}$.*

Proof. Since $\mathscr{A}_{al}$ is norm-dense in $\mathscr{A}$, we have $\psi(VB) = \psi(BV)$ for any $B \in \mathscr{A}$. Let $A \in \mathscr{A}_{al}$ and let $(\mathcal{H},\, \pi,\, \Omega)$ be the GNS triple of ψ. Since ψ is pure, π is irreducible. In particular $\pi(\mathscr{A})$ is weakly dense in the bounded operators on $\mathcal{H}_\psi$, so there is a sequence $\{P_k\}_{k\in\mathbb{Z}_{\geq 0}}$ of elements of $\mathscr{A}$ such that $\pi(P_k)$ converges weakly to $P = |\Omega\rangle\langle\Omega|$, and we have

$$\begin{aligned} \psi(VA) &= \lim_{k\to\infty} \psi(VAP_k) \\ &= \lim_{k\to\infty} \psi(AP_kV) \\ &= \psi(A)\psi(V), \end{aligned} \tag{2.14}$$

which proves the second statement. The first follows from $\overline{\psi(V)}\psi(V) = \psi(V^*V) = 1$. □

The space $\mathfrak{D}_{al}^\psi \subset \mathfrak{D}_{al}$ is a Lie subalgebra which can be resolved to a dg-Lie subalgebra $C_\psi^\bullet \subset C^\bullet$. We put $C_\psi^0 := \mathfrak{D}_{al}^\psi \subset \mathfrak{D}_{al}$, while for $k > 0$ we define C_ψ^{-k} to be the (closed) subspace of k-chains f for which $\mathsf{f}_{j_1,\dots,j_k} \in \mathscr{A}_{al}^\psi$ for all $j_1,\dots,j_k \in \mathbb{Z}^d$. It is easy to see that $C_\psi^\bullet$ is preserved by the differential ∂ and is closed with respect to the bracket $\{\,,\}$.

We will be interested in several special classes of pure states. For states ψ,ψ' on quasilocal algebras $\mathscr{A}$ and $\mathscr{A}'$, we write $\psi \otimes \psi'$ for the resulting state on the quasilocal algebra $\mathscr{A} \otimes \mathscr{A}'$.

Definition 2.2.1. *Let ψ be a pure state of $\mathscr{A}$. We say ψ is*

i) ***factorized*** *if for each $j \in \mathbb{Z}^d$ there is a pure state ψ_j on $\mathscr{A}_j$ such that $\psi|_{\mathscr{A}_j} = \psi_j$,*

ii) ***short-range entangled*** *(SRE for short) if there exists an LGA α such that $\psi \circ \alpha$ is a factorized pure state,*

iii) ***invertible*** *if there is another state ψ' such that $\psi \otimes \psi'$ is SRE,*

iv) ***gapped*** *if there is a $\mathsf{H} \in \mathfrak{D}_{al}$ such that ψ is a gapped ground state of H. That is, there exists $\Delta > 0$ such that $-i\psi(A^*\mathsf{H}(A)) \geq \Delta(\psi(A^*A) - |\psi(A)|^2)$ for all $A \in \mathscr{A}_{a\ell}$.*

Factorized states model trivial systems. Short-range entangled states model systems in a trivial topological phase as they can be prepared from factorized states by a local Hamiltonian evolution [Zen+19]. Invertible states model systems in invertible topological phases as introduced by A.Kitaev [Kit]. These are phases that have inverses, i.e., it is possible to stack the system with another system, such that the composite is in a trivial phase.

Proposition 2.2.1. *Every invertible state is gapped.*

Proof. Given a state $\psi \otimes \psi'$ and an observable $A \in \mathscr{A} \otimes \mathscr{A}'$, one can define a partial average $\psi'(A) \in \mathscr{A}$ that on observables of the form $\mathcal{O} \otimes \mathcal{O}' \in \mathscr{A} \otimes \mathscr{A}'$ is given by $\psi'(\mathcal{O} \otimes \mathcal{O}') := \psi'(\mathcal{O}')\mathcal{O}$. The value on general observables is obtained by linear extension, and it is a standard fact that the resulting map is a conditional expectation; in particular, we have $\|\psi'(A)\| \leq \|A\|$. For any $A \in \mathscr{A}_{a\ell}$ and $r \geq 0$, we have

$$\inf_{B \in \mathscr{A}_{B_j(r)}} \|B - \psi'(A)\| \leq \inf_{B \in (\mathscr{A} \otimes \mathscr{A}')_{B_j(r)}} \|\psi'(B - A)\| \leq \inf_{B \in (\mathscr{A} \otimes \mathscr{A}')_{B_j(r)}} \|B - A\|, \tag{2.15}$$

and so partial averaging takes almost-local observables to almost-local observables. We also define partial averaging of a derivation $\mathsf{F} \in \mathfrak{D}_{al}$ by $\psi'(\mathsf{F})(A) = \psi'(\mathsf{F}(A \otimes \mathbf{1}))$ for any $A \in \mathscr{A}_{a\ell}$, which is again a derivation because ψ' is a conditional expectation.

Let $(\psi', \mathscr{A}')$ be an inverse of $(\psi, \mathscr{A})$, and let α be an LGA on the composite system $\mathscr{A} \otimes \mathscr{A}'$ such that $\Psi_0 := (\psi \otimes \psi') \circ \alpha$ is factorized. Let us choose a

UAL derivation F for the composite system such that Ψ_0 is a gapped ground state for F with a gap greater than $\Delta > 0$ (we can choose F to be $\partial\mathsf{f}$ for an on-site $\mathsf{f} \in C^1$). Then $(\psi \otimes \psi')$ is a gapped ground state for $\alpha(\mathsf{F})$. Let H be a UAL derivation of $\mathscr{A}$ obtained from $\alpha(\mathsf{F})$ by partial averaging over ψ'. Then for any $A \in \mathscr{A}_{a\ell}$ we have

$$\begin{aligned} - i\psi(A^*\mathsf{H}(A)) = -i(\psi \otimes \psi')(\alpha(B^*)\alpha(\mathsf{F}(B))) = -i\Psi_0(B^*\mathsf{F}(B)) \geq \\ \geq \Delta\left(\Psi_0(B^*B) - |\Psi_0(B)|^2\right) = \Delta\left(\psi(A^*A) - |\psi(A)|^2\right), \quad (2.16) \end{aligned}$$

where $B = \alpha^{-1}(A \otimes 1)$. Thus, ψ is a gapped ground state for H with a gap greater than $\Delta > 0$. □

It is believed that every 1d gapped state is invertible. For $d > 1$ there are many examples of gapped states which are not invertible (for example, topologically ordered states).

We now turn to the situation when the state is a smooth function of some parameter space M, which we take to be a smooth manifold. The set $C^\infty(M, C^\bullet)$ of smooth functions[7] $M \to C^\bullet$ is a cochain complex valued in $C^\infty(M)$-modules. Suppose that $\{\psi_x\}_{x\in M}$ is a family of states parametrized by points of M. Then the set

$$C^\infty(M, C^\bullet_\psi) := \{f \in C^\infty(M, C^\bullet) : f(x) \in C^\bullet_{\psi_x}\ \forall x \in M\} \quad (2.17)$$

is another cochain complex valued in $C^\infty(M)$-modules. For any $k > 0$, we set $\Omega^k(M, C^\bullet) := \mathrm{Hom}_{C^\infty(M)}(\wedge^k TM, C^\infty(M, C^\bullet))$. Similarly, we define $\Omega^k(M, C^\bullet_\psi) := \mathrm{Hom}_{C^\infty(M)}(\wedge^k TM, C^\infty(M, C^\bullet_\psi))$.

Definition 2.2.2. *Let $\psi = \{\psi_x\}_{x\in M}$ be family of states indexed by points of a smooth manifold M. We say ψ is **smooth** if for every $A \in \mathscr{A}_{al}$ the function $x \mapsto \psi_x(A)$ is a smooth function on M, and there is a $\mathsf{G} \in \Omega^1(M, \mathfrak{D}_{al})$ such that*

$$d\psi(A) = \psi(\mathsf{G}(A)) \quad \forall A \in \mathscr{A}_{al}. \quad (2.18)$$

We say ψ is **parallel** with respect to G if (2.18) holds. We will sometimes write (ψ, G) for a smooth family when we want to specify a particular G with respect to which it is parallel.

[7]That is, functions $f^k : M \to C^k$ for each $k \leq 0$ such that in any set of smooth coordinates on M all partial derivatives of f^k exist and are continuous.

We say a smooth family of states is factorized, SRE, or invertible if it is so pointwise. If M is connected, then a smooth family ψ is SRE or invertible if it is so for any one $x_0 \in M$. This happens because two states connected by a smooth path $\gamma : [0,1] \to M$ are related by the LGA obtained by exponentiating (as in (2.12)) G along γ.

We say a smooth family ψ is gapped if there is a $\mathsf{H} \in C^\infty(M, \mathfrak{D}_{al})$ such that ψ_x is a gapped groundstate of $\mathsf{H}(x)$ for each $x \in M$. If M is connected, then ψ is gapped iff it is gapped for any one $x_0 \in M$ (this follows from a partition of unity argument, but we do not prove this here since we will not need this fact). Conversely, if ψ is a family of states such that $\psi_x(A)$ is a smooth function of $x \in M$ for every $A \in \mathscr{A}_{al}$, and if there is a $\mathsf{H} \in C^\infty(M, \mathfrak{D}_{al})$ such that ψ_x is a gapped groundstate of $\mathsf{H}(x)$ for each $x \in M$, then under some extra technical assumptions[8] ψ can be shown to be smooth [KS22; MO20].

We conclude this section with a discussion of smooth families of LGAs.

Definition 2.2.3. *A family of LGAs $\alpha = \{\alpha_x\}_{x \in M}$ is **smooth** if for every $A \in \mathscr{A}_{al}$ the map $M \to \mathscr{A}_{al}$ taking $x \mapsto \alpha_x(A)$ is smooth, and there is a $\mathsf{G} \in \Omega^1(M, \mathfrak{D}_{al})$ such that*

$$d\alpha(A) = \alpha(\mathsf{G}(A)) \quad \forall A \in \mathscr{A}_{al}. \tag{2.19}$$

If such a G exists, it is unique, and we denote it by $\alpha^{-1} d\alpha$.

The most natural way to produce an LGA is to integrate a $\mathfrak{D}_{al}$-valued 1-form along a path, as in (2.12). As we will see below, this can be extended coherently to the setting of smooth families of LGAs. Let M be a manifold and $I = [0, r]$ an interval. Define the vertical complex $\Omega^\bullet(M \times I, C^\bullet)_{vert}$ as the quotient of $\Omega^\bullet(M \times I, C^\bullet)$ by the set of elements a for which $\iota_{\frac{\partial}{\partial \theta}} \mathsf{a} = 0$, and we write a_{vert} for the image of a under the projection to $\Omega^\bullet(M \times I, C^\bullet)_{vert}$, followed by the obvious inclusion back into $\Omega^\bullet(M \times I, C^\bullet)$. Write $j_s : M \to M \times I$ for the inclusion as $M \times \{s\}$.

Proposition 2.2.2. *Let M be a manifold and let $\mathsf{G} \in \Omega^1(M \times I, \mathfrak{D}_{al})$. Then there is a unique smooth family of LGAs α on $M \times I$ satisfying $\alpha \circ j_0 = \mathbf{1}$ and*

$$\frac{d}{ds} \alpha(A) = \alpha(\iota_{\frac{\partial}{\partial s}} \mathsf{G}(A)) \quad \forall A \in \mathscr{A}_{al}, \tag{2.20}$$

where s is the coordinate on I.

[8] See Assumption 1.2 in [MO20].

Proof. Let $\gamma_x : I \to M$ be the function taking $s \mapsto (x, s)$. By [KS22] Prop. E.1, for each $x \in M$ there is a unique solution to (2.20) with $\alpha \circ j_0 = \mathbf{1}$ which we denote by $\alpha_{(x,s)}$ By [KS22] Proposition E.2 we have

$$(\alpha^{-1} d\alpha)_{(x,t)} = -\int_0^t \alpha^{-1}_{(x,t)} \circ \alpha_{(x,s)}(\iota_{\frac{\partial}{\partial s}} d(\mathsf{G}_{vert})_{(x,s)}) ds + \mathsf{G}_{vert} \quad \in \Omega^1(M \times I, \mathfrak{D}_{al}). \tag{2.21}$$

□

Definition 2.2.4. *Given $\mathsf{G} \in \Omega^1(M \times I, \mathfrak{D}_{al})$ and α as in Proposition 2.2.2, we denote $\tau \exp\left(\int_0 \mathsf{G}\right) := \alpha$, while for $s \in I$ we write $\tau \exp\left(\int_0^s \mathsf{G}\right) := \alpha \circ j_s$.*

Notice that $\tau \exp \int_0 \mathsf{G}$ depends only on the vertical component G_{vert} of G. We close this section with a description of a gauge action of smooth families of LGA on on smooth families of states (the proof is straightforward and is omitted):

Proposition 2.2.3. *If (ψ, G) is a smooth family of states on M and α is a smooth family of LGAs on M, then $\psi^\alpha = \psi \circ \alpha$ is parallel with respect to*

$$\mathsf{G}^\alpha := \alpha^{-1}(\mathsf{G}) + \alpha^{-1} d\alpha. \tag{2.22}$$

Higher Berry curvatures and classes

We can now state the main result of [KS22], which allows for the construction of the invariants which are the subject of this paper. Recall that a cochain complex $(K^\bullet, \partial)$ is nullhomotopic if there is a map $h : K^\bullet \to K^{\bullet-1}$ (which we call a contracting homotopy) satisfying $h \circ \partial + \partial \circ h = \mathbf{1}$.

Theorem 2.2.1. *Let M be a smooth manifold.*

i) The cochain complex $C^\bullet$ is nullhomotopic via a contracting homotopy $h : C^\bullet \to C^{\bullet-1}$. For any $k \geq 0$ the unique $C^\infty(M)$-linear extension $h : \Omega^k(M, C^\bullet) \to \Omega^k(M, C^{\bullet-1})$ is also a contracting homotopy.

ii) Suppose ψ is a smooth gapped family of states. Then for every $k \geq 0$ the complex $\Omega^k(M, C^\bullet_\psi)$ is nullhomotopic via a $C^\infty(M)$-linear contracting homotopy $h^\psi : \Omega^k(M, C^\bullet_\psi) \to \Omega^k(M, C^{\bullet-1}_\psi)$.

We can extend the graded bracket on $C^\bullet$ to $\Omega^\bullet(M, C^\bullet)$ by defining the bracket between $\mathsf{a} \in \Omega^p(M, C^k)$ and $\mathsf{b} \in \Omega^q(M, C^\ell)$ as

$$\{\mathsf{a}, \mathsf{b}\}(X_1, \dots, X_{p+q}) = (-1)^{kq} \sum_\sigma \frac{\operatorname{sgn}\sigma}{p!q!} \{\mathsf{a}(X_{\sigma(1)}, \dots X_{\sigma(p)}), \mathsf{b}(X_{\sigma(p+1)}, \dots X_{\sigma(p+q)})\} \tag{2.23}$$

for any vector fields $X_1, \dots, X_{p+q}$. The differentials d and ∂ on $\Omega^\bullet(M)$ and $C^\bullet$ extend naturally to $\Omega^\bullet(M, C^\bullet)$, and we get a total differential which acts on $\mathsf{a} \in \Omega^p(M, C^k)$ by

$$\boldsymbol{d}(\mathsf{a}) := d(\mathsf{a}) + (-1)^p \partial(\mathsf{a}). \tag{2.24}$$

This graded bracket and total differential make $\operatorname{Tot}(\Omega^\bullet(M, C^\bullet))$ into a dg-Lie algebra over $C^\infty(M)$, with $\operatorname{Tot}(\Omega^\bullet(M, C^\bullet_\psi))$ as a dg-Lie subalgebra.

Note that our sign conventions differ from those in [KS22] — in particular our ∂ and d commute instead of anticommuting[9]. This choice will make the explicit calculations in Section 2.5 easier. The price we pay is that although d is a graded derivation of $\operatorname{Tot}(\Omega^\bullet(M, C^\bullet))$, ∂ is not. Instead, $(-1)^p\partial : \Omega^p(C^q) \to \Omega^p(C^{q+1})$ is.

The element $\mathsf{G} \in \Omega^1(M, \mathfrak{D}_{al})$ can be interpreted as a connection 1-form on the trivial graded bundle $M \times C^\bullet$. Its covariant derivative is the graded derivation D of $\operatorname{Tot}(\Omega^\bullet(M, C^\bullet))$ given by $d + \{\mathsf{G}, \cdot\}$. Its curvature $\mathsf{F} \in \Omega^2(M, \mathfrak{D}^\psi_{al})$ satisfies

$$D \circ D(A) = \{\mathsf{F}, A\} \quad \forall A \in \Omega^\bullet(M, C^\bullet) \tag{2.25}$$

and is given by the usual formula $\mathsf{F} = d\mathsf{G} + \frac{1}{2}\{\mathsf{G}, \mathsf{G}\}$.

The higher Berry invariants are constructed by solving the following Maurer-Cartan equation. Recall that $\boldsymbol{d}$ is the total differential on $\operatorname{Tot}(\Omega^\bullet(M, C^\bullet))$, given by (2.24).

Proposition 2.2.4. *Suppose that (ψ, G) is a gapped smooth family. Then there exists an element $\mathsf{g}^\bullet \in \operatorname{Tot}^1(\Omega^\bullet(M, C^\bullet))$, whose component in $\Omega^{n+1}(M, C^{-n})$ we denote*[10] *$\mathsf{g}^{(n)}$, that satisfies $\mathsf{g}^{(0)} = \mathsf{G}$ and*

$$\boldsymbol{d}\mathsf{g}^\bullet + \frac{1}{2}\{\mathsf{g}^\bullet, \mathsf{g}^\bullet\} = 0. \tag{2.26}$$

Furthermore we have $\mathsf{g}^{(n)} \in \Omega^{n+1}(M, C^{-n}_\psi)$ for all $n > 0$.

[9] Explicitly, what we call C^q is called $\mathcal{N}^q$ in [KS22], and what we call $\partial : C^q \to C^{q+1}$ is $(-1)^q\partial : \mathcal{N}^q \to \mathcal{N}^{q+1}$ in the notation of [KS22].

[10] What we call $\mathsf{g}^{(n)}$ was called $g^{(n-1)}$ in [KS22].

We call (2.26) the Maurer-Cartan equation or alternatively the descent equation. The proof of Prop. 2.2.4 in [KS22] involves writing out eq. (2.26) as a system of equations for $\mathsf{g}^{(n)}$

$$d\mathsf{g}^{(n-1)} + (-1)^n \partial \mathsf{g}^{(n)} + \frac{1}{2}\sum_{k=0}^{n-1} \{\mathsf{g}^{(k)}, \mathsf{g}^{(n-k-1)}\} = 0. \tag{2.27}$$

and solving (2.27) successively for $n = 1, 2, \ldots,$ using the exactness of the bi-complex $\Omega^\bullet(M, C_\psi^{-\bullet})$ with respect to ∂ in positive degrees. For this reason, $\mathsf{g}^{(n+1)}$ will be called the descendant of $\mathsf{g}^{(n)}$. Notice that (2.27), together with the fact that $\mathsf{g}^{(n)} \in \Omega^{n+1}(M, C_\psi^{-n})$ for $n > 0$, imply that $d\psi(\mathsf{g}^{(n)}) = \psi(\partial \mathsf{g}^{(n+1)})$.

In Section 2.3 we introduce an operation we call "evaluating against the origin" (equation (2.38)). The evaluation of $\mathsf{g}^{(d+1)}$ at the origin is an element of $\Omega^{d+2}(M, \mathscr{A}_{al})$ denoted by $\langle \mathsf{g}^{(d+1)}, [*] \rangle$. Evaluating $\mathsf{g}^{(d+1)}$ against the origin and applying the family of states ψ to this observable-valued form we obtain a $(d+2)$-form on M:

$$\omega^{(d+2)} := \psi(\langle \mathsf{g}^{(d+1)}, [*] \rangle) \in \Omega^{d+2}(M, \mathbb{C}) \tag{2.28}$$

which is closed because

$$-d\omega^{(d+2)} = (-1)^{d+2}\psi(\langle \partial \mathsf{g}^{(d+2)}, [*] \rangle) + \frac{1}{2}\sum_{k=1}^{d} \psi\big(\langle \{\mathsf{g}^{(k)}, \mathsf{g}^{(d-k+1)}\}, [*] \rangle\big).$$

The first term above vanishes because $\langle \mathsf{h}, [*] \rangle = 0$ wheneverif h is ∂-exact and the second term vanishes because $\psi(\langle \mathsf{h}, [*] \rangle) = 0$ if $\psi(\mathsf{h}_{j_1,\ldots,j_{d+1}}) = 0$ for all $j_1, \ldots, j_{d+1} \in \mathbb{Z}^d$.

Definition 2.2.5. *Suppose (ψ, G) is a smooth family of states such that a solution $\mathsf{G}^\bullet$ of the MC equation (2.26) exists. Then the cohomology class $[\omega^{(d+2)}] \in H_{dR}^{d+2}(M, i\mathbb{R})$ is independent of the choice of G and $\mathsf{G}^\bullet$. It is called the **higher Berry class** of the smooth family ψ.*

By Proposition 2.2.4 all gapped smooth families (and thus all SRE and invertible smooth families) have a solution to (2.26) and thus a higher Berry class.

For $d = 0$, this is just the usual Berry curvature (Chern number) of a line bundle. For $d = 1$ the higher Berry curvature is a closed 3-form $\omega^{(3)}$ whose cohomology class measures the flow of Berry curvature from the right half of the spin chain to the left half [Wen+23].

When the system under consideration is equipped with an on-site action of a compact Lie group G we can consider equivariant smooth families (ψ, G) parametrized by a G-manifold[11] and there is an equivariant version of the above descent procedure. We describe it here in the case that $G = U(1)$ and the $U(1)$-action on the parameter space M is trivial — in other words, (ψ, G) is a smooth family of states on M that is $U(1)$-invariant for each $x \in M$, and G is a $U(1)$-invariant element of $\Omega^1(M, \mathfrak{D}_{al})$.

The generators of the on-site $U(1)$ actions form a 1-chain $\mathsf{q}^{(1)}$ such that the derivation $\mathsf{Q} := \partial \mathsf{q}^{(1)}$ preserves ψ_x for every $x \in M$. Consider the Cartan complex $\Omega^{\bullet,\bullet}(M, C^\bullet)_{U(1)} := \Omega^\bullet(M) \otimes S^\bullet \mathbb{R} \hat{\otimes} (C^\bullet)_{U(1)}$, where $S^\bullet \mathbb{R}$ is the algebra of polynomials $\mathbb{R}[t]$ on one generator t, which we assign degree 2, and $(C^\bullet)_{U(1)}$ are the $U(1)$-invariant chains. If ψ is a $U(1)$-invariant smooth family of states, we define $\Omega^{\bullet,\bullet}(M, C^\bullet_\psi)_{U(1)}$ similarly.

The equivariant descent equation reads

$$\boldsymbol{d}\mathsf{g}^\bullet + \frac{1}{2}\{\mathsf{g}^\bullet, \mathsf{g}^\bullet\} + \mathsf{Q} \otimes t = 0, \tag{2.29}$$

where $\mathsf{g}^\bullet \in \mathrm{Tot}^1(\Omega^{\bullet,\bullet}(M, C^\bullet)_{U(1)})$ and the component of g in $\Omega^{1,0}(M, C^0)$ is G. As before, the components of $\mathsf{g}^\bullet$ in $\Omega^{\bullet,\bullet}(M, C^{d+1})_{U(1)}$ can be evaluated against the origin (as in (2.38)) to produce closed forms on M which altogether form a class in the equivariant cohomology $H^{d+2}_{U(1)}(M)$, and it can be shown that this cohomology class is independent of the choice of solution $\mathsf{g}^\bullet$ of the equivariant Maurer-Cartan equation.

The components of g in various degrees encode various cohomology invariants one can assign to a $U(1)$-invariant smooth family of states. Letting $\mathsf{g}^{(n,k)}$ be the component of $\Omega^{n+1-2k,2k}(M, C^{-n})_{U(1)}$, the first few components of $\mathsf{g}^\bullet$ can be arranged in the following table:

$$\begin{matrix} \mathsf{g}^{(0,0)} & & \\ \mathsf{g}^{(1,0)} & \mathsf{g}^{(1,1)} & \\ \mathsf{g}^{(2,0)} & \mathsf{g}^{(2,1)} & \\ \mathsf{g}^{(3,0)} & \mathsf{g}^{(3,1)} & \mathsf{g}^{(3,2)} \end{matrix} \tag{2.30}$$

[11]The 1-form G is assumed to be G-equivariant too.

Each component $\mathsf{g}^{(n,k)}$ associates a closed $n+1-2k$-form to a smooth family of $U(1)$-invariant states in $n-1$ dimensions. For instance, for a family of 1-dimensional $U(1)$-invariant states $\psi(\langle \mathsf{g}^{(2,0)}, [*]\rangle) = \omega^{(3)} \in \Omega^3(M)$ is the higher Berry curvature discussed above. For a family of 0-dimensional $U(1)$-invariant states $\psi(\langle \mathsf{g}^{(1,0)}, [*]\rangle) \in \Omega^2(M)$ is the ordinary Berry curvature. In general, the invariant corresponding to $\mathsf{g}^{(n+1,k)}$ is the descendant of the one corresponding to $\mathsf{g}^{(n,k)}$.

The rest of the terms in (2.30) represent the following invariants. As we just described, the first column contains the Berry curvature $\mathsf{g}^{(1,0)}$ and its descendants[12]. At the top of the second column is the $U(1)$ charge $\mathsf{g}^{(1,1)}$ (which can be thought of as giving a locally constant function on a family of 0d systems). The descendant $\mathsf{g}^{(2,1)}$ of charge gives the usual Thouless pump for 1d systems, while $\mathsf{g}^{(n,1)}$ for $n > 2$ give the higher Thouless pump invariants. Finally $\mathsf{g}^{(3,2)}$ is the Hall conductance (whose descendants $\mathsf{g}^{(n,2)}$ for $n \geq 4$ are not pictured).

The main results of this work deal with the entries $\mathsf{g}^{(2,0)}$ (1d Berry curvature) and $\mathsf{g}^{(3,1)}$ (2d Thouless pump) in the above table. The proof of quantization of the 2d Thouless invariant will hinge on showing that these two are related by the process of inserting a flux at infinity. We remark that this pattern holds more generally. We will not treat these rigorously in this work, but let us simply state a few other instances of this "diagonal" relationship. Beginning with a single 2d $U(1)$-invariant state we obtain an S^1-family by inserting a θ-domain wall at the x-axis for every $\theta \in U(1)$, and the charge pumped along the domain wall as one cycles $\theta \in S^1$ from 0 to 2π, which can be interpreted as the charge of a fluxon, can be shown to equal the Hall conductance. This is the original Laughlin argument and relates $\mathsf{g}^{(3,2)}$ (Hall conductance) to $\mathsf{g}^{(2,1)}$ (1d Thouless pump). By inserting another domain wall, along the y-axis this time, we obtain a $S^1 \times S^1$-family of states whose ordinary Berry curvature (given by $\mathsf{g}^{(1,0)}$) is again the Hall conductance: this is the basis of the proof of the Hall conductance quantization [HM14].

This paper is only concerned with the first two columns of (2.30), so we will use a simplified notation for their entries. Instead of $\mathsf{g}^{(n,0)}$ we will simply write $\mathsf{g}^{(n)}$, while $\mathsf{g}^{(n,1)}$ will be denoted $\mathsf{t}^{(n)}$. Then $\mathsf{g}^{(n)}$ satisfy the ordinary descent

[12]One might wonder if $\mathsf{g}^{(0,0)}$ corresponds to some invariant. It should associate a 1-form to a family of (-1)-dimensional states. If one interprets a (-1)-dimensional state as a phase, then $\mathsf{g}^{(0,0)}$ is nothing but the pullback of the form $d\theta$ on $U(1)$.

equations (2.27), of which we will need only the first two:

$$\begin{aligned} \partial \mathsf{g}^{(1)} &= \mathsf{F} \\ \partial \mathsf{g}^{(2)} &= -D\mathsf{g}^{(1)}. \end{aligned} \tag{2.31}$$

Meanwhile the first three descent equations for $\mathsf{t}^{(n)}$ are

$$\begin{aligned} \partial \mathsf{t}^{(1)} &= \mathsf{Q} \\ \partial \mathsf{t}^{(2)} &= -D\mathsf{t}^{(1)} \\ \partial \mathsf{t}^{(3)} &= D\mathsf{t}^{(2)} + \{\mathsf{t}^{(1)}, \mathsf{g}^{(1)}\}. \end{aligned} \tag{2.32}$$

2.3 Localization properties

In this section we introduce a few tools to deal with localization properties of chains, derivations, and automorphisms. We begin in Section 2.3 by defining the notion of a derivation, chain, or automorphism that is confined on a given region in $\mathbb{Z}^d$, then in Section 2.3 we discuss some ways to produce derivations confined on a given region.

Confined maps

Definition 2.3.1. *A linear map $F : \mathscr{A}_{al} \to \mathscr{A}_{al}$ is h-**confined** on a region $X \subset \mathbb{Z}^d$ if for every finite $Y \subset \mathbb{Z}^d$ it satisfies*

$$\|F(B)\| \leq \sum_{z \in X} h(d(z, Y)) \|B\| \tag{2.33}$$

for all B localized on Y. If we omit h and say F is confined on X, we mean that it is h-confined on X for some function h with superpolynomial decay.

Definition 2.3.2. *For $n > 0$, an n-chain f is h-**confined** on a region $X \subset \Lambda$ if*

$$\|\mathsf{f}_{j_1,\ldots,j_n}\| \leq \min_{k=1,\ldots,n} h(d(X, j_k)). \tag{2.34}$$

As before we say f is confined on X if it is h-confined on X for some superpolynomially decreasing h.

For $\mathsf{f} \in \Omega^\bullet(M, C^\bullet)$, being pointwise confined on a region $X \subset \mathbb{Z}^d$ is rarely a sufficiently strong condition — one must impose some kind of uniformity on the decay function h: we say $\mathsf{f} \in C^\infty(\mathbb{R}^n, C^\bullet)$ is **smoothly confined** on X if for any multi-index $\mu \geq 0$ and any $x \in \mathbb{R}^n$, there is a neighbourhood $V \ni x$

and a superpolynomially decaying function h such that $\partial^\mu \mathsf{f}(x)$ is h-confined on X for all $x \in V$. Since this is a local property we extend this definition to $\mathsf{f} \in \Omega^\bullet(M, C^\bullet)$ for a manifold M by requiring f to be smoothly confined on X in any chart. Finally, a chain-valued form $\mathsf{f} \in \Omega^k(M, C^\bullet)$ is defined to be smoothly confined on X if $\mathsf{f}(\sigma)$ is smoothly confined on X for any multivector field σ. Lastly, if $\mathsf{f}, \mathsf{g}, \mathsf{h} \in \Omega^\bullet(M, C^\bullet)$ we say f **smoothly interpolates** between g on X and h on X^c if $\mathsf{f} - \mathsf{g}$ is smoothly confined on X^c and $\mathsf{f} - \mathsf{h}$ is smoothly confined on X.

The notion of confinement is compatible with many operations typically applied to chains, as summarized in Proposition 2.3.1 below, whose proof appears in Section 2.7.

For $X, X' \subset \Lambda$, we say Y is a **stable intersection** of X and X' if there exist a $c > 0$ such that $X(r) \cap X'(r) \subset Y(cr)$ for all $r \geq 0$ [note: this is not the only definition, and maybe there is a better one]. Note in particular that the origin is a stable intersection of the set $\{x \geq 0\} \subset \mathbb{Z}$ and its complement, and the positive y-axis is a stable intersection of the upper half-space in $\mathbb{Z}^2$ with the y-axis.

Proposition 2.3.1. *Let* $\mathsf{a}, \mathsf{b} \in \Omega^\bullet(M, C^\bullet)$. *Let* X, X' *be any subsets of* $\mathbb{Z}^d$ *and let* Y *be a stable intersection of* X *and* X'.

i) If a *is smoothly confined on* X *then* $\partial \mathsf{a}$ *is smoothly confined on* X.

ii) If a *is smoothly confined on both* X *and* X' *then it is smoothly confined on* Y.

iii) If a *and* b *are smoothly confined on* X *and* X', *respectively, then* $\{\mathsf{a}, \mathsf{b}\}$ *is smoothly confined on* Y.

LGAs also have some desirable localization properties if they are produced by integrating a confined derivation:

Proposition 2.3.2. *Let* $\mathsf{G} \in \Omega^1(M \times [0,1], \mathfrak{D}_{al})$ *and suppose* G_{vert} *is smoothly confined on* $X \subset \mathbb{Z}^d$. *Let* $\alpha := \tau \exp \int_0 \mathsf{G}$. *Then* $\alpha^{-1} d\alpha$ *is smoothly confined on* X, *and* $\alpha(\mathsf{F}) - \mathsf{F}$ *is smoothly confined on* X *for any* $\mathsf{F} \in \Omega^\bullet(M, \mathfrak{D}_{al})$.

We call an element of $\mathsf{G} \in \mathfrak{D}_{al}$ **inner** if it is inner as a derivation of $\mathscr{A}_{al}$, in other words there is some $A \in \mathscr{A}_{al}$ such that $\mathsf{G}(B) = [A, B]$ for all $B \in \mathscr{A}_{al}$ (we say

A is **associated** to G). Since $\mathscr{A}_{al}$ has trivial center, any two elements of $\mathscr{A}_{al}$ associated to the same G are related by a multiple of $\mathbf{1}$. The notion of confined derivations allows an explicit description of the set of inner UAL derivations: a derivation $\mathsf{G} \in \mathfrak{D}_{al}$ is inner iff it is confined on a bounded $X \subset \mathbb{Z}^d$. This is a consequence of the more general statement:

Proposition 2.3.3. *Let M be a smooth manifold and suppose $\mathsf{F} \in \Omega^\bullet(M, \mathfrak{D}_{al})$. Then F is of the form $\mathsf{F} = ad_A$ for some antiselfadjoint $A \in \Omega^\bullet(M, \mathscr{A}_{al})$ iff it is confined on a bounded region of $\mathbb{Z}^d$.*

Let ψ be a state on $\mathscr{A}$. If $\mathsf{F} \in \mathfrak{D}_{al}$ is inner we may unambiguously define $\psi(\mathsf{F})$ as $\psi(A) - \overline{\mathrm{tr}}(A)$ for any $A \in \mathscr{A}_{al}$ associated to F. This procedure is covariant with respect to automorphisms of $\mathscr{A}$. Indeed, since $\overline{\mathrm{tr}}$ is the unique tracial state on $\mathscr{A}$[13], we have $\overline{\mathrm{tr}}^\alpha = \overline{\mathrm{tr}}$ for any automorphism of $\mathscr{A}$. Thus

$$\psi^\alpha(\mathsf{F}) = \psi^\alpha(A) - \overline{\mathrm{tr}}(A) = \psi(\alpha(A)) - \overline{\mathrm{tr}}(\alpha(A)) = \psi(\alpha(\mathsf{F})) \tag{2.35}$$

for any $A \in \mathscr{A}_{al}$ associated to F.

Restricting and evaluating chains

Given a subset $X \subset \mathbb{Z}^d$ and an n-chain f define the **restriction** of f to X as the n-chain $\mathrm{res}_X(\mathsf{f})$ given by

$$\mathrm{res}_X(\mathsf{f})_{j_1,\dots,j_n} = \begin{cases} \mathsf{f}_{j_1,\dots,j_n} & \text{if } j_i \in X \text{ for every } i = 1,\dots,n \\ 0 & \text{otherwise.} \end{cases} \tag{2.36}$$

It is easy to see that res_X commutes with F for any $\mathsf{F} \in \mathfrak{D}_{al}$, and that for $k > 0$ and a smooth manifold M the obvious extension of res_X to $\Omega^\bullet(M, C^k)$ commutes with the exterior derivative d. Notice also that $\mathrm{res}_X(\mathsf{f})$ is confined on X, and if f is confined on $Y \subset \mathbb{Z}^d$ then $\mathrm{res}_X(\mathsf{f})$ is also.

Suppose h is an n-chain and let $X \subset \mathbb{Z}^d$. We may form the $(n-1)$-chain $\partial\,\mathrm{res}_X\,\mathsf{h} - \mathrm{res}_X\,\partial\mathsf{h}$, or $[\partial, \mathrm{res}_X]\mathsf{h}$ for short. This chain measures the current of the quantity h across the boundary of the region X. Since $[\partial, \mathrm{res}_X] = -[\partial, \mathrm{res}_{X^c}]$, it is clear that this $(n-1)$-chain is confined on both X and X^c (and thus, by Proposition 2.3.1, on any stable intersection of X and X^c). In what follows, we will most often set X to be one of the half-spaces $\mathbb{H}_i := \{(x_1,\dots,x_n) : x_i \leq 0\} \subset \mathbb{Z}^d$.

[13]Indeed any finite-dimensional matrix algebra has a unique tracial state, and $\mathscr{A}$ is a norm-limit of these.

We end this section by establishing some notation which will be useful throughout the rest of this work. If $\mathsf{h}^{(2)}$ is a 2-chain that is confined on a region which has bounded stable intersection with $\partial\mathbb{H}_i = \{(x_1, \ldots, x_n) : x_i = 0\} \subset \mathbb{Z}^d$, then we define

$$\langle \mathsf{h}^{(2)}, [\partial\mathbb{H}_i]\rangle := \sum_{j\in\mathbb{Z}^d} ([\partial, \mathrm{res}_{\mathbb{H}_i}]\mathsf{h}^{(2)})_j \in \mathscr{A}_{al}, \tag{2.37}$$

the sum on the right-hand side being absolutely convergent in $\mathscr{A}_{al}$.

Now suppose $\mathsf{h}^{(d+1)}$ is any $d+1$-chain. Then $[\partial, \mathrm{res}_{\mathbb{H}_d}]...[\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{h}^{(d+1)}$ is a 1-chain that measures the d-dimensional circulation of h around the origin[14], and we define

$$\langle \mathsf{h}^{(d+1)}, [*]\rangle := \sum_{j\in\mathbb{Z}^d} ([\partial, \mathrm{res}_{\mathbb{H}_d}]...[\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{h}^{(d+1)})_j \in \mathscr{A}_{al}, \tag{2.38}$$

where the sum is again absolutely convergent. Notice that the observable $\langle \mathsf{h}, [*]\rangle$ is traceless and associated to the inner derivation $\partial[\partial, \mathrm{res}_{\mathbb{H}_d}]...[\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{h}$. Since ∂ commutes with $[\partial, \mathrm{res}_X]$ for any X, it follows that $\langle \mathsf{h}, [*]\rangle = 0$ if h is ∂-closed.

2.4 1d higher Berry quantization

We are now ready to prove our first main result: that for invertible families the higher Berry class has an integral refinement. Recall that the exponential exact sequence $0 \to 2\pi i\,\mathbb{Z} \to i\mathbb{R} \to U(1) \to 0$ gives rise to an isomorphism $H^2(M, \underline{U(1)}_M) \cong H^3(M, 2\pi i\,\mathbb{Z})$, where $\underline{U(1)}_M$ is the sheaf of continuous $U(1)$-valued functions on M [DF99; Bry08]. Let $\iota : H^2(M, \underline{U(1)}_M) \hookrightarrow H^3(M, i\mathbb{R})$ denote the composition of this isomorphism with the usual Čech-de Rham map. For a gapped smooth family ψ of 1d states, let $\omega^{(3)} = \psi(\langle \mathsf{g}^{(2)}, [*]\rangle) \in \Omega^3(M, i\,\mathbb{R})$ denote its higher Berry curvature.

Theorem 2.4.1. *To any smooth family (ψ, G) of invertible 1d states on M we can associate a class $[h] \in H^2(M, \underline{U(1)}_M)$ such that $\iota([h]) = [\omega^{(3)}]$. In particular, the class $[\omega^{(3)}/2\pi i] \in H^3(M, \mathbb{R})$ is integral.*

We will first prove the result when ψ is SRE, then extend the result to the case when ψ is invertible. Let $\{U_a\}_{a\in J}$ be an open cover of M such that for any

[14] In the language of [KS22] this is the same as contracting with the conical partition $\{X_k\}_{k=1}^{d+1}$ with $X_k = \mathbb{H}_k \backslash (\mathbb{H}_1 \cup \ldots \cup \mathbb{H}_{k-1})$ for $1 \le k \le d$ and $X_{d+1} = \mathbb{H}_1^c \cap \ldots \cap \mathbb{H}_d^c$.

$a_1, \ldots, a_n \in J$ the intersection $U_{a_1} \cap \ldots \cap U_{a_n}$ is either empty or contractible. Write $U_{ab} := U_a \cap U_b$ and $U_{abc} := U_a \cap U_b \cap U_c$.

The proof will proceed by constructing a Deligne-Beilinson cocycle whose curvature is $\omega^{(3)}$. Recall [DF99; Bry08] that a Deligne-Beilinson 2-cocycle is a triple $(h_{abc} \in C^\infty(U_{abc}, U(1)), a_{ab} \in \Omega^1(U_{ab}, i\mathbb{R}), b_a \in \Omega^2(U_a, i\mathbb{R}))$ such that

$$h_{abc}h_{acd} = h_{abd}h_{bcd} \tag{2.39}$$

$$h_{abc}^{-1}dh_{abc} = a_{ab} - a_{ac} + a_{bc} \tag{2.40}$$

$$da_{ab} = b_a - b_b. \tag{2.41}$$

In the physics literature, such 2-cocycles are called 2-form gauge fields and define a connection on a line bundle gerbe over M [Mur07]. The existence of such a cocycle with $db_a = \omega^{(3)}|_{U_a}$ implies quantization of $[\omega^{(3)}/2\pi i]$ [DF99; Bry08].

Pick a basepoint $x_0 \in M$. For each $a \in J$ let $H_a : U_a \times [0,1] \to M$ be a smooth homotopy from the constant map $U_a \to \{x_0\}$ to the identity map $U_a \to U_a$. Let $L = \mathbb{Z}_{\leq 0} \subset \mathbb{Z}$ and $R = L^c$.

For $a \in J$, define $\tilde{\alpha}_a^{-1} := \tau \exp\left(\int_0^1 H_a^* \mathsf{G}\right)$[15]. This is a smooth family of automorphisms on U_a that provides a local trivialization of ψ in the sense that for every $x \in U_a$ we have $\psi_x = \psi_{x_0} \circ (\tilde{\alpha}_a)_x^{-1}$. Next, define $\alpha_a^{-1} := \tau \exp\left(\int_0^1 H_a^* \partial \operatorname{res}_L h\mathsf{G}\right)$ (where h is the contracting homotopy from Theorem 2.2.1 i)), which can be thought of as a restriction of $\tilde{\alpha}_a^{-1}$ to the left half-line. Define $\alpha_{ab} := \alpha_a \circ \alpha_b^{-1}$.

The family of states $\psi \circ \alpha_{ab}^{-1}$ differs from ψ appreciably only near the origin. In fact, there exists a smooth family of unitaries $V_{ab} \in C^\infty(U_{ab}, \mathscr{A}_{al})$ satisfying $\psi \circ \alpha_{ab}^{-1} = \psi \circ \operatorname{Ad}_{V_{ab}^{-1}}$ and $\overline{\operatorname{tr}}(V_{ab}^{-1} dV_{ab}) = 0$. To see this, note first that we have $\psi \circ \alpha_{ab}^{-1} = \psi \circ \tilde{\alpha}_a \circ \tilde{\alpha}_b^{-1} \circ \alpha_{ab}^{-1}$. It is clear that α_{ab}^{-1} is of the form $\tau \exp\left(\int_0^1 \mathsf{H}\right)$ for some H confined on L. On the other hand, we have $\tilde{\alpha}_a^{-1} \circ \alpha_a = \tau \exp(\alpha_a^{-1}(\partial \operatorname{res}_R h(\mathsf{G})))$ and $\tilde{\alpha}_a \circ \tilde{\alpha}_b^{-1} \circ \alpha_b \circ \tilde{\alpha}_a^{-1} = \tau \exp\left(\tilde{\alpha}_a \circ \alpha_b^{-1}(\partial \operatorname{res}_R h(\mathsf{G}))\right)$. Since both of these are of the form $\tau \exp\left(\int_0^1 \mathsf{H}\right)$ for a H confined on R their product is also of this form. Thus we may use Lemma 2.6.2 to guarantee that such a V_{ab} exists.

Define $W_{abc} := V_{ac}^{-1} \alpha_{ab}(V_{bc}) V_{ab}$, which is a smooth $U(\mathscr{A}_{al})$-valued function satisfying $\overline{\operatorname{tr}}(W_{abc}^{-1} dW_{abc}) = 0$. We also define LGAs $\beta_{ab} := \operatorname{Ad}_{V_{ab}^{-1}} \circ \alpha_{ab}$ and the

[15] Here and below, for a map $f : M \to N$ between smooth manifolds M, N and a differential form $\mathsf{A} \in \Omega^\bullet(N)$ we write $f^*\mathsf{A} \in \Omega^\bullet(M)$ for the pullback of differential forms.

derivation-valued forms $\mathsf{B}_{ab} := \beta_{ab}^{-1} d\beta_{ab}$. It is easy to check that β_{ab} and B_{ab} preserve ψ, and that β_{ab} and W_{abc} satisfy the following two relations:

$$\beta_{ab} \circ \beta_{bc} \circ \beta_{ac}^{-1} = \mathrm{Ad}_{W_{abc}}^{-1}, \tag{2.42}$$

$$W_{abd}^{-1} W_{acd} W_{abc} = \beta_{ab}(W_{bcd}). \tag{2.43}$$

From the first equation above it follows that W_{abc} preserves ψ, so $h_{abc} := \psi(W_{abc})$ is a smooth $U(1)$-valued function on U_{abc}. From the second it follows that $h_{abc}h_{acd} = h_{abd}h_{bcd}$, i.e., h_{abc} is a cocycle (both this and the previous statements use Lemma 2.2.1, which we will continue to use throughout).

Suppose V'_{ab} is another smooth choice of unitaries satisfying $\psi \circ \alpha_{ab}^{-1} := \psi \circ \mathrm{Ad}_{V'_{ab}{}^{-1}}$. Then $Y_{ab} := V_{ab}^{-1} V'_{ab}$ preserves ψ, so $g_{ab} := \psi(Y_{ab})$ is a smooth $U(1)$-valued function on U_{ab}. Writing $W'_{abc} := V'_{ac}{}^{-1} \alpha_{ab}(V'_{bc}) V'_{ab}$, we have

$$W'_{abc} = Y_{ac}^{-1} W_{abc} \beta_{ab}(Y_{bc}) Y_{ab}, \tag{2.44}$$

and so $\psi(W'_{abc}) = g_{ab} g_{bc} g_{ac}^{-1} \psi(W_{abc})$. Thus the 2-cocycle constructed from Y_{ab} differs from the 2-cocycle h_{abc} constructed from V_{ab} by a 2-coboundary, and so h_{abc} defines an element $[h_{abc}] \in \check{H}^2(M, \underline{U(1)}_M) \cong H^3(M, \mathbb{Z})$ which is independent of the choice of V_{ab}'s.

Differentiating (2.42) gives

$$\mathrm{ad}_{W_{abc}^{-1} dW_{abc}} = \mathrm{Ad}_{W_{abc}}^{-1} \, d \, \mathrm{Ad}_{W_{abc}} = \mathsf{B}_{ac} - \mathsf{B}_{bc} - \beta_{bc}^{-1}(\mathsf{B}_{ab}). \tag{2.45}$$

Since $W_{abc}^{-1} dW_{abc}$ is traceless, this implies that

$$h_{abc}^{-1} dh_{abc} = \psi\left(\mathsf{B}_{ac} - \mathsf{B}_{bc} - \beta_{bc}^{-1}(\mathsf{B}_{ab})\right), \tag{2.46}$$

where on the right-hand side we are evaluating a state on an inner derivation as in Section 2.3.

Below we write $\mathsf{F}_{\mathsf{H}} := d\mathsf{H} + \frac{1}{2}\{\mathsf{H}, \mathsf{H}\}$ for any $\mathsf{H} \in \Omega^1(M, \mathfrak{D}_{al})$. Since $\psi = \psi_0 \circ \tilde{\alpha}_a^{-1}$, the family ψ is parallel with respect to $\tilde{\alpha}_a d\tilde{\alpha}_a^{-1}$. By Lemma 2.7.7 there is a $\mathsf{C}_a \in \Omega^1(U_a, \mathfrak{D}_{al})$ such that ψ is parallel with respect to C_a, C_a smoothly interpolates between $\tilde{\alpha}_a d\tilde{\alpha}_a^{-1}$ on L and G on R, and $\mathsf{F}_{\mathsf{C}_a}$ smoothly interpolates between 0 and F. Now define

$$a_{ab} := \psi(\mathsf{B}_{ab} - \mathsf{C}_b + \beta_{ab}{}^{-1}(\mathsf{C}_a)), \tag{2.47}$$

$$b_a := \psi(d\mathsf{C}_a + \frac{1}{2}\{\mathsf{C}_a, \mathsf{C}_a\} - \partial \, \mathrm{res}_R \, \mathsf{g}^{(1)}). \tag{2.48}$$

Using Proposition 2.3.2 one can check that $\mathsf{B}_{ab} - \mathsf{C}_b + {\beta_{ab}}^{-1}(\mathsf{C}_a)$ is smoothly confined on both L and R, ensuring that a_{ab} is well-defined and smooth. A similar argument shows this for b_a as well.

Lemma 2.4.1. *We have*

$$h_{abc}^{-1} dh_{abc} = a_{ab} - a_{ac} + a_{bc}. \tag{2.49}$$

Proof. Using the fact that $\psi \circ \beta_{bc}^{-1} = \psi$ we have

$$a_{ab} - a_{ac} + a_{bc} = \psi(\beta_{bc}^{-1}(\mathsf{B}_{ab}) - \mathsf{B}_{ac} + \mathsf{B}_{bc})) + \psi(\beta_{bc}^{-1}(\beta_{ab}^{-1}(\mathsf{C}_a)) - \beta_{ac}^{-1}(\mathsf{C}_a)). \tag{2.50}$$

The second term equals $\psi(\mathrm{Ad}_{W_{abc}}(\mathsf{C}_a) - \mathsf{C}_a) = 0$, and so (2.50) agrees with the expression (2.46). □

Lemma 2.4.2. *We have*

$$da_{ab} = b_a - b_b. \tag{2.51}$$

Proof. On an overlap U_{ab}, ψ is parallel with respect to both C_a and C_b. by Proposition 2.2.3 it is parallel with respect to $(\mathsf{C}_b)^{\beta_{ab}}$. Thus it is parallel with respect to $\frac{1}{2}((\mathsf{C}_a)^{\beta_{ab}} + \mathsf{C}_b) = \frac{1}{2}(\beta_{ab}^{-1}(\mathsf{C}_a) + \mathsf{B}^{ab} + \mathsf{C}_b)$. Using this we get

$$\begin{aligned} da_{ab} &= \psi(\mathsf{B}_{ab} + \frac{1}{2}\{\mathsf{B}_{ab}, \mathsf{B}_{ab}\} - d\mathsf{C}_b - \frac{1}{2}\{\mathsf{C}_b, \mathsf{C}_b\} + {\beta_{ab}}^{-1}(d\mathsf{C}_a + \frac{1}{2}\{\mathsf{C}_a, \mathsf{C}_a\})) \\ &= \psi(-\mathsf{F}_{\mathsf{C}_b} + {\beta_{ab}}^{-1}(\mathsf{F}_{\mathsf{C}_a})), \end{aligned} \tag{2.52}$$

where as before we write $\mathsf{F}_{\mathsf{C}_a} := d\mathsf{C}_a + \frac{1}{2}\{\mathsf{C}_a, \mathsf{C}_a\}$, and we used the fact that $\mathsf{F}_{\mathsf{B}_{ab}} = 0$. To split the last line into two terms, we regularize $-\mathsf{F}_{\mathsf{C}_b} + {\beta_{ab}}^{-1}(\mathsf{F}_{\mathsf{C}_a})$ by adding $\partial \operatorname{res}_R \mathsf{g}^{(1)} - {\beta_{ab}}^{-1}(\partial \operatorname{res}_R \mathsf{g}^{(1)})$. Since $\operatorname{res}_R \mathsf{g}^{(1)} - {\beta_{ab}}^{-1}(\operatorname{res}_R \mathsf{g}^{(1)})$ is a 1-chain confined at the origin, each of whose terms is traceless and has zero expectation under ψ, we have $\psi(\partial \operatorname{res}_R \mathsf{g}^{(1)} - {\beta_{ab}}^{-1}(\partial \operatorname{res}_R \mathsf{g}^{(1)})) = 0$. Thus,

$$\begin{aligned} da_{ab} &= \psi(-\mathsf{F}_{\mathsf{C}_b} + {\beta_{ab}}^{-1}(\mathsf{F}_{\mathsf{C}_a}) - \partial \operatorname{res}_R \mathsf{g}^{(1)} + {\beta_{ab}}^{-1}(\partial \operatorname{res}_R \mathsf{g}^{(1)})) \\ &= b_a - b_b. \end{aligned} \tag{2.53}$$

□

Lemma 2.4.3. $db_a = -\psi(\langle \mathsf{g}^{(2)}, [*] \rangle)$

Proof.

$$\begin{aligned} db_a &= \psi(D_{\mathsf{C}_a}\mathsf{F}_{\mathsf{C}_a} + \{\mathsf{G}-\mathsf{C}_a, \mathsf{F}_{\mathsf{C}_a}\} + D_{\mathsf{G}}\partial \mathsf{g}^{(1)}_R) \\ &= \psi(\{\mathsf{G}-\mathsf{C}_a, \mathsf{F}_{\mathsf{C}_a}\}) + \psi(\partial[\partial, \mathrm{res}_R]\mathsf{g}^{(2)}). \end{aligned} \tag{2.54}$$

The first term in (2.54) is zero since $\{\mathsf{G}-\mathsf{C}_a, \mathsf{F}_{\mathsf{C}_a}\}$ is associated to the absolutely convergent $\sum_{j\in\mathbb{Z}^d} \mathsf{F}_{C_a}(h(\mathsf{G}-\mathsf{C}_a)_j))$ and $\mathsf{F}_{\mathsf{C}_a}$ preserves ψ. The result then follows from the fact that $\langle \mathsf{g}^{(2)}, [*]\rangle$ is associated to $\partial[\partial, \mathrm{res}_L]\mathsf{g}^{(2)} = -\partial[\partial, \mathrm{res}_R]\mathsf{g}^{(2)}$. □

This concludes the proof of Theorem 2.4.1 in the case that the family ψ is SRE.

Although so far we defined the refined higher Berry class $[h_{abc}] \in H^3(M, 2\pi i\mathbb{Z})$ only for SRE families, it is easy to extend the definition as well as the proof of Theorem 2.4.1 to arbitrary smooth invertible families. Let ψ be such a family. Pick $x_0 \in M$, let ψ'_{x_0} be an inverse for ψ_{x_0}, and consider the family $\psi \otimes \psi'_{x_0} = \{\psi_x \otimes \psi'_{x_0}\}_{x\in M}$. This family is SRE at the point $x_0 \in M$ and thus it is SRE on the whole M. Define the refined higher Berry class $[h_{abc}]$ of ψ as that of $\psi \otimes \psi'_{x_0}$. It is independent of the choice of ψ'_{x_0}. Indeed, suppose ψ''_{x_0} is another inverse for ψ_{x_0}. Since the SRE families $\psi_{x_0} \otimes \psi'_{x_0}$ and $\psi_{x_0} \otimes \psi''_{x_0}$ are constant, their refined higher Berry class vanish. Further, it is easy to see that for any two smooth SRE families ψ, ψ' the refined higher Berry class of $\psi \otimes \psi'$ is the sum of the refined higher Berry classes of ψ and ψ'. Therefore the refined higher Berry class of the SRE family $\psi \otimes \psi'_{x_0} \otimes \psi''_{x_0} \otimes \psi_{x_0}$ is equal to both the refined higher Berry class of $\psi \otimes \psi'_{x_0}$ and the refined higher Berry class of $\psi \otimes \psi''_{x_0}$.

Example: Let us describe an example of the family of SRE states for which the class $[\omega^{(3)}/2\pi i] \in H^3(M, \mathbb{R})$ is non-trivial. It is essentially the example from [Wen+23] adapted for our setting. Let $(\chi \in [0, \pi], \theta \in [0, \pi], \phi \in [0, 2\pi))$ be spherical coordinates on S^3 with (θ, ϕ) being spherical coordinates on S^2 at fixed $0 < \chi < \pi$. The equatorial S^2 is located at $\chi = \pi/2$. The regions $\chi \leq \pi/2$ and $\chi \geq \pi/2$ correspond to the upper S^3_+ and the lower hemisphere S^3_-, respectively. Let $B : S^2 \to \mathcal{B}(\mathbb{C}^2)$ defined by $B(\theta, \phi) = \vec{n}(\theta, \phi) \cdot \vec{\sigma}$ with $\vec{n}$ being a unit vector in $\mathbb{R}^3$ pointed in the direction $(\theta, \phi) \in S^2$ and $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ being Pauli matrices, and let $p_\pm = (1 \pm B)/2$. Let us choose $\epsilon \in (0, \pi/4)$. Let us choose a smooth family of rank one projections $P^{(+)} : S^3_+ \to \mathcal{B}(\mathbb{C}^2) \otimes \mathcal{B}(\mathbb{C}^2)$ such that in the neighbourhood $0 \leq \chi \leq \epsilon$ it is some constant rank one projection, while in the neighbourhood $(\pi/2-\epsilon)\le\chi\le\pi/2$ it is given by

$$P^{(+)}(\theta,\phi,\chi)=p_+(\theta,\phi)\otimes p_-(\theta,\phi).$$

Similarly, we define a smooth family of rank one projections $P^{(-)}:S^3_-\to\mathcal{B}(\mathbb{C}^2)\otimes\mathcal{B}(\mathbb{C}^2)$ such in the neighbourhood $(\pi-\epsilon)\le\chi\le\pi$ it is some constant rank one projection, while in the neighbourhood $\pi/2\le\chi\le(\pi/2+\epsilon)$ it is given by

$$P^{(-)}(\theta,\phi,\chi)=p_-(\theta,\phi)\otimes p_+(\theta,\phi).$$

Let us consider a one-dimensional lattice system with $\mathscr{A}_j\cong\mathcal{B}(\mathbb{C}^2)$. For $k\in\mathbb{Z}$, we let $P^{(+)}_k\in\mathscr{A}_{a\ell}$ be a smooth family of local observables on S^3_+ corresponding to $P^{(+)}$ under the isomorphism $\mathscr{A}_{2k}\otimes\mathscr{A}_{2k+1}\cong\mathcal{B}(\mathbb{C}^2)\otimes\mathcal{B}(\mathbb{C}^2)$. Similarly, let $P^{(-)}_k\in\mathscr{A}_{a\ell}$ be a smooth family of observables on S^3_- corresponding to $P^{(-)}$ via the isomorphism $\mathscr{A}_{2k-1}\otimes\mathscr{A}_{2k}\cong\mathcal{B}(\mathbb{C}^2)\otimes\mathcal{B}(\mathbb{C}^2)$. We let $\{\psi_x\}_{x\in S^3_+}$ be a family of pure states of $\mathscr{A}$ uniquely defined by the requirement that when restricted to $\mathscr{A}_{2k}\otimes\mathscr{A}_{2k+1}$ it is given by $A\mapsto \mathrm{T}rP^{(+)}_kA$. This is a smooth family of states on S^3_+ which is parallel with respect to $\mathsf{G}'^{(+)}\in\Omega^1(S^3_+,\mathfrak{D}_{al})$ given by

$$\mathsf{G}'^{(+)}=\sum_{k\in\mathbb{Z}}[P^{(+)}_k,dP^{(+)}_k]. \tag{2.55}$$

Similarly, we consider a family of pure states $\{\psi_x\}_{x\in S^3_-}$ of $\mathscr{A}$ defined by the requirement that when restricted to $\mathscr{A}_{2k-1}\otimes\mathscr{A}_{2k}$ it is given by $A\mapsto \mathrm{T}rP^{(-)}A$. This is a smooth family of states on S^3_- which is parallel with respect to $\mathsf{G}'^{(-)}\in\Omega^1(S^3_+,\mathfrak{D}_{al})$ given by

$$\mathsf{G}'^{(-)}=\sum_{k\in\mathbb{Z}}[P^{(-)}_k,dP^{(-)}_k]. \tag{2.56}$$

It is easy to see that the two families of states agree on the equatorial S^2. Moreover, the resulting family of states on the whole S^3 is smooth. To see this, consider an open neighbourhood E of the equatorial S^2 given by $\pi/2-\epsilon/2<\chi<\pi/2+\epsilon/2$. $\psi|_E$ is a family of product states whose restriction to $\mathscr{A}_{2k}$ (resp. $\mathscr{A}_{2k+1}$) is given by $A\mapsto \mathrm{T}rp_+A$ (resp. $A\mapsto \mathrm{T}rp_-A$). Therefore $\psi|_E$ is parallel with respect to a derivation-valued 1-form $\mathsf{A}\in\Omega^2(E,\mathfrak{D}_{al})$ given by the sum of on-site terms $[p_+,dp_+]$ on $\mathscr{A}_{2k}$ and $[p_-,dp_-]$ on $\mathscr{A}_{2k+1}$ for $k\in\mathbb{Z}$. Since S^3_+,S^3_-, and E form an open cover of S^3, there exists a partition of unity $1=\rho_++\rho_-+\rho_E$, where ρ_+,ρ_-,ρ_E are smooth functions supported on S^3_+,S^3_-,E, respectively. We get a globally-defined 1-form $\mathsf{G}\in\Omega^1(S^3,\mathfrak{D}_{al})$ such that ψ is parallel with respect to $D=d+\mathsf{G}$ by letting $\mathsf{G}=\rho_+\mathsf{G}'^{(+)}+\rho_-\mathsf{G}'^{(-)}+\rho_E\mathsf{A}$.

For such G, we can choose $\mathsf{g}^{(1)} \in \Omega^2(S^3, C_\psi^{-1})$ such that 1) $\mathsf{g}^{(1)}_{2k}, \mathsf{g}^{(1)}_{2k+1} \in \mathscr{A}_{2k} \otimes \mathscr{A}_{2k+1}$ on S^3_+; 2) $\mathsf{g}^{(1)}_{2k}, \mathsf{g}^{(1)}_{2k-1} \in \mathscr{A}_{2k-1} \otimes \mathscr{A}_{2k}$ on S^3_-; 3) on E, $\mathsf{g}^{(1)}_{2k}$ and $\mathsf{g}^{(1)}_{2k+1}$ are given by $\frac{1}{2}[dp_+, dp_+] \in \mathscr{A}_{2k}$ and $\frac{1}{2}[dp_-, dp_-] \in \mathscr{A}_{2k+1}$, respectively. Note that for any k, $D(\mathsf{g}^{(1)}_{2k} + \mathsf{g}^{(1)}_{2k+1}) = 0$ on S^3_+ and $D(\mathsf{g}^{(1)}_{2k-1} + \mathsf{g}^{(1)}_{2k}) = 0$ on S^3_-. Therefore $\langle \mathsf{g}^{(2)}, [*]\rangle$ vanishes on S^3_- and coincides with $D\mathsf{g}^{(1)}_0$ on S^3_+. The integral of the higher Berry curvature over S^3 is

$$\int_{S^3} \psi(\langle \mathsf{g}^{(2)}, [*]\rangle) = \int_{S^3_+} \psi(D\mathsf{g}^{(1)}_0) = \int_{S^2 = \partial S^3_+} \psi(\mathsf{g}^{(1)}_0) = \int_{S^2} \frac{1}{2} \mathrm{Tr}\,(p_+[dp_+, dp_+]) = 2\pi i. \tag{2.57}$$

2.5 2d Thouless pump

Let ψ_M be a smooth gapped family of 2d $U(1)$-invariant states over a compact manifold M. The 2d Thouless pump invariant $\langle \mathsf{t}^{(3)}, [*]\rangle$ associates to it a class in de Rham cohomology $H^2(M, i\mathbb{R})$. In this section we show, using a proof analogous to Laughlin's flux insertion argument, that this class can be refined to a class in integral cohomology. Here is a roadmap of the argument.

We extend ψ_M to a family of states ψ on $M \times S^1$ by performing a $U(1)$ gauge transformation on the right half-plane, which we interpret as implementing a 2π-flux insertion at a point at infinity on the y-axis $\partial\mathbb{H}_1$. Although the 3-form $\psi(\langle \mathsf{g}^{(1)}, [\partial\mathbb{H}_2]\rangle)$ which measures the Berry curvature flux across the x-axis is divergent, its vertical component $\psi(\langle \mathsf{g}^{(1)}_{vert}, [\partial\mathbb{H}_2]\rangle)$ is finite because varying the S^1-parameter $\theta \in [0, 2\pi)$ changes ψ appreciably only near the y-axis in $\mathbb{Z}^2$. In Section 2.5 below we compute this form and show that it equals $d\theta \wedge \langle \mathsf{t}^{(3)}, [*]\rangle$. Thus in particular the total Berry curvature pumped across the x-axis during the flux insertion is equal to 2π times the 2d Thouless invariant. This result is true for any gapped U(1)-invariant smooth family ψ_M.

Then, in Section 2.5 we use an argument analogous to the proof of Berry flux quantization in Section 2.4 to show that if ψ_M is invertible then the total Berry curvature transported across the x-axis along the flux insertion, which is given by the fiber integral $\int_{S^1} \psi(\langle \mathsf{g}^{(1)}_{vert}, [\partial\mathbb{H}_2]\rangle)$ and thus equals $2\pi\langle \mathsf{t}^{(3)}, [*]\rangle$, is integral.

2d Thouless pump as a higher Berry curvature

Throughout this section we will use the following action of the de Rham complex $\Omega^\bullet(M)$ on $\Omega^\bullet(M, C^\bullet)$: for $\eta \in \Omega^p(M)$ and $\mathsf{a} \in \Omega^q(M, C^k)$ we put

$$\eta \wedge \mathsf{a}(X_1, \dots, X_{p+q}) := \sum_\sigma \frac{\mathrm{sgn}(\sigma)}{p!q!} \eta(X_{\sigma(1)}, \dots X_{\sigma(p)}) \mathsf{a}(X_{\sigma(p+1)}, \dots X_{\sigma(p+q)}), \tag{2.58}$$

for any vector fields $X_1, \dots, X_{p+q}$. It is easy to check that $d(\eta \wedge \mathsf{a}) = d\eta \wedge \mathsf{a} + (-1)^p \eta \wedge d\mathsf{a}$ and if $\mathsf{b} \in \Omega^r(M, C^\ell)$ then $\{\mathsf{b}, \eta \wedge \mathsf{a}\} = (-1)^{p(r+\ell)} \eta \wedge \{\mathsf{b}, \mathsf{a}\}$.

Let (ψ_M, G_M) be a gapped $U(1)$-invariant smooth family of 2d states on M. View it as a family of states on $M \times S^1$ that is constant in the S^1 direction, which we will also call (ψ_M, G_M). We will often refer to a (chain-valued) differential form on M and its pullback by the projection $M \times S^1 \to M$ by the same symbol; it should be clear by context which is meant.

Define $\rho = \tau \exp\big(\int_0 \partial \operatorname{res}_{\mathbb{H}_1} \mathsf{q}^{(1)} d\theta\big)$, where $\mathsf{q}^{(1)}$ is the 1-chain consisting of the generators of the onsite $U(1)$ action, and θ is the coordinate on S^1. This is a smooth family of automorphisms on $M \times S^1$. Define $\psi := \psi_M \circ \rho^{-1}$. This is a $U(1)$-invariant family of gapped states which represents the threading of a flux "at infinity" into the original family ψ_M (see Figure 2.1 below). By Proposition

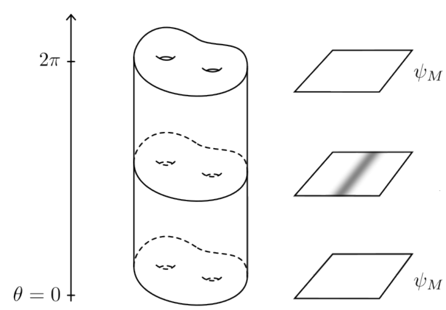

Figure 2.1: A schematic depiction of $\psi := \psi_M \circ \rho^{-1}$. The shaded areas on the right side indicate regions in $\mathbb{Z}^2$ where ψ differs from ψ_M. For $x \in M$ and $0 \le \theta \le 2\pi$, the state $\psi_{(x,\theta)}$ is the state $(\psi_M)_x$ with a θ-domain wall on the y-axis. Cycling θ from 0 to 2π performs a flux insertion at infinity.

2.2.3 ψ is parallel with respect to the $U(1)$-invariant connection $\mathsf{G}_M^{\rho^{-1}} = \rho(\mathsf{G}_M - \partial \operatorname{res}_{\mathbb{H}_1} \mathsf{q}^{(1)} d\theta)$. However, we will use a slightly different connection. Define $\mathsf{G} \in \Omega^1(M \times S^1, \mathfrak{D}_{al})$ by

$$\mathsf{G} := \rho(\mathsf{G}_M - \partial \operatorname{res}_{\mathbb{H}_1} (\mathsf{q}^{(1)} - \mathsf{t}^{(1)}) d\theta), \tag{2.59}$$

where $\mathsf{t}^{(1)} := h^{\psi_M}(\mathsf{Q})$, with h^{ψ_M} the contracting homotopy from Theorem 2.2.1 *ii*). This differs from $\mathsf{G}_M^{\rho^{-1}}$ by the term $\rho(\partial \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)})d\theta$ which preserves ψ and is $U(1)$-invariant, so ψ is still parallel with respect to G, and G is still $U(1)$-invariant. The reason we choose G instead of $\mathsf{G}_M^{\rho^{-1}}$ is that its vertical component is confined on the y-axis $\partial\mathbb{H}_1$. In what follows, we will need to choose all our derivation-valued forms to satisfy this constraint.

Theorem 2.5.1. *The smooth gapped family* (ψ, G) *admits a solution to the MC equation (2.26) such that* $\mathsf{g}^\bullet_{vert}$ *is smoothly confined on the y-axis* $\partial\mathbb{H}$*, and*

$$\psi(\langle \mathsf{g}^{(2)}_{vert}, [\partial\mathbb{H}_2]\rangle) = d\theta \wedge \psi_M(\langle \mathsf{t}^{(3)}\rangle, [*]) \tag{2.60}$$

where $\mathsf{t}^{(3)}$ *is a solution to the equivariant Maurer-Cartan equation (2.29) for* (ψ_M, G_M)*.*

Proof. We proceed as though we were computing the 1d Berry invariant for the family ψ by solving the MC equation for G. At each step this will require adding a counterterm to ensure that the vertical component of $\mathsf{g}^{(k)}$ is confined on $\partial\mathbb{H}_1$. As it turns out, choosing these counterterms will precisely involve solving the equivariant descent equations (2.32). Indeed, the first counterterm $d\theta \wedge \rho(\partial \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)})$, which was required to regularize the vertical component of G, already involved solving $\partial \mathsf{t}^{(1)} = \mathsf{Q}$.

Let $\mathsf{g}^\bullet_M$ be a solution of the Maurer-Cartan equation (2.26) for (ψ_M, G_M). Below we write $D_M = d + \{\mathsf{G}_M, \cdot\}$ and $\mathsf{F}_M = d\mathsf{G}_M + \frac{1}{2}\{\mathsf{G}_M, \mathsf{G}_M\}$. We begin by computing the curvature of G:

$$\mathsf{F} = \rho(\mathsf{F}_M + D_M(d\theta \wedge \partial \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)})). \tag{2.61}$$

The first step in the descent equation is to find a $\mathsf{g}^{(1)} \in \Omega^2(M \times S^1, C^{-1}_\psi)$ with $\partial \mathsf{g}^{(1)} = \mathsf{F}$. We will choose a $\mathsf{g}^{(1)}$ of the form

$$\mathsf{g}^{(1)} = \rho(\mathsf{g}^{(1)}_M + d\theta \wedge \mathsf{f}^{(1)}), \tag{2.62}$$

where $\partial \mathsf{f}^{(1)} = -D_M(\partial \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)})$. Since $-D_M(\partial \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}) = -\partial D_M \operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}$, we could use the naive expression

$$\mathsf{f}^{(1)}_{naive} := -D_M(\operatorname{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}). \tag{2.63}$$

However, since $\mathsf{f}^{(1)}_{naive}$ isn't confined on $\partial\mathbb{H}_1$, it needs to be regularized. To do this, let $\mathsf{t}^{(2)} \in \Omega^1(M, C^{-2}_{\psi_M})$ be a $U(1)$-invariant chain with $\partial \mathsf{t}^{(2)} = -D_M \mathsf{t}^{(1)}$, and set

$$\mathsf{f}^{(1)} := -[\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{t}^{(2)}. \tag{2.64}$$

For the next step in the descent procedure, we seek $\mathsf{g}^{(2)} \in \Omega^3(M \times S^1, C_\psi^{-2})$ which satisfies $\partial \mathsf{g}^{(2)} = -D\mathsf{g}^{(1)}$. Calculating $D\mathsf{g}^{(1)}$ gives

$$D\mathsf{g}^{(1)} = \rho\Bigg(D_M \mathsf{g}_M^{(1)} + d\theta \wedge \left(\{\partial\, \mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} - D_M(\mathsf{f}^{(1)}) \right) \Bigg), \tag{2.65}$$

so we choose the following ansatz for $\mathsf{g}^{(2)}$:

$$\mathsf{g}^{(2)} = \rho(\mathsf{g}_M^{(2)} + d\theta \wedge \mathsf{f}^{(2)}), \tag{2.66}$$

where $\mathsf{f}^{(2)} \in \Omega^2(M \times S^1, C_\psi^{-2})$ must satisfy

$$\begin{aligned} \partial \mathsf{f}^{(2)} &= -\{\partial\, \mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} + D_M(\mathsf{f}^{(1)}) \\ &= -\partial\Bigg(\{\mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} + \mathrm{res}_{\mathbb{H}_1} D_M \mathsf{t}^{(2)} \Bigg). \end{aligned} \tag{2.67}$$

This gives an unregularized expression for $\mathsf{f}^{(2)}$:

$$\begin{aligned} \mathsf{f}_{naive}^{(2)} &= -\{\mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} - \mathrm{res}_{\mathbb{H}_1} D_M \mathsf{t}^{(2)} \\ &= -\{\mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathrm{res}_{\mathbb{H}_1^c} \mathsf{g}_M^{(1)}\} - \mathrm{res}_{\mathbb{H}_1} \left(\{\mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} + D_M \mathsf{t}^{(2)} \right). \end{aligned} \tag{2.68}$$

Only the second term in (2.68) needs regularization, giving

$$\mathsf{f}^{(2)} = -\{\mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathrm{res}_{\mathbb{H}_1^c} \mathsf{g}_M^{(1)}\} + [\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{t}^{(3)}, \tag{2.69}$$

where $\mathsf{t}^{(3)} \in \Omega^2(M, C_{\psi_M}^{-3})$ is chosen such that

$$\partial \mathsf{t}^{(3)} = \{\mathsf{t}^{(1)}, \mathsf{g}_M^{(1)}\} + D_M \mathsf{t}^{(2)}. \tag{2.70}$$

Clearly $d\theta \wedge \rho(\mathsf{f}^{(2)})$ is the vertical component of $\mathsf{g}^{(2)}$ and we have

$$\begin{aligned} \psi(\langle d\theta \wedge \rho(\mathsf{f}^{(2)}), [\partial \mathbb{H}_2]\rangle) &= d\theta \wedge \psi_M(\partial[\partial, \mathrm{res}_{\mathbb{H}_2}]\mathsf{f}^{(2)}) \\ &= d\theta \wedge \psi_M(\partial[\partial, \mathrm{res}_{\mathbb{H}_2}][\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{t}^{(3)})) \\ &= d\theta \wedge \psi_M(\langle \mathsf{t}^{(3)}, [*]\rangle). \end{aligned} \tag{2.71}$$

The first equality holds because $\psi_M = \psi \circ \rho$ and the second because $\psi_M(\langle\{\mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}, \mathrm{res}_{\mathbb{H}_1^c} \mathsf{g}_M^{(1)}\}, [\partial \mathbb{H}_2]\rangle) =$ 0, since both $\mathsf{t}^{(1)}$ and $\mathsf{g}_M^{(1)}$ preserve ψ_M. □

2d Thouless pump quantization

Having expressed the 2d Thouless invariant as the Berry curvature transport during flux insertion, we proceed to proving that this invariant is quantized if ψ_M is SRE. The proof is along the lines of the proof of ordinary Berry curvature quantization in Section 2.4, but some modifications must be made because ψ is not a family of 1d states — instead it is only 1d in the θ direction. Let $\eta^{(2)} := \psi_M(\langle \mathsf{t}^{(3)}, [*]\rangle)$ be the 2d Thouless invariant of a family of states ψ_M on M, and recall that we write $\iota : H^2(M, \underline{U(1)}_M) \cong H^2(M, 2\pi i\,\mathbb{Z}) \hookrightarrow H^3(M, i\mathbb{R})$ for the Čech-de Rham map.

Theorem 2.5.2. *To any smooth family (ψ_M, G_M) of invertible $U(1)$-invariant 2d states on M we can associate a class $[h_{ab}] \in H^1(M, \underline{U(1)}_M)$ such that $\iota([h_{ab}]) = 2\pi[\eta^{(2)}]$. In particular, the class $-i[\eta^{(2)}] \in H^2(M, \mathbb{R})$ is integral.*

Before we begin, we will need the following Lemma:

Lemma 2.5.1. *Let G and G_M be as in Section 2.5. Then $\mathsf{G} - \mathsf{G}_M$ is smoothly confined on $\partial\mathbb{H}_1$. In particular, G_{vert} is smoothly confined on $\partial\mathbb{H}_1$.*

Proof. We have

$$\mathsf{G} - \mathsf{G}_M = \rho(\mathsf{G}) - \mathsf{G}_M + d\theta \wedge \rho(\partial\, \mathrm{res}_{\mathbb{H}_1}(\mathsf{q}^{(1)}) - \mathsf{t}^{(1)}). \tag{2.72}$$

By $U(1)$-invariance of G_M we have

$$\mathsf{G} - \mathsf{G}_M = \tau \exp\left(\int_0^{2\pi} \partial\, \mathrm{res}_{\mathbb{H}_1} \mathsf{q}^{(1)}\right)(\mathsf{G}_M) - \mathsf{G}_M = \tau \exp\left(\int_0^{2\pi} -\partial\, \mathrm{res}_{\mathbb{H}_1^c} \mathsf{q}^{(1)}\right)(\mathsf{G}_M) - \mathsf{G}_M, \tag{2.73}$$

so by Proposition 2.3.2, $\mathsf{G} - \mathsf{G}_M$ is smoothly confined on both $\mathbb{H}_1$ and $\mathbb{H}_1^c$, and thus it's confined on $\partial\mathbb{H}_1$. Next, since $\partial\mathsf{q}^{(1)} = \mathsf{Q} = \partial\mathsf{t}^{(1)}$, there is a $\mathsf{k}^{(2)}$ satisfying $\partial\mathsf{k}^{(2)} = \mathsf{q}^{(1)} - \mathsf{t}^{(1)}$, and we have

$$d\theta \wedge \rho(\partial\, \mathrm{res}_{\mathbb{H}_1}(\mathsf{q}^{(1)} - \mathsf{t}^{(1)})) = -d\theta \wedge \rho(\partial[\partial, \mathrm{res}_{\mathbb{H}_1}]\mathsf{k}^{(2)}) \tag{2.74}$$

which is confined on $\partial\mathbb{H}_1$ by the results of Section 2.3. □

Let us introduce a key ingredient of the proof of Theorem 2.5.2. Define the following smooth families of LGAs on $M \times [0, 2\pi]$:

$$\tilde{\gamma} := \tau \exp\left(\int_0 \mathsf{G}\right), \tag{2.75}$$

$$\gamma := \tau \exp\left(\int_0 \partial\, \mathrm{res}_{\mathbb{H}_2} h\mathsf{G}\right), \tag{2.76}$$

where h is the contracting homotopy from Theorem 2.2.1 i). Notice that we have

$$\psi_M \circ \tilde{\gamma} \circ \rho = \psi_M \tag{2.77}$$

since $\tilde{\gamma} \circ \rho = \tau \exp\left(\int_0 \partial\, \mathrm{res}_{\mathbb{H}_1} \mathsf{t}^{(1)}\right)$ and $\mathsf{t}^{(1)}$ preserves ψ_M. This means that $\psi_M \circ \tilde{\gamma}$ is nothing but the family of states $\psi := \psi_M \circ \rho^{-1}$ on $M \times [0, 2\pi]$ describing a flux-insertion at infinity which was used in Section 2.5. On the other hand, $\psi_M \circ \gamma$ inserts a flux at the origin in $\mathbb{Z}^2$ (see Figure 2.2). We are now ready to

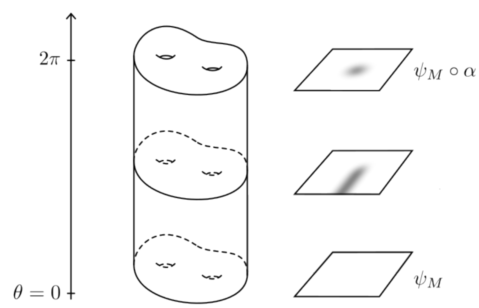

Figure 2.2: $\psi_M \circ \gamma$ performs a flux insertion at the origin.

begin the proof of Theorem 2.5.2:

Proof. As before let $\{U_a\}_{a \in J}$ be an open cover of M such all U_a and all nonempty intersections $U_{ab} := U_a \cap U_b$ are contractible. Let $\tilde{\alpha}$ and α be the families of LGAs on M given by $\tilde{\alpha} := \tilde{\gamma} \circ j_{2\pi}$ and $\alpha := \gamma \circ j_{2\pi}$, where $j_\theta : M \to M \times [0, 2\pi]$ is the embedding $x \mapsto (x, \theta)$.

The family of states $\psi_M \circ \alpha$ differs from ψ_M only near the origin. In fact, on each neighbourhood in M the family $\psi_M \circ \alpha$ can be produced from ψ_M by the action of an almost-local unitary, as we now show. Notice that we have $\psi_M \circ \alpha^{-1} = \psi_M \circ \tilde{\alpha} \circ \alpha^{-1}$, and that $\tilde{\alpha} \circ \alpha^{-1} = \tau \exp\left(\int_0^{2\pi} \alpha^{-1}(\partial\, \mathrm{res}_{\mathbb{H}_2^c} h\mathsf{G})\right)$. Since G_{vert} is confined on $\partial\mathbb{H}_1$ (Lemma 2.5.1), by Lemma 2.6.2 on each U_a we can find a smooth map $V_a : U_a \to U(\mathscr{A}_{al})$ such that $\psi_M \circ \alpha^{-1} = \psi_M \circ \mathrm{Ad}_{V_a^{-1}}$ and $\overline{\mathrm{tr}}(V_a^{-1} dV_a) = 0$.

On an overlap U_{ab} we have the smooth unitary $V_a^{-1} V_b$ which preserves ψ_M, and we define

$$h_{ab} := \psi_M(V_a^{-1} V_b) \in C^\infty(U_{ab}, U(1)) \tag{2.78}$$

which satisfies the cocycle condition $h_{ab}h_{bc} = h_{ac}$. As in Section 2.4 define $\beta_a := \mathrm{Ad}_{V_a^{-1}} \circ \alpha$ and $\mathsf{B}_a := \beta_a^{-1} d\beta_a$, both of which preserve ψ_M. Since $\beta_a\beta_b^{-1} = \mathrm{Ad}_{V_a^{-1}V_b}$, a straightforward calculation shows

$$h_{ab}^{-1} dh_{ab} = \psi_M(\mathsf{B}_a - \mathsf{B}_b). \tag{2.79}$$

By Lemma 2.7.7, ψ_M is parallel with respect to a $\mathsf{C} \in \Omega^1(M, \mathfrak{D}_{al})$ that smoothly interpolates between G_M on $\mathbb{H}_2^c$ and $\mathsf{G}_M^{\tilde{\alpha}}$ on $\mathbb{H}_2$. Defining

$$a_a := -\psi_M(\mathsf{C} - \mathsf{G}_M^{\beta_a}), \tag{2.80}$$

we obtain, from (2.79),

$$\begin{aligned} h_{ab}^{-1} dh_{ab} &= \psi_M(\mathsf{B}_a - \mathsf{B}_b) + \psi_M((\beta_a^{-1}(\mathsf{G}_M) - \beta_b^{-1}(\mathsf{G}_M)) \\ &= a_a - a_b, \end{aligned} \tag{2.81}$$

where the second line is because $\psi_M((\beta_a^{-1}(\mathsf{G}_M) - \beta_b^{-1}(\mathsf{G}_M)) = \psi_M((\mathsf{G}_M - \mathrm{Ad}_{V_a^{-1}V_b}(\mathsf{G}_M)) = 0$. Since ψ_M is parallel with respect to $\frac{1}{2}(\mathsf{G}_M^{\beta_a} + \mathsf{C})$ we have

$$\begin{aligned} da_a &= -\psi_M(d(\mathsf{C} - \mathsf{G}_M^{\beta_a}) + \frac{1}{2}\{\mathsf{G}_M^{\beta_a} + \mathsf{C}, \mathsf{C} - \mathsf{G}_M^{\beta_a}\}) \\ &= -\psi_M(\mathsf{F}_{\mathsf{C}} - \beta_a^{-1}(\mathsf{F}_M)). \end{aligned} \tag{2.82}$$

This collection of closed 2-forms is a Čech 0-cocycle in $\Omega^2(M, i\mathbb{R})$ and thus defines a closed 2-form on M. This can be seen in two different ways. First, one can compute the Čech coboundary using the expressions on the r.h.s.:

$$\psi_M\left(\beta_a^{-1}(\mathsf{F}_M) - \beta_b^{-1}(\mathsf{F}_M)\right) = \psi(\mathsf{F}_M - \beta_a(\beta_b^{-1}(\mathsf{F}_M))) = \psi(\mathsf{F}_M - \mathrm{Ad}_{V_a^{-1}V_b}(\mathsf{F}_M)) = 0, \tag{2.83}$$

where we used the fact that the automorphisms $\beta_a^{-1}, \beta_b^{-1}$ and $\mathrm{Ad}_{V_a^{-1}V_b}$ preserve ψ_M. Second, from the definition of a_a we have $da_a - da_b = d(h_{ab}^{-1}dh_{ab}) = 0$. Thus da_a is a restriction of a globally defined closed 2-form ω. In addition, the second argument shows that the cohomology class of $\omega/2\pi i$ is integral (it is the de Rham representative of the first Chern class of the line bundle defined by the Čech 2-cocycle h_{ab}).

Finally, let us show that $-\omega$ is cohomologous to $2\pi\psi_M(\langle \mathsf{t}^{(3)}, [*]\rangle)$. The strategy will be to define a form $b \in \Omega^2(M \times [0,1], \mathbb{C})$ with $j_0^* b - j_{2\pi}^* b = -\omega$ and

$db = \psi_M(\langle \mathsf{t}^{(3)}, [*]\rangle)\wedge d\theta$. Then the result will follow from the following formula:

$$\begin{aligned} -\omega &= j_{2\pi}^* b - j_0^* b \\ &= d\int_0^{2\pi} b - \int_0^{2\pi} db \\ &= d\int_0^{2\pi} b + 2\pi\psi_M(\langle \mathsf{t}^{(3)}, [*]\rangle). \end{aligned} \tag{2.84}$$

Begin by defining

$$\hat{\mathsf{C}} := \mathsf{G} - \partial\,\mathrm{res}_{\mathbb{H}_2}(h^{\psi}(\mathsf{G} - \mathsf{G}_M^{\tilde{\gamma}})) \in \Omega^1(M\times[0,2\pi], \mathfrak{D}_{al}), \tag{2.85}$$

$$\mathsf{E} := \partial\,\mathrm{res}_{\mathbb{H}_2^c}\,\mathsf{g}^{(1)} + \partial\,\mathrm{res}_{\mathbb{H}_2}\,\tilde{\gamma}^{-1}(\mathsf{g}_M^{(1)}) \in \Omega^2(M\times[0,2\pi], \mathfrak{D}_{al}), \tag{2.86}$$

where $\mathsf{g}^{(1)}, \mathsf{g}_M^{(1)}$ are as in Section 2.5. These definitions have been chosen so that $\hat{\mathsf{C}}$ and E satisfy the following properties:

i) ψ is parallel with respect to $\hat{\mathsf{C}}$.

ii) $\hat{\mathsf{C}}$ smoothly interpolates between G on $\mathbb{H}_2^c$ and $\mathsf{G}_M^{\tilde{\gamma}}$ on $\mathbb{H}_2$.

iii) $\mathsf{F}_{\hat{\mathsf{C}}}$ smoothly interpolates between F on $\mathbb{H}_2^c$ and $\tilde{\gamma}^{-1}(\mathsf{F}_M)$ on $\mathbb{H}_2$.

iv) $j_0^*\hat{\mathsf{C}} = \mathsf{G}_M$ and $j_{2\pi}^*\hat{\mathsf{C}} = \mathsf{C}$.

v) $\psi_M(j_{2\pi}^*\mathsf{E} - \beta_a^{-1}(j_0^*\mathsf{E})) = 0$ for any $a \in J$.

vi) $\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{E}$ is smoothly confined at the origin in $\mathbb{Z}^2$.

The first three follow from Lemma 2.7.7, and the fourth is easy to verify. Property v) follows from the identity

$$\psi_M(j_{2\pi}^*\mathsf{E} - \beta_a^{-1}(j_0^*\mathsf{E})) = \psi_M(\partial\,\mathrm{res}_{\mathbb{H}_2}(\beta_a^{-1}(\mathsf{g}_M^{(1)}) - \tilde{\alpha}^{-1}(\mathsf{g}_M^{(1)}))). \tag{2.87}$$

The right-hand side of the above expression is well-defined since $\beta_a^{-1}(\mathsf{g}_M^{(1)}) - \tilde{\alpha}^{-1}(\mathsf{g}_M^{(1)})$ is smoothly confined on $\mathbb{H}_1^c \cap \mathbb{H}_2$, and it is zero because both β_a and $\tilde{\alpha}_a$ preserve ψ_M. Finally, property vi) is proved in the following:

Lemma 2.5.2. $\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{E}$ *is smoothly confined at the origin in* $\mathbb{Z}^2$.

Proof. Since both $\mathsf{F}_{\hat{\mathsf{C}}}$ and E interpolate between F on $\mathbb{H}_2^c$ and $\tilde{\gamma}^{-1}(\mathsf{F}_M)$ on $\mathbb{H}^c$, it follows that $\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{E}$ is smoothly confined on $\partial\mathbb{H}_2$. Next, using the fact that both $\mathsf{G} - \mathsf{G}_M$ and $\mathsf{G}_M^{\tilde{\gamma}} - \mathsf{G}_M$ are is smoothly confined on the vertical line

$\partial\mathbb{H}_1$, one can show that $\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{F}_M$ is too. Similarly, since both $\mathsf{g}^{(1)} - \mathsf{g}_M^{(1)}$ and $\tilde{\gamma}^{-1}(\mathsf{g}_M^{(1)}) - \mathsf{g}_M^{(1)}$ and are smoothly confined on $\partial\mathbb{H}_1$, one can show that $\mathsf{E} - \mathsf{F}_M$ is too. Thus $\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{E} = (\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{F}_M) - (\mathsf{E} - \mathsf{F}_M)$ smoothly confined on $\partial\mathbb{H}_1$. Thus it is smoothly confined on the origin. □

Property vi) allows us to define

$$b := \psi(\mathsf{F}_{\hat{\mathsf{C}}} - \mathsf{E}) \in \Omega^2(M \times [0, 2\pi]). \tag{2.88}$$

Lemma 2.5.3. *With* b *defined as above, we have*

$$j_0^* b - j_{2\pi}^* b = -\omega \tag{2.89}$$

and

$$db = \psi(\langle \mathsf{g}^{(2)} - \rho(\mathsf{g}_M^{(2)}), [\partial\mathbb{H}_2]\rangle). \tag{2.90}$$

Proof. First, from property v) above we have

$$\begin{aligned} -\omega|_{U_a} &= \psi_M(\mathsf{F}_{\mathsf{C}} - j_{2\pi}^*\mathsf{E} - \beta_a^{-1}(\mathsf{F}_M - j_0^*\mathsf{E})) \\ &= j_{2\pi}^* b|_{U_a} - j_0^* b|_{U_a}, \end{aligned} \tag{2.91}$$

and so (2.89) is established. Next, we have

$$\begin{aligned} db &= \psi\left(D_{\hat{\mathsf{C}}}\mathsf{F}_{\hat{\mathsf{C}}} + (D - D_{\hat{\mathsf{C}}})\mathsf{F}_{\hat{\mathsf{C}}} - D\mathsf{E}\right) \\ &= \psi\left(\{\mathsf{G} - \hat{\mathsf{C}}, \mathsf{F}_{\hat{\mathsf{C}}}\} - D\mathsf{E}\right), \end{aligned} \tag{2.92}$$

where the second line is due to the Bianchi identity $D_{\hat{\mathsf{C}}}\mathsf{F}_{\hat{\mathsf{C}}} = 0$. Inserting the definitions of $\hat{\mathsf{C}}$ and E into the above, and adding and subtracting the term $\tilde{\gamma}^{-1}\left(D_M \partial \operatorname{res}_{\mathbb{H}_2} \mathsf{g}_M^{(1)}\right)$, we get

$$\begin{aligned} db &= \psi\left(\{\mathsf{G} - \hat{\mathsf{C}}, \mathsf{F}_{\hat{\mathsf{C}}}\} + D\partial \operatorname{res}_{\mathbb{H}_2} \mathsf{g}^{(1)} - D\partial \operatorname{res}_{\mathbb{H}_2} \tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right) \\ &= \psi\left(D\partial \operatorname{res}_{\mathbb{H}_2} \mathsf{g}^{(1)} - \tilde{\gamma}^{-1}\left(D_M \partial \operatorname{res}_{\mathbb{H}_2} \mathsf{g}_M^{(1)}\right)\right) \\ &\quad + \psi\left(\{\mathsf{G} - \hat{\mathsf{C}}, \mathsf{F}_{\hat{\mathsf{C}}}\} + \tilde{\gamma}^{-1}\left(D_M \partial \operatorname{res}_{\mathbb{H}_2} \mathsf{g}_M^{(1)}\right) - D\partial \operatorname{res}_{\mathbb{H}_2} \tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right). \end{aligned} \tag{2.93}$$

The first term in (2.93) is

$$-\psi\left(\partial \operatorname{res}_{\mathbb{H}_2} \partial(\mathsf{g}^{(2)} - \tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)}))\right) = \psi(\langle \mathsf{g}^{(2)} - \tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)}), [\partial\mathbb{H}_2]\rangle), \tag{2.94}$$

while the second one is

$$\begin{aligned}&\psi\left(\{\mathsf{G}-\hat{\mathsf{C}},\mathsf{F}_{\hat{\mathsf{C}}}\}+(\tilde{\gamma}^{-1}\circ D_M\circ\tilde{\gamma}-D)\partial\operatorname{res}_{\mathbb{H}_2}\tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right)\\=&\psi\left(\{\mathsf{G}-\hat{\mathsf{C}},\mathsf{F}_{\hat{\mathsf{C}}}\}+\left\{\mathsf{G}_M^{\tilde{\gamma}}-\mathsf{G},\partial\operatorname{res}_{\mathbb{H}_2}\tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right\}\right).\end{aligned}$$

Splitting $\mathsf{G}_M^{\tilde{\gamma}}-\mathsf{G}$ in the above into $\partial\operatorname{res}_{\mathbb{H}_2}h^{\psi}(\mathsf{G}_M^{\tilde{\gamma}}-\mathsf{G})+\partial\operatorname{res}_{\mathbb{H}_2^c}h^{\psi}(\mathsf{G}_M^{\tilde{\gamma}}-\mathsf{G})$ gives

$$\begin{aligned}&\psi\left(\left\{\partial\operatorname{res}_{\mathbb{H}_2}(h^{\psi}(\mathsf{G}-\mathsf{G}_M^{\tilde{\gamma}})),\mathsf{F}_{\hat{\mathsf{C}}}-\partial\operatorname{res}_{\mathbb{H}_2}\tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right\}\right)\\&\quad-\psi\left(\left\{\partial\operatorname{res}_{\mathbb{H}_2^c}(h^{\psi}(\mathsf{G}-\mathsf{G}_M^{\tilde{\gamma}})),\partial\operatorname{res}_{\mathbb{H}_2}\tilde{\gamma}^{-1}\left(\mathsf{g}_M^{(1)}\right)\right\}\right).\end{aligned}$$

Both terms above are of the form $\psi(\{\mathsf{A},\mathsf{B}\})$ where A and B preserve ψ and are smoothly confined on regions with bounded stable intersection. Thus it is well-defined and zero, and so we have

$$db=\psi(\langle\mathsf{g}^{(2)}-\tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)}),[\partial\mathbb{H}_2]\rangle).\tag{2.95}$$

Finally, (2.90) follows from the following claim:

$$\psi(\langle\rho(\mathsf{g}_M^{(2)})-\tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)}),[\partial\mathbb{H}_1]\rangle)=\psi_M(\langle\mathsf{g}_M^{(2)}-\rho^{-1}\circ\tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)},[\partial\mathbb{H}_1]\rangle))=0.\tag{2.96}$$

(The terms in the above equation are well-defined because $\rho\circ\tilde{\gamma}^{-1}(\mathsf{g}_M^{(2)})-\mathsf{g}_M^{(2)}$ is smoothly confined on $\partial\mathbb{H}_1$ by $U(1)$-invariance of $\mathsf{g}_M^{(2)}$). The first equality in (2.96) is by definition of ψ, and the second follows from (2.77). □

We are now ready to conclude the proof of Theorem 2.5.2. Looking at (2.66) it is clear that $\mathsf{g}^{(2)}-\rho(\mathsf{g}^{(2)})=\mathsf{g}_{vert}^{(2)}$, and so by Theorem 2.5.1 we have $db=\psi_M(\langle\mathsf{t}^{(3)},[*]\rangle)\wedge d\theta$. By (2.84) this concludes the proof that the 2D Thouless form is quantized when ψ is a smooth family of $U(1)$-invariant SRE states. To extend this to smooth families of $U(1)$-invariant invertible states is a matter of applying the same argument as the one appearing at the end of Section 2.4. □

Remark 2.5.1. *One can construct an example of a family of 2d states with a non-trivial 2d Thouless pump invariant in a way similar to the example from Section 2.4. The family is parameterized by S^2. At the north pole, it is a product state with vanishing ground-state $U(1)$ charges on each site. At the south pole, it is a product state with the ground-state charge $(-1)^{x+y}$ on* *a site* $(x,y) \in \mathbb{Z}^2$*. There are four different pairings of neighbouring sites that correspond to four different directions* $0, \pi/2, \pi$ *and* $3\pi/2$*: 1)* $(2k,l)$ *with* $(2k+1,l)$*; 2)* $(2k-1,l)$ *with* $(2k,l)$*; 3)* $(k,2l)$ *with* $(k,2l+1)$*; 4)* $(k,2l-1)$ *with* $(k,2l)$*. There are also four different ways to form quadruples of neighbouring sites:* $\{(2k,2l),(2k+1,2l),(2k,2l+1),(2k+1,2l+1)\}$*, and its shifts. The meridians of* S^2 *at* $0, \pi/2, \pi,$ *and* $3\pi/2$ *correspond to the families of states between the poles such that at each point the state is a product of pure states on pairs of sites for the corresponding pairing. Four different quarters of the sphere between the meridians correspond to the families of states such that at each point the state is a product of pure states on quadruples of sites. The family can be made smooth by choosing partitions of unity and has a unit 2d Thouless pump invariant. We omit the precise formulas.*

2.6 Asymptotically equal states

It is a standard result in the theory of spin systems that two pure states on $\mathscr{A}$ unitarily equivalent if they are "equal at infinity" (see for instance Corollary 2.6.11 in [BR87]). Below we prove two versions of this theorem that are adapted to our needs. Namely, first we show that if one of the states is SRE and the states rapidly approach each other at infinity, then the two states are related by the action of an almost-local unitary. Then we show that for certain smooth families of SRE states this almost-local unitary can be chosen to be a smooth function of parameters on any contractible neighbourhood in the parameter space. The first of these statements was proved in [KSY21], but we include its proof here for completeness.

Lemma 2.6.1. *Let* $|\chi^1\rangle$ *and* $|\chi^2\rangle$ *be two vectors in a Hilbert space* $\mathcal{H}$ *such that* $\langle\chi^i|\chi^i\rangle = 1$*,* $i = 1,2$*, and* $\langle\chi^1|\chi^2\rangle > 0$*. Then there exists a unitary* $U \in U(\mathcal{H})$ *such that* $U|\chi^1\rangle = |\chi^2\rangle$ *and* $\|U - \mathbf{1}\| = \||\chi^1\rangle - |\chi^2\rangle\|$*.*

We omit the proof of this elementary lemma.

Proposition 2.6.1. *Suppose* ψ *is an SRE state and* ϕ *is another pure state such that there exists a superpolynomially decreasing function* f *for which*

$$|\psi(A) - \phi(A)| \leq f(R)\|A\| \tag{2.97}$$

holds for any A *localized outside of* $B_R(0)$*. Then there is a unitary* $V \in \mathscr{A}_{al}$ *such that* $\phi = \psi \circ \mathrm{Ad}_V$*.*

Proof. Since ψ is SRE, we have $\psi = \psi_{fact} \circ \alpha^{-1}$ for a factorized pure state ψ_{fact} and some LGA α. Then $|\psi_{fact}(A) - \phi \circ \alpha|$ decays superpolynomially, as in (2.97), and if we find a unitary $V \in \mathscr{A}_{al}$ with $\phi \circ \alpha = \psi_{fact} \circ \mathrm{Ad}_{V^{-1}}$ then we would have $\phi = \psi_{\alpha(V^{-1})}$. So we may assume without loss of generality that ψ is a factorized state.

Let $(\mathcal{H}, \pi, |0\rangle)$ be the GNS triple of ψ. From (2.97) and Corollary 2.6.11 in [BR87] it follows that ϕ is given by a vector state $|\phi\rangle\langle\phi|$ in $\mathcal{H}$. For each positive integer R let B_R be the ball of radius R around zero, $|0\rangle_{B_R}$ and $|0\rangle_{B_R^c}$ the (pure) restrictions of $|0\rangle$ to B_R and B_R^c, respectively. Since ψ is factorized we have $\mathcal{H} = \mathcal{H}_{B_R} \otimes \mathcal{H}_{B_R^c}$, where $\mathcal{H}_{B_R}$ and $\mathcal{H}_{B_R^c}$ are the GNS Hilbert spaces of $\psi|_{B_R}$ and $\psi|_{B_R^c}$.

Pick an $R_0 > 0$ with $f(R_0) < 1$ and let $R \geq R_0$. Notice that the purifications of $|0\rangle_{B_R^c}$ in $\mathcal{H}$ are precisely the unit-norm vectors in $\mathcal{H}_{B_R} \otimes |0\rangle_{B_R^c}$, and that $|\phi\rangle$ is a purification of $\phi|_{B_R^c}$ in $\mathcal{H}$. By Uhlmann's theorem [Uhl76] we have

$$\max\left\{ |\langle\psi|\chi\rangle| \;\middle|\; |\chi\rangle \in \mathcal{H}_{B_R} \otimes |0\rangle_{B_R^c} \text{ and } \langle\chi|\chi\rangle = 1 \right\} = F(\phi|_{B_R^c}, \psi|_{B_R^c}). \quad (2.98)$$

Let $|\chi^R\rangle$ be a maximizer with $\langle\phi|\chi_x^R\rangle \geq 0$. It satisfies

$$\begin{aligned} \langle\phi|\chi^R\rangle &= F(\phi|_{B_R^c}, \psi|_{B_R^c}) \\ &\geq 1 - f(R)/2, \end{aligned} \quad (2.99)$$

where the second line is due to the Fuchs-Van de Graaf inequality. Since $f(R) < 1$, $|\phi\rangle$ and $|\chi^n\rangle$ aren't orthogonal, and since $|\chi^R\rangle$ maximizes (2.98) it follows that $|\chi^R\rangle$ is the normalized projection of $|\phi\rangle$ onto $\mathcal{H}_{B_R} \otimes |0\rangle_{B_R^c}$.

By Lemma 2.6.1 there is a unitary U^{R_0} localized on B_{R_0} such that $U^{R_0}|0\rangle_{B_{R_0}} = |\chi^{R_0}\rangle$. Next, by (2.99) we have

$$\begin{aligned} \| |\chi^{R-1}\rangle - |\chi^R\rangle \| &\leq \| |\chi^{R-1}\rangle - |\phi\rangle \| + \| |\chi^R\rangle - |\phi\rangle \| \\ &\leq 2\sqrt{f(R-1)}, \end{aligned} \quad (2.100)$$

so for any $R \geq R_0$, Lemma 2.6.1 guarantees unitary U^R localized on B_R with $U^R|\chi^{R-1}\rangle = |\chi^R\rangle$, and

$$\|U^R - \mathbf{1}\| = 2\sqrt{f(R-1)}. \quad (2.101)$$

Then

$$V := \lim_{R\to\infty} U^R \dots U^{R_0} = \sum_{R=R_0+1}^{\infty} (U^{R-1} - 1)U^{R-1} \dots U^{R_0} \quad (2.102)$$

is unitary and satisfies $V|0\rangle = |\phi\rangle$, and for any $S \geq R_0$ we have $\|V - \sum_{R=R_0+1}^{S}(U^{R-1} - 1)U^{R-1} \dots U^{R_0}\| \leq \sum_{r \geq S} 2\sqrt{f(r)}$, so $V \in \mathscr{A}_{al}$. $\square$

For the following Lemma, let $\Gamma_1, \Gamma_2 \subset \mathbb{Z}^d$ be two regions such that $\Gamma_1 \subset \mathbb{H}_d$, $\Gamma_2 \subset \mathbb{H}_d^c$, and $\Gamma_1 \cup \Gamma_2$ has bounded stable intersection with $\partial\mathbb{H}_d$.

Lemma 2.6.2. *Let K be a contractible open subset of $\mathbb{R}^n$ for some $n \geq 0$, and let γ_1 and γ_2 be families of automorphisms on K such that each γ_i is obtained as the path-ordered integral of a derivation-valued 1-form on $K \times [0,1]$ that is smoothly confined on Γ_i. Suppose that (ψ, G) a smooth family of SRE states on K such that $\psi \circ \gamma_1 = \psi \circ \gamma_2$. Then there is a smooth family of unitary observables $V \in C^\infty(K, \mathscr{A}_{al})$ with $\psi \circ \gamma_i = \psi \circ \mathrm{Ad}_V$ and $\overline{\mathrm{tr}}(V^{-1}dV) = 0$.*

Remark 2.6.1. *This lemma is used twice in the text: once in Section 2.4 with $\Gamma_1 = L \subset \mathbb{Z}^1$ and $\Gamma_2 = R \subset \mathbb{Z}^1$, and once in Section 2.5 with $\Gamma_1 = (\partial\mathbb{H}_1) \cap \mathbb{H}_2 \subset \mathbb{Z}^2$ and $\Gamma_2 = (\partial\mathbb{H}_1) \cap \mathbb{H}_2^c \subset \mathbb{Z}^2$.*

Proof. Choose an arbitrary basepoint $x_* \in K$ and let $F : K \times [0,1] \to K$ be a smoooth nullhomotopy to the point x_*. Then $\beta := \tau \exp\left(\int_0^1 F^*\mathsf{G}\right)$ satisfies $\psi_x = \psi_{x_*} \circ \beta_x$ for any $x \in K$. Define $\tilde{\gamma}_i := \beta \circ \gamma_i \circ \beta^{-1}$. Since γ_i is of the form $\tau \exp\left(\int_0^1 \mathsf{G}\right)$ for a $\mathsf{G} \in \Omega^1(K \times [0,1], \mathfrak{D}_{al})$ that is smoothly confined on Γ_i, the LGA $\beta \circ \gamma_i \circ \beta^{-1} = \tau \exp\left(\int_0^1 \beta(\mathsf{G})\right)$ is of that form too. By Proposition 2.3.2, $\tilde{\gamma}_i^{-1} d\tilde{\gamma}_i$ is smoothly confined on Γ_i.

Let $\chi := \psi \circ \gamma_i \circ \beta^{-1}$. Then χ is parallel with respect to $\tilde{\gamma}_i^{-1} d\tilde{\gamma}_i$ for $i = 1, 2$. By Lemma 2.7.7, χ is parallel with respect to a $\mathsf{H} \in \Omega^1(K, \mathfrak{D}_{al})$ that is confined on $\Gamma_1 \cup \Gamma_2$ and smoothly interpolates between $\tilde{\gamma}_2^{-1} d\tilde{\gamma}_2$ on $\mathbb{H}_2$ and $\tilde{\gamma}_1^{-1} d\tilde{\gamma}_1$ on $\mathbb{H}_2^c$. It follows that H is smoothly confined on a bounded region, so by Proposition 2.3.3 it has a lift to $\Omega^1(K, \mathscr{A}_{al})$, which by abuse of notation we will also call H. Then the path-ordered integral of H along F is an almost-local unitary $W := \tau \exp\left(\int_0^1 F^*\mathsf{H}\right)$ and we have $\chi_x = \chi_{x_*} \circ \mathrm{Ad}_{W_x}$ for any $x \in K$.

By the definition of χ it is apparent that it asymptotically equals ψ_{x_*} away from a stable intersection of Γ_1 and Γ_2, as in (2.97). Thus by Proposition 2.6.1 there is a unitary $V_* \in \mathscr{A}_{al}$ with $\chi_{x_*} = \psi_{x_*} \circ \mathrm{Ad}_{V_*}$. Letting $V_x := \beta_x^{-1}(V_* W_x)$

we have

$$\begin{aligned}\psi_x \circ (\gamma_i)_x &= \chi_x \circ \beta_x \\ &= \chi_{x_*} \circ \mathrm{Ad}_{W_x} \circ \beta_x \\ &= \psi_{x_*} \circ \mathrm{Ad}_{V_* W_x} \circ \beta_x \\ &= \psi_x \circ \mathrm{Ad}_{V_x} . \end{aligned} \tag{2.103}$$

Finally, since $\overline{\mathrm{tr}}(V^{-1}dV)$ is a closed 1-form and K is contractible, there is a smooth function $g : K \to U(1)$ with $g^{-1}dg = \overline{\mathrm{tr}}(V^{-1}dV)$, and multiplying V by g^{-1} ensures that $\overline{\mathrm{tr}}(V^{-1}dV) = 0$. □

2.7 Confined chains

The goals of this section is to prove Propositions 2.3.1, 2.3.2, and 2.3.3, as well as to introduce Lemma

Lemma 2.7.1. *A 1-chain* f *is confined on* $X \subset \mathbb{Z}^d$ *iff there is another 1-chain* g *whose entries* g_j *vanish outside* X *such that* $\partial\mathsf{g} = \partial\mathsf{f}$*.*

Proof. For each $j \in X$ define $S_j := \{k \in X^c : d(k, X) = d(k, j)\}$. Choose any total order on $\mathbb{Z}^d$ and define $\tilde{S}_j := S_j \setminus \bigcup_{k<j} S_k$. Then the $\tilde{S}_j$ are disjoint and $\bigsqcup_{j\in X} \tilde{S}_j = X^c$. Define the 1-chain g by

$$\mathsf{g}_j := \begin{cases} \mathsf{f}_j + \sum_{k\in\tilde{S}_j} \mathsf{f}_k & \text{if } j \in X \\ 0 & \text{otherwise.} \end{cases} \tag{2.104}$$

Then $\partial\mathsf{g} = \partial\mathsf{f} = \mathsf{F}$ and it remains only to show that g is a 1-chain. Since f is confined on X we have a superpolynomially decaying h such that $\|\mathsf{f}_k\| \leq h(d(k, X))$. Thus for $k \in \tilde{S}_j$ we have $\|\mathsf{f}_k\| \leq h(d(k, j))$ and it follows that $\sum_{k\in\tilde{S}_j} \mathsf{f}_k$ is absolutely convergent and the g_j's have uniformly bounded norm. Finally let us show that $\sum_{k\in\tilde{S}_j} \mathsf{f}_k$ is f-confined on j for a function f which is the same for all j. Since f is a 1-chain there is a superpolynomially decaying g_1 such that every f_k is g_1-confined at k. Let $r > 0$ be even. For each $k \in \tilde{S}_j \cap B_j(r/2)$ pick $A_k \in \mathscr{A}_{B_k(r/2)}$ with $\|A_k - \mathsf{f}_k\| \leq g_1(r/2)$, and let $B := \sum_{k\in\tilde{S}_j\cap B_j(r/2)} A_k \in \mathscr{A}_{B_j(r)}$. Then we have

$$\begin{aligned}\Big\| \sum_{k\in\tilde{S}_j} \mathsf{f}_k - B \Big\| &\leq \sum_{k\in\tilde{S}_j\cap B_j(r/2)} \|\mathsf{f}_k - A_k\| + \sum_{k\in\tilde{S}_j\cap B_j(r/2)^c} \|\mathsf{f}_k\| \\ &\leq r^d g_1(r) + \sum_{R\geq r/2} (2R)^d h(R) := g_2(r). \end{aligned} \tag{2.105}$$

Thus g_j is $(g_1 + g_2)$-confined on j. □

Below we will often use the following family of seminorms on traceless almost-local observables:

Lemma 2.7.2 ([KS22] Proposition D.1). *Let $V \subset \mathscr{A}_{al}$ be the subspace of traceless observables. Then for any $j \in \mathbb{Z}^d$ the family of seminorms $\{\|\cdot\|_{j,\alpha}\}_{\alpha\in\mathbb{N}}$ on V is equivalent to the family $\{\|\cdot\|^{br}_{j,\alpha}\}_{\alpha\in\mathbb{N}}$ given by*

$$\|A\|^{br}_{j,\alpha} := \sup_X \|A^X\|(1 + \mathrm{diam}(\{j\} \cup X))^\alpha, \tag{2.106}$$

where the supremum is taken over all bricks in $\mathbb{Z}^d$ and $\sum_Z A^Z$ is the brick decomposition of the inner derivation corresponding to $A \in \mathscr{A}_{al}$.

The following lemma shows that if an observable is h-confined on two faraway points $j, k \in \mathbb{Z}^d$ then its norm decays superpolynomially with $d(j, k)$.

Lemma 2.7.3. *For any traceless $A \in \mathscr{A}_{al}$ and any positive integer α we have*

$$\|A\| \le 2^{2d+1}(\|A\|^{br}_{j,\alpha+2d+1} + \|A\|^{br}_{k,\alpha+2d+1}) \left(\frac{d(j,k)}{2}\right)^{-\alpha} \tag{2.107}$$

Proof. Let $R := d(j, k)$.

$$\begin{aligned}
\|A\| &\le \sum_{X\neq\emptyset} \|A^X\| \\
&\le \sum_{X\neq\emptyset} \min\Big((1 + \mathrm{diam}(X \cup \{j\}))^{-\alpha-2d-1}\|A\|^{br}_{j,\alpha+2d+1},\ (1 + \mathrm{diam}(X \cup \{k\}))^{-\alpha-2d-1}\|A\|^{br}_{k,\alpha+2d+1}\Big) \\
&\le (\|A\|^{br}_{j,\alpha+2d+1} + \|A\|^{br}_{k,\alpha+2d+1}) \Bigg(\sum_{\mathrm{diam}(X\cup\{j\})\ge R/2} (1 + \mathrm{diam}(X \cup \{j\}))^{-\alpha-2d-1} \\
&\qquad + \sum_{\mathrm{diam}(X\cup\{k\})\ge R/2} (1 + \mathrm{diam}(X \cup \{k\}))^{-\alpha-2d-1} \Bigg).
\end{aligned} \tag{2.108}$$

Since there are at most $(2r)^{2d}$ bricks X with $\mathrm{diam}(X \cup \{j\}) = r$ for any $r > 0$, we get

$$\begin{aligned}\sum_{\text{diam}(X\cup\{j\})\geq R/2}(1+\text{diam}(X\cup\{j\}))^{-\alpha-2d-1} &\leq \sum_{r\geq R/2}(2r)^{2d}(1+r)^{-\alpha-2d-1}\\ &\leq 4^d\sum_{r\geq R/2}(1+r)^{-\alpha-1}\\ &\leq 4^d\int_{r\geq R/2}^{\infty} r^{-\alpha-1}dr\\ &= 4^d\alpha^{-1}(R/2)^{-\alpha}\\ &\leq 4^d(R/2)^{-\alpha}. \end{aligned}\tag{2.109}$$

□

The following lemma shows that the definitions of confinement for derivations and chains are compatible.

Lemma 2.7.4. *Let $\mathsf{F}\in\mathfrak{D}_{al}$ and $X\subset\mathbb{Z}^d$. The following are equivalent:*

i) *F is confined on X.*

ii) *For every $\alpha\in\mathbb{Z}_{>0}$ there is a C_α such that*

$$\|\mathsf{F}^Z\|(1+\text{diam}(Z))^\alpha(1+d(Z,X))^\alpha\leq C_\alpha \tag{2.110}$$

for every brick Z.

iii) *The 1-chain $\mathsf{f}_j:=\sum_{X\ni j}\frac{1}{|X|}\mathsf{F}^X$ is confined on X.*

Proof. *i)* $\implies$ *ii)*. Let $\mathsf{F}=\sum_Z\mathsf{F}^Z$ be the brick decomposition of F. Fix a brick Z. There is an operator A supported in Z with $\|A\|=1$ and $\|\mathsf{F}_Z(A)\|=\|\mathsf{F}_Z\|$. From this it follows that

$$\begin{aligned}\|\mathsf{F}_Z\| &= \|\mathsf{F}_Z(A)\|\\ &= \|\overline{\text{tr}}_{Z^c}\mathsf{F}(A)\|\\ &\leq \|\mathsf{F}(A)\|. \end{aligned}\tag{2.111}$$

Since F is confined on X we have

$$\|\mathsf{F}_Z\|\leq\|\mathsf{F}(A)\|\leq\sum_{j\in X}h_1(d(j,Z)) \tag{2.112}$$

for some superpolynomially decaying function h_1. By Proposition C.1 in [KS22] we have

$$\|\mathsf{F}^Z\| \leq 4^d \|\mathsf{F}_Z\| \leq 4^d \sum_{j\in X} h_1(d(j,Z)). \tag{2.113}$$

Letting $h_2(R) := \sum_{r\geq R} 2^d r^d h_1(r)$, we have

$$\begin{aligned} \sum_{j\in X} h_(d(j,Z)) &\leq \sum_{\substack{j\in X\\k\in Z}} h_1(d(j,k)) \\ &\leq \sum_{k\in Z} h_2(d(k,X)) \\ &\leq \operatorname{diam}(Z)^d h_2(d(Z,X)), \end{aligned} \tag{2.114}$$

and so

$$\|\mathsf{F}^Z\| \leq 4^d \operatorname{diam}(Z)^d h_2(d(Z,X)). \tag{2.115}$$

If $\operatorname{diam}(Z)^d h_2(d(Z,X)) \leq (1+d(X,Z))^{-\alpha}(1+\operatorname{diam}(Z))^{-\alpha}$ then we have

$$\|\mathsf{F}^Z\|(1+d(X,Z))^{\alpha}(1+\operatorname{diam}(Z))^{\alpha} \leq 4^d. \tag{2.116}$$

Otherwise if $\operatorname{diam}(Z)^d h_2(d(Z,X)) > (1+d(X,Z))^{-\alpha}(1+\operatorname{diam}(Z))^{-\alpha}$ we have

$$\begin{aligned} \|\mathsf{F}^Z\|(1+d(Z,X))^{\alpha}(1+\operatorname{diam}(Z))^{\alpha} &\leq \|\mathsf{F}\|_{2\alpha+d}(1+\operatorname{diam}(Z))^{-\alpha-d}(1+d(Z,X))^{\alpha} \\ &\leq \|\mathsf{F}\|_{2\alpha+d} h_2(d(Z,X))(1+d(Z,X))^{2\alpha} \\ &\leq \|\mathsf{F}\|_{2\alpha+d} \sup_r (1+r)^{2\alpha} h_2(r). \end{aligned} \tag{2.117}$$

$ii) \implies iii)$. First, f is a 1-chain because

$$\|\mathsf{f}_j\|^{br}_{j,\alpha} = \sup_{Z\ni j} \frac{1}{|Z|} \|\mathsf{F}^Z\|(1+\operatorname{diam}(Z))^{\alpha} \leq \|\mathsf{F}\|_{\alpha}. \tag{2.118}$$

To show f is confined on X we use the bound

$$\|\mathsf{f}_j\| \leq \sum_{r>0} \sum_{\substack{Z\ni j\\ \operatorname{diam}(Z)=r}} r^{-1}\|\mathsf{F}^Z\|. \tag{2.119}$$

Consider an arbitrary term in the above sum. When $r \leq d(j,X)/2$ we have

$$\|\mathsf{F}^Z\| \leq C_{\alpha}(1+r)^{-\alpha}(1+d(j,X)/2)^{-\alpha} \tag{2.120}$$

since $d(Z,X)+r \geq d(j,X)$. On the other hand when $r \geq d(j,X)/2$ we will use the bound

$$\|\mathsf{F}^Z\| \leq C_\alpha(1+r)^{-\alpha}. \tag{2.121}$$

Putting these together and using the fact that there are at most $d(r+1)^{d+1}$ bricks of diameter r containing j, we have

$$\|\mathsf{f}_j\| \leq C_\alpha(1+d(j,X)/2)^{-\alpha} \sum_{0<r\leq d(j,X)/2} d(1+r)^{-\alpha+d} + C_\alpha \sum_{r>d(j,X)/2} d(1+r)^{-\alpha+d}. \tag{2.122}$$

When $\alpha \geq d+2$ we obtain

$$\|\mathsf{f}_j\| \leq dC_\alpha(1+c)(1+d(j,X)/2)^{-\alpha+d+1}, \tag{2.123}$$

where c is a constant with $\sum_{r>R}(1+r)^{-\alpha+d} \leq cR^{-\alpha+d+1}$. Thus $\sup_j \|\mathsf{f}_j\|$ decays superpolynomially with $d(j,X)$.

iii) $\implies$ *ii)*. Suppose $\mathsf{F} = \partial\mathsf{f}$ for some 1-chain f confined on X. By Lemma 2.7.1 above, we may assume that the entries of f vanish outside X. Let $Y \subset \mathbb{Z}^d$ be a finite region and let $A \in \mathscr{A}_Y$ be arbitrary. Since f is a chain we have $\|[\mathsf{f}_j, A]\| \leq \|A\| h(d(j,A))$ for some superpolynomially decaying h. Summing these over all $j \in X$ we find that F is h-confined on X. □

Recall that every $\mathsf{F} \in \mathfrak{D}_{al}$ has $\|\mathsf{F}^X\| \leq h(\mathrm{diam}(X))$ for some superpolynomially decreasing h. For such a derivation we have

$$\|\mathsf{F}(A)\| \leq C|\operatorname{supp}(A)|\|A\| \tag{2.124}$$

for any strictly local observable A, where $C = d\sum_{R>0} R^d h(R)$. By integrating this bound one can see that it continues to hold when F is replaced by an LGA α.

Lemma 2.7.5. *Let $F : \mathscr{A}_{al} \to \mathscr{A}_{al}$ be a linear map that satisfies the bound (2.124). Suppose F is h_2-confined on a region X. If A is an observable that is h_1-confined at a site j then $\|F(A)\|$ is bounded by a superpolynomially decreasing function of $d(j,X)$ that depends only on h_1, h_2, and $\|A\|$.*

Remark 2.7.1. *If F is trace-preserving then this implies that for any p-chain f, $F(\mathsf{f})$ is a p-chain that is confined on X if F is.*

Proof. For any site ℓ and any $R > 0$ we have

$$\sum_{k \in B_\ell(r)^c} h_2(d(\ell, k)) \leq \sum_{R>r} (2R)^d h_2(R) := h_3(r), \tag{2.125}$$

where evidently h_3 decays superpolynomially if h_2 does. It follows that for any bounded set $Y \subset \mathbb{Z}^d$ we have

$$\sum_{k \in X} h_2(d(k, Y)) \leq |Y| h_3(d(X, Y)). \tag{2.126}$$

Since A is h_1-confined at j we have $\|A - \overline{\mathrm{tr}}_{B_j(r)^c} A\| \leq 2h_1(r)$. Defining $A_r := \overline{\mathrm{tr}}_{B_j(r)^c} A - \overline{\mathrm{tr}}_{B_j(r-1)^c} A$ for $r \geq 1$ and $A_0 := \overline{\mathrm{tr}}_{\{j\}^c} A - \overline{\mathrm{tr}}(A)\mathbf{1}$ we have

$$\begin{aligned} \|A_r\| &= \|\overline{\mathrm{tr}}_{B_j(r)^c}(A - \overline{\mathrm{tr}}_{B_j(r-1)^c} A)\| \\ &\leq 2h_1(r-1), \end{aligned} \tag{2.127}$$

for $r \geq 1$ while $\|A_0\| \leq 2\|A\|$. Writing $R := d(j, X)$, we have

$$\begin{aligned} \|\mathsf{F}(A)\| &\leq \sum_{r \geq 0} \|\mathsf{F}(A_r)\| \\ &\leq \|\mathsf{F}(A_0)\| + \sum_{1 \leq r < R} \|\mathsf{F}(A_r)\| + \sum_{r \geq R} \|\mathsf{F}(A_r)\| \\ &\leq h_2(R)\|A\| + \sum_{1 \leq r < R} \sum_{k \in A} h_3(d(k, B_j(r)))\|A_r\| + \sum_{r \geq R} C(2r)^d h_1(r-1) \\ &\leq h_2(R)\|A\| + \sum_{1 \leq r < R} (2r)^d h_1(r-1) h_3(R-r) + \sum_{r \geq R} C(2r)^d h_1(r-1), \end{aligned} \tag{2.128}$$

where we used (2.126) in the last line. □

Proof of Proposition 2.3.1. The proofs involving $\mathsf{a} \in C^p$ for some $p \geq 0$ will need to be split into cases according to whether $p = 0$ or $p > 0$, i.e. whether a is a derivation or a chain.

i): When $\mathsf{a} \in C^1$ this follows from Lemma 2.7.1. When $\mathsf{a} \in C^p$ for $p > 1$ it follows from Lemma 2.7.3.

ii): Consider first the case $p > 0$ and let f be a p-chain that is h_1-confined on X and h_2-confined on X'. Since Y is a stable intersection of X and X' there is a $c > 0$ such that $d(j, Y) \leq c \max(d(j, X), d(j, X'))$. For any $j_1 \ldots, j_k \in \mathbb{Z}^d$

and any $1 \leq \ell \leq k$ we have

$$\begin{aligned}\|f_{j_1,\ldots,j_k}\| &\leq \min(h_1(d(j_\ell, X)), h_2(d(j_\ell, X'))) \\ &\leq g(\max(d(j_\ell, X), d(j_\ell, X'))) \\ &\leq g(c^{-1}d(j, Y))\end{aligned} \tag{2.129}$$

where $g = \max(h_1, h_2)$. Next, if $p = 0$ (i.e. a is a derivation) the result follows from Lemma 2.7.5 and the $p = 1$ case.

iii): Suppose first that $\mathsf{a} \in C^p$ and $\mathsf{b} \in C^q$ for $p, q > 0$. Then the bound $\|[\mathsf{a}_{j_1,\ldots,j_p}, \mathsf{b}_{j_{p+1},\ldots,j_{p+q}}]\| \leq 2\|\mathsf{a}_{j_1,\ldots,j_p}\|\|\mathsf{b}_{j_{p+1},\ldots,j_{p+q}}\|$ shows that $\|\{\mathsf{a}, \mathsf{b}\}_{j_1,\ldots,j_{p+q}}\|$ decays superpolynomially with both $d(j_i, X)$ and $d(j_i, X'))$ for any $1 \leq i \leq p+q$, and so by part *i)* it decays polynomially with $d(j_i, Y)$.

Next, suppose $p = 0$ and $q > 0$. Then by Lemma 2.7.5 and Proposition D.4 in [KS22], $\|\{\mathsf{a}, \mathsf{b}\}_{j_1 \ldots, j_q}\|$ decays superpolynomially with both $d(j_i, X)$ and $d(j_i, X'))$ for any $1 \leq i \leq q$, so again by part *i)* we are done.

Finally if $p = q = 0$ then the result follows from the $p = 0, q = 1$ case together with Lemma 2.7.4. □

Proposition 2.3.2 now follows easily from Proposition 2.3.1.

Proof of Proposition 2.3.2. The fact that $\alpha^{-1}d\alpha$ is smoothly confined on X follows from the explicit expression (2.21). The second fact follows from the expression

$$\alpha(\mathsf{F}) - \mathsf{F} = \int_0^1 \alpha_s(\iota_{\frac{\partial}{\partial s}} \mathsf{G}(\mathsf{F}))ds. \tag{2.130}$$

By Proposition 2.3.1 the integrand is confined on X, so $\alpha(\mathsf{F}) - \mathsf{F}$ is confined there too. Differentiating the equation (2.130) and using the fact that $\alpha^{-1}d\alpha$ and G are confined on X, together with Proposition 2.3.1, shows that the partial derivatives of $\alpha(\mathsf{F}) - \mathsf{F}$ are also confined on X. □

We now move on to proving Proposition 2.3.3.

Lemma 2.7.6. *Suppose* $\mathsf{F} \in \mathfrak{D}_{al}$ *is* h*-confined on a bounded set* $X \subset \mathbb{Z}^d$*. Then the sum* $A := \sum_Z \mathsf{F}^Z$ *is absolutely convergent in* $\mathscr{A}_{al}$ *and for any* $j \in X$ *we have* $\|A\|^{br}_{j,\alpha} \leq (1 + \mathrm{diam}(X))^\alpha(4^d + C_\alpha\|\mathsf{F}\|_{2\alpha+d})$ *for some constants* C_α *that depend only on* α *and* h*.*

Proof. From the proof of Lemma 2.7.4 we have constants C'_α depending only on h and F such that

$$\|\mathsf{F}^Z\| \leq C'_\alpha(1+\mathrm{diam}(Z))^{-\alpha}(1+d(X,Z))^{-\alpha}. \tag{2.131}$$

In fact, from the proof of Lemma 2.7.4, we see that these constants are of the form $C'_\alpha = 4^d + C_\alpha\|\mathsf{F}\|_{2\alpha+d}$ for some constants C_α depending only on h.

For any $j \in X$ we have an inclusion $X \subset B_j(R)$, where we denoted $R = \mathrm{diam}(X)$ for brevity. Therefore

$$\begin{aligned}\|\mathsf{F}^Z\| &\leq C'_\alpha(1+\mathrm{diam}(Z))^{-\alpha}(1+d(Z,X))^{-\alpha}\\ &\leq C'_\alpha(1+\mathrm{diam}(Z)+d(Z,X))^{-\alpha}\\ &\leq C'_\alpha(1+\mathrm{diam}(Z)+\max(0,d(j,Z)-R))^{-\alpha}\\ &\leq (1+R)^\alpha C'_\alpha(1+\mathrm{diam}(Z)+d(j,Z))^{-\alpha}.\end{aligned} \tag{2.132}$$

From this bound, and the fact that for sufficiently large α we have $\sum_X (1+\mathrm{diam}(X\cup\{j\})^{-\alpha} < \infty$ (the sum being over all bricks X) it follows that $\sum_Z \mathsf{F}^Z$ is absolutely convergent in $\mathscr{A}_{al}$. Furthermore,

$$\|A^Z\|(1+\mathrm{diam}(\{j\}\cup Z))^\alpha = \|\mathsf{F}^Z\|(1+\mathrm{diam}(\{j\}\cup Z))^\alpha \leq C'_\alpha(1+\mathrm{diam}(X))^\alpha. \tag{2.133}$$

□

We are now ready to prove Proposition 2.3.3.

Proof of Proposition 2.3.3. Suppose $\mathsf{F} = \mathrm{ad}_A$ for an antiselfadjoint $A \in \Omega^\bullet(M, \mathscr{A}_{al})$, and let $X = \{0\} \subset \mathbb{Z}^d$. Regarding A as a 1-chain f with f_j equal to A if $j = 0$ and 0 otherwise and applying Proposition 2.3.1 $i)$ we find that F is smoothly confined on X.

Conversely, suppose F is smoothly confined on F. Since this is a local statement we may assume without loss that $M = \mathbb{R}^n$. By Lemma 2.7.6, for each $x \in \mathbb{R}^n$ and each multi-index μ the sum $A_\mu(x) := \sum_Z \partial^\mu \mathsf{F}^Z \in \mathscr{A}_{al}$ is well-defined and for any μ, α, j the seminorm $\|A_\mu(x)\|_{j,\alpha}$ is a continuous function of x.

To show that $A \in C^\infty(U, \mathscr{A}_{al})$ it suffices to show that for any μ and any $0 \leq i \leq n$ the equation $\partial_i A_\mu = A_{\mu+i}$ holds in $C^\infty(U, \mathscr{A}_{al})$. For any brick Z

and any μ the expression $(\partial^\mu \mathsf{F})^Z = \partial^\mu(\mathsf{F}^Z)$ is a smooth function $\mathbb{R}^n \to \mathscr{A}_Z$, and so for any $x \in \mathbb{R}^n$, $1 \leq i \leq n$, and $h > 0$ we have

$$\begin{aligned} \left\| \frac{\partial^\mu \mathsf{F}^Z(x + he_i) - \partial^\mu \mathsf{F}^Z(x)}{h} - \partial^{\mu+i}\mathsf{F}^Z(x) \right\| &\leq \frac{1}{h}\int_{h_0=0}^{h} dh_0 \|\partial^{\mu+i}\mathsf{F}^Z(x+h_0e_i) - \partial^{\mu+i}\mathsf{F}^Z(x)\| \\ &\leq \sup_{0\leq h_0 \leq h} \|\partial^{\mu+i}\mathsf{F}^Z(x+h_0e_i) - \partial^{\mu+i}\mathsf{F}^Z(x)\| \\ &\leq h \sup_{0\leq h_0\leq h} \|\partial^{\mu+2i}\mathsf{F}^Z(x+h_0e_i)\|, \end{aligned} \tag{2.134}$$

and so for any $j \in \mathbb{Z}^d$ we have

$$\left\| \frac{A_\mu(x+he_i) - A_\mu(x)}{h} - A_{\mu+i} \right\|_{j,\alpha}^{br} \leq h \sup_{0\leq h_0\leq h} \|A_{\mu+2i}(x+h_0e_i)\|_{j,\alpha}^{br}, \tag{2.135}$$

which approaches 0 as $h \to 0$. □

We conclude this section with a lemma which we will often use to create derivations that interpolate on the lattice between one derivation and another.

Lemma 2.7.7. *Suppose ψ is a gapped family of states on M that is parallel with respect to both $\mathsf{G}_1 \in \Omega^1(M, \mathfrak{D}_{al})$ and $\mathsf{G}_2 \in \Omega^1(M, \mathfrak{D}_{al})$. Then for any $X \subset \mathbb{Z}^d$ there exists $\mathsf{G}_3 \in \Omega^1(M, \mathfrak{D}_{al})$ such that ψ is parallel with respect to G_3, and G_3 (resp. $\mathsf{F}_{\mathsf{G}_3}$) smoothly interpolates between G_1 (resp. $\mathsf{F}_{\mathsf{G}_1}$) on X and G_2 (resp. $\mathsf{F}_{\mathsf{G}_2}$)on X^c. If in addition G_1 and G_2 are both smoothly confined on some $Y \subset \mathbb{Z}^d$, then G_3 and $\mathsf{F}_{\mathsf{G}_3}$ are smoothly confined there too.*

Proof. Since ψ is parallel with respect to both G_1 and G_2, their difference lies in $\Omega^1(M, \mathfrak{D}_{al}^\psi)$. Define

$$\mathsf{G}_3 := \mathsf{G}_1 - \partial \operatorname{res}_{X^c}(h^\psi(\mathsf{G}_1 - \mathsf{G}_2)) \tag{2.136}$$

$$= \mathsf{G}_2 - \partial \operatorname{res}_X(h^\psi(\mathsf{G}_2 - \mathsf{G}_1)). \tag{2.137}$$

Since $\operatorname{res}_{X^c}(h^\psi(\mathsf{G}_1 - \mathsf{G}_2))$ (resp. $\operatorname{res}_X(h^\psi(\mathsf{G}_2 - \mathsf{G}_1))$) is smoothly confined on X (resp. X^c), by Proposition 2.3.1 *i*) and *ii*), G_3 interpolates between G_1 on X and G_2 on X^c.

Next, we have

$$\mathsf{F}_{\mathsf{G}_3} = \mathsf{F}_{\mathsf{G}_1} - \partial \operatorname{res}_{X^c} D_{\mathsf{G}}(h^\psi(\mathsf{G}_1 - \mathsf{G}_2)) \tag{2.138}$$

$$= \mathsf{F}_{\mathsf{G}_2} - \partial \operatorname{res}_X D_{\mathsf{G}}(h^\psi(\mathsf{G}_2 - \mathsf{G}_1)). \tag{2.139}$$

By the same reasoning as above $\mathsf{F}_{\mathsf{G}_3} - \mathsf{F}_{\mathsf{G}_1}$ (resp. $\mathsf{F}_{\mathsf{G}_3} - \mathsf{F}_{\mathsf{G}_2}$) is smoothly confined on X^c (resp. X). □

References

[Bac+19] Sven Bachmann et al. "A Many-Body Index for Quantum Charge Transport". In: *Communications in Mathematical Physics* 375.2 (July 2019), pp. 1249–1272. ISSN: 1432-0916. DOI: 10.1007/s00220-019-03537-x. URL: http://dx.doi.org/10.1007/s00220-019-03537-x.

[Bac+22] Sven Bachmann et al. "A classification of G-charge Thouless pumps in 1D invertible states". In: *arXiv e-prints*, arXiv:2204.03763 (Apr. 2022), arXiv:2204.03763. DOI: 10.48550/arXiv.2204.03763. arXiv: 2204.03763 [math-ph].

[BBR24] Sven Bachmann, Alex Bols, and Mahsa Rahnama. "Many-body Fu-Kane-Mele index". In: *arXiv e-prints*, arXiv:2406.19463 (June 2024), arXiv:2406.19463. DOI: 10.48550/arXiv.2406.19463. arXiv: 2406.19463 [math-ph].

[Ber84] Michael V. Berry. "Quantal Phase Factors Accompanying Adiabatic Changes". In: *Proceedings of the Royal Society of London Series A* 392 (1984), pp. 45–57. DOI: 10.1098/rspa.1984.0023.

[BR87] Ola Bratteli and Derek W. Robinson. *Operator algebras and quantum statistical mechanics. 1. C^*- and W^*-algebras, symmetry groups, decomposition of states.* 2nd ed. Texts and Monographs in Physics. Springer-Verlag, New York, 1987.

[Bry08] Jean-Luc Brylinski. *Loop spaces, characteristic classes and geometric quantization*. Modern Birkhäuser Classics. Reprint of the 1993 edition. Birkhäuser Boston, Inc., Boston, MA, 2008, pp. xvi+300. ISBN: 978-0-8176-4730-8. DOI: 10.1007/978-0-8176-4731-5. URL: https://doi.org/10.1007/978-0-8176-4731-5.

[D23] Spiegel Daniel D. "A C*-Algebraic Approach to Parametrized Quantum Spin Systems and Their Phases in One Spatial Dimension". PhD thesis. University of Colorado, 2023.

[DF99] Pierre Deligne and Daniel S. Freed. "Classical field theory". In: *Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997).* Amer. Math. Soc., Providence, RI, 1999, pp. 137–225. ISBN: 0-8218-1198-3.

[HKT20] Po-Shen Hsin, Anton Kapustin, and Ryan Thorngren. "Berry phase in quantum field theory: Diabolical points and boundary phenomena". In: *Physical Review B* 102.24, 245113 (2020), p. 245113.

[HM14] Matthew B. Hastings and Spyridon Michalakis. "Quantization of Hall Conductance for Interacting Electrons on a Torus". In: *Communications in Mathematical Physics* 334.1 (Sept. 2014), pp. 433–

471. ISSN: 1432-0916. DOI: 10.1007/s00220-014-2167-x. URL: http://dx.doi.org/10.1007/s00220-014-2167-x.

[Kit] Alexei Kitaev. "On the classificaton of Short-Range Entangled states". Talk at Simons Center for Geometry and Physics, June 2013. URL: http://scgp.stonybrook.edu/archives/7874.

[KS20a] Anton Kapustin and Nikita Sopenko. "Hall conductance and the statistics of flux insertions in gapped interacting lattice systems". In: *J. Math. Phys.* 61.10 (2020), pp. 101901, 24.

[KS20b] Anton Kapustin and Lev Spodyneiko. "Higher-dimensional generalizations of Berry curvature". In: *Phys. Rev. B* 101 (2020), p. 235130. DOI: 10.1103/PhysRevB.101.235130. arXiv: 2001.03454 [cond-mat.str-el].

[KS20c] Anton Kapustin and Lev Spodyneiko. "Higher-dimensional generalizations of the Thouless charge pump". In: *arXiv e-prints*, arXiv:2003.09519 (Mar. 2020), arXiv:2003.09519. DOI: 10.48550/arXiv.2003.09519. arXiv: 2003.09519 [cond-mat.str-el].

[KS22] Anton Kapustin and Nikita Sopenko. "Local Noether theorem for quantum lattice systems and topological invariants of gapped states". In: *Journal of Mathematical Physics* 63 (2022), p. 091903. DOI: 10.1063/5.0085964. arXiv: 2201.01327 [math-ph].

[KSY21] Anton Kapustin, Nikita Sopenko, and Bowen Yang. "A classification of invertible phases of bosonic quantum lattice systems in one dimension". In: *Journal of Mathematical Physics* 62.8 (2021).

[Lau81] Robert B. Laughlin. "Quantized Hall conductivity in two dimensions". In: *Phys. Rev. B* 23 (1981), pp. 5632–5633.

[Lau83] Robert B. Laughlin. "Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations". In: *Phys. Rev. Lett.* 50 (1983), pp. 1395–1398. DOI: 10.1103/PhysRevLett.50.1395.

[MO20] Alvin Moon and Yoshiko Ogata. "Automorphic equivalence within gapped phases in the bulk". In: *Journal of Functional Analysis* 278.8 (2020), p. 108422.

[Mur07] Michael K. Murray. "An Introduction to Bundle Gerbes". In: *arXiv e-prints*, arXiv:0712.1651 (Dec. 2007), arXiv:0712.1651. DOI: 10.48550/arXiv.0712.1651. arXiv: 0712.1651 [math.DG].

[OK] Yoshiko Ogata and Yosuke Kubota. *unpublished*.

[OR23] Shuhei Ohyama and Shinsei Ryu. "Higher structures in matrix product states". In: *arXiv e-prints*, arXiv:2304.05356 (Apr. 2023), arXiv:2304.05356. DOI: 10.48550/arXiv.2304.05356. arXiv: 2304.05356 [cond-mat.str-el].

[OTS23] Shuhei Ohyama, Yuji Terashima, and Ken Shiozaki. "Discrete Higher Berry Phases and Matrix Product States". In: *arXiv e-prints*, arXiv:2303.04252 (Mar. 2023), arXiv:2303.04252. DOI: 10.48550/arXiv.2303.04252. arXiv: 2303.04252 [cond-mat.str-el].

[Sak67] Shôichirô Sakai. "Derivations of uniformly hyperfinite C^*-algebras". In: *Publ. Res. Inst. Math. Sci. Ser. A* 3 (1967), pp. 167–175. DOI: 10.2977/prims/1195195562.

[Sim83] Barry Simon. "Holonomy, the Quantum Adiabatic Theorem, and Berry's phase". In: *Phys. Rev. Lett.* 51 (1983), pp. 2167–2170. DOI: 10.1103/PhysRevLett.51.2167.

[Tho83] D. J. Thouless. "Quantization of particle transport". In: *Physical Review B* 27.10 (May 1983), pp. 6083–6087. ISSN: 0163-1829. DOI: 10.1103/physrevb.27.6083. URL: http://dx.doi.org/10.1103/PhysRevB.27.6083.

[Uhl76] Armin Uhlmann. "The "transition probability" in the state space of a *-algebra". In: *Reports on Mathematical Physics* 9.2 (1976), pp. 273–279.

[Wen+23] Xueda Wen et al. "Flow of higher Berry curvature and bulk-boundary correspondence in parametrized quantum systems". In: *Physical Review B* 108.12 (2023), p. 125147.

[Zen+19] Bei Zeng et al. *Quantum information meets quantum matter: From quantum entanglement to topological phases of many-body systems.* Quantum Science and Technology. Springer, New York, 2019.

Chapter 3

A MATHEMATICAL THEORY OF TOPOLOGICAL INVARIANTS OF QUANTUM SPIN SYSTEMS

This Chapter is available as a preprint at

[AKY24] Adam Artymowicz, Anton Kapustin, and Bowen Yang. "A mathematical theory of topological invariants of quantum spin systems". In: *arXiv e-prints*, arXiv:2410.19287 (Oct. 2024), arXiv:2410.19287. DOI: 10.48550/arXiv.2410.19287. arXiv: 2410.19287 [math-ph].

3.1 Introduction

The study of gapped phases of quantum matter at zero temperature is an important area of theoretical physics. Much conceptual progress has been made by assuming that gapped phases can be described by topological quantum field theory (TQFT). For example, the celebrated Quantum Hall Effect is captured by Chern-Simons field theory. However, the precise relation between gapped phases of matter and TQFTs is not understood. Recently, new mathematically rigorous approaches to classifying gapped phases of matter have been developed (see [Oga19b; Oga19a; BO20; KSY21] for the case of one-dimensional systems, [Oga21; Sop21; KS20; AKS24; BBR24; Bac+24] for the case of two-dimensional systems, and [KS22] for systems in an arbitrary number of dimensions). They enable one to assign indices to gapped states of infinite-volume quantum systems invariant under symmetries. The main property of these indices, also referred to as topological invariants, is that they do not vary along suitably-defined continuous paths in the space of states. In some cases, the indices can be related to physical quantities, such as the zero-temperature Hall conductance, thereby explaining the robustness of the latter.

The methods of [KS20; KS22; AKS24; BBR24] apply to arbitrary gapped states of infinite-volume quantum spin systems with rapidly decaying interactions and employ C^*-algebraic techniques, some well-established and some relatively new. The construction of topological invariants in [KS22; AKS24] also uses some algebraic and geometric ingredients . The algebraic ingredient is a pointed (or curved) Differential Graded Lie Algebra (DGLA) and an associated Maurer-Cartan equation. The geometric ingredient is a collection of conical subsets of the Euclidean space triangulating the sphere at infinity. The appearance of these ingredients in the context of quantum statistical mechanics has not been motivated, and consequently the mathematical meaning of the invariants remains obscure.

The primary goal of this paper is provide a proper mathematical framework for the constructions of [KS22; AKS24] and to interpret topological invariants of gapped states as lattice analogs of 't Hooft anomalies in Quantum Field Theory. The secondary goal is to generalize the construction in various directions. In particular, we show how to define topological invariants of lattice spin systems confined to well-behaved subsets of the lattice. This generalization makes explicit that the invariants take values in a vector space which is determined by the asymptotic geometry of the subset.

While our work concerns quantum lattice systems, we take inspiration from Quantum Field Theory (QFT). These two subjects are connected via the bulk-boundary correspondence. One aspect of this conjectural correspondence is that topological invariants of gapped states with symmetries are related to 't Hooft anomalies of symmetries of the boundary field theory.[1] It is usually said that 't Hooft anomalies are obstructions to gauging a global symmetry of a QFT [t H80]. A possible mathematical interpretation of this statement is that an 't Hooft anomaly is an obstruction to defining a local action of the group of gauge transformations on the algebra of local observables of a QFT. Assuming this interpretation, the presence of an 't Hooft anomaly is a purely kinematic statement which involves neither the Hamiltonian nor the vacuum state of the field theory. It is not clear if conventional markers of 't Hooft anomalies, such as anomalous Ward identities for vacuum correlators of currents, are implied by a kinematic statement. Proving or disproving this is currently out of reach because of gaps in the mathematical foundations of QFT. The mathematical theory of quantum lattice systems, on the other hand, is sufficiently mature and enables us to address the problem of 't Hooft anomalies from the bulk side of the bulk-boundary correspondence. In this paper we show that topological invariants of gapped states of lattice systems, such as the zero-temperature Hall conductance, can be interpreted as obstructions to promoting a symmetry

[1] This assumes, of course, that a field-theoretic description of boundary degrees of freedom exists, which is far from obvious.

of a gapped state to a gauge symmetry. Dynamics enters this statement only though the state.

The main novelty of the paper is a new formulation of locality on a lattice. Building on ideas introduced in [KS20; KS22; AKS24], we define for any (possibly unbounded) region of the lattice a space of derivations that are approximately localized on that region. For sufficiently regular regions, we show that these spaces behave as expected under natural operations like the commutator. To combine them into a single geometric object we show that they form a cosheaf on a certain *site*, i.e. a category with a Grothendieck topology. The utility of Grothendieck topologies in describing spaces of functions with a prescribed asymptotic behavior is well-known to analysts, see e.g. [KS01; GS16], and here we apply the same idea in a non-commutative context. We call the resulting global geometric object a *local Lie algebra*. An on-site action of a Lie group on a lattice system yields a representation of a certain local Lie algebra by derivations, and we show that the invariants defined in [KS22] can be phrased as purely algebraic invariants of this representation. Namely, an obstruction exists to defining a representation which acts by state-preserving derivations, and this obstruction takes value in the homology of a certain DGLA associated naturally to the local Lie algebra of state-preserving derivations. The invariants defined in [KS22] then arise from a natural pairing of this homology with the Čech cohomology of the sphere at infinity. Aside from clarifying their mathematical meaning, this also shows that the invariants defined in [KS22] do not depend on certain choices present in their construction.

The content of the paper is as follows. In Section 3.2 we axiomatize the notion of an infinitesimal local symmetry by defining local Lie algebras abstractly in terms of cosheaves on a site. We also introduce the Čech functor which assigns a DGLAs to a local Lie algebra, and will serve as the main link between lattice geometry and algebraic topology. In Section 3.3 we turn to infinitesimal symmetries on the lattice, introducing the space of derivations approximately localized on a region, and prove the main properties of these spaces, some of which hold only for sufficiently regular regions. In Section 3.4 we identify a suitable category of such regular regions in $\mathbb{R}^n$, the category $\mathcal{CS}_n$ of *fuzzy semilinear sets* which comes with a natural Grothendieck topology. In Section 3.5 we show that infinitesimal symmetries of any gapped state ψ of a quantum lattice system on $\mathbb{R}^n$ can be described by a local Lie algebra $\mathfrak{D}^{\psi}_{al}$ over $\mathcal{CS}_n$.

We also study gapped states invariant under an action of a compact Lie group G and define a G-equivariant analog of $\mathfrak{D}^{\psi}_{al}$. In Section 3.6 we construct invariants of G-invariant gapped states. The construction is along the lines of [KS22; AKS24] and uses an inhomogeneous Maurer-Cartan equation. We show that these invariants are obstructions for promoting the symmetry G to a local symmetry of the state ψ. We also explain how to generalize the construction of invariants to lattice systems defined on sufficiently nice (asymptotically conical) subsets of $\mathbb{R}^n$ and show that their invariants take values in a space which depends on the asymptotic geometry of the subset. This goes beyond what one can access using the TQFT heuristics. In Section 3.7 we isolate some proofs necessary for Section 3.3, and Section 3.8 develops some properties of the inhomogeneous Maurer-Cartan equation.

We are grateful to Owen Gwilliam, Ezra Getzler, and Bas Janssens for discussions. The work of A. A. and A. K. was supported by the Simons Investigator Award. B. Y. would like to thank Yu-An Chen and Peking University for hospitality during the final stages of this work. A. K. would like to thank Yau Mathematical Sciences Center, Tsinghua University, for the same.

3.2 Local Lie algebras

Locality and (pre-)cosheaves

Let M be a (compact) manifold and $Open(M)$ be the category whose objects are open subsets of M, and the set of morphisms from an open U to an open V is the singleton or the empty set depending on whether $U \subseteq V$ or $U \nsubseteq V$. Composition of morphisms is uniquely defined. A pre-cosheaf $\mathfrak{F}$ on M with values in a category $\mathcal{C}$ is a functor $\mathfrak{F} : Open(M) \to \mathcal{C}$. Thus for every inclusion of opens $U \subseteq V$ one is given a co-restriction morphism $e_{VU} : \mathfrak{F}(U) \to \mathfrak{F}(V)$ such that for any three opens $U \subseteq V \subseteq W$ one has $e_{WV} \circ e_{VU} = e_{WU}$. Pre-cosheaves (as well as pre-sheaves, which are functors from the opposite category of $Open(M)$ to $\mathcal{C}$) can be used to describe local data on M. This form of locality is rather weak, since it does not require $\mathfrak{F}(U \cup V)$ to be expressible through $\mathfrak{F}(U)$ and $\mathfrak{F}(V)$.

As an example, consider the Lie algebra of gauge transformations, i.e. the Lie algebra $\mathfrak{G}(M) := C^\infty(M, \mathfrak{g})$ of smooth functions on M with values in a finite-dimensional Lie algebra $\mathfrak{g}$. It is a global object attached to M. To "localize" it, for any open $U \subseteq M$ we define the Lie algebra $\mathfrak{G}(U)$ to be the space of smooth $\mathfrak{g}$-valued functions on M whose closed support is contained in U. In particular, $\mathfrak{G}(\varnothing) = 0$. For any inclusion of opens $U \subseteq V$ we have a homomorphism of Lie algebras $\iota_{VU} : \mathfrak{G}(U) \to \mathfrak{G}(V)$ such that the Lie algebras $\mathfrak{G}(U)$ assemble into a pre-cosheaf $\mathfrak{G}$ of Lie algebras on M. This is a *coflasque* pre-cosheaf, i.e. all its structure maps ι_{VU} are injective.[2]

Continuing with the example, for any two opens U, V the following sequence is exact:

$$\mathfrak{G}(U \cap V) \to \mathfrak{G}(U) \oplus \mathfrak{G}(V) \to \mathfrak{G}(U \cup V) \to 0. \tag{3.1}$$

Here the first arrow is $\iota_{U,U\cap V} \oplus (-\iota_{V,U\cap V})$ and the second arrow is $\iota_{U\cup V,U} \oplus \iota_{U\cup V,V}$. Exactness follows from the existence of a partition of unity for the cover $\mathfrak{U} = \{U, V\}$ of $U \cup V$. In words, the exactness of the sequence (3.1) means that any element of $\mathfrak{G}(U \cup V)$ can be decomposed as a sum of elements of sub-algebras attached to U and V modulo ambiguities which take values in the sub-algebra attached to $U \cap V$.

More generally, for a compact M the existence of a partition of unity implies that for any collection of opens U_i, $i \in I$, the following sequence is exact:

$$\oplus_{i<j}\mathfrak{G}(U_i \cap U_j) \to \oplus_i \mathfrak{G}(U_i) \to \mathfrak{G}(\cup_i U_i) \to 0. \tag{3.2}$$

By definition, this means that the pre-cosheaf of vector spaces $\mathfrak{G}$ is a cosheaf of vector spaces. The cosheaf property is a compatibility of the pre-cosheaf with the notions of intersection and union of opens and expresses a stronger form of locality.

Note that the maps in the above exact sequences are not Lie algebra homomorphisms. Hence $\mathfrak{G}$ is not a cosheaf of Lie algebras. Nevertheless, the following additional property of $\mathfrak{G}$ can be regarded as a form of locality of the Lie bracket: for any U, V, $[\mathfrak{G}(U), \mathfrak{G}(V)] \subseteq \mathfrak{G}(U \cap V)$. We will call this "Property I", where "I" stands for "intersection". In particular, elements of $\mathfrak{G}(M)$ which are supported on non-intersecting opens U and V commute.

Symmetries of gapped states of quantum lattice spin systems are typically local only approximately. To phrase locality of symmetries in lattice systems in a similar language, one needs to replace the set $Open(M)$ of open subsets

[2]The terminology comes from sheaf theory, where a pre-sheaf $\mathcal{F} : Open(M)^{opp} \to \mathcal{C}$ is called flasque if for any $U \subseteq V$ the restriction morphism $\mathcal{F}(V) \to \mathcal{F}(U)$ is a surjection.

of M with a more general structure which admits the notions of intersection, union, and cover.

The first thing to note is that the category $\mathit{Open}(M)$ is rather special: its objects form a pre-ordered set (i.e. the set of objects carries a relation $\subseteq$ which is reflexive and transitive), and the category structure is determined by the pre-order. The relation $\subseteq$ is also anti-symmetric: $U \subseteq V$ and $V \subseteq U$ implies $U = V$. In other words, $\mathit{Open}(M)$ is a poset. In general, we will not require the pre-order to be anti-symmetric. From the categorical viewpoint, $U \subseteq V$ and $V \subseteq U$ means that U and V are isomorphic objects of the category $\mathit{Open}(M)$, and as a general rule, it is not advisable to identify isomorphic objects.

For any pre-ordered set $(X, \leq)$ there is a natural notion of intersection and union. The intersection of $U, V \in X$ can be defined as the greatest lower bound (or meet) of both U and V, i.e. a $W \in X$ such that $W \leq U$, $W \leq V$, and for any $W' \leq U, V$ we have $W' \leq W$. The meet of U and V is denoted $U \wedge V$. Similarly, the union of U and V can be defined as the smallest upper bound (or join) of both U and V. It is denoted $U \vee V$. For a general pre-ordered set, the meet and join may not exist for all pairs of objects. If they exist, they are unique up to isomorphism. We will assume that $(X, \leq)$ is such that $U \wedge V$ and $U \vee V$ exist for all $U, V \in X$.[3] The existence of all pairwise meets and joins implies the existence of all finite meets and joins. In the case of the pre-ordered set $\mathit{Open}(M)$ arbitrary (i.e. not necessarily finite) joins make sense.

Finally, to define covers of elements of X, let us assume that $U \wedge (V \vee W) \leq (U \wedge V) \vee (U \wedge W)$ for all $U, V, W \in X$.[4] We will say that X is a distributive pre-ordered set. This condition is certainly satisfied for $\mathit{Open}(M)$. We say that a collection $\mathfrak{U} = \{U_i\}_{i \in I}$ of elements of X covers $A \in X$ iff $U_i \leq A$ for all $i \in I$ and $A \leq \bigvee_{i \in I} U_i$. This definition ensures that if $\mathfrak{U}$ covers A, then for any $B \leq A$ the collection $\mathfrak{U} \wedge B = \{U_i \wedge B\}_{i \in I}$ covers B.

In the case of the pre-ordered set $\mathit{Open}(M)$, the standard topological definition of a cover allows I to be infinite. In general, if X admits only finite joins, I needs to be finite. Also, we may or may not allow I to be empty. This

[3] If we turn X into a poset by identifying isomorphic objects, then this means that the poset is a lattice in the sense of order theory.

[4] The opposite relation is automatic, so this condition ensures that $U \wedge (V \vee W) \simeq (U \wedge V) \vee (U \wedge W)$ for all $U, V, W \in X$. This is equivalent to saying that the poset corresponding to X is a distributive lattice.

possibility only arises when A is the smallest element of X, i.e. $A \leq U$ for any $U \in X$. In the case of the pre-ordered set $Open(M)$, the smallest element is the empty set $\varnothing$, and the standard choice is to allow the empty cover of the empty set. For a general pre-ordered set, it is up to us whether to allow I to be empty.

From a categorical perspective, this notion of a cover equips any distributive pre-ordered set $(X, \leq)$ admitting pairwise meets and joins with a Grothendieck topology, thus making it into a *site* [MM94]. Apart from the option of allowing the labeling set I to be empty, this Grothendieck topology is canonical.

For any $W \in X$ we may consider the subset $X^W = \{U \in X \mid U \leq W\}$ with the pre-order inherited from $(X, \leq)$. It is a distributive pre-ordered set in its own right. When equipped with its canonical Grothendieck topology, it can be regarded as a sub-site of the site associated to $(X, \leq)$.

Given any distributive pre-ordered set $(X, \leq)$, we can define the notion of a pre-cosheaf of vector spaces, a pre-cosheaf of Lie algebras, a cosheaf of vector spaces, and a coflasque pre-cosheaf of Lie algebras with Property I exactly as before, i.e. by mechanically replacing $\cup$ with $\vee$ and $\cap$ with $\wedge$. Motivated by the above example, we introduce the following definition.

Definition 3.2.1. *A local Lie algebra over $(X, \leq)$ is a coflasque pre-cosheaf of Lie algebras with Property I which is also a cosheaf of vector spaces over the corresponding site. A morphism of local Lie algebras is a morphism of the underlying pre-cosheaves of Lie algebras.*

Remark 3.2.1. *Let $\mathfrak{F}$ be a local Lie algebra. Then for any $U \leq V$ the Lie algebra $\mathfrak{F}(U)$ is an ideal in $\mathfrak{F}(V)$. One can equivalently define a local Lie algebra as a pre-cosheaf of Lie algebras over $(X, \leq)$ which is a cosheaf of vector spaces and such that all co-restriction maps are inclusions of Lie ideals.*

Remark 3.2.2. *In this paper all Lie algebras will be Fréchet-Lie algebras and all morphisms will be continuous. We define a local Fréchet-Lie algebra over $(X, \leq)$ to be a coflasque pre-cosheaf of Fréchet-Lie algebras with Property I which is also a cosheaf of vector spaces.*

The following Lemma will be useful in future sections to check the cosheaf property:

Lemma 3.2.1. *Let $\mathfrak{F}$ be a pre-cosheaf of vector spaces on a distributive lattice X, with co-restriction maps $\iota_{U,V} : U \to V$. Then $\mathfrak{F}$ is a cosheaf on X (with the topology of finite covers) iff for any $U, V \in X$ the following sequence is exact:*

$$\mathfrak{F}(U \wedge V) \xrightarrow{\alpha} \mathfrak{F}(U) \oplus \mathfrak{F}(V) \xrightarrow{\beta} \mathfrak{F}(U \vee V) \to 0, \tag{3.3}$$

where $\alpha = \iota_{U\wedge V,U} - \iota_{U\wedge V,V}$ and $\beta = \iota_{U,U\vee V} + \iota_{V,U\vee V}$.

The following proof is essentially a restatement of the proof of Proposition 1.3 in [Bre68], adapted to the site L:

Proof. We must show that for any $U \in X$ and every covering $U_1 \vee \ldots \vee U_n = U$, the sequence of vector spaces

$$\bigoplus_{i<j} \mathfrak{F}(U_i \wedge U_j) \xrightarrow{\alpha} \bigoplus_{i} \mathfrak{F}(U_i) \xrightarrow{\beta} \mathfrak{F}(\vee_i U_i) \to 0 \tag{3.4}$$

is exact, where $\alpha = \sum_{i<j} \iota_{U_i\wedge U_j,U_i} - \iota_{U_i\wedge U_j,U_j}$ and $\beta = \sum_i \iota_{U_i,U}$. Exactness of the last three terms follows from an easy induction and the associativity of the join operation. For exactness of the first three terms of the sequence, we also proceed by induction: suppose the result holds for all covers of cardinality $n-1$, and let $U_1, \ldots, U_n \in L$ be a cover of U. Suppose $(s_1, \ldots, s_n) \in \bigoplus_{i=1}^n \mathfrak{F}(U_i)$ lies in the kernel of β. Let $V := \bigvee_{i=1}^{n-1} U_i$. An application of (3.3) with U_n and V shows that $s_n = \iota_{U_n\cap V,U}(t)$ for some $t \in V \wedge U_n = (U_1 \wedge U_n) \vee ... \vee (U_{n-1} \vee U_n)$, and by right-exactness of (3.4) this shows that $s_n = \sum_{i=1}^{n-1} \iota_{U_i\cap U_n,U_n}(v_i)$ for some $v_i \in \mathfrak{F}(U_i)$. Finally we write

$$(s_1, \ldots, s_n) = (s_1 + w_1, \ldots, s_{n-1} + w_{n-1}, 0) + (-w_1, \ldots, -w_{n-1}, s_n),$$

where $w_i := \iota_{U_i\cap U_n,U_n}(v_i)$. Both terms above the first term lies in the image of α by the inductive hypothesis, while the second term equals $\sum_{i=1}^{n-1} \iota_{U_i\wedge U_n,U_n}(v_i) - \iota_{U_i\wedge U_n,U_i}(v_i)$, which evidently is also in the image of α. ☐

DGLA attached to a cover

Let X be a distributive pre-ordered set. Let $W \in X$ and $\mathfrak{U} = \{U_i\}_{i\in I}$ be a cover of W. Let $\mathfrak{F}$ be a pre-cosheaf of vector spaces over X. The Čech chain complex $C_\bullet(\mathfrak{U}, W; \mathfrak{F})$ is defined by

$$C_n(\mathfrak{U}, W; \mathfrak{F}) = \oplus_{i_0<\ldots<i_n} \mathfrak{F}(U_{i_0} \wedge \ldots \wedge U_{i_n}), \quad n \geq 0,$$

where some linear order on I has been chosen. The differential is the Čech differential $\partial : C_{n+1} \to C_n$ given by $\partial = \sum_{j=0}^{n}(-1)^j \lambda_j$, where λ_j is the canonical map

$$\mathfrak{F}(U_{i_0} \wedge \ldots \wedge U_{i_n}) \to \mathfrak{F}(U_{i_0} \wedge \ldots \widehat{U_{i_j}} \ldots \wedge U_{i_n}).$$

Lemma 3.2.2. *If $\mathfrak{F}$ is a coflasque cosheaf of vector spaces over X, the homology of the Čech complex is 0 for $n > 0$ and $\mathfrak{F}(W)$ for $n = 0$.*

Proof. See [Bre68], Corollary 4.3. Note that [Bre68] uses the term "flabby" instead of "coflasque". □

Let $C^{aug}(\mathfrak{U}, W; \mathfrak{F}) = \{C_\bullet(\mathfrak{U}, W; \mathfrak{F}) \to \mathfrak{F}(W)\}$ be the augmented Čech complex.

Proposition 3.2.1. *Let $\mathfrak{F}$ be a local Lie algebra over X. Then for any $W \in X$ and any cover $\mathfrak{U}$ of W the 1-shifted augmented Čech complex $C^{aug}_{\bullet+1}(\mathfrak{U}, W; \mathfrak{F})$ has a natural structure of a non-negatively graded acyclic DGLA.*

Proof. Let $\mathfrak{U}$ be a cover of W indexed by I. Let V be a vector space with a basis e_i, $i \in I$ and let $f^i, i \in I$, be the dual basis of V^*. The 1-shifted augmented Čech complex of $\mathfrak{F}$ with respect to $\mathfrak{U}$ is naturally identified with a sub-complex of the DGLA $(\mathfrak{F}(W) \otimes \Lambda^\bullet V, \partial)$, where ∂ is contraction with $\sum_i f^i$. It is easy to check that this sub-complex is closed with respect to the graded Lie bracket thanks to Property I. By Lemma 3.2.2, the resulting DGLA is acyclic. □

Covers of $W \in X$ form a category whose morphisms are refinements. A refinement of a cover $\mathfrak{U} = \{U_i\}_{i \in I}$ to a cover $\mathfrak{V} = \{V_j\}_{j \in J}$ is a map $\phi : J \to I$ such that $V_j \leq U_{\phi(j)}$. Refinements are composed in an obvious way.

Proposition 3.2.2. *For a fixed $W \in X$, the map which sends a local Lie algebra $\mathfrak{F}$ and a cover $\mathfrak{U}$ of W to the DGLA $C^{aug}_{\bullet+1}(\mathfrak{U}, W; \mathfrak{F})$ is functorial in both $\mathfrak{F}$ and $\mathfrak{U}$.*

Proof. Functoriality in $\mathfrak{F}$ is clear. Functoriality in $\mathfrak{U}$ is written Čech componentwise for $\mathsf{p}^{\mathfrak{V}} \in C_k(\mathfrak{V}, W; \mathfrak{F})$:

$$(\phi_* \mathsf{p}^{\mathfrak{V}}_k)_{i_0,\ldots,i_k} := \sum_{j_0 \in \phi^{-1}(i_0)} \cdots \sum_{j_k \in \phi^{-1}(i_k)} (\mathsf{p}^{\mathfrak{V}}_k)_{j_0,\ldots,j_k},$$

for $i_0 < i_2 < \cdots < i_k$. □

We will call $C^{aug}_{\bullet+1}(-,W;-)$ the Čech functor. We will need some variants of the Čech functor. First, we can define a *graded* local Lie algebra over a distributive pre-ordered set $(X,\leq)$ in an obvious manner. The construction of the acyclic DGLA $C^{aug}_{\bullet+1}(\mathfrak{U},W;\mathfrak{F})$ works in this case as well, except that it may have components in negative degrees.

Second, we define a pointed DGLA as a DGLA equipped with a distinguished central cycle of degree -2 (which we call the curvature). A morphism of pointed DGLAs is a DGLA morphism which preserves the distinguished central cycle.[5] We say that a graded local Lie algebra $\mathfrak{F}$ over $(X,\leq)$ with a terminal object $T\in X$ is pointed if it is equipped with a distinguished central element $\mathsf{B}\in\mathfrak{F}(T)$ of degree -2. Morphisms in the category of pointed graded local Lie algebras are required to preserve the distinguished element. Then the DGLA $C^{aug}_{\bullet+1}(\mathfrak{U},T;\mathfrak{F})$ is an acyclic pointed DGLA, the distinguished central cycle being $\mathsf{B}\in C^{aug}_{-1}(\mathfrak{U},T;\mathfrak{F})$. Of course, since the DGLA is acyclic, this central cycle is exact. The construction of a pointed DGLA from a pointed graded local Lie algebra and a cover of T is functorial in both arguments.

3.3 Quantum lattice systems

Observables and derivations

We use the ℓ^∞ metric on $\mathbb{R}^n$, i. e. $d(x,y):=\max_{i=1,\dots,n}|x_i-y_i|$. For any $U,V\subset\mathbb{R}^n$ we write $\mathrm{diam}(U):=\sup_{x,y\in U}d(x,y)$ and $d(U,V):=\inf_{x\in U,y\in V}d(x,y)$. They take values in extended non-negative reals $[0,\infty]$. Thus $\mathrm{diam}(\varnothing)=0$ and $d(U,\varnothing)=\infty$ for any $U\subset\mathbb{R}^n$. For a nonempty set U and $r\geq 0$ we define $U^r:=\{x\in\mathbb{R}^n : d(x,U)\leq r\}$ while we set $\varnothing^r=\varnothing$.

A quantum lattice system consists of a countable subset $\Lambda\subset\mathbb{R}^n$ ("the lattice") and a finite-dimensional complex Hilbert space V_j for every $j\in\Lambda$. We make the following assumption on the lattice system[6]: there is a $C_\Lambda>0$ such that the number of points of Λ in any hypercube of diameter d is bounded by $C_\Lambda(d+1)^n$.

For any bounded nonempty $X\subset\mathbb{R}^n$ let $\mathscr{A}(X):=\bigotimes_{j\in X\cap\Lambda}\mathrm{Hom}_{\mathbb{C}}(V_j,V_j)$. For

[5] The category of pointed DGLAs as defined here is a full subcategory of the category of curved DGLAs as defined in [CLM14]. There, for a curved DGLA with curvature B, B is not required to be central and the derivation ∂ satisfies $\partial^2=\mathrm{ad}_{\mathsf{B}}$.

[6] In [KS22] Λ was assumed to be a Delone set, i.e. it was required to be uniformly filling and uniformly discrete. These assumptions were imposed on physical grounds. All the results proved in [KS22] hold under weaker assumptions adopted in this paper. In [AKS24] Λ was taken to be $\mathbb{Z}^n$ for simplicity.

any $X \subset Y$ there is an inclusion $\mathscr{A}(X) \hookrightarrow \mathscr{A}(Y)$ and the algebras $\mathscr{A}(X)$ form a direct system with respect to these inclusions. We extend this direct system to include the empty set by setting $\mathscr{A}(\varnothing) = \mathbb{C}$ and letting the inclusion $\mathscr{A}(\varnothing) \hookrightarrow \mathscr{A}(X)$ take $\alpha \mapsto \alpha\mathbf{1}$. Each $\mathscr{A}(X)$ is a finite-dimensional C^*-algebra with the operator norm, and the inclusions $\mathscr{A}(X) \hookrightarrow \mathscr{A}(Y)$ preserve this norm. The normed *-algebra of local observables is

$$\mathscr{A}_\ell = \varinjlim_X \mathscr{A}(X).$$

The algebra of quasi-local observables $\mathscr{A}$ is the norm-completion of $\mathscr{A}_\ell$; it is a C^*-algebra.

For any bounded $X \subset \mathbb{R}^n$, define the normalized trace $\overline{tr} : \mathscr{A}(X) \to \mathbb{C}$ as $\overline{tr}(\mathcal{A}) = \mathrm{tr}(\mathcal{A})/\sqrt{\dim(\mathscr{A}(X))}$. For any bounded $X \subset Y$ the *partial trace* $\overline{tr}_{X^c} : \mathscr{A}(Y) \to \mathscr{A}(X)$ is uniquely specified by the condition $\overline{tr}_{X^c}(\mathcal{A} \otimes \mathcal{B}) = \overline{tr}(\mathcal{A})\mathcal{B}$ for any $\mathcal{A} \in \mathscr{A}(Y \backslash X)$ and $\mathcal{B} \in \mathscr{A}(X)$. Besides forming a direct system with respect to inclusions, the spaces $\mathscr{A}(X)$ are also an *inverse* system with respect to the partial trace. $\overline{tr}$ extends to a normalized positive linear functional on $\mathscr{A}$, i.e. a state. We say that $\mathcal{A} \in \mathscr{A}$ is traceless if $\overline{tr}(\mathcal{A}) = 0$. The space of traceless anti-hermitian elements of $\mathscr{A}(X)$ will be denoted $\mathfrak{d}_l(X)$. $\mathfrak{d}_l(X)$ is a real Lie algebra with respect to the commutator. The Lie algebras $\mathfrak{d}_l(X)$ form a direct system over the directed set of bounded subsets of $\mathbb{R}^n$, and its limit will be denoted $\mathfrak{d}_l$. Equivalently, $\mathfrak{d}_l$ is the Lie algebra of traceless anti-hermitian elements of $\mathscr{A}_\ell$. Note that $\mathscr{A}_\ell = \mathbb{C}\mathbf{1} \oplus (\mathfrak{d}_l \otimes \mathbb{C})$.

Definition 3.3.1. *A brick in $\mathbb{R}^n$ is a non-empty subset of the form*

$$Y = \{(x_1, \ldots, x_n) \mid \ell_i \leq x_i \leq m_i, i = 1, \ldots, n\}, \tag{3.5}$$

where $(k_1, \ldots, k_n)$, $(\ell_1, \ldots, \ell_n)$, and $(m_1, \ldots, m_n)$ are n-tuples of integers. We write $\mathbb{B}_n$ for the set of all bricks in $\mathbb{R}^n$.

The set of bricks exhausts the collection of bounded subsets of $\mathbb{R}^n$ in the sense that any bounded subset is contained in a brick. In addition, the set of bricks satisfies the following regularity property:

Lemma 3.3.1. *For any $j \in \mathbb{R}^n$ we have*

$$\sum_{Y \in \mathbb{B}_n} (1 + \mathrm{diam}(Y) + d(Y, j))^{-2n-2} \leq \frac{\pi^4 4^n (n+1)^2}{36}.$$

Proof. Any pair of points $x, y \in \mathbb{Z}^n$ specifies a brick with x and y on opposing corners, and any brick can be specified this way (not uniquely). With X the brick corresponding to x and y it is easy to see that $\max(d(x,j), d(y,j)) \leq \operatorname{diam}(X) + d(X,j)$, and so $(1+d(x,j))(1+d(y,j)) \leq (1+\operatorname{diam}(X)+d(X,j))^2$. Thus we have

$$\begin{aligned}\sum_{Y \in \mathbb{B}_n} (1 + \operatorname{diam}(Y) + d(Y,j))^{-2n-2} &\leq \sum_{x,y \in \mathbb{Z}^n} (1 + d(x,j))^{-n-1}(1 + d(y,j))^{-n-1} \\ &= \left(\sum_{x \in \mathbb{Z}^n} (1 + d(x,j))^{-n-1} \right)^2,\end{aligned}$$

and it remains only to bound the above sum. Let $f(k) := (1+k)^{-n-1}$ and $g(k) := \#(\mathbb{Z}^n \cap B_k(j)) \leq (1+2k)^n$. Using summation by parts we have

$$\begin{aligned}\sum_{j \in \Lambda} (1 + d(x,j))^{-n-1} &\leq \sum_{k \geq 0} f(k)(g(k+1) - g(k)) \\ &= \lim_{k \to \infty} f(k)g(k) - \sum_{k \geq 0} g(k)(f(k+1) - f(k)).\end{aligned}$$

It is easy to check that $f(k)g(k) \to 0$ and that $-(f(k+1) - f(k)) \leq (n+1)(1+k)^{-n-2}$, and so

$$\begin{aligned}\sum_{j \in \Lambda} (1 + d(x,j))^{-n-1} &\leq 2^n(n+1) \sum_{k \geq 0} (1+k)^{-2} \\ &\leq \frac{\pi^2 2^n (n+1)}{6}\end{aligned}$$

which proves the Lemma. □

For any brick Y we define the following subspace of $\mathfrak{d}_l(Y)$:

$$\mathfrak{d}_l{}^Y := \{\mathcal{A} \in \mathfrak{d}_l(Y) \mid \overline{\operatorname{tr}}_{X^c}(\mathcal{A}) = 0 \text{ for any brick } X \subsetneq Y\}.$$

Each $\mathfrak{d}_l(Y)$ decomposes as a direct sum $\mathfrak{d}_l(Y) = \bigoplus_{X \subseteq Y} \mathfrak{d}_l{}^X$ over bricks contained in Y, and for any brick $X \subseteq Y$ the partial trace $\overline{\operatorname{tr}}_{Y \setminus X^c}$ is the projection onto $\bigoplus_{Z \subseteq X} \mathfrak{d}_l{}^Z \subseteq \mathfrak{d}_l(Y)$. Intuitively, $\mathfrak{d}_l{}^Y$ consists of elements of $\mathfrak{d}_l(Y)$ which are not localized on any brick properly contained in Y.

Derivations of $\mathscr{A}$ which appear in the physical context are typically only densely defined and have the form

$$\mathsf{F} : \mathcal{A} \mapsto \sum_{Y \in \mathbb{B}_n} [\mathsf{F}^Y, \mathcal{A}],$$

where $\mathsf{F}^Y \in \mathfrak{d}_l{}^Y$. We are now going to define for every $U \subset \mathbb{R}^n$ a real Lie algebra $\mathfrak{D}_{al}(U)$ which consists of derivations approximately localized on U and such that all $\mathfrak{D}_{al}(U)$ have a common dense domain. Moreover, they form a pre-cosheaf of Lie algebras over a certain category of subsets of $\mathbb{R}^n$.

Definition 3.3.2. *For any element* $\mathsf{F} = \{\mathsf{F}^Y\}_{Y\in\mathbb{B}_n}$ *of* $\prod_{Y\in\mathbb{B}_n} \mathfrak{d}_l{}^Y$ *and every* $U \subset \mathbb{R}^n$ *we let*

$$\|\mathsf{F}\|_{U,k} := \sup_{Y\in\mathbb{B}_n} \|\mathsf{F}^Y\|(1 + \mathrm{diam}(Y) + d(U, Y))^k \tag{3.6}$$

and define $\mathfrak{D}_{al}(U) \subset \prod_{Y\in\mathbb{B}_n} \mathfrak{d}_l{}^Y$ *as the set of elements* F *with* $\|\mathsf{F}\|_{U,k} < \infty$ *for all* $k \geq 0$.

If U is empty, then for $k > 0$ $\|\mathsf{F}\|_{U,k} < \infty$ if and only if $\mathsf{F}^Y = 0$ for all $Y \in \mathbb{B}_n$. Thus $\mathfrak{D}_{al}(\emptyset) = 0$. We also denote $\mathfrak{D}_{al}(\mathbb{R}^n) = \mathfrak{D}_{al}$.

It is easy to see that (3.6) is a norm on $\mathfrak{D}_{al}(U)$ for each $k \geq 0$. We endow $\mathfrak{D}_{al}(U)$ with the locally convex topology given by the norms (3.6) ranging over all $k \geq 0$. Recall that a topological vector space is called a Fréchet space if it is Hausdorff, and if its topology can be generated by a countable family of seminorms with respect to which it is complete.

Proposition 3.3.1. $\mathfrak{D}_{al}(U)$ *is a Fréchet space.*

Proof. The Hausdorff property follows from the fact that if $\|\mathsf{F}\|_{U,k} = 0$ for any $k \geq 0$ then $\mathsf{F} = 0$. To show completeness, suppose $\{\mathsf{F}_m\}_{m\in\mathbb{N}} \subset \mathfrak{D}_{al}(U)$ is Cauchy, i.e. that for any $k \geq 0$ and any $\epsilon > 0$ there is an $N \in \mathbb{N}$ such that $m, m' \geq N \implies \|\mathsf{F}_m - \mathsf{F}_{m'}\|_{U,k} < \epsilon$. For any fixed $Y \in \mathbb{B}_n$ this implies that $\{\mathsf{F}^Y_n\}$ is Cauchy in $\mathfrak{d}_l{}^Y$ (with the operator norm) and thus converges to a limit F^Y. Let $\mathsf{F} := \{\mathsf{F}^Y\}_{Y\in\mathbb{B}_n}$.

Fix $k \in \mathbb{N}$ and $\epsilon > 0$. For every $\ell = 0, 1, 2, ...,$ choose $N_\ell \in \mathbb{N}$ so that $m, m' \geq N_\ell \implies \|\mathsf{F}_m - \mathsf{F}_{m'}\|_{U,k} < 2^{-\ell-1}\epsilon$. For any $Y \in \mathbb{B}_n$, any $m \geq N_1$, and any $M > 1$, we have

$$\begin{aligned}\|\mathsf{F}^Y_m - \mathsf{F}^Y\| &\leq \|\mathsf{F}^Y_m - \mathsf{F}^Y_{N_1}\| + \sum_{i=1}^{M-1} \|\mathsf{F}^Y_{N_i} - \mathsf{F}^Y_{N_{i+1}}\| + \|\mathsf{F}^Y_{N_M} - \mathsf{F}^Y\| \\ &\leq \epsilon(1 + \mathrm{diam}(Y) + d(U, Y))^{-k} + \|\mathsf{F}^Y_{N_M} - \mathsf{F}^Y\|.\end{aligned}$$

Taking $M \to \infty$ shows that $\|\mathsf{F}_m^Y - \mathsf{F}^Y\|(1 + \mathrm{diam}(Y) + d(U,Y))^k < \epsilon$. Since Y was arbitrary, we have $\|\mathsf{F}_m - \mathsf{F}\|_{U,k} < \epsilon$. Since k was arbitrary, $\{\mathsf{F}_m\}$ converges to F in the topology of $\mathfrak{D}_{al}(U)$. □

Recall that for a nonempty $U \subset \mathbb{R}^n$ we write $U^r := \{x \in \mathbb{R}^n : d(x,U) \leq r\}$. The norms $\|\cdot\|_{U,k}$ obey the following dominance relation.

Lemma 3.3.2. *Let U, V be subsets of the lattice and suppose that $U \subseteq V^r$. Then for any $\mathsf{F} \in \mathfrak{D}_{al}(U)$ we have*

$$\|\mathsf{F}\|_{V,k} \leq (r+1)^k \|\mathsf{F}\|_{U,k}. \tag{3.7}$$

In particular, $\mathfrak{D}_{al}(U) \subseteq \mathfrak{D}_{al}(V)$ and the inclusion is continuous.

Proof. Let Y be any subset of the lattice. Then (3.7) follows from

$$\begin{aligned} 1 + \mathrm{diam}(Y) + d(Y,V) &\leq 1 + \mathrm{diam}(Y) + d(Y,V^r) + r \\ &\leq 1 + \mathrm{diam}(Y) + d(Y,U) + r \\ &\leq (r+1)(1 + \mathrm{diam}(Y) + d(Y,U)), \end{aligned}$$

where in the second line we used the triangle inequality and in the third we used $U \subseteq V^r$. □

The above Lemma shows that the space $\mathfrak{D}_{al}(U)$ only depends on the asymptotic geometry of the region U in the following sense: if $U \subseteq V^r$ and $V \subseteq U^r$ for some $r \geq 0$ then $\mathfrak{D}_{al}(U) = \mathfrak{D}_{al}(V)$ (as subsets of $\prod_Y \mathfrak{d}_l{}^Y$) and are isomorphic as Fréchet spaces. In particular, for any non-empty bounded $U \subset \mathbb{R}^n$, the space $\mathfrak{D}_{al}(U)$ coincides with $\mathfrak{D}_{al}(\{0\})$.

To relate the spaces $\mathfrak{D}_{al}(U)$ to the traditional C^*-algebraic picture we prove the following:

Proposition 3.3.2. *Suppose $U \subset \mathbb{R}^n$ is non-empty and bounded and let $\mathsf{F} \in \mathfrak{D}_{al}(U)$. Then the sum $\sum_{X \in \mathbb{B}_n} \mathsf{F}^X$ is absolutely convergent and defines a continuous dense embedding of $\mathfrak{D}_{al}(U)$ into the subspace of traceless anti-hermitian elements of the algebra $\mathscr{A}$.*

Proof. We can assume without loss of generality that $U = \{0\}$. We have

$$\sum_{Y \in \mathbb{B}_n} \|\mathsf{F}^Y\| \leq \|\mathsf{F}\|_{\{0\},2n+2} \sum_{Y \in \mathbb{B}_n} (1 + \mathrm{diam}(Y) + d(Y,0))^{-2n-2},$$

and by Lemma 3.3.1 the above sum is finite. This shows that the map $\mathfrak{D}_{al}(\{0\}) \to \mathscr{A}$ is well-defined and continuous. Its image is dense in the space of traceless anti-hermitian elements of $\mathscr{A}$ because it contains the dense subspace $\mathfrak{d}_l$. Finally, to show that it is injective, writing $\mathcal{A} := \sum_{Y \in \mathbb{B}_n} \mathsf{F}^Y$ we have

$$\mathsf{F}^Y = \overline{\mathrm{tr}}_{Y^c}(\mathcal{A}) - \sum_{X \subsetneq Y} \overline{\mathrm{tr}}_{X^c}(\mathcal{A})$$

and so $\mathcal{A} = 0 \implies \mathsf{F}^Y = 0$ for all $Y \in \mathbb{B}_n$. □

Definition 3.3.3. *We let $\mathfrak{d}_{al} \subset \mathscr{A}$ be the image of $\mathfrak{D}_{al}(\{0\})$ under the embedding of Prop. 3.3.2, with the Fréchet topology of $\mathfrak{D}_{al}(\{0\})$.*

In [KS22], the algebra $\mathscr{A}_{a\ell}$ of *almost-local* operators was defined as a subspace of $\mathscr{A}$ where a countable family of norms similar to (3.6) takes finite values. Here we equivalently define $\mathscr{A}_{a\ell}$ as the set of elements of $\mathscr{A}$ whose traceless hermitian and anti-hermitian parts live in $\mathfrak{d}_{al}$, topologized as $\mathscr{A}_{a\ell} = \mathbb{C}\mathbf{1} \oplus (\mathfrak{d}_{al} \otimes \mathbb{C})$.

Proposition 3.3.3. *$\mathscr{A}_{a\ell}$ is a dense sub-algebra of $\mathscr{A}$.*

Proof. $\mathscr{A}_{a\ell}$ contains all local observables and these are dense in $\mathscr{A}$. The fact that $\mathscr{A}_{a\ell}$ is closed under multiplication is proven in [KS22]. □

In view of Prop. 3.3.2 it is natural to make the following definition.

Definition 3.3.4. *An element $\mathsf{F} \in \mathfrak{D}_{al}$ is inner iff it is contained in $\mathfrak{D}_{al}(U)$ for some bounded U.*

For any two bounded sets U, V, a local observable is strictly localized on both U and V iff it is localized on their intersection, i.e. $\mathscr{A}(U) \cap \mathscr{A}(V) = \mathscr{A}(U \cap V)$. An analogous relation for the spaces $\mathfrak{D}_{al}(U)$ does not hold in general[7], but it does hold if we assume that U and V satisfy the following transversality condition:

[7]Indeed, for any two bounded U, V the spaces $\mathfrak{D}_{al}(U)$ and $\mathfrak{D}_{al}(V)$ coincide and are nontrivial but if U and V are disjoint then $\mathfrak{D}_{al}(U \cap V) = 0$.

Definition 3.3.5. *Let $U, V \subseteq \mathbb{R}^n$ and $C > 0$. We say U and V are C-*transverse *if*

$$d(x, U \cap V) \leq C \max(d(x, U), d(x, V))$$

for all $x \in \mathbb{R}^n$.

We will say U and V are transverse if they are C-transverse for some $C > 0$.

Proposition 3.3.4. *If $U, V \subseteq \mathbb{R}^n$ are C-transverse then*

$$\max(\|\mathsf{F}\|_{U,k}, \|\mathsf{F}\|_{V,k}) \leq \|\mathsf{F}\|_{U\cap V,k} \leq (C+1)^k \max(\|\mathsf{F}\|_{U,k}, \|\mathsf{F}\|_{V,k}) \tag{3.8}$$

for all $k > 0$. In particular, $\mathfrak{D}_{al}(U \cap V)$ is a topological pullback: it is the set $\mathfrak{D}_{al}(U) \cap \mathfrak{D}_{al}(V)$ with the topology of simultaneous convergence in $\mathfrak{D}_{al}(U)$ and $\mathfrak{D}_{al}(V)$.

Proof. The first inequality is true even without assuming transversality — it follows from Lemma 3.3.2. For the second, let $Z \in \mathbb{B}_n$ and choose $x^*, y^* \in Z$ so that $d(x^*, U) = d(Z, U)$ and $d(y^*, V) = d(Z, V)$. Then we have

$$\begin{aligned} d(Z, U \cap V) &= \inf_{z \in Z} d(z, U \cap V) \\ &\leq C \inf_{z \in Z} \max(d(z, U), d(z, V)) \\ &\leq C \inf_{z \in Z} \max(d(z, x^*) + d(x^*, U), d(z, y^*) + d(y^*, V)) \\ &\leq C(\operatorname{diam}(Z) + \max(d(Z, U), d(Z, V)), \end{aligned}$$

and thus

$$\begin{aligned} &1 + \operatorname{diam}(Z) + d(Z, U \cap V) \leq \\ &\qquad \leq (C+1)(1 + \operatorname{diam}(Z) + \max(d(Z, U), d(Z, V))), \end{aligned} \tag{3.9}$$

which proves (3.8). □

The next proposition relates $\mathfrak{D}_{al}(U \cup V)$ with $\mathfrak{D}_{al}(U)$ and $\mathfrak{D}_{al}(V)$ for any $U, V \subseteq \mathbb{R}^n$.

Proposition 3.3.5. *For any $U, V \subset \mathbb{R}^n$ consider the sequence of vector spaces*

$$\mathfrak{D}_{al}(U \cap V) \xrightarrow{\alpha} \mathfrak{D}_{al}(U) \oplus \mathfrak{D}_{al}(V) \xrightarrow{\beta} \mathfrak{D}_{al}(U \cup V) \to 0, \tag{3.10}$$

where $\alpha(\mathsf{F}) = (\mathsf{F}, -\mathsf{F})$ and $\beta(\mathsf{F}, \mathsf{G}) = \mathsf{F} + \mathsf{G}$.

i) The sequence (3.10) admits a right splitting, i.e. a map $\gamma : \mathfrak{D}_{al}(U \cup V) \to \mathfrak{D}_{al}(U) \oplus \mathfrak{D}_{al}(V)$ *with* $\beta \circ \gamma = \mathrm{id}$*. In particular, it is exact on the right.*

ii) If U *and* V *are transverse, then (3.10) is exact on the left.*

Proof. i). For any $Y \in \mathbb{B}_n$, define

$$\chi(Y) := \begin{cases} 1 & \text{if } d(Y,U) < d(Y,V) \\ 1/2 & \text{if } d(Y,U) = d(Y,V) \\ 0 & \text{if } d(Y,U) > d(Y,V) \end{cases} .$$

For any $\mathsf{F} \in \mathfrak{D}_{al}(U \cup V)$ define $\gamma_1(\mathsf{F}) := \sum_{Y \in \mathbb{B}_n} \chi(Y)\mathsf{F}^Y$, and $\gamma_2(\mathsf{F}) = \mathsf{F} - \gamma_1(\mathsf{F})$. Then it is not hard to show that $\|\gamma_1(\mathsf{F})\|_{U,k} \leq \|\mathsf{F}\|_{U \cup V,k}$ and $\|\gamma_2(\mathsf{F})\|_{V,k} \leq \|\mathsf{F}\|_{U \cup V,k}$ and that $\gamma = (\gamma_1, \gamma_2)$ is a right splitting of (3.10).

ii). Follows immediately from Proposition 3.3.4. □

Next we will show how to endow $\mathfrak{D}_{al}(U)$ with the Lie algebra structure.

Proposition 3.3.6. *Let* $U, V \subset \mathbb{R}^n$*. For any* $\mathsf{F} \in \mathfrak{D}_{al}(U)$ *and* $\mathsf{G} \in \mathfrak{D}_{al}(V)$ *the sum*

$$[\mathsf{F}, \mathsf{G}]^Z := \sum_{X,Y \in \mathbb{B}_n} [\mathsf{F}^X, \mathsf{G}^Y]^Z \tag{3.11}$$

is absolutely convergent for every $Z \in \mathbb{B}_n$*. The resulting bracket* $[\cdot,\cdot]$ *satisfies the Jacobi identity and*

$$\|[\mathsf{F}, \mathsf{G}]\|_{U,k} \leq C 3^k \|\mathsf{F}\|_{U,k+4n+4} \|\mathsf{G}\|_{V,k+4n+4} \tag{3.12}$$

for some constant $C > 0$ *that depends only on* n*.*

To prove Proposition 3.3.6 we will need several lemmas. For any $X, Y \in \mathbb{B}_n$, define[8] the join $X \vee Y \in \mathbb{B}_n$ as the smallest brick that contains X and Y.

Lemma 3.3.3. *For any* $X, Y \in \mathbb{B}_n$ *with* $X \cap Y \neq \varnothing$ *we have*

$$\mathrm{diam}(X \vee Y) \leq \mathrm{diam}(X) + \mathrm{diam}(Y) \tag{3.13}$$

and for any $z \in X \vee Y$ *we have*

$$d(z, X) \leq \mathrm{diam}(Y).$$

[8]This is well-defined since the intersection of an arbitrary number of bricks is either empty or a brick, so $X \vee Y$ is the intersection of all bricks containing X and Y.

Proof. Let $\pi_i : \mathbb{R}^n \to \mathbb{R}$ be the projection onto the ith coordinate. The following identites hold for any bricks $X, Y \in \mathbb{B}_n$:

$$\begin{aligned} \pi_i(X \vee Y) &= \pi_i(X) \vee \pi_i(Y), \\ \operatorname{diam}(X) &= \max_{i=1,\dots n} \operatorname{diam}(\pi_i(X)), \\ d(X,Y) &= \max_{i=1,\dots n} d(\pi_i(X), \pi_i(Y)). \end{aligned}$$

When $n = 1$ the results are clear. When $n > 1$ they follow from the $n = 1$ case via the above identities. □

Lemma 3.3.4. *Let $X, Y, Z \in \mathbb{B}_n$ and let $\mathsf{F} \in \mathfrak{d}_l(X)$ and $\mathsf{G} \in \mathfrak{d}_l(Y)$. Then $[\mathsf{F}^X, \mathsf{G}^Y]^Z = 0$ unless $X \cap Y \neq \varnothing$ and $Z \subseteq X \vee Y$.*

Proof. The requirement that $X \cap Y \neq \varnothing$ is clear, since F^X and G^Y would commute otherwise. Suppose $Z \nsubseteq X \vee Y$. Then $Z' := (X \vee Y) \cap Z$ is a brick that is strictly contained in Z, so $[\mathsf{F}^X, \mathsf{G}^Y]^Z \in {\mathfrak{d}_l}^Z \cap \mathfrak{d}_l(Z') = \{0\}$. □

We make the following definitions for the next lemma. For any $U \subset \mathbb{R}^n$ and any brick X write $\tilde{d}(X,U) := 1 + \operatorname{diam}(X) + d(X,U)$ and $\tilde{d}(X) := 1 + \operatorname{diam}(X)$.

Lemma 3.3.5. *For any $U \subset \mathbb{R}^n$, $Z \in \mathbb{B}_n$, and $k \geq 0$ we have*

$$\sum_{\substack{X,Y \in \mathbb{B}_n \\ X \cap Y \neq \varnothing \\ Z \subset X \vee Y}} \tilde{d}(X,U)^{-k-4n-4} \tilde{d}(Y)^{-k-4n-4} \leq \frac{\pi^8 16^n (n+1)^4 3^k}{1296} \tilde{d}(Z,U)^{-k}.$$

Proof. Let $X, Y \in \mathbb{B}_n$ with $X \cap Y \neq \varnothing$ and let $Z \subset X \vee Y$ be a brick. Pick an arbitrary point $w \in X \cap Y$. We have

$$\begin{aligned} d(Z,U) &\leq d(Z,w) + d(w,U) \\ &\leq d(Z,w) + \operatorname{diam}(X) + d(X,U) \\ &\leq \operatorname{diam}(X \vee Y) + \operatorname{diam}(X) + d(X,U) \\ &\leq 2\operatorname{diam}(X) + \operatorname{diam}(Y) + d(X,U), \end{aligned}$$

and so, since by Lemma 3.3.3 $\operatorname{diam}(Z) \leq \operatorname{diam}(X \vee Y) \leq \operatorname{diam}(X) + \operatorname{diam}(Y)$, we have

$$\begin{aligned} \tilde{d}(Z,U) &\leq 1 + 3\operatorname{diam}(X) + 2\operatorname{diam}(Y) + d(X,U) \\ &\leq 3(1 + \operatorname{diam}(X) + d(X,U) + \operatorname{diam}(Y)) \\ &\leq 3(1 + \operatorname{diam}(X) + d(X,U))(1 + \operatorname{diam}(Y)) \\ &= 3\tilde{d}(X,U)\tilde{d}(Y). \end{aligned} \tag{3.14}$$

It follows that for any $k > 0$ we have

$$\tilde{d}(Z,U)^k \tilde{d}(X,U)^{-k} \tilde{d}(Y)^{-k} \leq 3^k$$

and so

$$\begin{aligned} \sum_{\substack{X,Y \in \mathbb{B}_n \\ X \cap Y \neq \varnothing \\ Z \subset X \vee Y}} \tilde{d}(X,U)^{-k-4n-4} \tilde{d}(Y)^{-k-4n-4} \leq \\ \leq 3^k \tilde{d}(Z,U)^{-k} \sum_{\substack{X,Y \in \mathbb{B}_n \\ X \cap Y \neq \varnothing \\ Z \subset X \vee Y}} \tilde{d}(X,U)^{-4n-4} \tilde{d}(Y)^{-4n-4}. \end{aligned} \tag{3.15}$$

It remains to bound the sum on the right-hand side. Fix an arbitrary $z \in Z$ and let $X, Y \in \mathbb{B}_n$ with $X \cap Y \neq \varnothing$ and $Z \subset X \vee Y$. Then by the second statement in Lemma 3.3.3 and the inequality $1 + a + b \leq (1+a)(1+b)$ for $a, b \geq 0$ we have

$$\begin{aligned} (1 + d(z,X) + \mathrm{diam}(X))(1 + d(z,Y) + \mathrm{diam}(Y)) \leq \\ \leq (1 + \mathrm{diam}(X))^2 (1 + \mathrm{diam}(Y))^2. \end{aligned} \tag{3.16}$$

Using (3.16) we can bound the sum (3.15) as follows:

$$\begin{aligned} \sum_{\substack{X,Y \in \mathbb{B}_n \\ X \cap Y \neq \varnothing \\ Z \subset X \vee Y}} \tilde{d}(X,U)^{-4n-4} \tilde{d}(Y)^{-4n-4} \leq \sum_{\substack{X,Y \in \mathbb{B}_n \\ X \cap Y \neq \varnothing \\ Z \subset X \vee Y}} (1+\mathrm{diam}(X))^{-4n-4} (1+\mathrm{diam}(Y))^{-4n-4} \\ \leq \sum_{X,Y \in \mathbb{B}_n} (1 + \mathrm{diam}(X) + d(X,z))^{-2n-2} (1 + \mathrm{diam}(Y) + d(Y,z))^{-2n-2} \\ \leq \left(\sum_{X \in \mathbb{B}_n} (1 + \mathrm{diam}(X) + d(X,z))^{-2n-2} \right)^2 \leq \frac{\pi^8 16^n (n+1)^4}{1296}. \end{aligned} \tag{3.17}$$

□

Now we are ready to prove Proposition 3.3.6.

Proof of Proposition 3.3.6. Notice that by Lemma 3.3.2 we have $\|\mathsf{G}\|_{V,k+2n+2} \leq \|\mathsf{G}\|_{\mathbb{R}^n,k+2n+2}$ so without loss of generality we set $V = \mathbb{R}^n$.

Let $Z \in \mathbb{B}_n$. By Lemmas 3.3.4 and 3.3.5 we have

$$\begin{aligned}\sum_{X,Y\in\mathbb{B}_n} \|[\mathsf{F}^X,\mathsf{G}^Y]^Z\| &= \sum_{\substack{X,Y\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ Z\subset X\vee Y}} \|[\mathsf{F}^X,\mathsf{G}^Y]^Z\| \\ &\leq 2\|\mathsf{F}\|_{U,k+4n+4}\|\mathsf{G}\|_{\mathbb{R}^n,k+4n+4} \sum_{\substack{X,Y\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ Z\subset X\vee Y}} \tilde{d}(X,U)^{-k-4n-4}\tilde{d}(Y)^{-k-4n-4} \\ &\leq C3^k\|\mathsf{F}\|_{U,k+4n+4}\|\mathsf{G}\|_{\mathbb{R}^n,k+4n+4}\tilde{d}(Z,U)^{-k},\end{aligned}$$

with $C = \frac{\pi^8 16^n(n+1)^4}{648}$. This proves that (3.11) is absolutely convergent and establishes the bound (3.12).

Next, let us prove the Jacobi identity. Let $\mathsf{F},\mathsf{G},\mathsf{H} \in \mathfrak{D}_{al}(\mathbb{R}^n)$. We have

$$[\mathsf{F},[\mathsf{G},\mathsf{H}]]^W = \sum_{X,Y\in\mathbb{B}_n}\sum_{X',Y'\in\mathbb{B}_n}\left[\mathsf{F}^X,\left[\mathsf{G}^{X'},\mathsf{H}^{Y'}\right]^Y\right]^W. \tag{3.18}$$

To show that this sum is absolutely convergent, we bound

$$\begin{aligned}&\sum_{X,Y\in\mathbb{B}_n}\sum_{X',Y'\in\mathbb{B}_n}\left\|\left[\mathsf{F}^X,\left[\mathsf{G}^{X'},\mathsf{H}^{Y'}\right]^Y\right]^W\right\| \\ \leq& 4\sum_{\substack{X,Y\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ W\subset X\vee Y}}\|\mathsf{F}^X\|\sum_{\substack{X',Y'\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ Y\subset X'\vee Y'}}\|\mathsf{G}^{X'}\|\|\mathsf{H}^{Y'}\| \\ \leq& C4\|\mathsf{G}\|_{\mathbb{R}^n,8n+8}\|\mathsf{H}\|_{\mathbb{R}^n,8n+8}\sum_{\substack{X,Y\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ W\subset X\vee Y}}\|\mathsf{F}^X\|\tilde{d}(Y)^{-4n-4} \\ \leq& C4\|\mathsf{F}\|_{\mathbb{R}^n,4n+4}\|\mathsf{G}\|_{\mathbb{R}^n,8n+8}\|\mathsf{H}\|_{\mathbb{R}^n,8n+8}\sum_{\substack{X,Y\in\mathbb{B}_n\\ X\cap Y\neq\varnothing\\ W\subset X\vee Y}}\tilde{d}(X)^{-4n-4}\tilde{d}(Y)^{-4n-4} \\ <&\infty.\end{aligned}$$

Here we used Lemma 3.3.5 in the second and fourth lines and C is a constant depending only on n. Thus the sum (3.18) is absolutely convergent. In particular, using the fact that $\sum_{Y\in\mathbb{B}_n}[\mathsf{G}^{X'},\mathsf{H}^{Y'}]^Y = [\mathsf{G}^{X'},\mathsf{H}^{Y'}]$ we have the following absolutely convergent expression

$$[\mathsf{F},[\mathsf{G},\mathsf{H}]]^W = \sum_{X,Y,Z\in\mathbb{B}_n}[\mathsf{F}^X,[\mathsf{G}^Y,\mathsf{H}^Z]]^W.$$

It is then easy to check that the Jacobi identity for the sum follows from the Jacobi identity for each term. □

From Propositions 3.3.4 and 3.3.6 we immediately get

Corollary 3.3.1. *Suppose $U, V \in \mathbb{R}^n$.*

i) $(\mathsf{F}, \mathsf{G}) \mapsto [\mathsf{F}, \mathsf{G}]$ *is a jointly continuous bilinear map from $\mathfrak{D}_{al}(U) \times \mathfrak{D}_{al}(V)$ to $\mathfrak{D}_{al}(U) \cap \mathfrak{D}_{al}(V)$.*

ii) If U and V are transverse, then this is jointly continuous bilinear map from $\mathfrak{D}_{al}(U) \times \mathfrak{D}_{al}(V)$ to $\mathfrak{D}_{al}(U \cap V)$.

In particular since $\{0\}$ and $\mathbb{R}^n$ are transverse, $\mathfrak{D}_{al}(\mathbb{R}^n)$ acts continuously on $\mathfrak{D}_{al}(\{0\})$ and this action is easily seen to extend to a continuous action of $\mathfrak{D}_{al}(\mathbb{R}^n)$ on the space $\mathscr{A}_{a\ell}$. We denote the action of $\mathsf{F} \in \mathfrak{D}_{al}(\mathbb{R}^n)$ on $\mathcal{A} \in \mathscr{A}_{a\ell}$ by $\mathcal{A} \mapsto \mathsf{F}(\mathcal{A})$. By Prop. 3.3.6, it is given by

$$\mathsf{F}(\mathcal{A}) = \sum_{Y \in \mathbb{B}_n} [\mathsf{F}^Y, \mathcal{A}]. \tag{3.19}$$

It is not hard to check that for any $X \in \mathbb{B}_n$ and any $\mathcal{A} \in \mathscr{A}(X)$ we have $\overline{tr}_{X^c}(\mathsf{F}(\mathcal{A})) = [\mathsf{F}_X, \mathcal{A}]$ and so the action of $\mathfrak{D}_{al}(\mathbb{R}^n)$ on $\mathscr{A}_{a\ell}$ is faithful. Thus, elements of $\mathfrak{D}_{al}(U)$ for any $U \subset \mathbb{R}^n$ may be identified with a subset of the Fréchet-continuous derivations of $\mathscr{A}_{a\ell}$. By Proposition 3.3.2, the Fréchet-Lie algebra $\mathfrak{D}_{al}(\{0\})$ is identified with the Fréchet-Lie algebra $\mathfrak{d}_{al}$ of traceless anti-hermitian elements of $\mathscr{A}_{a\ell}$ acting by inner derivations.

Automorphisms

In this section we recall certain automorphisms obtained by exponentiating elements of $\mathfrak{D}_{al}(\mathbb{R}^n)$ following [KS22]. One can develop the theory of such automorphisms that are almost-localized on regions in $\mathbb{R}^n$ in a similar spirit to the above, but since we do not have much occasion to use them in this work, we opt instead for a more minimal development. Let $\mathsf{F} : \mathbb{R} \to \mathfrak{D}_{al}(\mathbb{R}^n)$ be a smooth map. It is shown in [KS22] that for any $\mathcal{A} \in \mathscr{A}_{a\ell}$ the differential equation

$$\frac{d}{dt}\mathcal{A}(t) = \mathsf{F}(t)(\mathcal{A}(t))$$

with the initial condition $\mathcal{A}(0) = \mathcal{A}$ has a unique solution $\mathcal{A}(t) \in \mathscr{A}_{a\ell}$ for all $t \in \mathbb{R}$. Denote by α_t^{F} the map taking $\mathcal{A}$ to $\mathcal{A}(t)$. It is a continuous automorphism of the Lie algebra $\mathscr{A}_{a\ell}$ that preserves the $*$-operation.

Definition 3.3.6. *We call any automorphism of the form α_t^{F} for some smooth map $\mathsf{F} : \mathbb{R} \to \mathfrak{D}_{al}(\mathbb{R}^n)$ a locally-generated automorphism, or LGA for short.*

It is shown in [KS22] that every LGA extends to a continuous $*$-automorphism of the quasilocal algebra $\mathscr{A}$, and that the set of LGAs forms a group under composition.

States

By a state ψ we will mean a state on the quasilocal algebra $\mathscr{A}$. If F is an inner derivation (see Def. 3.3.4), we define its ψ-average as the evaluation of ψ on the corresponding element of $\mathfrak{d}_{al} \subset \mathscr{A}_{a\ell}$. The group of LGAs acts on states by pre-composition, which we denote $\psi^\alpha := \psi \circ \alpha$. We say an LGA α preserves a state ψ if $\psi^\alpha = \psi$. We say an element $\mathsf{F} \in \mathfrak{D}_{al}(\mathbb{R}^n)$ preserves ψ if $\psi(\mathsf{F}(\mathcal{A})) = 0$ for any $\mathcal{A} \in \mathscr{A}_{a\ell}$, which is equivalent to the one-parameter group of automorphisms $t \mapsto \alpha_t^{\mathsf{F}}$ corresponding to a constant map $t \mapsto \mathsf{F}$ preserving ψ.

Definition 3.3.7. *For any $U \subset \mathbb{R}^n$ define $\mathfrak{D}_{al}^{\psi}(U)$ as the set of all elements of $\mathfrak{D}_{al}(U)$ that preserve ψ.*

It is easy to check that $\mathfrak{D}_{al}^{\psi}(U)$ is a closed subset of $\mathfrak{D}_{al}(U)$, and that if F and G preserve ψ, then $[\mathsf{F}, \mathsf{G}]$ preserves ψ. Thus the analog of Propositions 3.3.4 and 3.3.6 and Corollary 3.3.1 hold for the spaces $\mathfrak{D}_{al}^{\psi}(U)$. Proposition 3.3.5 on the other hand, does not hold for the spaces $\mathfrak{D}_{al}^{\psi}(U)$ for a general state ψ. To circumvent this, we will restrict to gapped states, where quasiadiabatic evolution [Has04; Kit06; Osb07] can be used to prove the analog of Proposition 3.3.5.

Definition 3.3.8. *A state ψ is gapped if there exists $\mathsf{H} \in \mathfrak{D}_{al}(\mathbb{R}^n)$ and $\Delta > 0$ such that for any $\mathcal{A} \in \mathscr{A}_{a\ell}$ one has*

$$-i\psi(\mathcal{A}^*\mathsf{H}(\mathcal{A})) \geq \Delta \left(\psi(\mathcal{A}^*\mathcal{A}) - \psi(\mathcal{A}^*)\psi(\mathcal{A})\right). \tag{3.20}$$

Remark 3.3.1. *The meaning of this condition becomes more transparent if one recalls that any $\mathsf{H} \in \mathfrak{D}_{al}$ is a generator of a one-parameter group of $*$-automorphisms of $\mathscr{A}$ [KS22]. The condition (3.20) implies that ψ is invariant under this one-parameter group of automorphisms [BR87], and that the corresponding one-parameter group of unitaries in the GNS representation of $\mathscr{A}$ has* *a generator whose spectrum in the orthogonal complement to the GNS vacuum vector is contained in* $[\Delta, +\infty)$*. The condition (3.20) also implies that* ψ *is pure [KS24].*

Remark 3.3.2. *If* ψ *is a gapped state of* $\mathscr{A}$ *and* α *is an LGA, then* ψ^α *is also a gapped state. In [KS22] it was proposed to define a gapped phase as an orbit of gapped state under the action of the group of LGAs.*

In Section 3.7 we prove the following.

Proposition 3.3.7. *Suppose* ψ *is gapped, the corresponding Hamiltonian is* H*. Then there are linear functions*

$$\mathcal{J} : \mathfrak{D}_{al}(\mathbb{R}^n) \to \mathfrak{D}_{al}^{\psi}(\mathbb{R}^n)$$
$$\mathcal{K} : \mathfrak{D}_{al}(\mathbb{R}^n) \to \mathfrak{D}_{al}(\mathbb{R}^n)$$

such that

i) If F *preserves* ψ *then* $\mathcal{K}(\mathsf{F})$ *preserves* ψ*.*

ii) For every $k > 0$*,* $U \subset \mathbb{R}^n$*, and* $\mathsf{F} \in \mathfrak{D}_{al}(U)$ *we have*

$$\|\mathcal{J}(\mathsf{F})\|_{U,k} \leq C_k \|\mathsf{F}\|_{U,k+4n+3}$$
$$\|\mathcal{K}(\mathsf{F})\|_{U,k} \leq C'_k \|\mathsf{F}\|_{U,k+4n+3}$$

for some constants C_k, C'_k *depending only on* k, n, H*, and* Δ*.*

iii) For every $\mathsf{F} \in \mathfrak{D}_{al}(\mathbb{R}^n)$ *we have*

$$\mathsf{F} = \mathcal{J}(\mathsf{F}) - \mathcal{K}([\mathsf{H}, \mathsf{F}]).$$

Using the above Lemma we will prove the analog of Proposition 3.3.5 for the spaces $\mathfrak{D}_{al}^{\psi}(U)$.

Proposition 3.3.8. *For any* $U, V \subset \mathbb{R}^n$ *consider the sequence*

$$\mathfrak{D}_{al}^{\psi}(U \cap V) \xrightarrow{\alpha} \mathfrak{D}_{al}^{\psi}(U) \oplus \mathfrak{D}_{al}^{\psi}(V) \xrightarrow{\beta} \mathfrak{D}_{al}^{\psi}(U \cup V) \to 0, \qquad (3.21)$$

where $\alpha(\mathcal{A}) = (\mathcal{A}, -\mathcal{A})$ *and* $\beta(\mathcal{A}, \mathcal{B}) = \mathcal{A} + \mathcal{B}$*.*

i) If ψ *is gapped then the sequence (3.10) admits a right splitting, and in particular it is exact on the right* *ii) If U and V are transverse, then (3.10) is exact on the left.*

To prove Proposition 3.3.8 we will need the following geometric result

Lemma 3.3.6. *Let $U, V \subset \mathbb{R}^n$ and define $U' := \{x \in \mathbb{R}^n : d(x, U) \leq d(x, V)\}$. Then U' and $U \cup V$ are transverse and their intersection is U.*

Proof. It is easy to check that $U' \cap (U \cup V) = U$. To prove transversality we will show

$$d(x, U) \leq 4 \max(d(x, U'), d(x, U \cup V)) \tag{3.22}$$

for every $x \in \mathbb{R}^n$. Suppose first that $d(x, U) \leq 2d(x, V)$. Then

$$\begin{aligned} d(x, U) &\leq 2 \min(d(x, U), d(x, V)) \\ &= 2d(x, U \cup V) \end{aligned}$$

which implies (3.22). Suppose instead that $d(x, U) > 2d(x, V)$, and let $y \in U'$ satisfy $d(x, y) = d(x, U')$. Notice $x \notin U'$ and so y lies in the boundary of U', which implies $d(y, U) = d(y, V)$. Thus we have

$$\begin{aligned} d(x, U) &\leq d(x, y) + d(y, U) \\ &= d(x, y) + d(y, V) \\ &\leq 2d(x, y) + d(x, V), \end{aligned}$$

where in the first and third lines we used the triangle inequality. Using $d(x, y) = d(x, U')$ and $d(x, V) < d(x, U)/2$, this gives $d(x, U) < 4d(x, U')$, which implies (3.22). □

Proof of Proposition 3.3.8. The proof of Proposition 3.3.5 goes through unmodified except for the definition of γ, which needs to be changed to ensure that the image of γ consists of derivations that preserve ψ. Suppose $U, V \subseteq \mathbb{R}^n$ and $\mathsf{F} \in \mathfrak{D}_{al}^{\psi}(U \cup V)$. Define

$$\begin{aligned} U' &:= \{x \in \mathbb{R}^n : d(x, U) \leq d(x, V)\}, \\ V' &:= \{x \in \mathbb{R}^n : d(x, V) \leq d(x, U)\}. \end{aligned}$$

Let $\gamma^{U,V}$ (resp. $\gamma^{U',V'}$) be the splitting from Proposition 3.3.5 with the sets U and V (resp. U' and V'). Define $\tilde{\gamma} = (\tilde{\gamma}_1, \tilde{\gamma}_2)$ as

$$\tilde{\gamma}_i(\mathsf{F}) := \mathcal{J}(\gamma_i^{U,V}(\mathsf{F})) - \mathcal{K}([\mathcal{J}(\gamma_i^{U',V'}(\mathsf{H})), \mathsf{F}])$$

for $i = 1, 2$. Using Prop. 3.3.7 and Lemma 3.3.6 and the fact that the commutator of two derivations that preserve ψ preserves ψ, one checks that $\tilde{\gamma}$ takes $\mathfrak{D}^{\psi}_{al}(U \cup V)$ to $\mathfrak{D}^{\psi}_{al}(U) \oplus \mathfrak{D}^{\psi}_{al}(V)$. Using Prop. 3.3.7 *iii*) and the fact that $\gamma_1^{U,V}(\mathsf{F}) + \gamma_2^{U,V}(\mathsf{F}) = \mathsf{F}$ and $\gamma_1^{U',V'}(\mathsf{H}) + \gamma_2^{U',V'}(\mathsf{H}) = \mathsf{H}$, we get $\tilde{\gamma}_1(\mathsf{F}) + \tilde{\gamma}_2(\mathsf{F}) = \mathsf{F}$, as desired. □

We showed that one can attach Fréchet-Lie algebras $\mathfrak{D}_{al}(U)$ and $\mathfrak{D}^{\psi}_{al}(U)$ to any $U \subset \mathbb{R}^n$. These form a pre-cosheaf over the pre-ordered set of subsets of $\mathbb{R}^n$. Moreover, Proposition 3.3.5, Corollary 3.3.1, and (when ψ is gapped) Proposition 3.3.8 show that these spaces satisfy the cosheaf condition and Property I for transverse pairs $U, V \subset \mathbb{R}^n$. What prevents the functors $\mathfrak{D}_{al}$ and $\mathfrak{D}^{\psi}_{al}$ from forming local Lie algebras is the fact that pairs of subsets $U, V \subset \mathbb{R}^n$ generally do not intersect transversely. This problem can be resolved by restricting to a suitable set of subsets of $\mathbb{R}^n$ that have well-behaved intersections. In the next section we identify one such set (the set of *semilinear subsets*) prove that they form a Grothendieck site, and discuss some properties of this site.

3.4 The site of fuzzy semilinear sets

Semilinear sets and their thickenings

A semilinear set in $\mathbb{R}^n$ is a subset of $\mathbb{R}^n$ which can be defined by means of a finite number of linear equalities and strict linear inequalities. More precisely, a basic semilinear set in $\mathbb{R}^n$ is an intersection of a finite number of hyperplanes and open half-spaces, and a semilinear set is a finite union of basic semilinear sets. The set of semilinear subsets of $\mathbb{R}^n$ will be denoted $\mathcal{S}_n$. Projections $\mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}^m$ map $\mathcal{S}_{m+n}$ to $\mathcal{S}_m$ [Dri98]. A map $\mathbb{R}^n \to \mathbb{R}^m$ is called semilinear iff its graph is a semilinear subset of $\mathbb{R}^{m+n}$. The composition of two semilinear maps is a semilinear map [Dri98].

Recall that we use the ℓ^∞ metric on $\mathbb{R}^n$.

Lemma 3.4.1. *The distance function $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is semilinear.*

Proof. The function $(x, y) \mapsto x_i - y_i$ is semilinear for any i. The function $|\cdot| : \mathbb{R} \to \mathbb{R}$ is semilinear. If $f, g : \mathbb{R}^n \to \mathbb{R}$ are semilinear, then $h = \max(f, g) : \mathbb{R}^n \to \mathbb{R}$ is semilinear. Since the set of semilinear functions is closed under composition, this proves the lemma. □

Recall that for any set $U \subset \mathbb{R}^n$, we write $U^r := \{x \in \mathbb{R}^n : \exists y \in U \text{ s.t } d(x,y) \leq r\}$ and call this the *r-thickening* of U. It is easy to see that if U is closed, then U^r is also closed for any $r \geq 0$.

Lemma 3.4.2. *If U is semilinear, U^r is semilinear for any r.*

Proof. Consider the set

$$\Delta_r = \{(x,y) \in \mathbb{R}^{2n} | d(x,y) \leq r\}.$$

By the previous lemma, Δ_r is semilinear. On the other hand, U^r is the projection to the first $\mathbb{R}^n$ of $\Delta_r \cap (\mathbb{R}^n \times U) \subset \mathbb{R}^n \times \mathbb{R}^n$. Since intersection and projection preserve the set of semilinear sets, the lemma is proved. □

Lemma 3.4.3. *If U is convex, then U^r is convex, for any $r \geq 0$.*

Proof. Suppose $x, y \in U^r$, and suppose $x', y' \in U$ satisfy $d(x,x') \leq r$ and $d(y,y') \leq r$. Then for any $t \in [0,1]$ we have $d(tx + (1-t)y, tx' + (1-t)x') \leq t^2 d(x,x') + (1-t)^2 d(y,y') \leq r$. □

A polyhedron in $\mathbb{R}^n$ is an intersection of a finite number of closed half-spaces. A polyhedron is closed, but not necessarily compact. A closed semilinear set is the same as a finite union of polyhedra. Conversely, according to Theorem 19.6 from [Roc70], a polyhedron can be described as a closed convex semilinear set. Combining this with the above lemmas, we get

Corollary 3.4.1. *If U is a polyhedron, then U^r is a polyhedron, for any $r \geq 0$.*

A category of fuzzy semilinear sets

Clearly, if for $X, Y \in \mathcal{S}_n$ we have $X \subseteq Y$, then for any $r \geq 0$ we have $X^r \subseteq Y^r$. Also, for any $r, s \geq 0$ and any $U \in \mathcal{S}_n$ we have $(U^r)^s \subseteq U^{r+s}$. Thus we can define a pre-order $\leq$ on $\mathcal{S}_n$ by saying that $U \leq V$ iff there exists $r \geq 0$ such that $U \subseteq V^r$. We will call this pre-order relation $f$uzzy inclusion. Equivalently, $\mathcal{S}_n$ can be made into a category, with a single morphism from U to V iff $U \leq V$. One can turn the pre-ordered set $(\mathcal{S}_n, \leq)$ into a poset by identifying isomorphic objects of the corresponding category, but for our purposes it is more convenient not to do so. On the other hand, every semilinear set is isomorphic to its closure, and we find it convenient to work with an equivalent category (or pre-ordered set) which contains only closed semilinear subsets.

We will denote it $\mathcal{CS}_n$ and call it the category (or pre-ordered set) of fuzzy semilinear sets.

Proposition 3.4.1. *$\mathcal{CS}_n$ has all pairwise joins: for any $U, V \in \mathcal{CS}_n$ the join is given by $U \cup V$.*

Proof. If $U \subseteq W^r$ and $V \subseteq W^s$ for some $r, s \geq 0$, then $U \subseteq W^{\max(r,s)}$ and $V \subseteq W^{\max(r,s)}$, and thus $U \cup V \subseteq W^{\max(r,s)}$. □

Let us show that $\mathcal{CS}_n$ has all pairwise meets, using the notion of transverse intersection from the previous section. Recall (Definition 3.3.5) that we say two sets $U, V \subset \mathbb{R}^n$ are transverse if for some $C > 0$ we have $d(x, U \cap V) \leq C \max(d(x, U), d(x, V))$ for all $x \in \mathbb{R}^n$.

We need the following geometric result [Pet][9]:

Lemma 3.4.4. *Let P and Q be polyhedra $\mathbb{R}^n$. If $P \cap Q \neq \varnothing$ then P and Q are transverse.*

Proposition 3.4.2. *For every $U, V \in \mathcal{CS}_n$ there is an $r > 0$ such that U^r and V^r are transverse.*

Proof. Let $U = \cup_i P_i$ and $V = \cup_j P_j$ be a decomposition of U and V into finite unions of polyhedra and choose $r > 0$ so that $P_i^r \cup Q_j^r$ is nonempty for each pair i, j. By Corollary 3.4.1 and Lemma 3.4.4 there are constants $C_{P_i Q_j} > 0$ such that

$$d(x, U^r \cap V^r) \leq C \max(d(x, U^r), d(x, V^r))$$

for each pair i, j. Since $U^r = \cup_i P_i^r$ and $V^r = \cup_i Q_i^r$, for any $x \in \mathbb{R}$ there are indices i^* and j^* such that $d(x, U^r) = d(x, P_{i^*}^r)$ and $d(x, V^r) = d(x, Q_{j^*}^r)$. Then we have

$$\begin{aligned} d(x, U^r \cap V^r) &= d(x, \cup_{ij}(P_i^r \cap Q_j^r)) \\ &\leq d(x, P_{i^*}^r \cap Q_{j^*}^r)) \\ &\leq C_{P_{i^*} Q_{j^*}} \max(d(x, P_{i^*}), d(x, Q_{j^*})) \\ &= C_{P_{i^*} Q_{j^*}} \max(d(x, U), d(x, V)), \end{aligned}$$

and so U^r, V^r are C-transverse for $C := \max_{i,j} C_{P_i Q_j}$. □

[9]The proof in [Pet] is for the Euclidean distance, but since the Euclidean distance function and $d(x, y) = \|x - y\|_\infty$ are equivalent (each one is upper-bounded by a multiple of the other), the result applies to $d(x, y)$ as well.

Corollary 3.4.2. *With U, V, r as above, $U^r \cap V^r$ is a meet of U and V. In particular, $\mathcal{CS}_n$ has all pairwise meets.*

Proof. Since U and U^r (resp. V and V^r) are isomorphic in $\mathcal{CS}_n$, it suffices to show that $U^r \cap V^r$ is a meet of U^r and V^r. It's clear that $U^r \cap V^r \leq U^r$ and $U^r \cap V^r \leq V^r$. Now suppose $W \in \mathcal{CS}_n$ satisfies $W \leq U^r$ and $W \leq V^r$. Then there is an $s > 0$ such that every $x \in W$ satisfies $\max(d(x, U^r), d(x, V^r)) \leq s$. Since $d(x, U^r \cap V^r) \leq C \max(d(x, U^r), d(x, V^r))$ for some $C > 0$ we have $W \subset (U^r \cap V^r)^{Cs}$. □

Proposition 3.4.3. *The pre-ordered set $\mathcal{CS}_n$ is distributive.*

Proof. We need to show that for any $U, V, W \in \mathcal{CS}_n$ we have $U \wedge (V \vee W) \leq (U \wedge V) \vee (U \wedge W)$. According to Corollary 3.4.2, there exists $r \geq 0$ such that $U \wedge (V \vee W) \simeq U^r \cap (V \cup W)^r$. Since $(V \cup W)^r = V^r \cup W^r$, we also have $U \wedge (V \vee W) \simeq (U^r \cap V^r) \cup (U^r \cap W^r)$. On the other hand, $U \wedge V \simeq U^r \wedge V^r \simeq (U^r)^s \cap (V^r)^s$ for some $s \geq 0$, and $U \wedge W \simeq U^r \wedge W^r \simeq (U^r)^t \cap (W^r)^t$ for some $t \geq 0$. Thus $(U \wedge V) \vee (U \wedge W) \simeq ((U^r)^s \cap (V^r)^s) \cup ((U^r)^t \cap (W^r)^t)$ for some $s, t \geq 0$. Since we have inclusions $U^r \cap V^r \subseteq (U^r)^s \cap (V^r)^s$ and $U^r \cap W^r \subseteq (U^r)^t \cap (W^r)^t$, the lemma is proved. □

We can now equip $\mathcal{CS}_n$ with a Grothendieck topology of Section 3.2. There are two versions of it which differ in whether we allow empty covers of an initial object or not. In the case of the pre-ordered set $\mathcal{CS}_n$, every bounded closed semilinear set is an initial object (they are all isomorphic objects of the category $\mathcal{CS}_n$). Since such sets are not empty, we will disallow empty covers. This choice is also forced on us if we want certain pre-cosheaves to be cosheaves (see below). Note that we only consider non-empty closed semilinear sets.

More generally, for any $W \in \mathcal{CS}_n$ we may consider a full sub-category $\mathcal{CS}_n/W$ whose objects are $U \in \mathcal{CS}_n$ such that $U \leq W$. This is a distributive pre-ordered set, and we will also have occasion to consider local Lie algebras on the associated site.

Spherical CS sets

Every two bounded elements of $\mathcal{CS}_n$ are isomorphic objects of the corresponding category. More generally, any two elements of $\mathcal{CS}_n$ which coincide outside some ball in $\mathbb{R}^n$ are isomorphic objects. Thus $\mathcal{CS}_n$ encodes the large-scale structure of $\mathbb{R}^n$. To make this explicit, we will show that the pre-ordered set $\mathcal{CS}_n$ is equivalent as a category to a certain poset of subsets of the "sphere at infinity" S^{n-1}.

A cone in $\mathbb{R}^n$ is a non-empty subset of $\mathbb{R}^n$ which is invariant under $x \mapsto \lambda x$, where $\lambda \geq 0$. Every cone contains the origin 0. Cones in $\mathbb{R}^n$ are in bijection with subsets of $S^{n-1} = (\mathbb{R}^n \backslash \{0\})/\mathbb{R}_+^*$ where $\mathbb{R}_+^*$ is the group of positive real numbers under multiplication. If $A \subset S^{n-1}$, we denote the corresponding cone $c(A)$. In particular, $c(\varnothing) = \{0\} \in \mathbb{R}^n$. If K is a cone in $\mathbb{R}^n$, we will denote the corresponding subset of S^{n-1} by $\hat{K}$.

Definition 3.4.1. *$A \subset S^{n-1}$ is a spherical polyhedron iff $c(A)$ is a polyhedron and A is contained in some open hemisphere of S^{n-1}. $A \subseteq S^{n-1}$ is a spherical CS set iff it is a union of a finite number of spherical polyhedra. The set of spherical CS sets in S^{n-1} is denoted $\mathcal{SCS}_n$.*

Every polyhedron is convex and thus contractible. This implies:

Proposition 3.4.4. *Any spherical polyhedron is contractible.*

Proof. Without loss of generality, we may assume that the spherical polyhedron is contained in the hemisphere $S_+^{n-1} = S^{n-1} \cap \{x_n > 0\}$. The map $\mathbb{R}^{n-1} \to S_+^{n-1}$ which sends $(x_1, \ldots, x_{n-1})$ to the equivalence class of $(x_1, \ldots, x_{n-1}, 1)$ is a homeomorphism which establishes a bijection between bounded polyhedra in $\mathbb{R}^{n-1}$ and spherical polyhedra contained in S_+^{n-1}. □

Proposition 3.4.5. *The intersection of two spherical polyhedra is a spherical polyhedron. The union and intersection of two spherical CS sets is a spherical CS set.*

Proof. Clear from definitions. □

Spherical CS sets form a poset $\mathcal{SCS}_n$ under inclusion. This poset has pairwise joins and meets given by unions and intersections, respectively.

Proposition 3.4.6. *The category $\mathcal{SCS}_n$ is equivalent to the category $\mathcal{CS}_n$.*

Proof. We proceed first by defining a functor from $\mathcal{CS}_n$ to $\mathcal{SCS}_n$. Notice, it is sufficient to define a functor on isomorphism classes of polyhedrons, then extend by joins. Every closed polyhedron is a finite intersection of closed half spaces $\bigcap_{i=1}^{k}\{n_i \cdot x \leq b_i\}$, where for each $i = 1, \dots k$, $n_i \in \mathbb{R}^n$ is the unit normal vector of the ith supporting hyperplane and $b_i \in \mathbb{R}$. By definition, $\bigcap_{i=1}^{k}\{n_i \cdot x \leq b_i\}$ is isomorphic to $\bigcap_{i=1}^{k}\{n_i \cdot x \leq 0\}$ in $\mathcal{CS}_n$. In other words, every polyhedron is isomorphic to a cone $\{Nx \preceq 0\}$, where N is the matrix with n_i as rows and we write $y \preceq 0$ for $y \in \mathbb{R}^n$ when $y_i \leq 0$ for all $i = 1, \dots n$. If $\{n_i\}_{i=1}^{k}$ spans $\mathbb{R}^n$, the set $\{Nx \preceq 0\}$, which contains no antipodal points, is mapped to its corresponding spherical polyhedron. Otherwise, complete $\{n_i\}_{i=1}^{k}$ into a spanning set $\{n_1, \dots, n_k, m_1, \dots, m_l\}$ and decompose $\{Nx \preceq 0\}$ into a union of cones $\{Nx \preceq 0\} \cap \bigcap_j \{\pm m_j \cdot x \leq 0\}$. By the universal property of the join, an arbitrary closed semilinear set is isomorphic to a union of conical polyhedra. For functoriality, it is sufficient to note that for any pair of closed cones U, V a fuzzy inclusion $U \subseteq V^r$ for some $r \geq 0$ implies $U \subseteq V$. It is easy to check that this functor is fully faithful and (essentially) surjective. □

Note that under this equivalence all bounded elements of $\mathcal{CS}_n$ correspond to $\varnothing \in \mathcal{SCS}_n$. The canonical Grothendieck topology on $\mathcal{CS}_n$ corresponds to a slightly unusual Grothendieck topology on the poset of spherical CS subsets of S^{n-1}: the one where empty covers of $\varnothing$ are not allowed. Consequently, a cosheaf of vector spaces on $\mathcal{SCS}_n$ equipped with this topology need not map $\varnothing$ to the zero vector space.

Spherical CS cohomology

Let $\mathfrak{U}$ be a spherical CS cover of a spherical CS set A. Spherical CS cohomology $\check{H}^{\bullet}_{CS}(\mathfrak{U}, A; \mathbb{R})$ is defined to be the simplicial cohomology of the Čech nerve $N(\mathfrak{U})$.

Definition 3.4.2. *Let A be a spherical CS set. The spherical CS cohomology $\check{H}^{\bullet}_{CS}(A, \mathbb{R})$ is defined as $\varinjlim \check{H}^{\bullet}_{CS}(\mathfrak{U}, A; \mathbb{R})$, where the colimit is taken over the directed set of all spherical CS covers.*

The following proposition connects spherical CS cohomology with singular cohomology using a functorial version of nerve theorems [Bor48; Ler45].

Proposition 3.4.7. *For any spherical CS set A the graded vector space $\check{H}^{\bullet}_{CS}(A, \mathbb{R})$ is isomorphic to the singular cohomology $H^{\bullet}(A, \mathbb{R})$.*

Proof. Every spherical CS cover can be refined to a cover by spherical polyhedra, so in the computation of $\varinjlim \check{H}^\bullet_{CS}(\mathfrak{U}, A; \mathbb{R})$ it suffices to take colimit over such covers. All intersections of elements of a spherical polyhedral cover $\mathfrak{U}$ are contractible. Also, since every polyhedron is a geometric realization of a simplicial complex, $\mathfrak{U}$ is a cover of a simplicial complex by subcomplexes. By Theorem C of [Bau+23] for such $\mathfrak{U}$ the direct system of groups $\mathfrak{U} \mapsto \check{H}^\bullet_{CS}(\mathfrak{U}, A; \mathbb{R})$ is constant and its limit is $H^\bullet(A, \mathbb{R})$. □

3.5 Local Lie algebras over fuzzy semilinear sets

Basic examples

Let ψ be a state of a quantum lattice system on $\mathbb{R}^n$. By Lemma 3.3.2 the maps sending $U \in \mathcal{CS}_n$ to $\mathfrak{D}_{al}(U)$ and $\mathfrak{D}^\psi_{al}(U)$ are pre-cosheaves of Fréchet spaces on $\mathcal{CS}_n$. We denote these pre-cosheaves by $\mathfrak{D}_{al}$ and $\mathfrak{D}^\psi_{al}$. Putting together Lemma 3.2.1, Proposition 3.3.5, Corollary 3.3.1, and Proposition 3.3.8, we have:

Theorem 3.5.1. *$\mathfrak{D}_{al}$ is a local Lie algebra over $\mathcal{CS}_n$. If ψ is gapped, then $\mathfrak{D}^\psi_{al}$ is a local Lie algebra over $\mathcal{CS}_n$.*

Our main object of study is the local Lie algebra $\mathfrak{D}^\psi_{al}$ attached to a gapped state ψ of a lattice system $(\Lambda, \{V_j\}_{j\in\Lambda})$.

A much simpler example of a local Lie algebra arises from a finite-dimensional Lie algebra $\mathfrak{g}$ and any subset $\Lambda \subset \mathbb{R}^n$. For any $U \in \mathcal{CS}_n$ let $\mathfrak{g}_{al}(U)$ be the space of bounded functions $U \cap \Lambda \to \mathfrak{g}$ which decay superpolynomially away from U. The subscript "al" stands for "almost localized". More precisely, $\mathfrak{g}_{al}(\mathbb{R}^n)$ is the space of bounded functions $\Lambda \to \mathfrak{g}$, while $\mathfrak{g}_{al}(U)$ is defined as a subspace of $\mathfrak{g}_{al}(\mathbb{R}^n)$ consisting of functions $f : \Lambda \to \mathfrak{g}$ such that the following seminorms are finite:

$$p_{k,U}(f) = \sup_{j\in\Lambda} |f(j)|(1 + d(U, j))^k, \quad k \in \mathbb{N}.$$

Proposition 3.5.1. *The assignment $U \mapsto \mathfrak{g}_{al}(U)$ is a local Lie algebra.*

Proof. It is easy to check that the assignment $U \mapsto \mathfrak{g}_{al}(U)$ it is a coflasque pre-cosheaf of Fréchet-Lie algebras satisfying Property I. The only thing left to check is that it is a cosheaf of vector spaces. By Lemma 3.2.1, it is sufficient to show that for any $U, V \in \mathcal{CS}_n$ the sequence

$$\mathfrak{g}_{al}(U \wedge V) \to \mathfrak{g}_{al}(U) \oplus \mathfrak{g}_{al}(V) \to \mathfrak{g}_{al}(U \vee V) \to 0$$

is exact. To show exactness at $\mathfrak{g}_{al}(U \vee V) = \mathfrak{g}_{al}(U \cup V)$, we note that every $f \in \mathfrak{g}_{al}(U \cup V)$ can be written as a sum $f_U + f_V$, where

$$f_U(x) = \begin{cases} f(x), & d(x,U) < d(x,V), \\ \frac{1}{2} f(x), & d(x,U) = d(x,V), \\ 0, & d(x,U) > d(x,V), \end{cases}$$

and $f_V(x)$ is defined by a similar expression with U and V exchanged. Using $d(x, U \cup V) = \min(d(x,U), d(x,V))$ it is easy to check that $p_{k,U}(f_U) \leq p_{k,U\cup V}(f)$ and $p_{k,V}(f_V) \leq p_{k,U\cup V}(f)$ for all k, and thus $f_U \in \mathfrak{g}_{al}(U)$ and $f_V \in \mathfrak{g}_{al}(V)$.

To show exactness at $\mathfrak{g}_{al}(U) \oplus \mathfrak{g}_{al}(V)$, suppose $f \in \mathfrak{g}_{al}(U) \cap \mathfrak{g}_{al}(V)$. From the proof of Prop. 3.4.2, there exist $r \geq 0, C_{UV} > 0$ such that $d(x, U^r \cap V^r) \leq C_{UV} \max(d(x,U), d(x,V))$. We may assume that $C_{UV} \geq 1$, in which case for any $x \in \mathbb{R}^n$ and any $k \in \mathbb{N}$

$$(1 + d(x, U^r \cap V^r))^k \leq C_{UV}^k (1 + \max(d(x,U), d(x,V))^k.$$

Therefore for any $f \in \mathfrak{g}_{al}(U) \cap \mathfrak{g}_{al}(V)$ we have

$$p_{k,U^r \cap V^r}(f) \leq C_{UV}^k \max(p_{k,U}(f), p_{k,V}(f)).$$

Since by Corollary 3.4.2 one can take $U \wedge V = U^r \cap V^r$, we conclude that $f \in \mathfrak{g}_{al}(U \wedge V)$. □

Symmetries of lattice systems

If $\Lambda \subset \mathbb{R}^n$ is countable, it can be viewed as a lattice in the physical sense, and the local Lie algebra $\mathfrak{g}_{al}$ over $\mathcal{CS}_n$ models infinitesimal gauge transformations of a lattice system on $\mathbb{R}^n$.

Definition 3.5.1. *A local action of a compact Lie group on a lattice system $(\Lambda, \{V_j\}_{j\in\Lambda})$ is a collection of homomorphisms $\rho_j : G \to U(V_j)$ such that the norms of the corresponding Lie algebra homomorphisms $\mathfrak{g} \to B(V_j)$ are bounded uniformly in j.*

A local action of G on $(\Lambda, \{V_j\}_{j\in\Lambda})$ gives rise to a homomorphism from G to the automorphism group of $\mathscr{A}$ via $g \mapsto \otimes_{j\in\Lambda} \mathrm{Ad}_{\rho_j(g)}$ which is smooth on $\mathscr{A}_{a\ell}$. The corresponding generator Q is a homomorphism from $\mathfrak{g}$ to the Lie algebra of derivations of $\mathscr{A}_{a\ell}$ defined by

$$\mathsf{Q} : (a, \mathcal{A}) \mapsto \sum_{j \in \Lambda} [\mathsf{q}_j(a), \mathcal{A}], \quad a \in \mathfrak{g},\ \mathcal{A} \in \mathscr{A}_{a\ell},$$

where q_j is the traceless part of the generator of ρ_j. The image of Q lands in $\mathfrak{D}_{al}(\mathbb{R}^n)$, with $\mathsf{Q}(a)^Y = \sum_{j \in \Lambda} \mathsf{q}_j(a)^Y$. We will regard Q as a homomorphism of Fréchet-Lie algebras $\mathfrak{g} \to \mathfrak{D}_{al}(\mathbb{R}^n)$.

This morphism of Fréchet-Lie algebras can be lifted to a morphism of local Lie algebras $\mathfrak{g}_{al} \to \mathfrak{D}_{al}$ over $\mathcal{CS}_n$. Indeed, for any $U \in \mathcal{CS}_n$ and any $f \in \mathfrak{g}_{al}(U)$ we let $\mathsf{Q}(f)$ be a derivation of $\mathscr{A}_{a\ell}$ given by

$$\mathsf{Q}(f)(\mathcal{A}) = \sum_{j \in \Lambda} [\mathsf{q}_j(f(j)), \mathcal{A}], \quad \mathcal{A} \in \mathscr{A}_{a\ell}.$$

It is easy to check that this derivation belongs to $\mathfrak{D}_{al}(U)$ and that the above map is a continuous homomorphism $\mathfrak{g}_{al}(U) \to \mathfrak{D}_{al}(U)$. The physical interpretation is that a local action of a compact Lie group on a quantum lattice system can be gauged on the infinitesimal level.

Definition 3.5.2. *A state ψ of $\mathscr{A}$ is said to be invariant under a local action of a compact Lie group G if it is invariant under the corresponding automorphisms of $\mathscr{A}$.*

Let ψ be a gapped state of $\mathscr{A}$ invariant under a local action of a Lie group G. In that case the image of $\mathsf{Q} : \mathfrak{g} \to \mathfrak{D}_{al}(\mathbb{R}^n)$ lands in $\mathfrak{D}^{\psi}_{al}(\mathbb{R}^n)$. One may ask if this morphism of Fréchet-Lie algebras can be lifted to a morphism of local Lie algebras $\mathfrak{g}_{al} \to \mathfrak{D}^{\psi}_{al}$. If this is the case, then the symmetry G of ψ can be gauged on the infinitesimal level. In the next section we construct obstructions for the existence of such a morphism of local Lie algebras and show that zero-temperature Hall conductance is an example of such an obstruction.

Equivariantization

As a preliminary step, for any G-invariant gapped state ψ we are going to define a graded local Lie algebra over $\mathcal{CS}_n$ which is a G-equivariant version of the local Lie algebra $\mathfrak{D}^{\psi}_{al}$. Recall that a graded local Lie algebra is a cosheaf of graded vector spaces that is a pre-cosheaf of graded Lie algebras satisfying the graded analogue of Property I. For example, if $\mathfrak{F}$ is a local Lie algebra and $A = \prod_{k \in \mathbb{Z}} A_k$ is a locally finite supercommutative graded algebra with finite-dimensional graded factors A_k,[10] then $U \mapsto \mathfrak{F}(U) \otimes A$ is a graded local

[10] A graded vector space is locally finite iff its graded components are finite-dimensional.

Lie algebra. We denote it $\mathfrak{F} \otimes A$.

Fix a compact Lie group G and a distributive pre-ordered set X and consider the category of graded local Lie algebras over X equipped with a G-action. An object of this category is a graded local Lie algebra $\mathfrak{F}$ on which G acts by automorphisms; morphisms are defined in an obvious manner. The first step is to define a functor $\mathfrak{F} \mapsto \mathfrak{F}^G$ from this category to the category of graded local Lie algebras over X such that $\mathfrak{F}^G(U)$ is the Lie algebra of G-invariant elements of $\mathfrak{F}(U)$. It is clear how to define such a functor for coflasque pre-cosheaves of Lie algebras with Property I, but the pre-cosheaf $\mathfrak{F}^G$ will not be a cosheaf of vector spaces without further assumptions about $\mathfrak{F}$ and the G-action.

Definition 3.5.3. *An action of G on a pre-cosheaf of Fréchet spaces $\mathfrak{F}$ is smooth if for each $U \in X$ the seminorms defining the topology of $\mathfrak{F}(U)$ can be chosen to be G-invariant and the map $G \times \mathfrak{F}(U) \to \mathfrak{F}(U)$ defining the action is smooth. An action of G on a pre-cosheaf of graded Fréchet spaces is smooth if the G-action on every graded component is smooth.*

Proposition 3.5.2. *Let $\mathfrak{F}$ be a pre-cosheaf of graded Fréchet spaces over X equipped with a smooth action of a compact Lie group G. The assignment $U \mapsto \mathfrak{F}^G(U) = (\mathfrak{F}(U))^G$ is a cosheaf of graded Fréchet spaces.*

Proof. It is sufficient to prove this in the ungraded case. We need to show that for any $U, V \in X$ the sequence

$$\mathfrak{F}^G(U \wedge V) \xrightarrow{\alpha} \mathfrak{F}^G(U) \oplus \mathfrak{F}^G(V) \xrightarrow{\beta} \mathfrak{F}^G(U \vee V) \to 0,$$

is exact. To show exactness at the rightmost term, let F be a G-invariant element of $\mathfrak{F}(U \vee V)$ and let $\mathsf{F}_U \in \mathfrak{F}(U)$ and $\mathsf{F}_V \in \mathfrak{F}(V)$ be such that $\iota_{U\cup V,U}\mathsf{F}_U + \iota_{U\cup V,V}\mathsf{F}_V = \mathsf{F}$. Averaging the action map $G \times \mathfrak{F}(U)$ over G with the Haar measure gives a linear map $h_U : \mathfrak{F}(U) \mapsto \mathfrak{F}^G(U)$ which is identity when restricted to $\mathfrak{F}^G(U)$. The co-restriction morphisms intertwine these maps. Thus $\iota_{U\cup V,U} \circ h_U(\mathsf{F}_U) + \iota_{U\cup V,V} \circ h_V(\mathsf{F}_V) = \mathsf{F}$ which proves that β is surjective. Exactness in the middle term is proved similarly. □

Remark 3.5.1. *For the proof to go through, it suffices to require the map $G \times \mathfrak{F}(U) \to \mathfrak{F}(U)$ to be continuous. However, if it is smooth, $\mathfrak{F}(U)$ becomes a $\mathfrak{g}$-module and all elements in $\mathfrak{F}^G(U) \subset \mathfrak{F}(U)$ are annihilated by the $\mathfrak{g}$-action. We will use this later on.*

Example 3.5.1. *If G acts locally on a lattice system, the action of G on the local Lie algebra $\mathfrak{D}_{al}$ is smooth. If ψ is a G-invariant gapped state of such a lattice system, the action of G on $\mathfrak{D}^{\psi}_{al}$ is smooth.*

Example 3.5.2. *Consider the local Lie algebra $\mathfrak{g}_{al}$ over $\mathcal{CS}_n$ associated to a finite-dimensional Lie algebra $\mathfrak{g}$ (see Section 3.4). Assume that $\mathfrak{g}$ is the Lie algebra of a compact Lie group G, then there is an obvious G-action on $\mathfrak{g}_{al}$:*

$$(g \cdot f)(j) = Ad_g f(j), \quad g \in G, j \in \Lambda.$$

This G-action is smooth.

Example 3.5.3. *If $\mathfrak{F}$ is a local Fréchet-Lie algebra with a smooth G-action and $A = \prod_{k\in\mathbb{Z}} A_k$ is a locally-finite supercommutative graded algebra on which G acts by automorphisms, then the G-action on $\mathfrak{F} \otimes A$ is smooth.*

Corollary 3.5.1. *Let $\mathfrak{F}$ be a graded local Fréchet-Lie algebra over X with a smooth G-action. The functor of G-invariant elements maps $\mathfrak{F}$ to a graded local FréchetLie algebra $\mathfrak{F}^G$ over X.*

Definition 3.5.4. *Let $\mathfrak{F}$ be a local Fréchet-Lie algebra over X with a smooth G-action. The G-equivariantization functor sends $\mathfrak{F}$ to the negatively-graded local Fréchet-Lie algebra $\mathfrak{F}^{\mathbf{G}}$ defined by*

$$U \mapsto \left(\mathfrak{F}(U) \otimes \prod_{k=1}^{\infty} Sym^k(\mathfrak{g}^*[-2]) \right)^G .$$

In the cases of interest to us, the G-action on a local Lie algebra over $\mathcal{CS}_n$ is infinitesimally inner, in the sense that the $\mathfrak{g}$-module structure mentioned in Remark 3.5.1 arises from a homomorphism $\rho : \mathfrak{g} \to \mathfrak{F}(\mathbb{R}^n)$. In such a case, the graded local Lie algebra $\mathfrak{F}^{\mathbf{G}}$ has an extra bit of structure: a central element in $\mathfrak{F}^{\mathbf{G}}(\mathbb{R}^n)$ of degree -2. This element is simply ρ re-interpreted as an element of $\mathfrak{F}(\mathbb{R}^n) \otimes \mathfrak{g}^*[-2]$. In the terminology of Section 3.2, $\mathfrak{F}^{\mathbf{G}}$ is a pointed graded local Fréchet-Lie algebra over $\mathcal{CS}_n$. It is easy to see that the G-equivariantization functor respects this extra structure. That is, if $f : \mathfrak{F} \to \mathfrak{F}'$ is a morphism of local Fréchet-Lie algebras over $\mathcal{CS}_n$ commuting with infinitesimally inner smooth G-actions on $\mathfrak{F}$ and $\mathfrak{F}'$, then $f^{\mathbf{G}}$ maps the central element $\rho \in \mathfrak{F}^{\mathbf{G}}(\mathbb{R}^n)_{-2}$ to the central element $\rho' \in \mathfrak{F}'^{\mathbf{G}}(\mathbb{R}^n)_{-2}$.

Example 3.5.4. *Let ψ be a G-invariant gapped state of a quantum lattice system with a local G-action which on the infinitesimal level is described by $\mathsf{Q} : \mathfrak{g} \to \mathfrak{D}^{\psi}_{al}(\mathbb{R}^n)$. Consider the graded local Lie algebra $\mathfrak{D}^{\psi}_{al}$ with its smooth G-action (Example 3.5.1) and its G-equivariantization $\mathfrak{D}^{\psi,\boldsymbol{G}}_{al}$. The distinguished central element of $\mathfrak{D}^{\psi,\boldsymbol{G}}_{al}(\mathbb{R}^n)$ is Q regarded as an element of $\mathfrak{D}^{\psi}_{al}(\mathbb{R}^n) \otimes \mathfrak{g}^*[-2]$.*

Example 3.5.5. *Consider the graded local Lie algebra $\mathfrak{g}^{\boldsymbol{G}}_{al}$ of Example 3.5.2. The degree -2 component of $\mathfrak{g}^{\boldsymbol{G}}_{al}(\mathbb{R}^n)$ is the space of G-invariant bounded functions on Λ with values in $\mathfrak{g} \otimes \mathfrak{g}^*$. The distinguished central element is the constant function on Λ which takes the value $id_{\mathfrak{g}}$.*

Armed with the equivariantization functor, we can now explain our strategy for constructing obstructions for the existence of a local Lie algebra morphism $\mathfrak{g}_{al} \to \mathfrak{D}^{\psi}_{al}$ which lifts the Fréchet-Lie algebra morphism $\mathsf{Q} : \mathfrak{g} \to \mathfrak{D}^{\psi}_{al}(\mathbb{R}^n)$. Suppose such a morphism ρ exists. Applying the G-equivariantization functor, we get a morphism of pointed negatively-graded local Fréchet-Lie algebras $\rho^{\mathbf{G}} : \mathfrak{g}^{\mathbf{G}}_{al} \to \mathfrak{D}^{\psi,\mathbf{G}}_{al}$. For any CS cover $\mathfrak{U}$ of $\mathbb{R}^n$ an application of the Čech functor gives a morphism of acyclic pointed DGLAs

$$C^{aug}_{\bullet+1}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{g}^{\mathbf{G}}_{al}) \to C^{aug}_{\bullet+1}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}^{\psi,\mathbf{G}}_{al}).$$

Consequently, a obstruction for the existence of such a pointed DGLA morphism is an obstruction for the existence of ρ. In the next section we use the twisted Maurer-Cartan equation for pointed DGLAs to construct such obstructions and identify them as topological invariants of gapped states defined in [KS22].

3.6 Topological invariants of G-invariant gapped states

The commutator class

Let $(\mathfrak{M}, \mathsf{B})$ be a pointed DGLA, i.e. a DGLA with a distinguished central cycle $\mathsf{B} \in \mathfrak{M}_{-2}$. Assume it is a limit of an inverse system of nilpotent pointed DGLAs $(\mathfrak{M}_N, \mathsf{B}_N)$, $N \in \mathbb{N}$.

Definition 3.6.1. *The commutator DGLA, denoted by $\overline{[\mathfrak{M}, \mathfrak{M}]}$, is defined to be the closure of the commutator subalgebra of $\mathfrak{M}$. Namely, $\mathsf{q} \in \overline{[\mathfrak{M}, \mathfrak{M}]}$ if and only if for any N its projection to $\mathfrak{M}_N$ is a finite linear combination of commutators in $\mathfrak{M}_N$.*

Even if $\mathfrak{M}$ is acyclic, the DGLA $\overline{[\mathfrak{M},\mathfrak{M}]}$ is not necessarily acyclic. We would like to construct an obstruction to finding an element $\mathsf{p} \in \mathfrak{M}_{-1}$ which satisfies $\partial\mathsf{p} = \mathsf{B}$ and $[\mathsf{p},\mathsf{p}] = 0$.

Definition 3.6.2. *Let* $(\mathfrak{M}, \mathsf{B})$ *be a pointed DGLA. A* B*-twisted Maurer-Cartan element in* $\mathfrak{M}$ *is* $\mathsf{p} \in \mathfrak{M}_{-1}$ *which satisfies*

$$\partial\mathsf{p} + \frac{1}{2}[\mathsf{p},\mathsf{p}] = \mathsf{B}.$$

We will denote the set of B-twisted MC elements of $\mathfrak{M}$ by $\mathrm{M}C(\mathfrak{M}, \mathsf{B})$. The map $(\mathfrak{M}, \mathsf{B}) \mapsto \mathrm{M}C(\mathfrak{M}, \mathsf{B})$ can be upgraded to a functor from the category of pointed DGLAs to the category of sets in an obvious way.

Let $(\mathfrak{M}, \mathsf{B})$ be pronilpotent pointed DGLA and $\mathsf{p} \in \mathrm{M}C(\mathfrak{M}, \mathsf{B})$. Then $[\mathsf{p},\mathsf{p}]$ is a cycle of the DGLA $\overline{[\mathfrak{M},\mathfrak{M}]}$.

Proposition 3.6.1. *Let* $(\mathfrak{M}, \mathsf{B})$ *be an acyclic pointed DGLA which is a limit of an inverse system of nilpotent acyclic pointed DGLAs* $(\mathfrak{M}_N, \mathsf{B}_N)$*,* $N \in \mathbb{N}$*. Assume further that the structure morphisms* $r_{N,N-1} : \mathfrak{M}_N \to \mathfrak{M}_{N-1}$ *are surjective and* $\mathfrak{j}_N = \ker r_{N,N-1}$ *is central in* $\mathfrak{M}_N$*. Finally, assume* $[\mathfrak{M}_1, \mathfrak{M}_1] = 0$*. Then* $MC(\mathfrak{M}, \mathsf{B})$ *is non-empty. Furthermore, the homology class of* $[\mathsf{p},\mathsf{p}]$ *in* $\overline{[\mathfrak{M},\mathfrak{M}]}$ *for* $\mathsf{p} \in MC(\mathfrak{M}, \mathsf{B})$ *is independent of the choice of* p*.*

A proof of this result can be found in Section 3.8. It uses some results from deformation theory. We will call the homology class of $[\mathsf{p},\mathsf{p}]$ the commutator class of the acyclic pointed DGLA $(\mathfrak{M}, \mathsf{B})$, for lack of a better name, and denote it $\mathbf{com}(\mathfrak{M}, \mathsf{B})$. The assignment $(\mathfrak{M}, \mathsf{B}) \mapsto (H_\bullet(\overline{[\mathfrak{M},\mathfrak{M}]}), \mathbf{com}(\mathfrak{M}, \mathsf{B}))$ is a functor from the full sub-category of the category of acyclic pointed DGLAs satisfying the conditions of Proposition 3.6.1, to the category $\mathsf{pVect}_{\mathbb{Z}}$ of pointed graded vector spaces.

The conditions of Prop. 3.6.1 apply to any pointed DGLA which is the value of the Čech functor on a graded local Lie algebra $\mathfrak{F}^{\mathbf{G}}$ over some $(X, \leq)$, where $\mathfrak{F}$ is a local Lie algebra equipped with a smooth infinitesimally inner G-action. Indeed, along with the graded algebra $A = \prod_{k=1}^{\infty} \mathrm{S}ym^k \mathfrak{g}^*[-2]$ used in the construction of $\mathfrak{F}^{\mathbf{G}}$ one can consider its quotient by the ideal $J_N = \prod_{k=N+1}^{\infty} \mathrm{S}ym^k \mathfrak{g}^*[-2]$. Replacing A with the nilpotent graded algebra A/J_N throughout, for any cover $\mathfrak{U}$ of the terminal object T one gets a sequence of nilpotent acyclic pointed DGLAs labeled by $N \in \mathbb{N}$. They assemble into an inverse system in an obvious manner, and its limit is the acyclic pointed DGLA $C^{aug}_{\bullet+1}(\mathfrak{U}, T; \mathfrak{F}^{\mathbf{G}})$. It is easy to see that the remaining conditions of Prop. 3.6.1 are also satisfied. In particular, Prop. 3.6.1 applies to the pointed DGLAs associated the graded local Lie algebras $\mathfrak{D}^{\psi,\mathbf{G}}_{al}$ and $\mathfrak{g}^{\mathbf{G}}_{al}$ and any CS cover of $\mathbb{R}^n$.

Proposition 3.6.2. *For any pointed DGLA* $(\mathfrak{M}(\mathfrak{U}), \mathsf{B})$ *obtained, as above, from the Čech functor with respect to a cover* $\mathfrak{U}$*, MC is functorial in* $\mathfrak{U}$*.*

Proof. Let $\mathfrak{V} = \{V_j\}_{j\in J}$ be a refinement of $\mathfrak{U}$. By definition, there exists a map $\phi : J \to I$ with $V_j \subset U_{\phi(j)}$. According to Prop. 3.2.2, there is a map from $\mathfrak{M}(\mathfrak{V})$ to $\mathfrak{M}(\mathfrak{U})$. As B is unaffected by ϕ_*, we deduce from $\mathsf{p}^{\mathfrak{V}} \in \mathrm{M}C(\mathfrak{M}(\mathfrak{V}), \mathsf{B})$ that $\phi_*\mathsf{p}^{\mathfrak{V}} \in \mathrm{M}C(\mathfrak{M}(\mathfrak{U}), \mathsf{B})$. □

Example 3.6.1. *Let* G *be a compact Lie group,* $\mathfrak{g}$ *be its Lie algebra, and* $\mathfrak{g}_{al}$ *be the pointed local Lie algebra over* $\mathcal{CS}_n$ *of Examples (3.5.2) and (3.5.5). The distinguished central cycle in* $C^{aug}_{\bullet+1}(\mathfrak{U}, \mathbb{R}^n, \mathfrak{g}^{G}_{al})$ *is the constant function on* Λ *with value* $id_{\mathfrak{g}}$ *. Here* $id_{\mathfrak{g}}$ *is regarded as a* G*-invariant element of* $\mathfrak{g}_{al}(\mathbb{R}^n) \otimes \mathfrak{g}^*[-2]$*. For any cover* $\mathfrak{U} = \{U_i\}_{i\in I}$ *one can construct a twisted MC element* q *as follows. Pick* $r > 0$ *large enough so that the interiors of* U_i^r*,* $i \in I$*, cover* $\mathbb{R}^n$ *in the usual sense and pick a partition of unity* χ_i*,* $i \in I$*, subordinate to this open cover. For any* $j \in \Lambda$ *and any* $i \in I$ *let* $\mathsf{q}_i(j) = \chi_i(j) id_{\mathfrak{g}}$*. It is easy to verify that this is a twisted MC element satisfying* $[\mathsf{q}, \mathsf{q}] = 0$*. Thus the commutator class vanishes in this case.*

Let G be a compact Lie group, ψ be a gapped G-invariant state of a lattice system on $\mathbb{R}^n$, and $U \in \mathcal{CS}_n$. The commutator class of the acyclic pointed DGLA $(C^{aug}_{\bullet+1}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}^{\psi,\mathbf{G}}_{al}), \mathsf{Q})$ is an obstruction for the existence of a morphism of local Lie algebras $\rho : \mathfrak{g}_{al} \to \mathfrak{D}^{\psi}_{al}$ which is a lift of the Lie algebra morphism $\mathsf{Q} : \mathfrak{g} \to \mathfrak{D}^{\psi}_{al}(\mathbb{R}^n)$. Indeed, as explained in Section 3.5, if ρ exists, it induces a morphism of pointed DGLAs $C^{aug}_{\bullet}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{g}_{al}) \to C^{aug}_{\bullet}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}^{\psi,\mathbf{G}}_{al})$ which in turn induces a morphism in the category $\mathsf{pVect}_{\mathbb{Z}}$ which maps the commutator class of $\mathfrak{g}_{al}$ to the commutator class of $\mathfrak{D}^{\psi,\mathbf{G}}_{al}$. Since the former class vanishes (see Example 3.6.1), so must the latter.

Construction of topological invariants

The commutator class defined in the previous section is not a useful invariant of a gapped G-invariant state ψ because it takes values in a set which itself depends on ψ. It is also not invariant under LGAs (defined in Section 3.3) and thus is not an invariant of a gapped phase (see Remark 3.3.2). In this section we define a pairing between the commutator classes of $\mathfrak{D}_{al}^{\psi,\mathbf{G}}$ and spherical CS cohomology classes of the sphere at infinity S^{n-1}, which takes values in the algebra of G-invariant symmetric polynomials on $\mathfrak{g}$. This gives a useful invariant of a gapped phase which is also an obstruction to promoting the global symmetry G of the state to a local symmetry. Additionally, we will show that the invariant does not depends on the choice of the cover $\mathfrak{U}$ and thus is essentially unique.

Keeping in view further generalizations, we work over a sub-site $\mathcal{CS}_n/W$[11] which depends on an arbitray $W \in \mathcal{CS}_n$. Let $\hat{W} \in \mathcal{SCS}_n$ be the image of W under the equivalence between $\mathcal{CS}_n$ and $\mathcal{SCS}_n$. We continue to denote by $\mathfrak{D}_{al}$ the local Fréchet-Lie algebra which maps $U \in \mathcal{CS}_n/W$ to $\mathfrak{D}_{al}$. For any cover $\mathfrak{U}$ of W we denote by $\hat{\mathfrak{U}}$ the corresponding cover of $\hat{W}$.

Definition 3.6.3. *For any $\mathfrak{U} = \{U_i\}_{i\in I}$ covering $W \in \mathcal{CS}_n$, any $\mathsf{f} \in C_p(\mathfrak{U}, W; \mathfrak{D}_{al})$, and any $\beta \in \check{C}^p(\hat{\mathfrak{U}}, \hat{W}; \mathbb{R})$ define an evaluation*

$$\langle \mathsf{f}, \beta\rangle = \sum_{s\in I_p} \beta_s \mathsf{f}_s \in \mathfrak{D}_{al}(W),$$

where $I_k := \{i_0 < i_1 < \cdots < i_k \in I^{k+1}\}$. We adopt the convention that $\beta_s = 0$ for $\bigwedge_{j\in s} U_j$ bounded. The definition implicitly uses co-restriction of the coflasque cosheaf.

Lemma 3.6.1. *For any $\mathfrak{U}$ covering $W \in \mathcal{CS}_n$, any cycle $\mathsf{f} \in C_p(\mathfrak{U}, W; \mathfrak{D}_{al})$, and any cocycle $\beta \in \check{C}^p(\hat{\mathfrak{U}}, \hat{W}; \mathbb{R})$ the derivation $\langle \mathsf{f}, \beta\rangle \in \mathfrak{D}_{al}(W)$ is inner.*

Proof. The chain complex

$$\ldots \to \bigoplus_{i<j} \mathfrak{D}_{al}(U_i \wedge U_j) \to \bigoplus_{i} \mathfrak{D}_{al}(U_i) \to \mathfrak{D}_{al}(W) \to 0 \qquad (3.23)$$

[11] This is the so-called overcategory whose objects are equipped with a morphism to W. Due to coflasqueness, this amounts to a restriction to objects fuzzily included in W.

is acyclic. Since f is a cycle, $\mathsf{f} = \partial \mathsf{g}$ for some $\mathsf{g} \in \bigoplus_{s\in I_{p+1}} \mathfrak{D}_{al}(\bigwedge_{j\in s} U_j)$. Thus

$$\begin{aligned}\langle \mathsf{f}, \beta\rangle =& \langle \partial \mathsf{g}, \beta\rangle \\ =& \langle \mathsf{g}, \partial^* \beta\rangle \\ =& \sum_{s\in I_{p+1}} \mathsf{g}_s (\partial^*\beta)_s \\ =& \sum_{\substack{s\in I_{p+1},\ \text{with} \\ \bigwedge_{j\in s} U_j \ \text{bounded}}} \mathsf{g}_s (\partial^*\beta)_s,\end{aligned}$$

where ∂^* is the adjoint of ∂ defined by

$$(\partial^*\beta)_{i_0\ldots i_p} = \sum_{k=0}^{p} (-1)^k \beta_{i_0\ldots\widehat{i_k}\ldots i_p}.$$

The last expression is clearly inner because each g_s is almost localized near some bounded region. The last equality depends on vanishing of

$$\sum_{\substack{s\in I_{p+1},\ \text{with} \\ \bigwedge_{j\in s} U_j \ \text{unbounded}}} \mathsf{g}_s (\partial^*\beta)_s,$$

because when $\bigwedge_{j\in s} U_j$ is unbounded $(\partial^*\beta)_s = (\check{\delta}\beta)_s = 0$ where $\check{\delta}$ is the coboundary of $\check{C}^p(\hat{\mathfrak{U}}, \hat{W}; \mathbb{R})$. □

Remark 3.6.1. *The above lemma remains true if one replaces $\mathfrak{D}_{al}$ with $\mathfrak{D}_{al}\otimes A$ where A is any locally-finite graded vector space. Then the pairing $\langle \mathsf{f}, \beta\rangle$ takes values in the space of inner derivations $\mathfrak{d}_{al}$ (Definition 3.3.3) tensored with A.*

Remark 3.6.2. *The relation between ∂^* and $\check{\delta}$ is as follows. They are equal for $s \in I_{p+1}$ with $\bigwedge_{j\in s} U_j$ unbounded. For s with $\bigwedge_{j\in s} U_j$ bounded, $\bigcap_{j\in s} \hat{U}_j = \varnothing$ and $(\partial^*\beta)_s$ is in general nonzero whereas $(\check{\delta}\beta)_s = 0$. This discrepancy arises because the Grothendieck topology on the poset of spherical CS sets induced by the coherent topology on $\mathcal{CS}_n$ does not allow the empty cover of the empty set. It is this discrepancy that makes the evaluation of DGLA cycles on spherical CS cocycles non-trivial.*

If U, V are closed semilinear sets with a bounded meet then any derivation in $[\mathfrak{D}_{al}(U), \mathfrak{D}_{al}(V)]$ is inner and thus has a well-defined average in any state on $\mathscr{A}$. More generally, if A is a locally-finite supercommutative graded algebra and $\mathfrak{F} = \mathfrak{D}_{al} \otimes A$ or some sub-algebra thereof, any element of $[\mathfrak{F}(U), \mathfrak{F}(V)]$ for $U \wedge V$ bounded has a well-defined average in any state of $\mathscr{A}$. The average takes values in A. We will need the following more refined result:

Lemma 3.6.2. *Let U and V be closed semilinear sets such that $U \wedge V$ is bounded. Let A be a locally-finite supercommutative graded algebra and ψ be a state. Then* $\psi([\mathfrak{D}^{\psi}_{al}(U) \otimes A, \mathfrak{D}_{al}(V) \otimes A]) = 0$.

Proof. It suffices to consider the case $A = \mathbb{R}$. Let $\mathsf{F} \in \mathfrak{D}^{\psi}_{al}(U)$ and $\mathsf{G} \in \mathfrak{D}_{al}(V)$. Propositions 3.3.2 and 3.3.6 give

$$\psi([\mathsf{F}, \mathsf{G}]) = \sum_{X \cap Y \neq \varnothing} \psi([\mathsf{F}^X, \mathsf{G}^Y]) = \sum_{Y} \psi(\mathsf{F}(\mathsf{G}^Y)) = 0,$$

where the last equality is because F preserves ψ. □

In what follows we will apply Lemma 3.6.1 to the graded local Lie algebra $\mathfrak{D}^{\psi}_{al} \otimes A$ (see Remark 3.6.1). The evaluation of cycles of $C^{aug}_{\bullet}(\mathfrak{U}, W; \mathfrak{D}^{\psi}_{al} \otimes A)$ on spherical CS cocycles has especially nice properties when DGLA cycles belong to the commutator DGLA

$$\overline{\left[C^{aug}_{\bullet+1}\left(\mathfrak{U}, W; \mathfrak{D}^{\psi}_{al} \otimes A\right), C^{aug}_{\bullet+1}\left(\mathfrak{U}, W, \mathfrak{D}^{\psi}_{al} \otimes A\right)\right]}. \tag{3.24}$$

Proposition 3.6.3. *If a cycle* f *lies in the commutator DGLA (3.24), then* $\psi(\langle \mathsf{f}, \beta \rangle)$ *depends only on the cohomology class of* β *and the homology class of* f *in the DGLA (3.24).*

Proof. Suppose $\mathsf{f} \in C^{aug}_{p}(\mathfrak{U}, W; \mathfrak{D}^{\psi}_{al} \otimes A)$ and $\mathsf{f} = \partial \mathsf{g}$ for some g in the commutator DGLA. Then the vanishing of $\psi(\langle \mathsf{f}, \beta \rangle) \in A$ follows from the proof of Lemma 3.6.1 and Lemma 3.6.2. Thus it remains to show that $\psi(\langle \mathsf{f}, \check{\delta} b \rangle) = 0$ for any $b \in C^{p-1}(\mathfrak{U}, \hat{W})$ if f is a cycle of the commutator DGLA. Indeed, since $\langle \mathsf{f}, \partial^* b \rangle = \langle \partial \mathsf{f}, b \rangle = 0$, we have

$$\langle \mathsf{f}, \check{\delta} b \rangle = \sum_{\substack{s \in I_p, \text{ with} \\ \bigwedge_{j \in s} U_j \text{ unbounded}}} \mathsf{f}_s (\partial^* b)_s = - \sum_{\substack{s \in I_p, \text{ with} \\ \bigwedge_{j \in s} U_j \text{ bounded}}} \mathsf{f}_s (\partial^* b)_s,$$

and the ψ-average of each term in the latter sum vanishes by Lemma 3.6.2. □

The evaluations of cycles of the commutator DGLA on spherical CS cocycles can be used to construct topological invariants of G-invariant gapped states on $\mathbb{R}^n$. We set $W = \mathbb{R}^n$. The cycle we use as an input is the commutator class of $C_{\bullet}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}^{\psi, \mathbf{G}}_{al})$ defined using the inhomogeneous Maurer-Cartan equation (Section 3.6). Since $\mathfrak{D}^{\psi, \mathbf{G}}_{al}$ is a sub-algebra of $\mathfrak{D}^{\psi}_{al} \otimes A$ with $A = \prod_{k=1}^{\infty} \mathrm{S}ym^k \mathfrak{g}^*[-2]$, Prop. 3.6.3 applies to such cycles.

Let $\mathfrak{U}$ be a CS cover of $\mathbb{R}^n$, and β be a spherical CS cocycle of $\hat{W} = S^{n-1}$ of degree l with respect to the cover $\hat{\mathfrak{U}}$. Let p be a Q-twisted MC element of $C^{aug}_{\bullet+1}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}^{\psi,\mathbf{G}}_{al})$. Evaluating $[\mathsf{p}, \mathsf{p}]$ on β and taking into account that the grading is shifted by 1 relative to the Čech grading, we get a G-invariant element of $\mathfrak{d}^{\psi}_{al} \otimes \mathrm{S}ym^k(\mathfrak{g}^*[-2])$ where $2k - 3 = l$. Since ψ is G-invariant, $\psi(\langle[\mathsf{p}, \mathsf{p}], \beta\rangle)$ is a G-invariant element of $\mathrm{S}ym^k(\mathfrak{g}^*[-2])$. Equivalently, it is the value of a degree 3 linear function on cocycles of $\check{C}^{\bullet}(\hat{\mathfrak{U}}, \mathbb{R})$ valued in $\mathrm{S}ym^{\bullet}\mathfrak{g}^*[2]$.

Theorem 3.6.1. *The function $\beta \mapsto \psi(\langle[\mathsf{p}, \mathsf{p}], \beta\rangle)$ depends only on ψ and the class of $(\mathfrak{U}, \beta)$ in the CS cohomology of S^{n-1}.*

Proof. For a fixed covering $\mathfrak{U}$, Prop. 3.6.1 and 3.6.3 implies $\psi(\langle[\mathsf{p}, \mathsf{p}], \beta\rangle)$ is independent of p. It depends on β solely through its cohomology class. It remains to show invariance under refinement of cover.

Let $(\mathfrak{V}, \phi)$ be a refinement of $\mathfrak{U}$ with $V_j \subset U_{\phi(j)}$. Cocycles $(\mathfrak{U}, \beta)$ and $(\mathfrak{V}, \phi^*\beta)$, where $(\phi^*\beta)_{j_0,\ldots,j_k} = \beta_{\phi(j_0),\ldots,\phi(j_k)}$, are in the same CS cohomology class. From Prop.3.6.1 there exists Q-twisted MC element p for the cover $\mathfrak{V}$. Prop.3.6.2 then implies that $\phi_*\mathsf{p}$ is a Q-twisted MC element p for the cover $\mathfrak{U}$. An easy expansion shows

$$\langle[\phi_*\mathsf{p}, \phi_*\mathsf{p}], \beta\rangle = \langle[\mathsf{p}, \mathsf{p}], \phi^*\beta\rangle.$$

Since any Q-twisted MC element gives the same answer, we have shown that this contraction of interest depends only on the CS cohomology class of $(\mathfrak{U}, \beta)$.

□

By Proposition 3.4.7, the cohomology group $H^l_{CS}(S^{n-1}, \mathbb{R})$ is one-dimensioal for $l = n - 1$ and vanishes otherwise. It is natural to take the class of $(\mathfrak{U}, \beta)$ to be a generator of $H^{n-1}_{CS}(S^{n-1}, \mathbb{Z})$. This generator is uniquely defined once an orientation of $\mathbb{R}^{n-1}$ has been chosen. Thus for any even n we obtain an invariant of gapped G-invariant states on $\mathbb{R}^n$ taking values in G-invariant polynomials on $\mathfrak{g}$ of degree $(n + 2)/2$, and this invariant changes sign when the orientation of $\mathbb{R}^n$ is changed. This is in agreement with Chern-Simons field theory.

The Hall conductance

For physics applications, the most important case is $G = U(1)$ and $n = 2$. Let us specialize the construction of topological invariants to this case.

Let ψ be a $U(1)$-invariant gapped state of a lattice system on $\mathbb{R}^n$. The generator of the $U(1)$ action is $\mathsf{Q} \in \mathfrak{D}_{al}^{\psi}(\mathbb{R}^n)$. Let $\mathfrak{D}_{al}^{\psi,\mathsf{Q}}$ be the sub-algebra of $U(1)$-invariant elements of $\mathfrak{D}_{al}^{\psi}$. Since $U(1)$ is connected, this the same as the sub-algebra of elements of $\mathfrak{D}_{al}$ which commute with Q. More generally, for any $U \in \mathcal{CS}_n$ $\mathfrak{D}_{al}^{\psi,\mathsf{Q}}(U) = \mathfrak{D}_{al}(U) \cap \mathfrak{D}_{al}^{\psi,\mathsf{Q}}$. This is a local Lie algebra over $\mathcal{CS}_n$. The graded local Lie algebra $\mathfrak{D}_{al}^{\psi,\mathbf{G}}$ reduces in this case to $\mathfrak{D}_{al}^{\psi,\mathsf{Q}} \otimes \mathbb{R}[[t]]$ where t is a variable of degree -2.

Pick a cover $\mathfrak{U} = \{U_i\}_{i \in I}$ of $\mathbb{R}^n$. To find a solution p of the inhomogenenous Maurer-Cartan equation with $\mathsf{B} = \mathsf{Q} \otimes t$, we write $\mathsf{p} = \sum_{k=1}^{\infty} \mathsf{p}_k \otimes t^k$, where $\mathsf{p}_k \in C_{k-1}(\mathfrak{U}, \mathbb{R}^n; \mathfrak{D}_{al}^{\psi,\mathsf{Q}})$. To compute the topological invariant of a state on $\mathbb{R}^2$ it is sufficient to solve for p_1.

p_1 is a solution of $\partial \mathsf{p}_1 = \mathsf{Q}$. Explicitly, $\mathsf{p}_1 = \{\mathsf{Q}_i \in \mathfrak{D}_{al}^{\psi,\mathsf{Q}}(U_i)\}_{i \in I}$ such that $\sum_{i \in I} \mathsf{Q}_i = \mathsf{Q}$. Such Q_i exist because $\mathfrak{D}_{al}^{\psi,\mathsf{Q}}$ is a cosheaf. Then the component of the commutator class in $C_1(U, \mathbb{R}^n; \mathfrak{D}_{al}^{\psi,\mathsf{Q}})$ is $\{[\mathsf{Q}_i, \mathsf{Q}_j]\}_{i<j}$. The topological invariant of the state ψ is obtained by evaluating it on a Čech 1-cocycle β on S^1 corresponding to the cover $\hat{\mathfrak{U}}$ and then averaging the resulting inner derivation:

$$\sigma(\beta) = \psi\left(\sum_{i<j} \beta_{ij} [\mathsf{Q}_i, \mathsf{Q}_j]\right).$$

Note that averaging over ψ must be performed after the summation over i, j because $[\mathsf{Q}_i, \mathsf{Q}_j]$ is not an inner derivation, in general.

The simplest CS cover of $\mathbb{R}^2$ which can represent a nontrivial class in $H^1_{CS}(S^1, \mathbb{R})$ is made of three cones with a common vertex. In this case the construction of the invariant reduces to that in [KS20; KS22]. It was shown there that the resulting invariant is proportional to the zero-temperature Hall conductance as determined by the Kubo formula.

Topological invariants of gapped states on subsets of $\mathbb{R}^n$

So far we assumed that Λ is an arbitrary countable subset of $\mathbb{R}^n$ with a uniform $O(r^n)$ bound on the number of points in a ball of radius r. Suppose $\Lambda \subset W^{\epsilon}$ for some CS set W and some $\epsilon > 0$. If this is the case, we will say the pair $(\Lambda, \{V_j\}_{j \in \Lambda})$ describes a quantum lattice system on W. Then for any $\mathsf{F} \in \mathfrak{D}_{al}$ the component F^X vanishes for any brick X which does not intersect $W^{\epsilon} \cap \Lambda$, and thus for any $U \in \mathcal{CS}_n$ we have $\mathfrak{D}_{al}(U) = \mathfrak{D}_{al}(U \wedge W)$ and

$\mathfrak{D}^{\psi}_{al}(U) = \mathfrak{D}^{\psi}_{al}(U \wedge W)$. Thus the assignment $U \mapsto \mathfrak{D}^{\psi}_{al}(U)$ can be regarded as a local Lie algebra over the site $\mathcal{CS}_n/W$.

In particular, if a compact Lie group G acts locally on the quantum lattice system on W and preserves a gapped state ψ, the generator of the action $\mathsf{Q} : \mathfrak{g} \to \mathfrak{D}^{\psi}_{al}$ takes values in the sub-algebra $\mathfrak{D}^{\psi}_{al}(W)$. Consequently $\mathfrak{D}^{\psi,\mathbf{G}}_{al}$ is a graded local Fréchet-Lie algebra over $\mathcal{CS}_n/W$ pointed by $\mathsf{Q} \in \mathfrak{D}^{\psi,\mathbf{G}}_{al}(W)$. Picking a cover $\mathfrak{U}$ of W and applying the Čech functor gives an acyclic pointed DGLA whose commutator class can be evaluated on any CS cocycle β of $\hat{W}$ to give an inner derivation. Its ψ-average is a G-invariant polynomial on $\mathfrak{g}$ which depends only on the class of $(\mathfrak{U}, \beta)$ in $H^\bullet(\hat{W}, \mathbb{R})$. Thus a quantum lattice system on W has a topological invariant which is a linear function of $H^\bullet(\hat{W}, \mathbb{R}) \to \mathrm{S}ym^\bullet \mathfrak{g}^*[2]$. It is easy to check that this linear function has degree 3.

For example, consider a $U(1)$-invariant gapped state of a quantum lattice system on $W = \mathbb{R}^2$ affinely embedded in $\mathbb{R}^3$. The topological invariant defined in Section 3.6 is obtained by contracting with a 2-cocycle of S^2 (the sphere at infinity) and vanishes for dimensional reasons. On the other hand, by contracting with the 1-cocycle of $\hat{W} = S^1$ one obtains the Hall conductance of this system.

For a more non-trivial example, for any $n > 2$ consider a finite graph $\Gamma \subset S^{n-1}$ whose edges are geodesics and take W to be the cone with base Γ and apex at an arbitrary point of $\mathbb{R}^n$. The invariants of $U(1)$-invariant gapped states of quantum lattice systems on $W \subset \mathbb{R}^n$ are labeled by generators of the free abelian group $H^1(\Gamma, \mathbb{Z})$. This example goes beyond TQFT since W need not be smooth or even locally Euclidean.

3.7 0-chains

In this section we use the results of [KS22] to derive the properties of LGAs which we used in Section 3.3.

0-chains on $\mathbb{Z}^n$

First let us characterize $\mathfrak{D}_{al}(U)$ in terms of 0-chains. A 0-chain on $\mathbb{Z}^n$ is an element $\mathsf{a} = \{\mathsf{a}_j\}_{j\in\mathbb{Z}^n} \in \prod_{j\in\mathbb{Z}^n} \mathfrak{D}_{al}(\{j\})$ such that

$$\|\mathsf{a}\|_k := \sup_{j\in\mathbb{Z}^n} \|\mathsf{a}_j\|_{\{j\},k} < \infty. \tag{3.25}$$

We say a 0-chain a is supported on U if $\mathsf{a}_i = 0$ whenever $i \notin U$, and write $C_0(U)$ for the set of U-supported 0-chains, endowed with the norms (3.25) for $k \geq 0$.

Proposition 3.7.1. *Let $U \subset \mathbb{R}^n$ be nonempty and let $U^1 := \{x \in \mathbb{R}^n : d(x,U) \leq 1\}$ be its 1-thickening.*

i) If $\mathsf{F} \in \mathfrak{D}_{al}(U)$ then $\mathsf{F} = \partial\mathsf{f}$ for a U^1-supported 0-chain f with $\|\mathsf{f}\|_k \leq 2^k\|\mathsf{F}\|_{U,k}$

ii) If $\mathsf{f} \in C_0(U)$, then for any $Y \in \mathbb{B}_n$ the sum

$$(\partial\mathsf{f})^Y := \sum_{j \in \mathbb{Z}^n \cap U} \mathsf{f}_j^Y$$

is absolutely convergent and defines a map $\partial : C_0(U) \to \mathfrak{D}_{al}(U)$ with $\|\partial\mathsf{f}\|_{U,k} \leq C\|\mathsf{f}\|_{k+2n+1}$, where the constant $C > 0$ depends only on n.

Lemma 3.7.1. *For any nonempty $U, Y \subset \mathbb{R}^n$ we have*

$$1 + d(Y, U^1 \cap \mathbb{Z}^n) + \operatorname{diam}(Y) \leq 2(1 + d(Y,U) + \operatorname{diam}(Y)).$$

Proof. Choose $y \in Y$ and $u \in U$ with $d(y,u) = d(Y,U)$, and choose $z \in \mathbb{Z}^n$ with $d(u,z) \leq 1$. Then since $z \in U^1 \cap \mathbb{Z}^n$ we have

$$\begin{aligned} d(Y, U^1 \cap \mathbb{Z}^n) &\leq \operatorname{diam}(Y) + d(y,z) \\ &\leq \operatorname{diam}(Y) + d(y,u) + d(u,z) \\ &\leq \operatorname{diam}(Y) + d(Y,U) + 1, \end{aligned}$$

and the Lemma follows. □

Proof of Proposition 3.7.1. i). Suppose $\mathsf{F} \in \mathfrak{D}_{al}(U)$. Choose any total order on $U^1 \cap \mathbb{Z}^n$ and for every $Y \in \mathbb{B}_n$ let $j^*(Y)$ be the closest point to Y in $U^1 \cap \mathbb{Z}^n$, using the total order as a tiebreaker. For every $i \in \Lambda$, define

$$\mathsf{f}_i := \sum_{\substack{Y \in \mathbb{B}_n \\ j^*(Y) = i}} \mathsf{F}^Y. \tag{3.26}$$

Then either $\mathsf{f}_i^Y = 0$ or $d(Y, U^1 \cap \mathbb{Z}^n) = d(Y,j)$ and $\|\mathsf{f}_i^Y\| = \|\mathsf{F}^Y\|$, and so

$$\begin{aligned} \|\mathsf{f}_i\|_k &= \sup_{Y \in \mathbb{B}_n \setminus \{\varnothing\}} (1 + \operatorname{diam}(Y) + d(Y,\{i\})^k \|\mathsf{f}_i^Y\| \\ &= \sup_{Y \in \mathbb{B}_n \setminus \{\varnothing\}} (1 + \operatorname{diam}(Y) + d(Y, U^1 \cap \mathbb{Z}^1))^k \|\mathsf{F}^Y\|, \end{aligned}$$

which by Lemma 3.7.1 is bounded by $2^k\|\mathsf{F}\|_{U,k}$.

ii). Suppose that f is a U-supported 0-chain. For any $k \geq 0$ we have

$$\begin{aligned}
\|\partial \mathsf{f}^Y\| &\leq \sum_{j\in\mathbb{Z}^n\cap U} \|\mathsf{f}_j^Y\| \\
&\leq \|\mathsf{f}\|_{k+2n+1} \sum_{j\in\mathbb{Z}^n\cap U} (1+\mathrm{diam}(Y)+d(j,Y))^{-k-2n-1} \\
&\leq \|\mathsf{f}\|_{k+2n+1}(1+\mathrm{diam}(Y)+d(U,Y))^{-k} \sum_{j\in\mathbb{Z}^n\cap U} (1+\mathrm{diam}(Y)+d(j,Y))^{-2n-1} \\
&\leq \|\mathsf{f}\|_{k+2n+1}(1+\mathrm{diam}(Y)+d(U,Y))^{-k}(1+\mathrm{diam}(Y))^{-n} \sum_{j\in\mathbb{Z}^n} (1+d(j,Y))^{-n-1} \\
&\leq \|\mathsf{f}\|_{k+2n+1}(1+\mathrm{diam}(Y)+d(U,Y))^{-k}(1+\mathrm{diam}(Y))^{-n} \sum_{j\in\mathbb{Z}^n} (1+d(j,Y))^{-n-1}.
\end{aligned}$$

It is not hard to show that for any brick Y the quantity $(1+\mathrm{diam}(Y))^{-n}\sum_{j\in\mathbb{Z}^n}(1+d(j,Y))^{-n-1}$ is bounded by a constant C depending only on n, which shows $\|\partial \mathsf{f}^Y\| \leq C\|\mathsf{f}\|_{k+2n+1}$. □

Proposition 3.7.1 will allow us to apply the results of [KS22] on 0-chains. The results in [KS22] are phrased in terms of the norms

$$\|\mathsf{a}\|_{x,k}^{KS} := \sup_{r>0}(1+r)^k \inf_{\mathsf{b}\in\mathfrak{d}(B_r(x))} \|\mathsf{a}-\mathsf{b}\|,$$

where $\mathfrak{d}(B_r(x))$ is the set of traceless anti-hermitian operators strictly localized on the ball of radius r around $x \in \mathbb{R}^n$. To apply their results we prove the equivalence of these norms:

Lemma 3.7.2. *For any $x \in \mathbb{Z}^n$ and $k > 0$, the norms $\|\cdot\|_{x,k}^{KS}$ and $\|\cdot\|_{\{x\},k}$ obey*

$$\|\mathsf{a}\|_{x,k}^{KS} \leq C\|\mathsf{a}\|_{\{x\},k+2n+2} \tag{3.27}$$

$$\|\mathsf{a}\|_{\{x\},k} \leq 8^k C'\|\mathsf{a}\|_{x,k}^{KS} \tag{3.28}$$

where C, C' are constants depending only on k.

Proof. Suppose $\|\mathsf{a}\|_{\{x\},k+2n+1} < \infty$ and let $r > 0$. Define $\mathsf{b} := \sum_{X\subset B_r(x)} \mathsf{a}^X$. Then

$$\|\mathsf{b}-\mathsf{a}\| \leq \|\mathsf{a}\|_{\{x\},k+2n+2} \sum_{X\not\subseteq B_r(x)} (1+\mathrm{diam}(X)+d(x,X))^{-k-2n-2}.$$

Since $X \nsubseteq B_r(x)$ means $\mathrm{diam}(X) + d(x,X) \geq r$, we continue this as follows:

$$\begin{aligned}
&\leq (1+r)^{-k} \|\mathsf{a}\|_{\{x\},k+2n+2} \sum_{X \nsubseteq B_r(x)} (1 + \mathrm{diam}(X) + d(x,X))^{-2n-2} \\
&\leq C(1+r)^{-k} \|\mathsf{a}\|_{\{x\},k+2n+2},
\end{aligned}$$

where in the last line we used Lemma 3.3.1. This proves (3.27). To prove (3.28) suppose $\|\mathsf{a}\|^{KS}_{x,k} < \infty$ and let X be any brick. Set $r := \lfloor (\mathrm{diam}(X) + d(x,X))/4 \rfloor$. Then $X \nsubseteq B_r(x)$. Indeed, if $X \subseteq B_r(x)$ then $d(x,X) \leq r$ and $\mathrm{diam}(X) \leq 2r$, implying $\mathrm{diam}(X) + d(x,X) \leq 3r$, which is impossible. Choose $\mathsf{b} \in \mathfrak{d}(B_r(x))$ with $\|\mathsf{a} - \mathsf{b}\| \leq (1+r)^{-k} \|\mathsf{a}\|^{KS}_{x,k}$. Since $X \nsubseteq B_r(x)$ we have $\mathsf{b}^X = 0$, and so

$$\begin{aligned}
\|\mathsf{a}^X\| &= \|(\mathsf{a} - \mathsf{b})^X\| \\
&\leq 4^n \|\mathsf{a} - \mathsf{b}\| \\
&\leq 4^n \|\mathsf{a}\|^{KS}_{x,k} (1+r)^{-k} \\
&\leq 4^{n+2k} \|\mathsf{a}\|^{KS}_{x,k} (1 + \mathrm{diam}(X) + d(x,X))^{-k},
\end{aligned}$$

where in the second line we used [KS22, Proposition C.1]. □

Proof of Lemma 3.3.7

We begin by describing the construction of $\mathcal{J}$ and $\mathcal{K}$. Suppose ψ is gapped with Hamiltonian H and gap Δ, and write τ_t for the one-parameter family of LGAs obtained by exponentiating H. There exists[12] a function $w_\Delta : \mathbb{R} \to \mathbb{R}$ such that $w_\Delta(t) = O(|t|^{-\infty})$, and the Fourier transform[13] $\widehat{w_\Delta}$ is supported in the interval $[-\Delta/2, \Delta/2]$ and satisfies $\widehat{w_\Delta}(0) = 1$. Let W_Δ be the odd function which on the positive real line is given by $W_\Delta(|t|) = -\int_{|t|}^\infty w_\Delta(u) du$. Then we define $\mathcal{F}$ and $\mathcal{G}$ as the following integral transforms:

$$\begin{aligned}
\mathcal{J}(\mathsf{F}) &:= \int w_\Delta(t) \tau_t(\mathsf{F}) dt, \\
\mathcal{K}(\mathsf{F}) &:= \int W_\Delta(t) \tau_t(\mathsf{F}) dt.
\end{aligned}$$

Proof of Lemma 3.3.7. $\mathcal{J}$ and $\mathcal{K}$ correspond to $\mathscr{I}_{\mathsf{H}, w_\Delta}$ and $\mathscr{I}_{\mathsf{H}, W_\Delta}$ in Section 4.1 of [KS22]. Part *i)* follows from the definition of $\mathcal{K}$ and the fact that H preserves ψ. Part *ii)* follows from Proposition 3.7.1 and Lemma 3.7.2, together with [KS22, Lemma F.1] (specifically line (177) therein). Part *iii)* is [KS22, line (72)]. □

[12]See for instance Lemma 2.3 in [BBR24].

[13]We use the convention $\widehat{f}(\xi) = \int f(t) e^{-i\omega t} dt$.

3.8 Inhomogeneous Maurer-Cartan equation

Let $(\mathfrak{M}, \mathsf{B})$ be a pointed pronilpotent DLGA which is a limit of an inverse system of nilpotent pointed DGLAs $(\mathfrak{M}_N, \mathsf{B}_N)$, $N \in \mathbb{N}$. The set $\mathrm{M}C(\mathfrak{M}, \mathsf{B})$ of B-twisted MC elements has an additional equivalence relation. This section revolves around this additional structure leading eventually to a proof of Prop. 3.6.1.

We have morphisms $r_{N,K} : \mathfrak{M}_N \to \mathfrak{M}_K$ for all $N > K$ and the DGLA $\mathfrak{M}$ is the inverse limit of the corresponding system of DGLAs. For any $N \in \mathbb{N}$ let $r_N : \mathfrak{M} \to \mathfrak{M}_N$ be the natural projection. Let $\mathsf{j}_N = \ker r_{N,N-1}$. The sets of B_N-twisted MC elements of $\mathfrak{M}_N$ will be denoted $\mathrm{M}C(\mathfrak{M}_N, \mathsf{B}_N)$.

A B-twisted MC element p gives rise to a degree -1 derivation $\partial_{\mathsf{p}} = \partial + \mathrm{a}d_{\mathsf{p}}$ of $\mathfrak{M}$ which squares to zero (twisted differential).

Lemma 3.8.1. *If $\mathsf{p} \in MC(\mathfrak{M}_N, \mathsf{B}_N)$, then $r_{N,K}(\mathsf{p}) \in MC(\mathfrak{M}_K, \mathsf{B}_K)$ for all $K < N$. Further, $\mathsf{p} \in MC(\mathfrak{M}, \mathsf{B})$ iff $\mathsf{p}^N = r_N(\mathsf{p}) \in MC(\mathfrak{M}_N, \mathsf{B}_N)$ $\forall N \in \mathbb{N}$.*

Proof. Straightforward. □

Thus $\mathrm{M}C(\mathfrak{M}, \mathsf{B})$ is the inverse limit of the system of sets $\mathrm{M}C(\mathfrak{M}_N, \mathsf{B}_N)$, $N \in \mathbb{N}$.

We are going to define an equivalence relations on $\mathrm{M}C(\mathfrak{M}, \mathsf{B})$ and $\mathrm{M}C(\mathfrak{M}_N, \mathsf{B}_N)$ for all N. This is done in the same way as for the ordinary (homogeneous) Maurer-Cartan equation [GM88; Man22].

First, $\mathfrak{M}_{N,0}$ is a nilpotent Lie algebra, so there is a well-defined nilpotent Lie group $\exp(\mathfrak{M}_{N,0})$ with the group law given by the Campbell-Baker-Hausdorff formula. Similarly, $\mathfrak{M}_0$ is pronilpotent (i.e. is an inverse limit of a system of nilpotent Lie algebras), so the CBH formula defines a group $\exp(\mathfrak{M}_0)$.

Second, there are Lie algebra homomorphisms from $\mathfrak{M}_0$ (resp. $\mathfrak{M}_{N,0}$) to the Lie algebras of affine-linear vector fields on $\mathfrak{M}_{-1}$ (resp. $\mathfrak{M}_{N,-1}$). This homomorphism maps $\mathsf{a} \in \mathfrak{M}_0$ or $\mathfrak{M}_{N,0}$ to the affine-linear vector field

$$\xi_{\mathsf{a}}(\mathsf{p}) = [\mathsf{a}, \mathsf{p}] - \partial \mathsf{a},$$

where $\mathsf{p} \in \mathfrak{M}_{-1}$ or $\mathfrak{M}_{N,-1}$. Here we used the identification of the space of affine-linear vector fields on a vector space V with the space of affine-linear maps $V \to V$. These homomorphisms exponentiate to actions of the groups

$\exp(\mathfrak{M}_0)$ and $\exp(\mathfrak{M}_{N,0})$ on $\mathfrak{M}_{-1}$ and $\mathfrak{M}_{N,-1}$ by affine-linear transformations. Explicitly, the actions are given by [GM88; Man22]:

$$\mathsf{p} \mapsto \exp(\mathsf{a}) * \mathsf{p} = \exp(\mathrm{ad}_{\mathsf{a}})(\mathsf{p}) + \frac{1 - \exp(\mathrm{ad}_{\mathsf{a}})}{\mathrm{ad}_{\mathsf{a}}}(\partial \mathsf{a}). \tag{3.29}$$

Lemma 3.8.2. *The actions of* $\exp(\mathfrak{M}_0)$ *on* $\mathfrak{M}_{-1}$ *(resp.* $\exp(\mathfrak{M}_{N,0})$ *on* $\mathfrak{M}_{N,-1}$*) preserve the sets* $MC(\mathfrak{M}, \mathsf{B})$ *(resp.* $MC(\mathfrak{M}_N, \mathsf{B}_N)$*).*

Proof. The proof in [GM88], Section 1.3, applies just as well in the inhomogeneous case. ☐

We say that elements p_1, p_2 of $MC(\mathfrak{M}, \mathsf{B})$ or $MC(\mathfrak{M}_N, \mathsf{B}_N)$ are equivalent if they belong to the same orbit of these actions.

Remark 3.8.1. *By analogy with the homogeneous case, one can define a* B*-twisted Deligne groupoid as the transformation groupoid for the action of* $\exp(\mathfrak{M}_0)$ *on* $MC(\mathfrak{M}, \mathsf{B})$*. Similarly, one can define "reduced" Deligne groupoids for every* $N \in \mathbb{N}$*.*

We observe an easy but useful lemma.

Lemma 3.8.3. *If* $\mathsf{p}_i \in MC(\mathfrak{M}_N, \mathsf{B}_N)$*,* $i = 1, 2$*, are equivalent, then* $r_{N,K}(\mathsf{p}_1)$ *is equivalent to* $r_{N,K}(\mathsf{p}_2)$ *for all* $K < N$*.*

Now come the interesting statements. Assume from now on that the DGLAs $\mathfrak{M}_N$ and $\mathfrak{M}$ are acyclic, that $\mathsf{j}_N \subset \mathfrak{M}_N$ is central for all $N > 1$, and that the morphisms $r_{N,N-1}$ are surjective for all $N > 1$.

Lemma 3.8.4. *With the above assumptions, the set* $MC(\mathfrak{M}, \mathsf{B})$ *is non-empty if and only if* $MC(\mathfrak{M}_1, \mathsf{B}_1)$ *is non-empty.*

Proof. The only if statement follows from Lemma 3.8.1. To prove the if direction, we use induction on N. Assume $MC(\mathfrak{M}_{N-1}, \mathsf{B}_{N-1})$ is non-empty. Let $\mathsf{p}_{N-1} \in MC(\mathfrak{M}_{N-1}, \mathsf{B}_{N-1})$. Pick $\tilde{\mathsf{p}}_N \in r^{-1}_{N,N-1}(\mathsf{p}_{N-1})$. Since p_{N-1} is a B_{N-1}-twisted MC element and $r_{N,N-1}(\mathsf{B}_N) = \mathsf{B}_{N-1}$, we must have

$$\partial \tilde{\mathsf{p}}_N + \frac{1}{2}[\tilde{\mathsf{p}}_N, \tilde{\mathsf{p}}_N] = \mathsf{B}_N + \mathsf{q}_N$$

for some $\mathsf{q}_N \in \mathsf{j}_N$. We look for a solution of the B_N-twisted MC equation of the form $\mathsf{p}_N = \tilde{\mathsf{p}}_N + \mathsf{b}_N$ where $\mathsf{b}_N \in \mathsf{j}_N$. Taking into account that j_N is central, the inhomogeneous MC equation reduces to $\partial \mathsf{b}_N = -\mathsf{q}_N$. Since by assumption $\mathsf{j}_N, \mathfrak{M}_N$, and $\mathfrak{M}_{N-1}$ form a short exact sequence and the latter two are acyclic, so is j_N. Hence such a b_N exists. This completes the inductive step proving that $\mathrm{M}C(\mathfrak{M}_N, \mathsf{B}_N) \neq \varnothing$ for all N. Moreover, we also proved that the morphisms $\mathrm{M}C(\mathfrak{M}_N, \mathsf{B}_N) \to \mathrm{M}C(\mathfrak{M}_{N-1}, \mathsf{B}_{N-1})$ are surjective. Therefore by Lemma 3.8.1 $\mathrm{M}C(\mathfrak{M}, \mathsf{B})$ is non-empty. □

The above lemma proves the first part of Prop. 3.6.1. Indeed when $[\mathfrak{M}_1, \mathfrak{M}_1] = 0$, $\mathrm{M}C(\mathfrak{M}_1, \mathsf{B}_1) \neq \varnothing$ is implied by acyclicity. Next we show that with the above assumption on $\mathfrak{M}_N$ and $\mathfrak{M}$ all B-twisted MC elements are equivalent.

Lemma 3.8.5. *Suppose* $\mathsf{a}, \mathsf{b} \in \mathfrak{M}_{N,0}$ *and* $\mathsf{a} \in \mathsf{j}_N$. *Then for any* $\mathsf{p} \in \mathfrak{M}_{N,-1}$ *one has*

$$\exp(\mathsf{b} + \mathsf{a})(\mathsf{p}) = \exp(\mathsf{b})(\mathsf{p}) - \partial \mathsf{a}.$$

Proof. See [GM88], Lemma 2.8. □

Lemma 3.8.6. *Let* $\mathsf{p}_i \in MC(\mathfrak{M}_N, \mathsf{B}_N)$, $i = 1, 2$ *such that* $r_{N,N-1}(\mathsf{p}_1) = r_{N,N-1}(\mathsf{p}_2)$. *Then* p_1 *and* p_2 *are equivalent.*

Proof. Let $\mathsf{q} = \mathsf{p}_2 - \mathsf{p}_1 \in \mathfrak{M}_{N,-1}$. By assumption, $\mathsf{q} \in \mathsf{j}_N$. Moreover, $\partial \mathsf{q} = 0$. Indeed,

$$\partial \mathsf{q} = \frac{1}{2}[\mathsf{p}_2, \mathsf{p}_2] - \frac{1}{2}[\mathsf{p}_1, \mathsf{p}_1] = [\mathsf{q}, \mathsf{p}_1] + \frac{1}{2}[\mathsf{q}, \mathsf{q}] = 0.$$

By acyclicity of j_N, we have $\mathsf{q} = \partial \mathsf{a}$ for some $\mathsf{a} \in \mathsf{j}_{N,0}$. Then Lemma 3.8.5 implies that $\exp(\mathsf{a}) \in \exp(\mathfrak{M}_{N,0})$ maps p_2 to p_1. □

Lemma 3.8.7. *Let* $\tilde{\mathsf{p}}_i \in MC(\mathfrak{M}_N, \mathsf{B}_N)$, $i = 1, 2$, *be such that* $\mathsf{p}_1 = r_{N,N-1}(\tilde{\mathsf{p}}_1)$ *and* $\mathsf{p}_2 = r_{N,N-1}(\tilde{\mathsf{p}}_2)$ *are equivalent. Then* $\tilde{\mathsf{p}}_1$ *and* $\tilde{\mathsf{p}}_2$ *are equivalent.*

Proof. Let $\mathsf{a} \in \mathfrak{M}_{N-1,0}$ be an equivalence between p_1 and p_2, i.e. $\exp(\mathsf{a}) * \mathsf{p}_2 = \mathsf{p}_1$. Let $\tilde{\mathsf{a}} \in \mathfrak{M}_{N,0}$ be any lift of a. Then $r_{N,N-1}(\exp(\tilde{\mathsf{a}}) * \tilde{\mathsf{p}}_2) = r_{N,N-1}(\tilde{\mathsf{p}}_1)$. By Lemma 3.8.6, $\exp(\tilde{\mathsf{a}}) * \tilde{\mathsf{p}}_2$ is equivalent to $\tilde{\mathsf{p}}_1$, therefore $\tilde{\mathsf{p}}_2$ is equivalent to $\tilde{\mathsf{p}}_1$. □

Proposition 3.8.1. *For any* $N \in \mathbb{N}$ *all elements of* $MC(\mathfrak{M}_N, \mathsf{B}_N)$ *are equivalent. All elements of* $MC(\mathfrak{M}, \mathsf{B})$ *are equivalent.*

The first statement is proved by induction on N, where the inductive step is Lemma 3.8.7. The second statement follows by passing to the inverse limit in N.

Theorem 3.8.1. *Let* $\mathsf{p} \in MC(\mathfrak{M}, \mathsf{B})$. *Then the homology class of* $[\mathsf{p}, \mathsf{p}]$ *in* $H_\bullet([\mathfrak{M}, \mathfrak{M}])$ *is independent of the choice of* p.

Proof. Let $\mathsf{p}, \mathsf{p}' \in \mathrm{M}C(\mathfrak{M}, \mathsf{B})$ and let $\mathsf{a} \in \mathfrak{M}_0$ be an equivalence between p and p'. Since p, p' satisfy the inhomogeneous Maurer-Cartan equation and B is a cycle, $[\mathsf{p}, \mathsf{p}]$ and $[\mathsf{p}', \mathsf{p}']$ are cycles as well. From (3.29) we have

$$\mathsf{p}' - \mathsf{p} = -\partial \mathsf{a} + \sum_{k=1}^{\infty} \frac{\mathrm{ad}_{\mathsf{a}}^k(\mathsf{p})}{k!} - \sum_{k=1}^{\infty} \frac{\mathrm{ad}_{\mathsf{a}}^k(\partial \mathsf{a})}{(k+1)!},$$

where

$$\mathsf{f} := \sum_{k=1}^{\infty} \frac{\mathrm{ad}_{\mathsf{a}}^k(\mathsf{p})}{k!} - \sum_{k=1}^{\infty} \frac{\mathrm{ad}_{\mathsf{a}}^k(\partial \mathsf{a})}{(k+1)!} \in \overline{[\mathfrak{M}, \mathfrak{M}]}.$$

Thus $[\mathsf{p}, \mathsf{p}] - [\mathsf{p}', \mathsf{p}'] = 2\partial(\mathsf{p}' - \mathsf{p}) = 2\partial \mathsf{f}$ is ∂-exact in $\overline{[\mathfrak{M}, \mathfrak{M}]}$. ☐

References

[AKS24] Adam Artymowicz, Anton Kapustin, and Nikita Sopenko. "Quantization of the Higher Berry Curvature and the Higher Thouless Pump". In: *Comm. Math. Phys.* 405.8 (2024), Paper No. 191.

[Bac+24] Sven Bachmann et al. "Tensor category describing anyons in the quantum Hall effect and quantization of conductance". In: *arXiv e-prints*, arXiv:2410.04736 (Oct. 2024), arXiv:2410.04736. DOI: `10.48550/arXiv.2410.04736`. arXiv: `2410.04736 [math-ph]`.

[Bau+23] Ulrich Bauer et al. "A unified view on the functorial nerve theorem and its variations". In: *Expositiones Mathematicae* 41.4 (2023), p. 125503.

[BBR24] Sven Bachmann, Alex Bols, and Mahsa Rahnama. "Many-body Fu-Kane-Mele index". In: *arXiv e-prints*, arXiv:2406.19463 (June 2024), arXiv:2406.19463. DOI: `10.48550/arXiv.2406.19463`. arXiv: `2406.19463 [math-ph]`.

[BO20] Chris Bourne and Yoshiko Ogata. "The classification of symmetry protected topological phases of one-dimensional fermion systems". In: *arXiv e-prints*, arXiv:2006.15232 (June 2020), arXiv:2006.15232. DOI: `10.48550/arXiv.2006.15232`. arXiv: `2006.15232 [math-ph]`.

[Bor48] Karol Borsuk. “On the imbedding of systems of compacta in simplicial complexes”. In: *Fundamenta Mathematicae* 35 (1948), pp. 217–234.

[BR87] Ola Bratteli and Derek W. Robinson. *Operator algebras and quantum statistical mechanics. 1. C^*- and W^*-algebras, symmetry groups, decomposition of states.* 2nd ed. Texts and Monographs in Physics. Springer-Verlag, New York, 1987.

[Bre68] Glen Bredon. “Cosheaves and homology”. In: *Pacific Journal of Mathematics* 25.1 (Apr. 1968), pp. 1–32.

[CLM14] J. Chuang, A. Lazarev, and Wajid Mannan. “Cocommutative coalgebras: homotopy theory and Koszul duality”. In: *arXiv e-prints*, arXiv:1403.0774 (Mar. 2014), arXiv:1403.0774. DOI: 10.48550/arXiv.1403.0774. arXiv: 1403.0774 [math.AT].

[Dri98] Lou van den Dries. *Tame topology and o-minimal structures.* Vol. 248. London Mathematical Society Lecture Note Series. Cambridge University Press, Cambridge, 1998.

[GM88] William M. Goldman and John J. Millson. “The deformation theory of representations of fundamental groups of compact Kähler manifolds”. In: *Inst. Hautes Études Sci. Publ. Math.* 67 (1988), pp. 43–96.

[GS16] Stéphane Guillermou and Pierre Schapira. “Construction of sheaves on the subanalytic site”. In: *Astérisque* 383 (2016), pp. 1–60.

[Has04] M. B. Hastings. “Lieb-Schultz-Mattis in higher dimensions”. In: *Physical Review B* 69.10, 104431 (2004), p. 104431.

[Kit06] Alexei Kitaev. “Anyons in an exactly solved model and beyond”. In: *Annals of Physics* 321.1 (2006), pp. 2–111.

[KS01] Masaki Kashiwara and Pierre Schapira. “Ind-sheaves”. In: *Astérisque* 271 (2001).

[KS20] Anton Kapustin and Nikita Sopenko. “Hall conductance and the statistics of flux insertions in gapped interacting lattice systems”. In: *J. Math. Phys.* 61.10 (2020), pp. 101901, 24.

[KS22] Anton Kapustin and Nikita Sopenko. “Local Noether theorem for quantum lattice systems and topological invariants of gapped states”. In: *Journal of Mathematical Physics* 63 (2022), p. 091903. DOI: 10.1063/5.0085964. arXiv: 2201.01327 [math-ph].

[KS24] Anton Kapustin and Nikita Sopenko. “Anomalous symmetries of quantum spin chains and a generalization of the Lieb-Schultz-Mattis theorem”. In: *arXiv e-prints*, arXiv:2401.02533 (Jan. 2024), arXiv:2401.02533. DOI: 10.48550/arXiv.2401.02533. arXiv: 2401.02533 [math-ph].

[KSY21] Anton Kapustin, Nikita Sopenko, and Bowen Yang. "A classification of invertible phases of bosonic quantum lattice systems in one dimension". In: *Journal of Mathematical Physics* 62.8 (2021), p. 081901.

[Ler45] Jean Leray. "Sur la forme des espaces topologiques et sur les points fixes des représentations". In: *Journal de Mathématiques Pures et Appliquées* 24 (1945), pp. 95–167.

[Man22] Marco Manetti. *Lie methods in deformation theory.* Springer Monographs in Mathematics. Springer, Singapore, 2022.

[MM94] Saunders Mac Lane and Ieke Moerdijk. *Sheaves in geometry and logic*. Universitext. A first introduction to topos theory, Corrected reprint of the 1992 edition. Springer-Verlag, New York, 1994.

[Oga19a] Yoshiko Ogata. "A $\mathbb{Z}_2$-index of symmetry protected topological phases with reflection symmetry for quantum spin chains". In: *arXiv e-prints*, arXiv:1904.01669 (Apr. 2019), arXiv:1904.01669. DOI: `10.48550/arXiv.1904.01669`. arXiv: `1904.01669 [math-ph]`.

[Oga19b] Yoshiko Ogata. "A Z_2-Index of Symmetry Protected Topological Phases with Time Reversal Symmetry for Quantum Spin Chains". In: *Communications in Mathematical Physics* 374.2 (2019), pp. 705–734.

[Oga21] Yoshiko Ogata. "A $H^3(G, \mathbb{T})$-valued index of symmetry protected topological phases with on-site finite group symmetry for two-dimensional quantum spin systems". In: *arXiv e-prints*, arXiv:2101.00426 (Jan. 2021), arXiv:2101.00426. DOI: `10.48550/arXiv.2101.00426`. arXiv: `2101.00426 [math-ph]`.

[Osb07] Tobias J Osborne. "Simulating adiabatic evolution of gapped spin systems". In: *Physical review A* 75.3 (2007), p. 032321.

[Pet] Fedor Petrov. *Bounding distance to an intersection of polyhedra.* MathOverflow. URL:https://mathoverflow.net/q/463857 (version: 2024-02-10).

[Roc70] R. Tyrrell Rockafellar. *Convex analysis*. Vol. No. 28. Princeton Mathematical Series. Princeton University Press, Princeton, NJ, 1970.

[Sop21] Nikita Sopenko. "An index for two-dimensional SPT states". In: *Journal of Mathematical Physics* 62.11 (2021), p. 111901.

[t H80] Gerard 't Hooft. "Naturalness, chiral symmetry, and spontaneous chiral symmetry breaking". In: *NATO Sci. Ser. B* 59 (1980). Ed. by Gerard 't Hooft et al., pp. 135–157.

Chapter 4

EFFICIENT HAMILTONIAN LEARNING FROM GIBBS STATES

This Chapter is available as a preprint at

[Art24] Adam Artymowicz. "Efficient Hamiltonian learning from Gibbs states". In: *arXiv e-prints*, arXiv:2403.18061 (Mar. 2024), arXiv:2403.18061. DOI: `10.48550/arXiv.2403.18061`. arXiv: `2403.18061 [quant-ph]`.

4.1 Introduction

In this work we consider the problem of learning a quantum Hamiltonian from its Gibbs state. Gibbs states are ubiquitous in quantum physics and represent systems in thermal equilibrium. They can be defined by a variational principle: they are the minimizers of free energy. This fact can in principle be used for Hamiltonian learning [SK14; Ans+21], but a naive implementation of this idea is impractical because the free energy is known to be classically exponentially difficult to compute [Mon15]. However, this does not preclude use of the variational principle in an efficient algorithm. Indeed, since the free energy is convex, the global variational principle is equivalent to a local one, which requires only knowledge of the derivatives of the free energy with respect to perturbations of the state. Linear response theory relates derivatives of free energy to locally measurable quantities, suggesting that they can be estimated without knowledge of the free energy itself. If such estimates can be made efficient, then the variational principle can be efficiently implemented.

The current work contains two main contributions. The first is a new lower bound on the entropy change due to a local perturbation of a quantum state (Theorem 4.2.1). We relate this to a hierarchy of semidefinite constraints known as the matrix EEB inequality [FFS] by showing that it is a relaxation of the free energy variational principle which can be enforced using polynomial classical resources.

Second, we use this to formulate a semidefinite algorithm for Hamiltonian learning. The algorithm either finds a local Hamiltonian respecting the matrix EEB inequality, or else it gives a proof that the given state is not a Gibbs state of any local Hamiltonian. We benchmark the algorithm by performing black-box learning of a nearest-neighbour Hamiltonian on 100 qubits from local expectation values with realistic levels of measurement noise.

These contributions are significant for several reasons. Hamiltonian learning is relevant in experimental settings [AA23]: near-term applications include studying frustrated systems by learning effective Hamiltonians [Sch+23] and probing entanglement properties of many-body states via their entanglement Hamiltonians [Dal+22]. For such applications, the problem of learning a Hamiltonian from local expectation values currently presents a practical bottleneck limiting the system sizes under consideration. Indeed, local expectation values of systems of $\sim$100 qubits can in many cases be obtained either numerically or using current NISQ technology. Meanwhile, practical algorithms for Hamiltonian learning that do not assume prior information or additional control over the state have so far achieved reliable learning only for systems of 10 or fewer qubits. The algorithm we propose in this work has the potential to remove this bottleneck.

The entropy lower bound in Theorem 4.2.1 is also of independent interest beyond Hamiltonian learning. For instance, efficient preparation of Gibbs states on a quantum computer remains an important open problem. A common approach is to thermalize an initial state using Lindbladian dynamics. The convergence speed can be related to the rate of change of free energy, which can be estimated using Theorem 4.2.1.

We begin in Section 4.2 by introducing the main entropy lower bound (Theorem 4.2.1) and the matrix EEB inequality (Corollary 4.2.1). Section 4.3 describes the semidefinite algorithm. In Section 4.4 we describe the results of numerical simulations on a 100-qubit spin chain. We conclude in Section 4.5 with a discussion of the results, and some future directions for research. This work additionally includes three appendices. In Section 4.6 we compare our algorithm to some existing approaches, with a focus on practical performance. In Section 4.7 we prove in detail the main theoretical results introduced in Section 4.2. Finally, Section 4.8 contains extra details about the numerical implementation described in Section 4.4.

The implementation of the learning algorithm used in this work is available for use at https://github.com/artymowicz/hamiltonian-learning

Aside from the learning algorithm itself, this repository also contains all routines used for performing the numerical tests in Section 4.4.

4.2 The lower bound on dS

In this section we begin by introducing Theorem 4.2.1 and derive the matrix EEB inequality as a consequence. We defer all proofs in this section to Section 4.7. Let $\mathcal{H}$ be the Hilbert space of a quantum system, and assume that $\dim \mathcal{H} < \infty$. Let $\mathcal{A}$ be the set of all operators on $\mathcal{A}$. As a rule, we will use lowercase letters to denote elements of $\mathcal{A}$. We will denote the adjoint of an operator a by a^*. We say a mixed state represented by a density matrix ρ is *faithful* if the matrix ρ is invertible. Let ρ be such a state.

We are interested in perturbations of ρ due to interactions with its environment. In the Lindblad formalism [Lin76; AL07] the evolution of the state ρ under open-system dynamics is given for $t \geq 0$ by

$$\rho_t = e^{tL}[\rho], \tag{4.1}$$

where L is the Lindbladian superoperator. Under the assumption that the environment is Markovian and interacts weakly with the system, L can be written in the form

$$L[\rho] := \sum_{i,j=1}^{r} \left\{ \frac{1}{2} \boldsymbol{M}_{ij} [a_j^* a_i, \rho] + \boldsymbol{\Lambda}_{ij} (a_i \rho a_j^* - \frac{1}{2} (a_j^* a_i \rho + \rho a_j^* a_i)) \right\}, \tag{4.2}$$

where $\boldsymbol{M}$ anti-Hermitian, $\boldsymbol{\Lambda}$ is positive-semidefinite, and $a_1, \ldots, a_r$ is a set of operators satisfying $\mathrm{tr}(\rho a_i^* a_j) = \delta_{ij}$ and $\mathrm{tr}(\rho a_i) = 0$ for all $i = 1, \ldots r$.

A straightforward calculation using the cyclic property of the trace yields the following expression for the first-order change in the expectation value of an observable under the evolution generated by the Lindbladian (4.2):

Lemma 4.2.1. *Let $h \in \mathcal{A}$ be selfadjoint and define the $r \times r$ matrix $\boldsymbol{H}_{ij} := \mathrm{tr}(\rho a_i^* [h, a_j])$. Then we have*

$$\left.\frac{d}{dt}\right|_{t=0} \mathrm{tr}(\rho_t h) = \mathrm{tr}(\boldsymbol{M}\boldsymbol{H}_-) + \mathrm{tr}(\boldsymbol{\Lambda}\boldsymbol{H}_+), \tag{4.3}$$

where $\boldsymbol{H}_\pm := (\boldsymbol{H} \pm \boldsymbol{H}^\dagger)/2$.

Notice that if $a_1, \dots, a_r$ and h are operators of bounded locality, then the expression (4.3) uses only expectation values of operators of bounded locality. One may ask if a similar expression exists for the first-order change in the von Neumann entropy $S(\rho) = -\operatorname{tr}(\rho \log \rho)$. In general, this cannot be expected, since entropy is not a local property of the state. However, instead of an exact expression, the following proposition bounds first-order change in entropy using only the correlations of the hopping operators:

Theorem 4.2.1. *We have*

$$\left.\frac{d}{dt}\right|_{t=0} S(\rho_t) \geq -\operatorname{tr}(\mathbf{\Lambda} \log \mathbf{\Delta}), \tag{4.4}$$

where the matrix $\mathbf{\Delta}$ *is defined as* $\mathbf{\Delta}_{ij} := \operatorname{tr}(\rho a_j a_i^*)$.

Let us remark on some ambiguities in the expression (4.2) and their effect on the above inequality. For a given Lindbladian L, the operators $a_1, \dots, a_r$ and the matrices $\boldsymbol{M}$ and $\mathbf{\Lambda}$ in (4.2) are not uniquely defined. Indeed, there are two ambiguities in their definition[1]:

1. Applying a change of basis $a_i' = \sum_{ij} Q_{ij} a_j$ that preserves the condition $\operatorname{tr}(\rho a_i^* a_j) = \delta_{ij}$ and applying the inverse change of basis to the matrices $\boldsymbol{M}$ and $\mathbf{\Lambda}$.
2. Appending additional operators $a_{r+1}, \dots, a_{r+q}$ to the list and setting all new matrix elements in $\boldsymbol{M}$ and $\mathbf{\Lambda}$ to zero.

While the first ambiguity does not change the right-hand side of (4.4), it turns out that the second ambiguity does. Indeed, adding operators to the list $a_1, \dots, a_r$ increases the right-hand side of (4.4). This can be seen as the result of the nonlinearity of the matrix logarithm $\log(\mathbf{\Delta})$. We summarize the above discussion as follows. Let $\mathcal{P} = \operatorname{span}\{a_1, \dots, a_r\} \subset \mathcal{A}$. Then the bound (4.4) depends only on L and $\mathcal{P}$. Growing $\mathcal{P}$ improves the bound, but requires knowledge of a larger number of correlations.

In the remainder of this section we describe one of the consequences of the bound (4.4). The free energy of a state ρ with respect to a Hamiltonian h and a temperature T is

$$F(\rho) := -TS(\rho) + \operatorname{tr}(\rho h). \tag{4.5}$$

[1] It is shown in Section 4.7 that these are the only ambiguities in the definition of $\mathbf{\Lambda}$.

Lemma 4.2.1 and Theorem 4.2.1 give an upper bound on the first-order change of free energy under the Lindbladian evolution generated by (4.2):

$$\left.\frac{d}{dt}\right|_{t=0} F(\rho_t) \leq \operatorname{tr}(\boldsymbol{M}\boldsymbol{H}_-) + \operatorname{tr}(\boldsymbol{\Lambda}(T \log \boldsymbol{\Delta} + \boldsymbol{H}_+)). \tag{4.6}$$

Given a Hamiltonian h and a temperature T, the Gibbs state $\rho := e^{-h/T} / \operatorname{tr}\left(e^{-h/T}\right)$ is the unique minimizer of the free energy. Let us call a Lindbladian L $\mathcal{P}$-*supported* if the operators $a_1, \ldots, a_r$ in the expression (4.2) can be chosen to lie in $\mathcal{P}$.

Corollary 4.2.1. *If ρ is the Gibbs state of a Hamiltonian h then*

$$T \log \boldsymbol{\Delta} + \boldsymbol{H} \succeq 0. \tag{4.7}$$

Moreover, if (4.7) fails, then there is a $\mathcal{P}$-supported Lindbladian that decreases the free energy of ρ with respect to h.

The inequality (4.7) is known as the matrix EEB inequality [FFS]. It is a hierarchy (depending on $\mathcal{P}$) of convex constraints that converges to the Hamiltonian of a Gibbs state.

4.3 Algorithm

In this section we apply the EEB inequality to the problem of learning the Hamiltonian of a Gibbs state. Given a set of selfadjoint traceless operators $h_1, \ldots, h_s$, we give an efficient algorithm that either finds a Hamiltonian in the span of $h_1, \ldots, h_s$ that satisfies the matrix EEB inequality, or else returns a Lindbladian that simultaneously rules out every h in the span of $h_1, \ldots, h_s$ by decreasing the free energy.

By adding a regularization parameter to the matrix EEB inequality and setting $T = 1$ we get the following linear semidefinite program:

$$\underset{\substack{h \in \operatorname{span}\{h_1, \ldots, h_s\} \\ \mu \in \mathbb{R}}}{\text{minimize}} \quad \mu \tag{4.8}$$

$$\text{subject to} \quad \log(\boldsymbol{\Delta}) + \boldsymbol{H} + \mu I \succeq 0, \tag{4.9}$$

As before, $\boldsymbol{\Delta}$ and $\boldsymbol{H}$ are defined as

$$\boldsymbol{\Delta}_{ij} := \operatorname{tr}(\rho a_j a_i^*), \tag{4.10}$$

$$\boldsymbol{H}_{ij} := \operatorname{tr}(\rho a_i^* [h, a_j]), \tag{4.11}$$

where $a_1, \ldots, a_r$ satisfy $\mathrm{tr}(\rho a_i^* a_j) = \delta_{ij}$ and $\mathrm{tr}(\rho a_i) = 0$. The convex dual of the above program reads:

$$\begin{aligned} \underset{\substack{\boldsymbol{\Lambda} \succeq 0 \\ \boldsymbol{M}^\dagger = -\boldsymbol{M}}}{\text{maximize}} \quad & -\mathrm{tr}(\boldsymbol{\Lambda} \log(\boldsymbol{\Delta})) & (4.12) \\ \text{subject to} \quad & \mathrm{tr}(\boldsymbol{M}\boldsymbol{H}_-) + \mathrm{tr}(\boldsymbol{\Lambda}\boldsymbol{H}_+) = 0, & (4.13) \\ & \mathrm{tr}(\boldsymbol{\Lambda}) = 1. & (4.14) \end{aligned}$$

In light of Lemma 4.2.1 and Theorem 4.2.1, the dual program seeks a $\mathcal{P}$-supported Lindbladian that maximizes dS/dt while preserving (to first order) the expectation values of the operators $h_1, \ldots, h_s$. Thus the dual program can be thought of as seeking the direction of steepest ascent for preparing the maximum-entropy state with prescribed expectation values of the operators $h_1, \ldots, h_s$.

A primal-dual pair is said to satisfy *Slater's condition* if the primal program has a strictly feasible point. Such a point can be found for (4.8) by setting $h = 0$ and taking μ sufficiently large. As a consequence, a standard result in convex optimization states that the optimal values of the primal and dual program coincide [BV04]. Thus we have:

Proposition 4.3.1. *Let μ, h be the optmizers of the primal program (4.8), and $\boldsymbol{M}, \boldsymbol{\Lambda}$ the optimizers of the dual program (4.12).*

1. *If $\mu \leq 0$, then h satisfies the matrix EEB inequality (4.7).*
2. *If $\mu > 0$ then the Lindbladian L corresponding to $\boldsymbol{M}$ and $\boldsymbol{\Lambda}$ increases the entropy of ρ while preserving $\mathrm{tr}(\rho h_\alpha)$ to first order for every $\alpha = 1, \ldots, s$.*

Thus, by running the primal-dual pair, we are guaranteed to get either a Hamiltonian h that satisfies the EEB inequality, or else get a $\mathcal{P}$-supported Lindbladian that a) acts as an interpretable guarantee that ρ is not the Gibbs state of any Hamiltonian in the search space, and b) is a heuristic for the best available Lindbladian for thermalizing the state ρ.

We conclude this section by discussing the computational complexity of the primal-dual pair. Interior-point methods produce solutions to the primal and dual problem whose objectives are within ϵ of the true optimum in $poly(r)\log(1/\epsilon)$ time, where r is the dimension of $\mathcal{P}$ [NN94]. In the remainder of the paper we will restrict our attention to a system of n spins on a lattice, where it is natural to choose an integer $k > 0$ and let $\mathcal{P}$ be the span of all k-local Pauli operators, and the variational Hamiltonian terms $h_1, \ldots, h_s$ to be the set of all k'-local Pauli operators. Here we mean k-local in the sense that the operator acts trivially outside a set of k *contiguous* qubits. With these choices we have $r = O(4^k n)$ and the algorithm requires $O(4^{k'+2k} n^2)$ expectation values of Paulis of weight at most $k + 2k$.

4.4 Numerical results

In this section, we describe a numerical implementation of the algorithm from Section 4.3, applied to the problem of learning a nearest-neighbour 100-qubit Hamiltonian from local expectation values of its Gibbs state. A variable amount of noise was added to the input of the algorithm. At zero noise, this acts as a test to how tightly the matrix EEB inequality constrains the set of possible Hamiltonians. At nonzero noise levels, this acts as a test of the number of independent samples of the state ρ required to accurately reconstruct the Hamiltonian.

Learning an XXZ Hamiltonian

The MPS purification technique [FW05] was used to prepare thermal states of the following anisotropic Heisenberg ferromagnet:

$$h_{XXZ} = -\sum_{i=1}^{n-1} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \frac{1}{2} \sigma_i^y \sigma_{i+1}^y), \tag{4.15}$$

with $n = 100$. Both the set of perturbing operators $b_1, \ldots, b_r$ and the set of variational Hamiltonian terms $h_1, \ldots, h_s$ were chosen to be the 1192 geometrically 2-local Pauli operators. Measurement error was simulated by adding Gaussian noise with variance σ_{noise} to the expectation value of each Pauli operator. The learning algorithm itself was implemented in Python, using the MOSEK solver [AA00] for the semidefinite optimization[2].

Hamiltonian recovery error was quantified using the overlap as in [QR19]: let $y \in \mathbb{R}^s$ be the vector of recovered Hamiltonian coefficients and $z \in \mathbb{R}^s$ the vector of true Hamiltonian coefficients. The Hamiltonian recovery error is then defined as the relative angle of the two, which for small angles approximately

[2] The convex modeling language CVXPy [DB16] and the open source solver SCS [ODo+16] were used in prototyping but not in the final code.

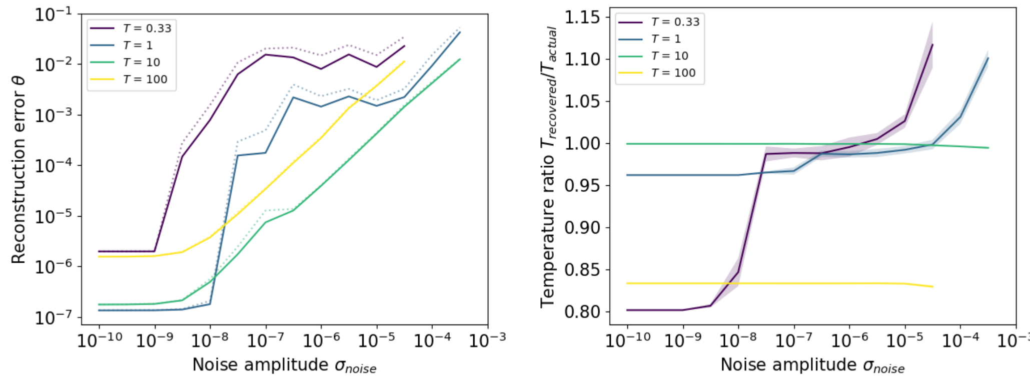

Figure 4.1: Numerical results for the 100-qubit anisotropic Heisenberg model (4.15) at several temperatures. Left: *Recovery error θ as a function of noise amplitude σ_{noise}, averaged over 10 runs. Dotted line is (mean) + (standard deviation).* Right: *Ratio of recovered temperature to actual temperature, averaged over 10 runs. Shaded region is (mean) $\pm$ (standard deviation).*

equals the reciprocal of the signal-to-noise ratio:

$$\theta = \arccos\left(\frac{|\langle y|z\rangle|}{\|y\|\|z\|}\right) \approx \frac{\|y-z\|}{\|z\|}. \tag{4.16}$$

Note that this metric is not sensitive to the overall scaling of the Hamiltonian. This degree of freedom is effectively the inverse temperature $1/T$. Interestingly, the algorithm reconstructed the “projective” degrees of freedom of the Hamiltonian terms much more accurately than it did its overall scale (or equivalently, the temperature).

The Hamiltonian recovery error θ and the recovered temperature T are plotted against σ_{noise} in Figure 4.1. A temperature-dependent noise threshold is found between $\sigma_{noise} \approx 10^{-5}$ and $\sigma_{noise} \approx 10^{-3}$ above which the matrix $\mathbf{\Delta}$ ceases to be positive definite — these are the right endpoints of the plots in Figure 4.1. The algorithm could possibly be emended to work for higher noise values by projecting onto the positive eigenspace of $\mathbf{\Delta}$, but we leave this to future work.

As one shrinks the noise amplitude, the recovery error first decreases (for high temperatures, this decrease is linear to a good approximation). This persists up until, at some temperature-dependent critical value of the noise amplitude, the recovery error plateaus. We interpret this two-stage behaviour as follows. In the limit of zero measurement error, perfect recovery is not guaranteed because the matrix EEB inequality (4.7) is weaker than the Gibbs condition. Instead, it defines a convex set of candidate Hamiltonians, and the algorithm picks one of these by maximizing the regularization parameter μ.

The recovery error is then on the order of the diameter of this convex set. Thus for low enough levels of measurement noise the recovery error is approximately noise-independent.

The only way to lower the levels of these plateaux is to enlarge $\mathcal{P}$, which tightens the matrix EEB constraint. This is relevant if one wants to prove asymptotic bounds on the number of copies of the state and the computational resources needed to specify the Hamiltonian up to an arbitrarily low error. Such results, however, do not necessarily have practical implications. Indeed, for the particular Hamiltonian under consideration, the plateaux start at noise amplitudes σ_{noise} of around 10^{-9} to 10^{-8}. Assuming that expectation values are estimated from independent copies of the state, this would require on the order of 10^{16} to 10^{18} samples, far beyond what is experimentally feasible anyway. So for practical applications it may be more important to understand the high-noise regime rather than the locations of the plateaux.

4.5 Outlook

Let us conclude by describing some directions for future research. While Proposition 4.7.3 establishes the correctness of the algorithm, it suffers from two important limitations which must be overcome if one is to prove sample complexity and computational complexity bounds. First, neither the feasibility nor the recoverability statements of Proposition 4.7.3 take into account measurement noise in the expectation values of the state, which is unavoidable whenever these are estimated using finitely many copies of the state. Second, the recoverability statement only holds when the set of perturbing operators is grown to a complete set of operators. The utility of this algorithm depends on approximate recoverability when the set of perturbing operators is far smaller than a complete set. Section 4.4 gives numerical evidence that this is indeed the case, but a proof is still lacking.

Acknowledgements

The author would like to thank Anton Kapustin, Hsin-Yuan (Robert) Huang, and Elliott Gesteau for helpful discussions and comments on the draft.

4.6 Comparison to other work

In this section we compare the Hamiltonian learning algorithm discussed in sections 4.3 and 4.4 to a few existing approaches, focusing on practical performance. We include only algorithms that learn from independent copies of an identical state ρ without assuming any other control over ρ. On the theoretical side, the recent series of works [Ans+21; HKT22; Bak+23] culminated with a proof by Bakshi et al. that this problem can be solved using polynomial classical resources [Bak+23]. However, their result is asymptotic and no implementation yet exists by which to assess its practical performance. Algorithms which have so far seen practical implementation either use exponential classical resources [Ans+21; Kok+21; Lif+21], or solve the more general problem of learning a Hamiltonian from a stationary state, which we show below is ill-posed in the setting of Gibbs states. Thus, so far a demonstration that the problem of learning a Hamiltonian from local expectations can reliably be solved in the noisy 100-qubit regime has been missing.

Local equilibrium criteria

On a theoretical level, the current work bears closest resemblance to the algorithm given by Bakshi et al in [Bak+23]. The *KMS condition* [BR97, Section 5.3] states that ρ is the Gibbs state of a Hamiltonian h at temperature $T = 1/\beta$ if and only if

$$\mathrm{tr}\left(\rho e^{-\beta H} a e^{\beta H} b\right) = \mathrm{tr}(\rho b a) \tag{4.17}$$

for all $a, b \in \mathcal{A}$. Another is the *EEB condition* [BR97, Theorem 5.3.15]: ρ is the Gibbs state of h at temperature $T = 1/\beta$ if and only if

$$\mathrm{tr}(\rho a^* a) \log\left(\frac{\mathrm{tr}(\rho a a^*)}{\mathrm{tr}(\rho a^* a)}\right) + \beta\, \mathrm{tr}(a^*[h, a]) \geq 0 \tag{4.18}$$

for all $a \in \mathcal{A}$. Both of these are local conditions in the sense that they can be checked for a subset of operators, yielding relaxations of the Gibbs condition. While the matrix EEB inequality used in the current work is a semidefinite relaxation of the EEB condition[FFS], the algorithm in [Bak+23] uses a sum-of-squares relaxation of the KMS condition.

Learning from steady states

The algorithms [BAL19] and [EHF19] learn a Hamiltonian from local expectation values of a steady state. This can be applied to a Gibbs state, since a Gibbs state is necessarily a steady state. Both these algorithms work by approximately enforcing the linear constraints

$$\mathrm{tr}(\rho[h, b_i]) = 0, \qquad i = 1, \ldots, m \tag{4.19}$$

for some choice of operators $b_1, \ldots, b_m$.

A constraint of this form can be seen to be implicit in the constraint used in the current algorithm. Indeed, by breaking the regularized EEB constraint

$$\log(\boldsymbol{\Delta}) + \boldsymbol{H} + \mu \mathbf{1} \succeq 0 \tag{4.20}$$

into its hermitean and anti-hermitean parts, (4.20) can be see to be equivalent to the pair of constraints

$$\boldsymbol{H}_- = 0 \tag{4.21}$$

$$\log(\boldsymbol{\Delta}) + \boldsymbol{H}_+ + \mu \mathbf{1} \succeq 0, \tag{4.22}$$

where $\boldsymbol{H}_\pm = (\boldsymbol{H} \pm \boldsymbol{H}^\dagger)/2$. It is not hard to check that $\boldsymbol{H}_- = 0$ if and only if

$$\mathrm{tr}(\rho[h, a_i^* a_j]) = 0 \text{ for all } 1 \leq i, j \leq r. \tag{4.23}$$

Let us remark on why the additional positive-semidefinite constraint is necessary. The linear constraint alone cannot recover h if the state ρ has any local symmetries other than the Hamiltonian. This happens, for instance, for Gibbs states of the XXZ model (4.15) considered in Section 4.4. A Gibbs state of h_{XXZ} at any temperature will commute with the generator $q := \sum_i \sigma_i^z$ of onsite z-rotations. This means that the linear constraint alone, and in general any algorithm that does not discriminate steady states from Gibbs states, cannot distinguish the Hamiltonians $h_{XXZ} + \lambda q$ for different values of the parameter λ.

Algorithms using loss functions

Several algorithms [Ans+21; Kok+21; Lif+21] work by minimizing a loss function which is intended to measure the discrepancy between the input state and the Gibbs state of a trial Hamiltonian. In [Ans+21] the loss function can be shown to equivalent to the relative entropy and requires computing the partition function of the trial Hamiltonian. In both [Kok+21] and [Lif+21], the loss function is a χ^2 statistic based on a random measurement scheme. In all three cases, the loss function requires exponential classical resources to compute, preventing these algorithms from being scaled beyond the ~ 10 qubit regime.

4.7 Proofs

In this section we prove the claims made in Section 4.2. First we prove a standard form for Markovian Lindbladians analogous to the GKSL standard form [GKS76; Lin76]. In what follows ρ will always refer to a faithful state.

Proposition 4.7.1 (Standard form for Lindbladians)**.** *Every Markovian Lindbladian can be written in the form*

$$L[\sigma] = \sum_{i,j=1}^{r} \left\{ \frac{1}{2}\boldsymbol{M}_{ij}[a_j^* a_i, \sigma] + \boldsymbol{\Lambda}_{ij}(a_i \sigma a_j^* - \frac{1}{2}(a_j^* a_i \sigma + \sigma a_j^* a_i)) \right\}, \tag{4.24}$$

where $\boldsymbol{M}$ *is anti-Hermitian,* $\boldsymbol{\Lambda}$ *is positive-semidefinite, and* $a_1, \dots, a_r$ *satisfy* $\operatorname{tr}(\rho a_i^* a_j) = \delta_{ij}$ *and* $\operatorname{tr}(\rho a_i) = 0$. *For a given* L*, the matrix* $\boldsymbol{\Lambda}$ *is uniquely determined by the choice of* $a_1, \dots, a_r$.

Next we prove a detailed version of the entropy bound in Theorem 4.2.1:

Proposition 4.7.2 (Entropy bound)**.** *Let* L *be a Lindbladian of the form given by Proposition 4.7.1 and define*

$$\mathscr{S} := -\operatorname{tr}(\boldsymbol{\Lambda} \log \boldsymbol{\Delta}), \tag{4.25}$$

where $\boldsymbol{\Delta}_{ij} := \operatorname{tr}(\rho a_j a_i^*)$. *Then*

i) $\mathcal{S}$ *depends only on* ρ*,* L*, and* $\mathcal{P} = \operatorname{span}\{a_1, \dots, a_r\}$.

ii) If $\mathcal{P} \subset \mathcal{P}'$ *then* $\mathcal{S}(\rho, L, \mathcal{P}) \leq \mathcal{S}(\rho, L, \mathcal{P}')$.

iii) If $\mathcal{P} = \{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$ *then*

$$\mathscr{S} = \frac{d}{dt}\bigg|_{t=0} S(\rho_t) \tag{4.26}$$

for $\rho_t = e^{tL}[\rho]$.

Finally, we state in detail the matrix EEB inequality.

Proposition 4.7.3 (Matrix EEB inequality)**.** *Let* $a_1, \dots, a_r$ *be operators satisfying* $\operatorname{tr}(\rho a_i^* a_j) = \delta_{ij}$ *and* $\operatorname{tr}(\rho a_i)$. *For a given* $T \geq 0$ *define* K *to be the convex set of all traceless selfadjoint operators* $h \in \mathcal{A}$ *such that*

$$T \log(\boldsymbol{\Delta}) + \boldsymbol{H} \succeq 0, \tag{4.27}$$

where $\boldsymbol{\Delta}_{ij} := \operatorname{tr}(\rho a_j a_i^*)$ *and* $\boldsymbol{H} = \operatorname{tr}(\rho a_i^* [h, a_j])$. *Then* *i) K depends only on ρ, T, and $\mathcal{P} := \operatorname{span}\{a_1, \ldots, a_r\}$.*

ii) If $\mathcal{P} \subset \mathcal{P}'$ then $K(\rho, T, \mathcal{P}') \subset K(\rho, T, \mathcal{P})$.

iii) If $\mathcal{P} = \{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$ then $K(\rho, T, \mathcal{P})$ is a singleton containing the unique traceless operator h such that $\rho = e^{-h/T} / \operatorname{tr}\big(e^{-h/T}\big)$.

Parts *iii*) of the above two propositions can be seen as convergence results. We remark however that when $\mathcal{P} = \{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$, the expressions (4.25) and (4.27) use the expectation values of all operators, and thus requires full tomography of the state ρ. As such, this result does not give a practical convergence proof for the Hamiltonian learning algorithm considered in Section 4.3. Instead it acts as a sanity check that the algorithm performs no worse than the naive algorithm using full state tomography.

The proofs of these three propositions will use the Gelfand-Naimark-Segal (GNS) construction, which we introduce briefly now. Although our introduction is entirely self-contained, readers wanting more details are referred to the standard references [BR87; Tak79], or to the lecture notes [Wit18] which contain an introduction aimed at physicists.

Let $\mathcal{A}$ be the space of all operators on the physical Hilbert space $\mathcal{H}$, and let ρ be a faithful state. The bilinear form $(a, b) \mapsto \operatorname{tr}(\rho a^* b)$ endows $\mathcal{A}$ with the structure of a Hilbert space. For an operator $a \in \mathcal{A}$ we write $|a\rangle$ when we view a as a vector in this Hilbert space[3]. The GNS vector $|1\rangle$ corresponding to the identity operator is usually denoted $|\Omega\rangle$.

The *modular operator* $\Delta : \mathcal{A} \to \mathcal{A}$ is defined by the equation

$$\langle a|\Delta|b\rangle = \operatorname{tr}(\rho b a^*). \tag{4.28}$$

It is easy to check that Δ is self-adjoint with respect to the GNS inner product. As the following calculation shows, an equivalent characterization of Δ is that it takes a GNS vector $|b\rangle$ to $|\rho b \rho^{-1}\rangle$:

$$\begin{aligned}
\langle a|\Delta|b\rangle &= \operatorname{tr}(\rho b a^*) && (4.29)\\
&= \operatorname{tr}\big((\rho b \rho^{-1}) \rho a^*\big) && (4.30)\\
&= \operatorname{tr}\big(\rho a^* (\rho b \rho^{-1})\big) && (4.31)\\
&= \langle a|\rho b \rho^{-1}\rangle. && (4.32)
\end{aligned}$$

[3] There is a close analogy between this notation and the state-operator correspondence in CFT.

We will use the following conventions: operators on the physical Hilbert space will be denoted by lowercase letters, operators on the GNS Hilbert space will be denoted by capital letters like Δ and Λ, and numerical matrices will be denoted by boldface captial letters like $\mathbf{\Delta}$ and $\mathbf{\Lambda}$.

Proof of Proposition 4.7.1

First let us show that every Markovian Lindbladian has a parametrization of the form (4.24). The GKSL theorem [GKS76; Lin76] says that every Markovian Lindbladian has an expression of the form (4.24) but where $a_1, \ldots, a_r$ don't necessarily satisfy $\mathrm{tr}(\rho a_i^* a_j) = \delta_{ij}$ and $\mathrm{tr}(\rho a_i) = 0$. Notice that the right-hand side of (4.24) is invariant under the following two operations,

1. Applying a coordinate transformation $a_i \mapsto \sum_j \boldsymbol{Q}_{ij} a_j$ while taking $\mathbf{\Lambda} \mapsto (\boldsymbol{Q}^{-1})^\dagger \mathbf{\Lambda} \boldsymbol{Q}^{-1}$ and $\boldsymbol{M} \mapsto (\boldsymbol{Q}^{-1})^\dagger \boldsymbol{M} \boldsymbol{Q}^{-1}$.
2. Adding new operators $a_{r+1}, \ldots, a_{r+q}$ to the list and setting all new matrix elements of $\boldsymbol{M}$ and $\mathbf{\Lambda}$ to zero.

Using the above operations we can ensure that $r = N^2$ (where N is the dimension of the physical Hilbert space $\mathcal{H}$), $a_{N^2} = 1_{\mathcal{H}}$, and $\mathrm{tr}(\rho a_i^* a_j) = \delta_{ij}$ for $1 \le i, j \le N^2$. Notice now that for every term in (4.24) where $i = N^2$, the dissipative part can be absorbed into the unitary part:

$$\frac{1}{2}\boldsymbol{M}_{N^2,j}[a_j^*, \sigma] + \mathbf{\Lambda}_{N^2,j}(\sigma a_j^* - \frac{1}{2}(a_j^* \sigma + \sigma a_j^*)) = \frac{1}{2}(\boldsymbol{M}_{N^2,j} - \mathbf{\Lambda}_{N^2,j})[a_j^*, \sigma]. \tag{4.33}$$

Together with an analogous calculation for terms where $j = N^2$, we have

$$L[\sigma] = [h, \sigma] + \sum_{i,j=1}^{N^2-1} \mathbf{\Lambda}_{ij}(a_i \sigma a_j^* - \frac{1}{2}(a_j^* a_i \sigma + \sigma a_j^* a_i)), \tag{4.34}$$

where

$$h = \frac{1}{2}\sum_{i,j=1}^{N^2} (\boldsymbol{M}_{ij} + (\delta_{i,N^2} - \delta_{j,N^2})\mathbf{\Lambda}_{ij}). \tag{4.35}$$

To conclude the existence proof, we need to replace h with $\sum_{i,j=1}^{N^2-1} \boldsymbol{M}'_{ij} a_i^* a_j$ for some antiselfadjoint matrix $\boldsymbol{M}'_{ij}$. We will use the following lemma:

Lemma 4.7.1. *Every $a \in \mathcal{A}$ can be written as $a = \sum_{i=1}^{m} b_i^* c_i + \gamma \mathbf{1}_{\mathcal{H}}$ where $\mathrm{tr}(\rho b_i) = \mathrm{tr}(\rho c_i) = 0$ and $\gamma \in \mathbb{C}$.*

Proof. For $N = 1$ this is immediate with $m = 0$ and $\gamma = a$. Suppose that $N > 1$. Let $\rho = \sum_{i=1}^{N} \rho_i |i\rangle\langle i|$. It suffices to prove the claim for $a = |i\rangle\langle j|$ for any $1 \leq i, j \leq N$. Choose any $k \neq j$. Then we have $a = b^* c$ where $b = |j\rangle\langle i|$ and $c = |j\rangle\langle j| - \frac{\rho_j}{\rho_k} |k\rangle\langle k|$. □

Since $a_1, \ldots, a_{N^2-1}$ form a basis for $\{a \in \mathcal{A} : \mathrm{tr}(\rho a) = 0\}$, by the above Lemma we can write

$$h = \sum_{i,j=1}^{N^2-1} c_{ij} a_i^* a_j + \gamma \mathbf{1}_{\mathcal{H}} \tag{4.36}$$

$$= \frac{1}{2} \sum_{i,j=1}^{N^2-1} (c_{ij} - \overline{c_{ji}}) a_i^* a_j + Im(\gamma) \mathbf{1}_{\mathcal{H}} \tag{4.37}$$

for some $\{c_{ij}\}_{i,j=1}^{N^2-1}$, where the second line is because h is anti-Hermitian. Thus finally we have

$$L[\sigma] = \frac{1}{2} \sum_{i,j=1}^{N^2-1} (c_{ij} - \overline{c_{ji}})[a_i^* a_j, \sigma] + \sum_{i,j=1}^{N^2-1} \mathbf{\Lambda}_{ij} (a_i \sigma a_j^* - \frac{1}{2}(a_j^* a_i \sigma + \sigma a_j^* a_i)) \tag{4.38}$$

which establishes the existence statement of Proposition 4.7.1.

The uniqueness statement will follow from the following result, which we will also use in the proof of Theorem 4.2.1. Let $\Lambda : \mathcal{A} \to \mathcal{A}$ be the positive-semidefinite operator

$$\Lambda := \sum_{i,j=1}^{r} \mathbf{\Lambda}_{ij} |a_i\rangle\langle a_j|. \tag{4.39}$$

Lemma 4.7.2. *Suppose a Lindbladian L is expressed in the form (4.24) where the operators $a_1, \ldots, a_r$ are unrestricted. Let $Q = 1 - |\Omega\rangle\langle\Omega|$.*

i) The operator $Q\Lambda Q$ is independent of parametrization, i.e. for a given L it does not depend on $(a_1, \ldots, a_r, \boldsymbol{M}, \mathbf{\Lambda})$.

ii) If $a_1, \ldots, a_r$ are required to satisfy $\mathrm{tr}(\rho a_i) = 0$, then $\Lambda = Q\Lambda Q$ and thus Λ is parametrization-independent.

Proof. To prove part i), suppose $(a_1,\dots,a_r,\,\boldsymbol{M},\,\boldsymbol{\Lambda})$ and $(a'_1,\dots,a'_{r'},\,\boldsymbol{M}',\,\boldsymbol{\Lambda}')$ are two parametrizations of L of the form (4.24). Notice that Λ is invariant under the operations 1 and 2 above. As a result we can assume without loss of generality that $r = r' = N^2$ and $a_1,\dots,a_{N^2} = a'_1,\dots,a'_{N^2}$ is a basis of $\mathcal{A}$ with $a_{N^2} = 1_{\mathcal{H}}/2^{N-1}$ and $\operatorname{tr}(a_i^* a_j) = \delta_{ij}$ for $1 \le 1, j \le N^2$. Then the trick used to obtain (4.34) shows that there are self-adjoint operators h and h' such that

$$L[\sigma] = -i[h,\sigma] + \sum_{i,j=1}^{N^2-1} \boldsymbol{\Lambda}_{ij}(a_i\sigma a_j^* - \frac{1}{2}(a_j^* a_i\sigma + \sigma a_j^* a_i)) \tag{4.40}$$

$$= -i[h',\sigma] + \sum_{i,j=1}^{N^2-1} \boldsymbol{\Lambda}'_{ij}(a_i\sigma a_j^* - \frac{1}{2}(a_j^* a_i\sigma + \sigma a_j^* a_i)), \tag{4.41}$$

for every σ. By adding a multiple of the identity, h and h' can be made traceless and so the uniqueness statement of Theorem 2.2 in [GKS76] shows that $\boldsymbol{\Lambda}_{ij} = \boldsymbol{\Lambda}'_{ij}$ for all $1 \le i, j \le N^2 - 1$. Thus we have

$$\Lambda' - \Lambda = \sum_{i=N^2 \text{ or } j=N^2} (\boldsymbol{\Lambda}'_{ij} - \boldsymbol{\Lambda}_{ij})|a_i\rangle\langle a_j| \tag{4.42}$$

$$= |\Omega\rangle\langle a| + |a\rangle\langle\Omega|, \tag{4.43}$$

for some $a \in \mathcal{A}$. The result then follows from the fact that $Q(|\Omega\rangle\langle a| + |a\rangle\langle\Omega|)Q = 0$.

Part ii) then follows immediately from part i) and the fact that $\operatorname{tr}(\rho a_i) = \langle\Omega|a_i\rangle$. □

The above lemma proves the uniqueness statement of Proposition 4.7.1, since the additional condition $\operatorname{tr}(\rho a_i^* a_j) = \delta_{ij}$ implies that $\boldsymbol{\Lambda}_{ij} = \langle a_i|\Lambda|a_j\rangle$.

Proof of Proposition 4.7.2

Part i).

Let $Q : \mathcal{A} \to \mathcal{A}$ be the orthogonal projection onto $\mathcal{P} := \operatorname{span}\{a_1,\dots,a_r\}$. Since $\boldsymbol{\Delta}$ is the coordinate expression for $Q\Delta Q$ in the basis $a_1,\dots,a_r$ and since $\langle a_i|a_j\rangle = \operatorname{tr}(\rho a_i^* a_j) = \delta_{ij}$ it is easy to check that

$$-\operatorname{tr}(\boldsymbol{\Lambda}\log(\boldsymbol{\Delta})) = -\operatorname{tr}(\Lambda Q\log(Q\Delta Q)Q). \tag{4.44}$$

By part ii) of Lemma 4.7.2, this expression depends only on L, ρ, and $\mathcal{P}$.

Part *ii*).

We will use the operator version of Jensen's inequality applied to the matrix logarithm, which follows from the main theorem in [Dav57] and the fact that log is operator convex [Cha15]:

Lemma 4.7.3 (Operator Jensen's inequality for log)**.** *Let $\mathcal{K}$ be a Hilbert space and let Q and Q' be projections in $\mathcal{K}$ such that the image of Q is contained in the image of Q'. Then for any positive operator M on $\mathcal{K}$ we have*

$$Q\log(QMQ)Q \succeq Q\log(Q'MQ')Q. \tag{4.45}$$

Let $(a_1,\ldots,a_r,\boldsymbol{M},\boldsymbol{\Lambda})$ and $(a'_1,\ldots,a'_r,\boldsymbol{M}',\boldsymbol{\Lambda}')$ be two parametrizations of L, and suppose $\mathcal{P}\subset\mathcal{P}$'. Letting Q and Q' be the orthogonal projections onto $\mathcal{P}$ and $\mathcal{P}'$, we have

$$\begin{aligned}-\operatorname{tr}(\boldsymbol{\Lambda}\log(\boldsymbol{\Delta})) &= -\operatorname{tr}(\Lambda Q\log(Q\Delta Q)Q) && (4.46)\\ &\le -\operatorname{tr}(\Lambda Q\log(Q'\Delta Q')Q) && (4.47)\\ &= -\operatorname{tr}(\Lambda Q'\log(Q'\Delta Q')Q') && (4.48)\\ &= -\operatorname{tr}(\boldsymbol{\Lambda}'\log(\boldsymbol{\Delta}')), && (4.49)\end{aligned}$$

where in the third line we used the fact that $\Lambda = Q\Lambda Q = Q'\Lambda Q'$.

Part *iii*).

We begin by computing a general expression for the derivative of the entropy:

Lemma 4.7.4. *Let σ_t, $t\ge 0$ be a smooth path of density matrices and suppose that σ_0 is faithful. Write $S_t = -\operatorname{tr}(\sigma_t\log\sigma_t)$. Then using a prime to denote a time-derivative at $t=0$, we have*

$$S' = -\operatorname{tr}(\sigma'\log(\sigma)). \tag{4.50}$$

Proof. We have

$$-\operatorname{tr}(\sigma\log(\sigma))' = -\operatorname{tr}(\sigma'\log(\sigma)) - \operatorname{tr}\big(\sigma\log(\sigma)'\big). \tag{4.51}$$

Using the power series of log about the identity operator and the cyclicity of the trace, the second term can be seen to equal $-\operatorname{tr}(\rho')=0$. □

Now we apply the above lemma to the time-evolution of our state ρ generated by the Lindbladian (4.24):

Lemma 4.7.5. *With $\rho_t = e^{tL}[\rho]$, we have*

$$\left.\frac{d}{dt}\right|_{t=0} S(\rho_t) = -\operatorname{tr}(\Lambda \log(\Delta)), \tag{4.52}$$

where $\Lambda := \sum_{ij} \mathbf{\Lambda}_{ij} |a_j\rangle\langle a_i|$

Proof. Since the first term of (4.24) generates a unitary evolution it does not contribute to the entropy and so we may set $\boldsymbol{M} = 0$ without loss of generality. Since $\Delta|a\rangle = |\rho a \rho^{-1}\rangle$, we have $\log(\Delta)|a\rangle = |[\log(\rho), a]\rangle$. Thus we can expand the right-hand of (4.52) as

$$\begin{aligned}
-\operatorname{tr}(\Lambda \log(\Delta)) &= -\sum_{ij} \mathbf{\Lambda}_{ij} \langle a_j| \log(\Delta) |a_i\rangle && (4.53)\\
&= -\sum_{ij} \mathbf{\Lambda}_{ij} \langle a_j | [\log(\rho), a_i]\rangle && (4.54)\\
&= -\sum_{ij} \mathbf{\Lambda}_{ij} \operatorname{tr}\big(\rho a_j^* [\log(\rho), a_i]\big) && (4.55)\\
&= -\sum_{ij} \mathbf{\Lambda}_{ij} \Big[\operatorname{tr}\big(a_i \rho a_j^* \log(\rho)\big) - \operatorname{tr}\big(\rho \log(\rho) a_j^* a_i\big)\Big] && (4.56)\\
&= -\sum_{ij} \mathbf{\Lambda}_{ij} \Big[\operatorname{tr}\big(a_i \rho a_j^* \log(\rho)\big) - \frac{1}{2}\operatorname{tr}\big(a_j^* a_i \rho \log(\rho)\big) - \frac{1}{2}\operatorname{tr}\big(\rho a_j^* a_i \log(\rho)\big)\Big] && (4.57)\\
&= -\operatorname{tr}(L[\rho]\log(\rho)), && (4.58)
\end{aligned}$$

which equals $\left.\frac{d}{dt}\right|_{t=0} S(\rho_t)$ by Lemma 4.7.4. □

Finally, we need the following lemma:

Lemma 4.7.6. *Let $Q = 1 - |\Omega\rangle\langle\Omega|$ be the orthogonal projection onto $\{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$. We have*

$$Q \log(Q \Delta Q) Q = \log(\Delta). \tag{4.59}$$

Proof. Since $\Delta|\Omega\rangle = |\Omega\rangle$, we have $\log(\Delta)|\Omega\rangle = 0$, which proves the lemma. □

We are now ready to prove part iii). Suppose $\mathcal{P} = \{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$. Then

$$\begin{aligned}
-\operatorname{tr}(\mathbf{\Lambda} \log(\mathbf{\Delta})) &= -\operatorname{tr}(\Lambda Q \log(Q\Delta Q) Q) && (4.60)\\
&= -\operatorname{tr}(\Lambda \log(\Delta)) && (4.61)\\
&= \left.\frac{d}{dt}\right|_{t=0} S(\rho_t). && (4.62)
\end{aligned}$$

Proof of Proposition 4.7.3

Parts *i*) and *ii*) follow from the corresponding parts of Proposition 4.7.2.

Part *iii*).

Suppose first that $\rho = e^{-h/T}/\operatorname{tr}\big(e^{-h/T}\big)$. Define $H : \mathcal{A} \to \mathcal{A}$ as $H : |a\rangle \to |[h,a]\rangle$. Since $T\log(\Delta) + H = 0$, Lemma 4.7.6 gives $TQ\log(Q\Delta Q)Q + H = 0$, and sandwiching this expression between $\langle a_i|$ and $|a_j\rangle$ for all $1 \le i, j \le N^2 - 1$ gives $T\log(\boldsymbol{\Delta}) + \boldsymbol{H} = 0$.

Conversely, suppose h satisfies the matrix EEB inequality for $\mathcal{P} = \{a \in \mathcal{A} : \operatorname{tr}(\rho a) = 0\}$. This implies in particular that $\boldsymbol{H}$ is self-adjoint, and the calculation

$$0 = \boldsymbol{H}_{ij} - \overline{\boldsymbol{H}}_{ji} \tag{4.63}$$

$$= \operatorname{tr}([\rho, h]a_i^* a_j) \tag{4.64}$$

together with Lemma 4.7.1 shows that $[h, \rho] = 0$. From this it is easy to show that $QHQ = H$, and so the matrix EEB inequality gives

$$T\log(\Delta) + H \succeq 0. \tag{4.65}$$

Let J be *the modular involution*, which is the complex-antilnear operator defined as

$$J|a\rangle := |\rho^{1/2}a^*\rho^{-1/2}\rangle. \tag{4.66}$$

For any $a \in \mathcal{A}$ we have

$$\langle Ja|H|Ja\rangle = \operatorname{tr}\big(\rho\,\rho^{-1/2}a\rho^{1/2}[h, \rho^{1/2}a^*\rho^{-1/2}]\big) \tag{4.67}$$

$$= \operatorname{tr}\big(a\rho^{1/2}h\rho^{1/2}a^*\big) - \operatorname{tr}\big(\rho^{1/2}a\rho a^*\rho^{-1/2}h\big) \tag{4.68}$$

$$= -\operatorname{tr}(\rho a^*[h,a]) \tag{4.69}$$

$$= -\langle a|H|a\rangle, \tag{4.70}$$

where in the third line we used the fact that $[\rho, h] = 0$. Thus $J^\dagger H J = -H$. The same calculation with $\log(\rho)$ replacing h shows that $J^\dagger \log(\Delta) J = -\log(\Delta)$. It follows that $-(T\log\Delta + H) = J^\dagger(T\log(\Delta) + H)J \succeq 0$ and thus $T\log(\Delta) + H = 0$. From this we see that $\log(\rho) - h/T$ commutes with every operator in $\mathcal{A}$, which means it is a multiple of the identity, and so $\rho = e^{-h/T}/\operatorname{tr}\big(e^{-h/T}\big)$.

4.8 Corrections to ideal algorithm

In this section we describe several modifications that were made to the idealized algorithm (4.8) for the numerical work in Section 4.4.

1. For any matrix M, a semidefnite constraint $M \succeq 0$ can be broken down to the constraints $M_- = 0$ and $M_+ \succeq 0$, where $M_\pm := (M \pm M^\dagger)/2$. Doing so with the semidefinite constraint (4.9) yields

$$\boldsymbol{H}_- = 0 \tag{4.71}$$

$$\log(\boldsymbol{\Delta}) + \boldsymbol{H}_+ \succeq 0. \tag{4.72}$$

   Instead of imposing these constraints simultaneously, we impose the linear constraint $\boldsymbol{H}_- = 0$ first. This greatly reduces the number of degrees of freedom in the semidefinite program, leading to a more computationally efficient algorithm.

2. In the presence of noise in the expectation values of ρ, it is not appropriate to impose the linear constraint $\boldsymbol{H}_- = 0$ exactly. Instead, the following matrix was computed

$$W_{\alpha\beta} := \mathrm{tr}\Big((\boldsymbol{H}_\alpha - \boldsymbol{H}_\alpha^\dagger)(\boldsymbol{H}_\beta - \boldsymbol{H}_\beta^\dagger)^\dagger\Big), \tag{4.73}$$

   where $(\boldsymbol{H}_\alpha)_{ij} := \mathrm{tr}(\rho a_i^*[h_\alpha, a_j])$ for $\alpha = 1, \ldots s$, and the search space of Hamiltonians was restricted to the span of the eigenvectors of W with eigenvalue below a threshold $\epsilon_W > 0$. This is equivalent to the matrix $\mathcal{K}$ used in [BAL19]. For sufficiently small values of σ_{noise}, the spectrum of W was found to have several near-zero eigenvalues and a spectral gap to the rest of the eigenvalues, and ϵ_W was chosen to lie in this gap. An empirical formula that was found to produce an ϵ_W lying in the spectral gap of W was

$$\epsilon_W = 400 \max(\sigma_{noise}^2 \sqrt{m},\ 10^{-11}), \tag{4.74}$$

   where m denotes the number of terms $a_i^*[h_\alpha, a_j]$ such that $[h_\alpha, a_j] \neq 0$. This formula is not expected to be universal across different values of n and choices of perturbing operators. We note that in practice, while choosing ϵ_W to be too low caused the output to be inaccurate, choosing ϵ_W to lie above the gap did not significantly affect the accuracy of the result.

3. Although the temperature can be thought of as the same degree of freedom as the overall scale of the Hamiltonian, we chose to explicitly isolate it by adding a variable $T \geq 0$ to the the semidefinite program and replacing the constraint

$$\log(\boldsymbol{\Delta}) + \boldsymbol{H}_+ - \mu I \succeq 0 \tag{4.75}$$

with

$$T \log(\boldsymbol{\Delta}) + \boldsymbol{H}_+ - \mu I \succeq 0, \tag{4.76}$$

$$\mathrm{tr}(\rho h) = -1. \tag{4.77}$$

Here the extra normalization (4.77) is necessary to eliminate the degree of freedom associated with simultaneously scaling T, h, and μ.

4. Although the MOSEK interior-point solver [AA00] solves the primal and dual programs simultaneously, it was found that the algorithm ran significantly faster when it was called explicitly with the dual program instead of the primal.

References

[AA00] Erling D. Andersen and Knud D. Andersen. "The Mosek Interior Point Optimizer for Linear Programming: An Implementation of the Homogeneous Algorithm". In: *High Performance Optimization*. Springer US, 2000, pp. 197–232. ISBN: 9781475732160. DOI: 10.1007/978-1-4757-3216-0_8. URL: http://dx.doi.org/10.1007/978-1-4757-3216-0_8.

[AA23] Anurag Anshu and Srinivasan Arunachalam. *A survey on the complexity of learning quantum states*. 2023. DOI: 10.48550/ARXIV.2305.20069. URL: https://arxiv.org/abs/2305.20069.

[AL07] Robert Alicki and Karl Lendi. *Quantum Dynamical Semigroups and Applications*. Springer Berlin Heidelberg, 2007. ISBN: 9783540708605. DOI: 10.1007/3-540-70861-8. URL: http://dx.doi.org/10.1007/3-540-70861-8.

[Ans+21] Anurag Anshu et al. "Sample-efficient learning of interacting quantum systems". In: *Nature Physics* 17.8 (May 2021), pp. 931–935. ISSN: 1745-2481. DOI: 10.1038/s41567-021-01232-0. URL: http://dx.doi.org/10.1038/s41567-021-01232-0.

[Bak+23] Ainesh Bakshi et al. *Learning quantum Hamiltonians at any temperature in polynomial time*. 2023. DOI: 10.48550/ARXIV.2310.02243. URL: https://arxiv.org/abs/2310.02243.

[BAL19] Eyal Bairey, Itai Arad, and Netanel H. Lindner. "Learning a Local Hamiltonian from Local Measurements". In: *Physical Review Letters* 122.2 (Jan. 2019). ISSN: 1079-7114. DOI: 10.1103/physrevlett.122.020504. URL: http://dx.doi.org/10.1103/PhysRevLett.122.020504.

[BR87] Ola Bratteli and Derek W. Robinson. *Operator algebras and quantum statistical mechanics. 1. C^*- and W^*-algebras, symmetry groups, decomposition of states.* 2nd ed. Texts and Monographs in Physics. Springer-Verlag, New York, 1987.

[BR97] Ola Bratteli and Derek W. Robinson. *Operator algebras and quantum statistical mechanics. 2. Equilibrium states. Models in quantum statistical mechanics.* 2nd ed. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1997.

[BV04] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization.* Cambridge University Press, Mar. 2004. ISBN: 9780511804441. DOI: 10.1017/cbo9780511804441. URL: http://dx.doi.org/10.1017/CBO9780511804441.

[Cha15] Pattrawut Chansangiam. "A Survey on Operator Monotonicity, Operator Convexity, and Operator Means". In: *International Journal of Analysis* 2015 (Nov. 2015), pp. 1–8. ISSN: 2314-4998. DOI: 10.1155/2015/649839. URL: http://dx.doi.org/10.1155/2015/649839.

[Dal+22] Marcello Dalmonte et al. "Entanglement Hamiltonians: From Field Theory to Lattice Models and Experiments". In: *Annalen der Physik* 534.11 (Aug. 2022). ISSN: 1521-3889. DOI: 10.1002/andp.202200064. URL: http://dx.doi.org/10.1002/andp.202200064.

[Dav57] Chandler Davis. "A Schwarz inequality for convex operator functions". In: *Proceedings of the American Mathematical Society* 8.1 (1957), pp. 42–44.

[DB16] Steven Diamond and Stephen Boyd. "CVXPY: a python-embedded modeling language for convex optimization". In: *J. Mach. Learn. Res.* 17.1 (Jan. 2016), pp. 2909–2913. ISSN: 1532-4435.

[EHF19] Tim J. Evans, Robin Harper, and Steven T. Flammia. *Scalable Bayesian Hamiltonian learning.* 2019. DOI: 10.48550/ARXIV.1912.07636. URL: https://arxiv.org/abs/1912.07636.

[FFS] Hamza Fawzi, Omar Fawzi, and Samuel O. Scalet. *Certified algorithms for equilibrium states of local quantum Hamiltonians.* DOI: 10.48550/arXiv.2311.18706. arXiv: 2311.18706 [quant-ph].

[FW05] Adrian E. Feiguin and Steven R. White. "Finite-temperature density matrix renormalization using an enlarged Hilbert space". In: *Physical Review B* 72.22 (Dec. 2005). ISSN: 1550-235X. DOI: 10.1103/physrevb.72.220401. URL: http://dx.doi.org/10.1103/PhysRevB.72.220401.

[GKS76] Vittorio Gorini, Andrzej Kossakowski, and E. C. G. Sudarshan. "Completely positive dynamical semigroups of N-level systems". In: *Journal of Mathematical Physics* 17.5 (May 1976), pp. 821–825. ISSN: 1089-7658. DOI: 10.1063/1.522979. URL: http://dx.doi.org/10.1063/1.522979.

[HKT22] Jeongwan Haah, Robin Kothari, and Ewin Tang. "Optimal learning of quantum Hamiltonians from high-temperature Gibbs states". In: *2022 IEEE 63rd Annual Symposium on Foundations of Computer Science (FOCS)*. IEEE, Oct. 2022. DOI: 10.1109/focs54457.2022.00020. URL: http://dx.doi.org/10.1109/FOCS54457.2022.00020.

[Kok+21] Christian Kokail et al. "Entanglement Hamiltonian tomography in quantum simulation". In: *Nature Physics* 17.8 (June 2021), pp. 936–942. ISSN: 1745-2481. DOI: 10.1038/s41567-021-01260-w. URL: http://dx.doi.org/10.1038/s41567-021-01260-w.

[Lif+21] Yotam Y. Lifshitz et al. *Practical Quantum State Tomography for Gibbs states*. 2021. DOI: 10.48550/ARXIV.2112.10418. URL: https://arxiv.org/abs/2112.10418.

[Lin76] G. Lindblad. "On the generators of quantum dynamical semigroups". In: *Communications in Mathematical Physics* 48.2 (June 1976), pp. 119–130. ISSN: 1432-0916. DOI: 10.1007/bf01608499. URL: http://dx.doi.org/10.1007/BF01608499.

[Mon15] Andrea Montanari. "Computational implications of reducing data to sufficient statistics". In: *Electronic Journal of Statistics* 9.2 (Jan. 2015). ISSN: 1935-7524. DOI: 10.1214/15-ejs1059. URL: http://dx.doi.org/10.1214/15-EJS1059.

[NN94] Yurii Nesterov and Arkadii Nemirovskii. *Interior-Point Polynomial Algorithms in Convex Programming*. Society for Industrial and Applied Mathematics, Jan. 1994. ISBN: 9781611970791. DOI: 10.1137/1.9781611970791. URL: http://dx.doi.org/10.1137/1.9781611970791.

[ODo+16] Brendan O'Donoghue et al. "Conic Optimization via Operator Splitting and Homogeneous Self-Dual Embedding". In: *Journal of Optimization Theory and Applications* 169.3 (Feb. 2016), pp. 1042–1068. ISSN: 1573-2878. DOI: 10.1007/s10957-016-0892-3. URL: http://dx.doi.org/10.1007/s10957-016-0892-3.

[QR19] Xiao-Liang Qi and Daniel Ranard. "Determining a local Hamiltonian from a single eigenstate". In: *Quantum* 3 (July 2019), p. 159. ISSN: 2521-327X. DOI: 10.22331/q-2019-07-08-159. URL: http://dx.doi.org/10.22331/q-2019-07-08-159.

[Sch+23] Henning Schlömer et al. "Quantifying hole-motion-induced frustration in doped antiferromagnets by Hamiltonian reconstruction". In: *Communications Materials* 4.1 (Aug. 2023). ISSN: 2662-4443. DOI: 10.1038/s43246-023-00382-3. URL: http://dx.doi.org/10.1038/s43246-023-00382-3.

[SK14] Brian Swingle and Isaac H. Kim. "Reconstructing Quantum States from Local Data". In: *Physical Review Letters* 113.26 (Dec. 2014). ISSN: 1079-7114. DOI: 10.1103/physrevlett.113.260501. URL: http://dx.doi.org/10.1103/PhysRevLett.113.260501.

[Tak79] Masamichi Takesaki. "Fundamentals of Banach Algebras and C*-Algebras". In: *Theory of Operator Algebras I*. Springer New York, 1979, pp. 1–57. ISBN: 9781461261889. DOI: 10.1007/978-1-4612-6188-9_1. URL: http://dx.doi.org/10.1007/978-1-4612-6188-9_1.

[Wit18] Edward Witten. "APS Medal for Exceptional Achievement in Research: Invited article on entanglement properties of quantum field theory". In: *Reviews of Modern Physics* 90.4 (Oct. 2018). ISSN: 1539-0756. DOI: 10.1103/revmodphys.90.045003. URL: http://dx.doi.org/10.1103/RevModPhys.90.045003.

Chapter 5

CERTIFIED ALGORITHMS FOR QUANTUM HAMILTONIAN LEARNING VIA ENERGY-ENTROPY INEQUALITIES

This Chapter is available as a preprint at

[Art+24] Adam Artymowicz et al. "Certified algorithms for quantum Hamiltonian learning via energy-entropy inequalities". In: *arXiv e-prints*, arXiv:2410.23284 (Oct. 2024), arXiv:2410.23284. DOI: 10.48550/arXiv.2410.23284. arXiv: 2410.23284 [quant-ph].

5.1 Introduction

In this work we consider the problem of Hamiltonian learning from a thermal state. Given the form of the Hamiltonian

$$h = \sum_{\alpha=1}^{m} \lambda_\alpha E_\alpha, \tag{5.1}$$

where local Hamiltonian terms E_α are known but their coefficients λ_α are not, we seek estimates of the λ_α's using measurements from the Gibbs state

$$\rho = \frac{e^{-\beta h}}{\mathrm{Tr}[e^{-\beta h}]}.$$

Hamiltonian learning is fundamental to validate our models of quantum physical systems [Wie+14; Wan+17], and plays an important role in certifying quantum devices. In addition, with the recent progress in quantum algorithms for Gibbs state preparation [Tem+11; Che+23], Hamiltonian learning is likely to be crucial to benchmark the future realizations of such algorithms. Aside from these applications, it can also directly be used to give physical insights about many-body quantum systems in both experimental and numerical contexts. For instance, Hamiltonian learning has already been applied to the study of *entanglement Hamiltonians* [Dal+22], which are sensitive probes of entanglement and have for instance been used to test CFT predictions in thermalizing systems [WRL18; Kok+21]. Applications like these demand a Hamiltonian learning algorithm that is efficient, reliable, and can provide rigorous bounds on the uncertainty.

Overview of the algorithm and results We propose an efficient Hamiltonian learning algorithm that provides rigorous error bounds. Our algorithm is based on a semidefinite constraint that generalizes a set of inequalities known as the *energy-entropy balance* or *EEB* inequalities [AS77]. These constraints were first applied to the forward problem in [FFS23] by three of us and to the inverse problem in [Art24] by one of us. In the latter work, it was benchmarked numerically, where it was found to scale well and to give accurate results when reconstructing a known Hamiltonian. However, this work did not include a theoretical analysis of the case with measurement noise, or any practically useful convergence guarantees. As such its output did not come with any guarantees of accuracy, which would be necessary for use in experiments. Here we solve this problem in two ways, with *a posteriori* and *a priori* guarantees.

Our algorithm computes rigorous lower and upper bounds on any linear functional $v{\cdot}\lambda$ of the unknown coefficients $\lambda \in \mathbb{R}^m$. By varying over different choices of v a convex relaxation of the Hamiltonian parameters can be obtained, i.e., a convex set including λ itself. In particular, by running the algorithm for all basis vectors in $\mathbb{R}^m$, we obtain intervals such that $\lambda_\alpha \in [a_\alpha, b_\alpha]$. Other interesting choices exist, however: if $\sum_\alpha v_\alpha E_\alpha$ is a symmetry of ρ, the quantity $v \cdot \lambda$ has the interpretation of a generalized *chemical potential* for this symmetry [Ara+77], an important physical quantity. This example includes the usual chemical potential when $\sum_\alpha v_\alpha E_\alpha$ is the number operator corresponding to a given particle type.

The algorithm is parametrized by a hierarchy level $\ell \in \mathbb{N}_+$ which governs the strength of the semidefinite constraint used. It is summarized in Figure 5.1. The details of the setup of the algorithm are described in Section 5.2 and the theorem is proved in Sections 5.3 and 5.4.

Theorem 5.1.1 (Informal version of Theorem 5.2.5)**.** *Consider a k-local Hamiltonian $h = \sum_{\alpha=1}^m \lambda_\alpha E_\alpha$ with unknown coefficients $\lambda \in \mathbb{R}^m$. Let $\beta = \max_\alpha |\lambda_\alpha|$ and let $\mathfrak{d}$ be the degree of the dual interaction graph (see Section 5.2 for the definition). Assume we have access to an oracle $\tilde{\omega}$ such that for the evaluated observables O, $|\tilde{\omega}(O) - \mathrm{tr}[\rho O]| \leq \varepsilon_0 \|O\|$, where $\rho = e^{-h}/\operatorname{Tr}\left[e^{-h}\right]$ is the Gibbs state of h. Let $v \in \mathbb{R}^m$ with $\|v\|_1 = 1$ and consider the problem of estimating the inner product $v \cdot \lambda$ given access to $\tilde{\omega}$.*

For each $\ell \in \mathbb{N}_+$, let $a^{(\ell)}$ and $b^{(\ell)}$ be the output of algorithm in Figure 5.1.

i) The pair of numbers $a^{(\ell)}$ and $b^{(\ell)}$ satisfy

$$a^{(\ell)} \leq v \cdot \lambda \leq b^{(\ell)}. \tag{5.5}$$

ii) If h is commuting and $\ell = \max(3, 1 + (1 + \mathfrak{d})^2)$, then we have

$$b^{(\ell)} - a^{(\ell)} \leq \varepsilon_0 / \sigma \tag{5.6}$$

provided $\varepsilon_0 \leq \sigma$ for some error threshold $\sigma = e^{-\mathcal{O}_{k,\mathfrak{d}}(\beta)} m^{-6}$.

Point (i) above shows that our algorithm returns *certified a posteriori bounds*, i.e., it returns an estimate of the parameter $v \cdot \lambda$ together with strict bounds on the error of these estimates, namely $b^{(\ell)} - a^{(\ell)}$. This type of algorithm is particularly beneficial for situations where no convergence guarantees can be proven or when *a priori* guarantees lead to overly pessimistic bounds. Moreover, if the program is infeasible, the dual program gives a certificate that ρ is not a Gibbs state of any Hamiltonian with the given structure. Point (ii) gives an a priori guarantee: for a constant value of ℓ and provided the noise ε_0 of the expectation values is below a certain threshold, the estimates of $v \cdot \lambda$ returned by the algorithm are proportional to ε_0. In particular, estimates can be obtained in *polynomial time* and using *polynomially many samples* in the system size and inverse error of the estimates.

Related work The version of the Hamiltonian learning problem we study has attracted wide interest over the past years, with several approaches being proposed. On the practical front, reliable algorithms which have been used in numerics and experiments have been limited to small system sizes [Ans+21; Kok+21; Lif+21]. More scalable approaches exist, including algorithms that only use the property that the Gibbs state is a steady state [BAL19; EHF19]. Even though such algorithms are efficient and can work for some instances, one can easily construct instances where such conditions are not enough to single out the Hamiltonian, even when the Hamiltonian is commuting and the expectation values are known perfectly [Art24]. We mention also the Hamiltonian learning algorithm [GCC22] (see also [Sti+24]) which has both a theoretical analysis of performance and has been implemented. However, it solves a different problem where Gibbs states with different temperatures can be queried.

From a theoretical perspective, the polynomial complexity of the commuting case follows from the simple approach in [Ans+]. Other polynomial complexity bounds have been proven in this and other contexts [HKT24; Kuw24; Bak+23; Nar24]. The best asymptotic computational and sample complexity bounds for the general problem are achieved in [Bak+23; Nar24], which give an algorithm with polynomial classical and sample complexity. It is interesting to compare their algorithm with ours. They use a convex hierarchy that is based on relaxations of the KMS condition [HHW67], which is physically related to the EEB condition used in this work. Both the KMS and the EEB conditions are interpretable in terms of local thermodynamic stability [CW87; AS77], and their ideal versions (i.e., taking all the possible conditions) have been shown to be equivalent [AS77; Sew77]. However, in order to obtain an efficient algorithm, only a subset of the conditions are imposed and this manifests differently for the KMS versus EEB conditions. Since the KMS conditions are non-linear in the Hamiltonian parameters, in [Bak+23], polynomial approximations are used to implement these constraints entailing an intricate error analysis already in the feasibility part. Furthermore, to deal with the resulting polynomial constraint systems, an additional hierarchy, the sum-of-squares relaxation, is introduced. In comparison, our constraints, which are linear in the parameters of the Hamiltonian, are much easier to implement.

5.2 Algorithmic framework and main results

Let $\mathcal{H}$ be a finite-dimensional Hilbert space. We write $\mathcal{B}(\mathcal{H})$ for the algebra of all linear operators on $\mathcal{H}$. The adjoint of an operator a will be denoted a^*. Let $m > 0$ and let $E_1, \ldots, E_m \in \mathcal{B}(\mathcal{H})$ be a collection of selfadjoint operators with $\|E_\alpha\| = 1$ for all $1 \leq \alpha \leq m$. Let

$$h = \sum_{\alpha=1}^{m} \lambda_\alpha E_\alpha \tag{5.7}$$

for some unknown coefficients $\lambda_1, \ldots, \lambda_m$, and set $\beta := \max_{\alpha=1,\ldots m} |\lambda_\alpha|$. Let ρ be the thermal state

$$\rho = \frac{e^{-h}}{\mathrm{Tr}[e^{-h}]}.$$

We will write thermal expectation values of observables as

$$\omega(A) := \mathrm{Tr}[\rho A].$$

Here and below, we use Tr to denote the usual trace and tr to denote the normalized trace $\mathrm{tr}(a) = \mathrm{Tr}(a)/\dim(\mathcal{H})$.

The matrix EEB constraint

We start by introducing the semidefinite constraint that forms the backbone of this work. It begins with a choice of selfadjoint operators $P_1, \dots, P_r \in \mathcal{B}(\mathcal{H})$ satisfying $\|P_i\| = 1$ which we call the *perturbing operators*. The constraint will depend on this choice, and adding operators to the list will yield a tighter constraint — in this sense we will say the constraints form a hierarchy depending on the choice of $P_1, \dots, P_r$[1]. Later, in sections 5.2 and 5.2 we will restrict to lattice models, where the perturbing operators will be chosen to be all the Pauli operators of a given locality, but in this section and the next we keep the choice of perturbing operators unrestricted.

Define the following $r \times r$ matrix C and $r \times r$ matrices $B_1, \dots, B_m$:

$$C_{ij} := \omega(P_i P_j) \qquad 1 \le i, j \le r \tag{5.8}$$

$$(B_\alpha)_{ij} := \omega(P_i [E_\alpha, P_j]) \qquad 1 \le i, j \le r \text{ and } 1 \le \alpha \le m. \tag{5.9}$$

Since $(P_i P_j)^* = P_j P_i$, the matrix C is automatically hermitian, and in fact it is guaranteed to be positive-definite because $\rho \succ 0$. This allows us to define the following matrices:

$$\boldsymbol{\Delta} := C^{-1/2} C^T C^{-1/2}, \tag{5.10}$$

$$\boldsymbol{H}_\alpha := C^{-1/2} B_\alpha C^{-1/2} \qquad 1 \le \alpha \le m. \tag{5.11}$$

We remark that although the *operators* E_α are hermitian, the *matrices* B_α and $\boldsymbol{H}_\alpha$ are not hermitian in general.

The conceptual starting point for this work is the following matrix inequality [FFS23]:

Theorem 5.2.1 (Matrix EEB inequality)**.**

$$\log(\boldsymbol{\Delta}) + \sum_{\alpha=1}^{m} \lambda_\alpha \boldsymbol{H}_\alpha \succeq 0. \tag{5.12}$$

Notice that since positive semidefinite matrices are by definition hermitian, the matrix EEB inequality subsumes the linear constraint $\sum_{\alpha=1}^m \lambda_\alpha \left(\boldsymbol{H}_\alpha - \boldsymbol{H}_\alpha^\dagger\right) = 0$, which is nontrivial because the matrices $\boldsymbol{H}_\alpha$ are (in general) not hermitian.

[1]The fact that adding perturbing operators strengthens the constraint was shown in a slightly different setting in [Art24, Proposition 4]. There, it was also shown that the constraint depends only on the *span* of the perturbing operators, and thus we have a hierarchy indexed by the poset of linear subspaces of $\mathcal{B}(\mathcal{H})$. We do not need either of these facts here.

Varying the choice of perturbing operators $P_1, \dots, P_r$, the matrix EEB inequality yields a hierarchy of semidefinite contraints that are satisfied for the true Hamiltonian coefficients $\lambda = (\lambda_1, \dots, \lambda_m)$. This is an idealized constraint using the quantities $\boldsymbol{\Delta}$ and $\boldsymbol{H}_\alpha$ built out of noise-free expectation values, which are not accessible to experiment. This is more than a practical concern, since shot noise is unavoidable given access to only finitely many copies of the state ρ, even in the absence of other sources of error like state preparation and measurement noise. Thus, in order to make practically useful statements we will need to consider an appropriate relaxation of this constraint, which we do below.

Relaxing the constraint

We assume access to an estimate of $\omega(A)$, which we call $\tilde{\omega}(A)$, for every observable A of the form

$$P_i P_j \qquad 1 \leq i, j \leq r, \tag{5.13}$$

$$P_i[E_\alpha, P_j] \qquad 1 \leq i, j \leq r \text{ and } 1 \leq \alpha \leq m. \tag{5.14}$$

We assume the following control over the errors in the estimates $\tilde{\omega}$: for some $\epsilon_0 \geq 0$ we have

$$|\tilde{\omega}(A) - \omega(A)| \leq \epsilon_0 \quad \text{for any operator } A \text{ of the form (5.13) or (5.14).} \tag{5.15}$$

We further assume that the estimates obey the following restrictions, which may be enforced without loss of generality:

$$\tilde{\omega}(1) = 1, \tag{5.16}$$

$$|\tilde{\omega}(P_i P_j)| \leq 1 \quad \text{for all } 1 \leq i, j \leq r \tag{5.17}$$

$$|\tilde{\omega}(P_i[E_\alpha, P_j])| \leq 2 \quad \text{for all } 1 \leq i, j \leq r \text{ and } 1 \leq \alpha \leq m. \tag{5.18}$$

Define the quantities $\tilde{C}, \tilde{B}_\alpha, \tilde{\boldsymbol{\Delta}}$, $\tilde{\boldsymbol{H}}_\alpha$ analogously to $C, B_\alpha, \boldsymbol{\Delta}, \boldsymbol{H}_\alpha$, but using the noisy estimates $\tilde{\omega}$ in place of ω. In order to do this, one needs $\tilde{C}$ to be positive-definite. We assume this for now, but as we will show in Theorem 5.2.3 below, this is guaranteed for sufficiently low noise levels. We relax the matrix EEB inequality as follows:

$$\log\left(\tilde{\boldsymbol{\Delta}}\right) + \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha + \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \succeq -\mu_1, \tag{5.19}$$

$$\pm i \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha - \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \preceq \mu_2, \tag{5.20}$$

for $\mu_1, \mu_2 \geq 0$. To show that this relaxation is useful, we need to find some relaxation parameters μ_1, μ_2 for which the true Hamiltonian coefficients are feasible. The following theorem is proved in Section 5.3:

Theorem 5.2.2 (A posteriori feasibility)**.** *Suppose $\tilde{C} \succ 0$ and let $K := 2r\|\tilde{C}^{-1}\|$. If $\varepsilon_0 \leq 1/K$ then the true Hamiltonian coefficients $\lambda' = \lambda$ are a feasible point for the relaxed matrix EEB constraints (5.19) and (5.20) with*

$$\mu_1 := \left(2K^3 + 3m\beta K^2\right)\varepsilon_0 \tag{5.21}$$

$$\mu_2 := 3m\beta K^2 \varepsilon_0. \tag{5.22}$$

We call this an *a posteriori* feasibility guarantee because it depends on the estimates $\tilde{\omega}$, which enter through the constant K. Thanks to this result, the inequalities (5.19) and (5.20) with μ_1 and μ_2 given by (5.21) and (5.22) place rigorous constraints on the set of potential Hamiltonian parameters λ'. If, for a given ansatz, the condition $\varepsilon_0 \leq 1/K$ is fulfilled, but the constraints are infeasible, this *guarantees* that the given state is not the Gibbs state in the family of Hamiltonians.

However, this guarantee only holds when $\varepsilon_0 \leq 1/K$ and it is not *a priori* clear that this condition can be satisfied by ensuring ε_0 is small enough because K depends on the measured data. The following Lemma shows that this is indeed the case if we assume that the perturbing operators are chosen to be Hilbert-Schmidt orthogonal:

Lemma 5.2.1. *Suppose the $P_1, \ldots, P_r$ satisfy $\mathrm{tr}(P_i P_j) = \delta_{ij}$ and let $\sigma = e^{-m\beta} d/3r$, where $d = \dim(\mathcal{H})$. Then if $\varepsilon_0 \leq \sigma$ then $K \leq 1/\sigma$ and in particular, Theorem 5.2.2 holds.*

Proof. Since $\rho \succeq e^{-\|h\|} \succeq e^{-m\beta}$ we have $w^\dagger C w \geq e^{-m\beta} d \|w\|^2$ for any $w \in \mathbb{C}^r$, and so $C \succeq e^{-m\beta} d = 3r\sigma$. An elementary bound gives $\|C - \tilde{C}\| \leq r\varepsilon_0$, so if $\varepsilon_0 \leq \sigma$ then $\|C - \tilde{C}\| \leq r\sigma$. It follows that $\tilde{C} \geq 2r\sigma$, and so $K = 2r\|\tilde{C}\| \leq 1/\sigma$. ∎

The exponential dependence on m is unavoidable in the general case. However, as we show in the next section, if we restrict to the setting of local Hamiltonians on a lattice, we can prove the analogous statement with an error threshold σ that does not depend on m or the Hilbert space dimension d at all.

The lattice setting

So far, we have made almost no assumptions on the structure of the problem and were able to give the *a posteriori* guarantee in Theorem 5.2.2 and the *a priori* guarantee in Lemma 5.2.1. In this section, we restrict to the setting of a quantum lattice system, where locality allows us to give much stronger *a priori* guarantees.

Suppose our Hilbert space is that of a collection of n qubits $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$. We say an operator E is *k-supported* if $|\operatorname{supp}(E)| \leq k$, and *$k$-local* if it is a sum of k-supported terms. Suppose the Hamiltonian terms $\{E_\alpha\}_{a=1}^m$ are k-supported for some $k > 0$, and define their *dual interaction graph* $\mathfrak{G}$ to have the vertex set $[m]$ and an edge between every pair of vertices $1 \leq \alpha, \alpha' \leq m$ with $\operatorname{supp}(E_\alpha) \cap \operatorname{supp}(E_b) \neq \emptyset$. We say $\{E_1, \ldots, E_m\}$ are *k-$\mathfrak{d}$-low-intersection* if the degree of the graph $\mathfrak{G}$ is bounded by $\mathfrak{d}$. Call an operator F *k-ℓ-$\mathfrak{G}$-supported* if $\operatorname{supp}(F) \subset \bigcup_S \operatorname{supp}(E_\alpha)$ for a set $S \subset \mathfrak{G}$ which satisfies $|S| \leq \ell$ and is connected in $\mathfrak{G}$. Note that a k-ℓ-$\mathfrak{G}$-supported operator is $k\ell$-supported.

Definition 5.2.1. *We define $\mathcal{P}_{k,\ell}$ to be the set of all k-ℓ-$\mathfrak{G}$-supported Paulis.*

In what follows, we will treat k and $\mathfrak{d}$ as constants that does not depend on the system size m. This scenario includes familiar examples of geometrically local Hamiltonians defined on a lattice.

The following theorem gives an *a priori* feasibility guarantee, by proving that Theorem 5.2.2 holds for sufficiently low error rate ε_0 without the need to incorporate measurement outcomes (which previously entered through the constant K) into the error threshold. The proof appears in Section 5.3.

Theorem 5.2.3 (A priori bound on K)**.** *Suppose that E_α are k-$\mathfrak{d}$-low-intersection for some constants $k, \mathfrak{d}$, and suppose that the operators $P_1, \ldots, P_r$ are all k-ℓ-$\mathfrak{G}$-supported for some $\ell > 0$. Then there is an error threshold*

$$\sigma = r^{-2} e^{-\mathcal{O}_{k,\mathfrak{d},\ell}(\beta)} \tag{5.23}$$

such that $\epsilon_0 \leq \sigma$ implies $K \leq 1/\sigma$. In particular, Theorem 5.2.2 holds.

Next, we give an *a priori* convergence result, i.e. a proof that our algorithm outputs estimates of the Hamiltonian parameters that are close to the true Hamiltonian parameters, in the case when the true Hamiltonian is *commuting*. The class of commuting Hamiltonians contains many interesting examples, including topologically ordered Hamiltonians.

Definition 5.2.2. *We say a Hamiltonian $h = \sum_\alpha \lambda_\alpha E_\alpha$ is* commuting *if there are selfadjoint operators $\{F_\alpha\}_{\alpha=1}^m$ with $\|F_\alpha\| = 1$ and real constants $\{\nu_\alpha\}_{\alpha=1}^m$ such that*

i) $h = \sum_{\alpha=1}^m \nu_\alpha F_\alpha$.

ii) $[F_\alpha, F_{\alpha'}] = 0$ *for any* $1 \leq \alpha, \alpha' \leq m$.

iii) $\operatorname{supp} F_\alpha \subset \operatorname{supp} E_\alpha$ *for all* $1 \leq \alpha \leq m$.

iv) $\max_{\alpha=1,\ldots m} |\nu_\alpha| \leq \mathcal{C} \max_{\alpha=1,\ldots m} |\lambda_\alpha|$ *for some constant* $\mathcal{C} > 0$.

Note that for the purpose of our algorithm it is not necessary to *know* the decomposition in Definition 5.2.2. A general ansatz of Pauli operators is used for the $\{E_\alpha\}_{\alpha=1}^m$, and Theorem 5.2.4 holds as long as a commuting decomposition exists. In order to prove a convergence guarantee, it is also necessary to ensure that the set $P_1, \ldots P_r$ is large enough, which we have not done so far. We require them to include all Pauli operators satisfying a k-ℓ-$\mathfrak{G}$-support assumption for a constant ℓ. The following Theorem is proven in Section 5.4

Theorem 5.2.4 (A priori convergence in the commuting case)**.** *Suppose E_α are Pauli operators with k-$\mathfrak{d}$-low-intersection and h is commuting. Set $\{P_1, \ldots, P_r\} = \mathcal{P}_{k,\ell}$ for $\ell = \max(3, 1 + (\mathfrak{d} + 1)^2)$. There is an error threshold*

$$\tau = m^{-6} e^{-\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} \tag{5.24}$$

such that if $\epsilon_0 \leq \tau$ then for any $\lambda' \in \mathbb{R}^m$ satisfying the constraints (5.19) and (5.20), we have

$$\sup_{\alpha=1,\ldots m} |\lambda'_\alpha - \lambda_\alpha| \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} \left(\mu_1 + m^{1/2}\mu_2\right) + \varepsilon_0/\tau. \tag{5.25}$$

Algorithms

Let us now describe how the above constraints lead to two algorithms for Hamiltonian learning. The first algorithm takes as input the set of perturbing operators $P_1, \ldots, P_r$, a choice of direction in the parameter space $v \in \mathbb{R}^m$, choices of nonnegative numbers μ_1, μ_2, and the estimates $\tilde{\omega}$. Assumptions on the errors in the estimates will enter through the choice of μ_1 and μ_2.

Algorithm A

Compute $K := 2r\|\tilde{C}^{-1}\|$. If $\tilde{C}$ is not positive definite or $K > 1/\varepsilon_0$, return the interval $[-\infty, +\infty]$. Otherwise, let

$$\mu_1 := \left(2K^3 + 3m\beta K^2\right)\varepsilon_0 \tag{5.26}$$

$$\mu_2 := 3m\beta K^2 \varepsilon_0, \tag{5.27}$$

and return the interval $[a, b]$ where a, b are minimum/maximum of the following SDP:

$$\underset{\lambda' \in \mathbb{R}^m}{\text{minimize/maximize}} \quad v \cdot \lambda' \tag{5.28}$$

$$\text{subject to} \quad \log\left(\tilde{\boldsymbol{\Delta}}\right) + \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha + \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \succeq -\mu_1, \tag{5.29}$$

$$\pm\, i \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha - \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \preceq \mu_2. \tag{5.30}$$

Theorems 5.2.2, 5.2.3, and 5.2.4 give the following guarantees:

Theorem 5.2.5 (Guarantees for Algorithm A)**.** *Suppose the input state ρ is the Gibbs state of $h = \sum_\alpha \lambda_\alpha E_\alpha$ for some unknown coefficients $\lambda \in \mathbb{R}^m$ with $\max_{\alpha=1,\ldots,m} |\lambda_\alpha| \leq \beta$, and Pauli operators E_α and consider Algorithm A for some $v \in \mathbb{R}^m$ with $\|v\|_1 = 1$. Then:*

i) The algorithm is feasible and its output $[a, b]$ satisfies

$$a \leq v \cdot \lambda \leq b. \tag{5.31}$$

If furthermore $P_1, \ldots, P_r = \mathcal{P}_{k,\ell}$, then:

ii) If h is commuting and $\ell = \max(3, 1 + (1 + \mathfrak{d})^2)$ then there is an error threshold

$$\sigma = e^{-\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} m^{-6} \tag{5.32}$$

such that $\varepsilon_0 \leq \sigma$ implies $b - a \leq \varepsilon_0/\sigma$.

Let us remark that in the above, increasing the error bound ε_0 can never violate the assumptions of the algorithm, but it does relax the constraints, producing worse bounds. As such, the practicality of the algorithm depends on access to error bounds that are not too conservative, and in some settings, such tight error bounds may be hard to obtain. In these settings, one of course cannot expect tight bounds on the λ_α, but one may be more interested in the qualitative structure of the Hamiltonian rather than in exact error bounds.

For such settings, we introduce a variant of the above algorithm, which does not assume any prior knowledge of the measurement error. It requires only a choice of hierarchy level $\ell \in \mathbb{N}_+$ and the estimates $\tilde{\omega}$.

Algorithm A (overview)

- **I**nput:
  - $v \in \mathbb{R}^m$ — coefficients of the linear functional $v \cdot \lambda$
  - $\tilde{\omega}$ — (noisy) oracle to Gibbs state observables
  - ε_0 — upper bound on the estimate of the noise
  - $\ell \in \mathbb{N}_+$ — level of the hierarchy
- **O**utput: Pair of numbers $a^{(\ell)}$, $b^{(\ell)}$

1. Evaluate $\tilde{\omega}$ on all operators of the form PQ and $P[E_\alpha, Q]$ for all $P, Q \in \mathcal{P}_{k,\ell}$ ($\mathcal{P}_{k,\ell}$ is a set of local Pauli operators defined in Definition 5.2.1) and $\alpha = 1, \ldots, m$ and collect the results in the matrices $\tilde{\boldsymbol{\Delta}}$ and $\tilde{\boldsymbol{H}}_\alpha$ according to Equations (5.11). Compute μ_1 and μ_2 according to Theorem 5.2.2.
2. Solve the semidefinite programs:

$$\underset{\lambda' \in \mathbb{R}^m}{\text{minimize/maximize}} \quad v \cdot \lambda' \tag{5.2}$$

$$\text{subject to} \quad \log\Big(\tilde{\boldsymbol{\Delta}}\Big) + \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha + \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \succeq -\mu_1, \tag{5.3}$$

$$\pm\, i \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha - \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \preceq \mu_2. \tag{5.4}$$

3. Return $a^{(\ell)}$ and $b^{(\ell)}$, the minimum and maximum values of the program respectively.

Figure 5.1: Algorithm to estimate parameters of local Hamiltonians from noisy observables of Gibbs states. We note that our presentation is slightly different from other works in Hamiltonian learning: instead of giving access to the copies of the state ρ, we have access to a noisy oracle computing expectation values of ρ. It is clear that having access to $O(\frac{1}{\varepsilon_0^2})$ copies of ρ, we can obtain an estimate of expectation values within ε_0 with high probability. We chose this presentation to avoid having probabilistic statements.

Algorithm B

Assume $\tilde{C} \succ 0$. Return the optimal parameters $\mu \in \mathbb{R}_{\geq 0}$, $\lambda' \in \mathbb{R}^m$ of the following program:

$$\underset{\substack{\lambda' \in \mathbb{R}^m \\ \mu \in \mathbb{R}}}{\text{minimize}} \qquad \mu \tag{5.33}$$

$$\text{subject to} \qquad \log\left(\tilde{\boldsymbol{\Delta}}\right) + \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha + \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \succeq -\mu, \tag{5.34}$$

$$\pm\, i \sum_{\alpha=1}^{m} \lambda'_\alpha (\tilde{\boldsymbol{H}}_\alpha - \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \preceq \mu. \tag{5.35}$$

The algorithm returns the putative Hamiltonian parameters $\lambda' \in \mathbb{R}^m$ and the parameter $\mu \geq 0$, which can be interpreted as a confidence parameter. A zero or near-zero value of μ indicates confidence that λ' are the true Hamiltonian parameters (a *positive result*) while a large value of μ indicates confidence that ρ is not the Gibbs state of any Hamiltonian in the span of $E_1, \dots, E_m$ (a *negative result*). Using Theorems 5.2.2, 5.2.3, and 5.2.4, we equip this algorithm with the following guarantees:

Theorem 5.2.6 (Guarantees for Algorithm B)**.** *Suppose the input state ρ is the Gibbs state of $h = \sum_\alpha \lambda_\alpha E_\alpha$ for some unknown coefficients $\lambda \in \mathbb{R}^m$ with $\max_{\alpha=1,\dots,m} |\lambda_\alpha| \leq \beta$, and let $\mu \in \mathbb{R}_{\geq 0}$ and $\lambda' \in \mathbb{R}^m$ be the output of Algorithm B. As before, let $K := 2r\|\tilde{C}^{-1}\|$.*

i) The algorithm is feasible and if $K \leq 1/\varepsilon_0$ returns $\mu \leq (2K^3 + 3m\beta K^2)\,\varepsilon_0$.

ii) If furthermore $P_1, \dots, P_r = \mathcal{P}_{k,\ell}$, with $\ell = \max(3, 1 + (1 + \mathfrak{d})^2)$ and h is commuting then there is an error threshold

$$\sigma = e^{-\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} m^{-6} \tag{5.36}$$

such that $\varepsilon_0 \leq \sigma$ implies $\sup_{\alpha=1,\dots,m} |\lambda'_\alpha - \lambda_\alpha| \leq \varepsilon_0/\sigma$.

Part *i*) is an a posteriori guarantee against *false negatives*: if $K \leq 1/\varepsilon_0$ then the program will never terminate with a value $\mu > (2K^3 + 3m\beta K^2)\,\varepsilon_0$ if the true Hamiltonian is in the span of $E_1, \dots, E_m$[2]. Part *ii*) and *iii*) show that

[2] Furthermore, a negative result is interpretable in terms of thermodynamic stability: the dual program produces Lindbladian that increases the entropy of ρ while keeping the expectation values of E_α fixed for all $\alpha = 1, \dots m$. This was shown in the noise-free case in [Art24].

the algorithm converges in the case of small systems (i.e. m constant) and commuting Hamiltonians, and that the convergence rate matches theoretical complexity bounds up to poly(m) factors.

5.3 Feasibility proofs

Now that we are finished stating the main results, we move on to the proofs. In this section we prove the main feasibility statements: Theorem 5.2.2 (a posteriori feasibility) and Theorem 5.2.3 (a priori feasibility). We will first prove a continuity bound for the matrix EEB inequality in terms of the condition number of the estimated correlation matrix $\tilde{C}$, and Theorem 5.2.2 will follow from the continuity bound and the matrix EEB inequality. Then Theorem 5.2.3 will follow from an *a priori* bound on the condition number of $\tilde{C}$.

Continuity of the matrix EEB constraint We begin with some elementary lemmas. A standard equivalence between finite-dimensional matrix norms goes as follows:

Lemma 5.3.1. *For an $n \times n$-matrix A*

$$\|A\| \leq n \max_{i,j} |a_{i,j}|. \tag{5.37}$$

We will make use of the following continuity bounds for matrix functions.

Lemma 5.3.2. *Let $A, B, \widetilde{A}, \widetilde{B}$ be matrices. Then*

i) If A and $\tilde{A}$ are positive definite then

$$\left\|\sqrt{A} - \sqrt{\tilde{A}}\right\| \leq \frac{\|A - \tilde{A}\|}{\|A^{-1/2}\|^{-1} + \|\tilde{A}^{-1/2}\|^{-1}} \tag{5.38}$$

and

$$\|\log(A) - \log(B)\| \leq \max\{\|A^{-1}\|, \|B^{-1}\|\}\|A - B\|. \tag{5.39}$$

ii) if A and B are invertible then

$$\|A^{-1} - B^{-1}\| \leq \|A^{-1}\|\|B^{-1}\|\|A - B\|. \tag{5.40}$$

iii)

$$\|AB - \widetilde{A}\widetilde{B}\| \leq \|A\|\|B - \widetilde{B}\| + \|\widetilde{B}\|\|A - \widetilde{A}\|. \tag{5.41}$$

Proof. Inequality (5.38) is proven in [Sch92, Lemma 2.2]. Inequality (5.39) follows from [Bha97, Theorem X.3.8]. The remaining inequalities are elementary from submultiplicativity and triangle inequality. □

Using the above lemmas, we will prove the main continuity bound:

Proposition 5.3.1 (Continuity bound for matrix EEB inequality)**.** *Let* $K := 2r\|\tilde{C}^{-1}\|$ *and suppose* $\varepsilon_0 \leq 1/K$*. Then we have*

$$\|\log \boldsymbol{\Delta} - \log \tilde{\boldsymbol{\Delta}}\| \leq 2K^3\varepsilon_0 \tag{5.42}$$

$$\|\boldsymbol{H}_\alpha - \tilde{\boldsymbol{H}}_\alpha\| \leq 3K^2\varepsilon_0. \tag{5.43}$$

Proof. By Lemma 5.3.1, the uniform bounds on measurement errors translate to the following error bounds on C and B_α:

$$\|C - \tilde{C}\| \leq r\varepsilon_0 \tag{5.44}$$

$$\|B_\alpha - \tilde{B}_\alpha\| \leq r\varepsilon_0. \tag{5.45}$$

Since $\epsilon_0 \leq 1/K$, Lemma 5.3.1 gives

$$C \succeq \tilde{C} - \|C - \tilde{C}\| \succeq \frac{2r}{K} - r\varepsilon_0 \succeq \frac{r}{K} \tag{5.46}$$

and so $\max(\|C^{-1}\|, \|\tilde{C}^{-1}\|) \leq K/r$. We also have $\|C\|, \|\tilde{C}\| \leq r$ and $\|B_\alpha\|, \|\tilde{B}_\alpha\| \leq 2r$ (using the assumptions (5.16) and (5.18) for the bounds on $\|\tilde{C}\|$ and $\|\tilde{B}_\alpha\|$). Using Lemma 5.3.2, we have

$$\|\boldsymbol{\Delta} - \tilde{\boldsymbol{\Delta}}\| \leq \|C^{-1/2} - \tilde{C}^{-1/2}\|(\|C\|\|C^{-1/2}\| + \|\tilde{C}\|\|\tilde{C}^{-1/2}\|) + \|C - \tilde{C}\|\|C^{-1/2}\|\|\tilde{C}^{-1/2}\| \tag{5.47}$$

$$\leq \|C - \tilde{C}\| \left(\frac{\|C\|\|C^{-1}\|\|\tilde{C}^{-1/2}\| + \|\tilde{C}\|\|\tilde{C}^{-1}\|\|C^{-1/2}\|}{\|C^{-1/2}\|^{-1} + \|\tilde{C}^{-1/2}\|^{-1}} + \|C^{-1/2}\|\|\tilde{C}^{-1/2}\| \right) \tag{5.48}$$

$$\leq \left(K^2 + K\right)\varepsilon_0 \tag{5.49}$$

$$\leq 2K^2\varepsilon_0, \tag{5.50}$$

where in the last line we used the fact that $K \geq 2r\operatorname{Tr}\left(\tilde{C}^{-1}\right) \geq 2r/\operatorname{Tr}\left(\tilde{C}\right) = 2 \geq 1$. The bounds $r/K \preceq C \preceq r$ (resp. $r/K \preceq \tilde{C} \preceq r$) imply that $\|\boldsymbol{\Delta}^{-1}\| \leq K$

(resp. $\| \tilde{\boldsymbol{\Delta}}^{-1} \| \le K$), which gives (5.42). Finally, a similar calculation gives (5.43):

$$\| \boldsymbol{H}_\alpha - \tilde{\boldsymbol{H}}_\alpha\| \le \|C - \tilde{C}\| \frac{\|B_\alpha\|\|C^{-1}\|\|\tilde{C}^{-1/2}\| + \|\tilde{B}_\alpha\|\|\tilde{C}^{-1}\|\|C^{-1/2}\|}{\|C^{-1/2}\|^{-1} + \|\tilde{C}^{-1/2}\|^{-1}} + \|B_\alpha - \tilde{B}_\alpha\|\|C^{-1/2}\|\|\tilde{C}^{-1/2}\| \tag{5.51}$$

$$\le (2K^2 + K)\varepsilon_0 \tag{5.52}$$

$$\le 3K^2\varepsilon_0. \tag{5.53}$$

□

Theorem 5.2.2 then follows immediately from Proposition 5.3.1 and the matrix EEB inequality (Theorem 5.2.1).

Proof of Theorem 5.2.3 This will follow from a lower bound on the local marginals of Gibbs states that was first proven in [Ans+21]. We use a form of this bound that was given in [Bak+23]:

Lemma 5.3.3 ([Bak+23, Corollary 2.14])**.** *Let E_α be k-local Paulis such that the Hamiltonian is k-$\mathfrak{d}$-low intersection and let $P_1, \ldots, P_r$ be distinct operators in $P_{k,\ell}$. There exist constants $\mathcal{C}_{k,\mathfrak{d},\ell}, \mathcal{D}_{k,\mathfrak{d},\ell}$ depending only $k, \mathfrak{d}\, \ell$ such that*

$$C \succeq \exp(-\mathcal{C}_{k,\mathfrak{d},\ell}\beta - \mathcal{D}_{k,\mathfrak{d},\ell})/r. \tag{5.54}$$

With this ingredient at hand we proceed to prove Theorem 5.2.3.

Set $\sigma := \exp(-\mathcal{C}_{k,\mathfrak{d},\ell}\beta - \mathcal{D}_{k,\mathfrak{d},\ell})/4r^2$ and suppose $\varepsilon_0 \le \sigma$. Then by Lemma 5.3.1 we have

$$\|\tilde{C} - C\| \le r\varepsilon_0 \tag{5.55}$$

$$\le \exp(-\mathcal{C}_{k,\mathfrak{d},\ell}\beta - \mathcal{D}_{k,\mathfrak{d},\ell})/2r. \tag{5.56}$$

By Lemma 5.3.3 we get $\tilde{C} \succeq \exp(-\mathcal{C}_{k,\mathfrak{d},\ell}\beta - \mathcal{D}_{k,\mathfrak{d},\ell})/2r = 2r\sigma$, and so $K = 2r\|\tilde{C}^{-1}\| \le 1/\sigma$. □

5.4 Convergence proofs

In this section we take on the proof of the main convergence guarantee, Theorem 5.2.4. The proof will crucially use some basic concepts from modular theory, which we recall now.

Modular theory

Consider a quantum system described by a finite-dimensional Hilbert space $\mathcal{H}$. In this section we will, as a rule, use lowercase letters for elements of $\mathcal{B}(\mathcal{H})$ and uppercase letters for operators $\mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ (sometimes called superoperators). Define a *state* as a complex-linear map $\omega : \mathcal{B}(\mathcal{H}) \to \mathbb{C}$ satisfying $\omega(1) = 1$ and $\omega(a^*a) \geq 0$ for every $a \in \mathcal{B}(H)$. These are in one-to-one correspondence with density matrices, i.e., positive-semidefinite trace-one operators ρ, via $\omega(a) = \mathrm{Tr}(\rho a)$ for any $a \in \mathcal{B}(H)$. A state ω is called *faithful* if $\omega(a^*a) > 0$ for every nonzero a, or equivalently, if its density matrix is positive-definite. This is the case for Gibbs states. For a faithful state ω, the inner product $\langle a|b\rangle := \omega(a^*b)$ is known as the *Gelfand-Naimark-Segal (GNS)* inner product, and endows $\mathcal{B}(\mathcal{H})$ with the structure of a Hilbert space [BR87]. We refer to an operator $a \in \mathcal{B}(\mathcal{H})$ as $|a\rangle$ when thought of a vector in this Hilbert space.

The $*$-operation $S : |a\rangle \to |a^*\rangle$ is an antilinear involution on $\mathcal{B}(\mathcal{H})$. Consider its polar decomposition[3]:

$$S = J\Delta^{1/2} = \Delta^{-1/2}J, \tag{5.57}$$

where $\Delta := S^\dagger S$ is positive-definite and $J := S\Delta^{-1/2}$ is anti-unitary. It is simple to check[4] that $\langle a|\Delta|b\rangle = \omega(ba^*)$ for every $a, b \in \mathcal{B}(\mathcal{H})$ and that Δ acts on any $|a\rangle \in \mathcal{B}(\mathcal{H})$ by

$$\Delta|a\rangle = |\rho a \rho^{-1}\rangle \tag{5.58}$$

$$\log(\Delta)|a\rangle = |[\log(\rho), h]\rangle. \tag{5.59}$$

By Lemma 5.5.1 in Section 5.5, the operators Δ and J satisfy

$$J\log(\Delta)J = -\log(\Delta). \tag{5.60}$$

If $h \in \mathcal{B}(\mathcal{H})$ is self-adjoint we denote by $H \in \mathcal{B}(\mathcal{H}_\omega)$ the operator $H : |a\rangle \mapsto |[h, a]\rangle$. We call it the GNS Hamiltonian corresponding to h. Note that even though h is hermitian, H in general is not. In fact, H is hermitian iff h is a *symmetry* of ω:

[3] Polar decomposition of antilinear operators is discussed in Section 5.5

[4] Recall the adjoint of an antilinear operator T is defined by the relation $\langle u|T^\dagger v\rangle := \overline{\langle Tu|v\rangle}$ for all vectors u and v.

Lemma 5.4.1. *Let $h \in \mathcal{B}(\mathcal{H})$ be hermitian and let $H : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be its GNS Hamiltonian. The following are equivalent:*

i) H *is hermitian.*

ii) $JHJ = -H$.

iii) $[h, \rho] = 0$.

Proof. *i)* $\iff$ *iii)*. It is easy to check that $\langle a|H - H^\dagger|a\rangle = \omega([h, a^*a])$ for any $a \in \mathcal{B}(\mathcal{H})$. Thus $H^\dagger = H$ iff $\mathrm{Tr}(\rho[h, a^*a]) = \mathrm{Tr}(a^*a[\rho, h]) = 0$ for all $a \in \mathcal{B}(\mathcal{H})$, which is equivalent to $[\rho, h] = 0$.

ii) $\iff$ *iii)*. It is easy to check that $SHS = -H$. By (5.58) we have $H + JHJ = H - \Delta^{1/2}H\Delta^{-1/2}$ which takes $|a\rangle \in \mathcal{B}(\mathcal{H})$ to $|[h - \rho^{1/2}h\rho^{-1/2}, a]\rangle$. Thus $H + JHJ = 0$ iff $h - \rho^{1/2}h\rho^{-1/2}$ is a multiple of the identity. But $\mathrm{Tr}\big(h - \rho^{1/2}h\rho^{-1/2}\big) = 0$ and so this can only happen when $[h, \rho^{1/2}] = 0$, which is equivalent to $[h, \rho] = 0$. □

The next lemma bounds the norm of the GNS Hamiltonian of a symmetry:

Lemma 5.4.2. *If $[\rho, h] = 0$ then the GNS Hamiltonian H of h satisfies*

$$\|H\|_{gns} \leq 2\|h\|. \tag{5.61}$$

In the above, we write $\|H\|_{gns}$ to indicate that this refers to the norm of H, which is an operator on the GNS Hilbert space $\mathcal{B}(\mathcal{H})$, while $\|h\|$ refers to the norm of h, which is an operator on the physical Hilbert space $\mathcal{H}$.

Proof. Denote the eigenbasis of h (in $\mathcal{H}$) by $h\psi_i = e_i\psi_i$. Then, an eigenbasis of H can be written as $|a_{ij}\rangle = |\psi_i\psi_j^*\rangle$, i.e., $H|a_{ij}\rangle = (e_i - e_j)|a_{ij}\rangle$. Since $[\rho, h] = 0$, H is hermitian, and so its operator norm can be bounded from its eigenvalues as $\|H\| \leq \max_{i,j}|e_i - e_j| \leq 2\|h\|$. □

A fundamental result in modular theory relates the modular operator Δ to the GNS Hamiltonian H:

Lemma 5.4.3. *Let $h \in \mathcal{B}(\mathcal{H})$ be hermitian. Then the following are equivalent:*

i) $\log(\Delta) + H \succeq 0$.

ii) $\log(\Delta) + H = 0$.

iii) $\rho = e^{-h}/\operatorname{Tr}\big(e^{-h}\big)$.

Proof. $i) \iff ii)$. Since $\log(\Delta)$ is automatically Hermitian, $i)$ implies $H^\dagger = H$, and so $JHJ = -H$, and so

$$0 \preceq J(\log(\Delta) + H)J \tag{5.62}$$

$$= -\log(\Delta) - H \tag{5.63}$$

which implies $ii)$. The inverse implication is obvious.

$ii) \iff iii)$. By (5.59), $ii)$ holds if and only if $\log(\rho) - h$ is a multiple of the identity, which is equivalent to $iii)$. □

Restricted GNS space

As we will show, our choice of perturbing operators selects a subspace of the GNS space, and the matrices appearing in the matrix EEB inequality are naturally interpreted as operators acting on this subspace. Let $P_1 \ldots, P_r \in \mathcal{B}(\mathcal{H})$ be a set of selfadjoint operators and let $h' \in \mathcal{B}(\mathcal{H})$ be hermitian. Define the $r \times r$ matrices

$$\boldsymbol{\Delta} := C^{-1/2} C^T C^{-1/2} \tag{5.64}$$

$$\boldsymbol{H'} := C^{-1/2} B' C^{-1/2}, \tag{5.65}$$

where $C_{ij} := \omega(P_i P_j)$ and $B'_{ij} := \omega(P_i[h', P_j])$. Define $|a_i\rangle := \sum_{i=1}^r (C^{-1/2})_{ij} |P_j\rangle$ for $i = 1, \ldots r$. It is easy to check that the vectors $|a_i\rangle$ form a basis of $\mathcal{P} := \operatorname{span}\{P_1, \ldots, P_r\}$ that is *orthonormal* in the GNS inner product, and that we have

$$\boldsymbol{\Delta}_{ij} := \langle a_i | \Delta | a_j \rangle \tag{5.66}$$

$$\boldsymbol{H'}_{ij} := \langle a_i | H' | a_j \rangle, \tag{5.67}$$

where H' is the GNS Hamiltonian of h'. Thus, with some abuse of notation we may write

$$\boldsymbol{\Delta} = Q \Delta Q \tag{5.68}$$

$$\boldsymbol{H'} = Q H' Q, \tag{5.69}$$

where $Q : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is the orthogonal projection onto $\mathcal{P}$. We also define the restricted $*$-operation $\boldsymbol{S}$ as

$$\boldsymbol{S} := QSQ, \tag{5.70}$$

which can equivalently be defined in terms of the correlation matrix C as $\boldsymbol{S} = C^{-1/2}\left(\overline{C}\right)^{-1/2}$, where $\overline{C}$ is the complex conjugate of C. Finally, we will use an operator $\boldsymbol{J}$, which is defined as

$$\boldsymbol{J} := \boldsymbol{S}\,\boldsymbol{\Delta}^{-1/2}. \tag{5.71}$$

It is important to stress that unlike $\boldsymbol{\Delta}$, $\boldsymbol{H}$, and $\boldsymbol{S}$, it turns out that the operator $\boldsymbol{J}$ is *not* simply the restriction of J to the span of $P_1, \ldots, P_r$, i.e. $\boldsymbol{J} \neq QJQ$. Instead, one can check that $\boldsymbol{\Delta} = \boldsymbol{S}^\dagger\,\boldsymbol{S}$ and it follows that $\boldsymbol{J}$ is the anti-unitary part in the polar decomposition of $\boldsymbol{S}$. Since $\boldsymbol{S}$ is an antilinear involution just like S, Lemma 5.5.1 gives

$$\boldsymbol{J}^2 = \mathbf{1}, \qquad \boldsymbol{J}^\dagger = \boldsymbol{J} \tag{5.72}$$

$$\boldsymbol{J}\,\boldsymbol{\Delta}\,\boldsymbol{J} = \boldsymbol{\Delta}^{-1}, \qquad \boldsymbol{J}\,\boldsymbol{\Delta}^{1/2}\,\boldsymbol{J} = \boldsymbol{\Delta}^{-1/2} \tag{5.73}$$

$$\boldsymbol{J}\log(\boldsymbol{\Delta})\,\boldsymbol{J} = -\log(\boldsymbol{\Delta}). \tag{5.74}$$

Proof of Theorem 5.2.4

In this section, we prove our main convergence theorem for commuting Hamiltonians. Fix $k, \mathfrak{d} > 0$ and suppose $E_1, \ldots E_m$ are k-supported Paulis with $\mathfrak{d}$-low-intersection. Fix $\ell > 0$, and let $P_1, \ldots P_r := \mathcal{P}_{k,\ell}$. Suppose ρ is the Gibbs state of a Hamiltonian $h = \sum_\alpha \lambda_\alpha E_\alpha$ for some parameters $\lambda \in \mathbb{R}^m$ with $\max_{\alpha=1,\ldots,m} |\lambda_\alpha| \leq \beta$. We do not assume that h is commuting throughout. Instead, we will state explicitly in the statement of each Lemma/Proposition/Theorem if we assume that h is commuting. Throughout this section $\lambda' \in \mathbb{R}^m$ will refer to an arbitray vector of parameters. We will write $h' = \sum_\alpha \lambda'_\alpha E_\alpha$ and H' for its GNS Hamiltonian. Finally, we will use the shorthand notations

$$\boldsymbol{H}' = \sum_{\alpha=1}^m \lambda'_\alpha\,\boldsymbol{H}_\alpha \quad \text{and} \quad \boldsymbol{H} = \sum_{\alpha=1}^m \lambda_\alpha\,\boldsymbol{H}_\alpha,$$

where $\boldsymbol{H}_\alpha$ are the $r \times r$ matrices defined in (5.11).

Let us now give an overview of the proof. The bulk of the proof will boil down to establishing convergence of the *relaxed* EEB constraints, for the *exact* expectation values, i.e. with no measurement noise. For each Hamiltonian parameter, the proof first identifies local witnesses of deviations: local operators a such that $\langle a| \boldsymbol{H}' - \boldsymbol{H} |a\rangle$ detects the difference in Hamiltonian parameters $|\lambda_\alpha - \lambda'_\alpha|$ for a given $\alpha = 1, \ldots, m$. While Lemma 5.4.1 above shows that $H'^\dagger = H'$ is equivalent to $JH'J = -H'$, we only enforce $\boldsymbol{H}^\dagger = \boldsymbol{H}$ up to some error, and in Lemma 5.4.7 and Corollary 5.4.1 we show that this gives an approximate version of $\boldsymbol{J}\,\boldsymbol{H}'\,\boldsymbol{J} = -\,\boldsymbol{H}'$. A crucial ingredient is the fact that the time-evolution, and thereby the J operation, for commuting Hamiltonians maps local operators to exactly local operators, preventing them from leaving the restricted GNS space, see Lemma 5.4.9. Using an antisymmetry argument based on the one in Lemma 5.4.3 find the desired bound on matrix elements of $H - H'$ (Proposition 5.4.1), which conclude the proof for the noiseless case. Finally, we prove Theorem 5.2.4 from the noiseless case via the continuity bounds proved in Section 5.3.

We begin with a bound on r, the number of perturbing operators, which has been shown in [Bak+23].

Lemma 5.4.4 ([Bak+23, Corollary 2.20])**.** *The size of the set $\mathcal{P}_{k,\ell}$ is bounded by $m\,\mathfrak{d}^\ell\,10^{k\ell}$.*

Since our constraints work with the GNS-Hamiltonian we need to relate its matrix elements to the coefficients of its parent Hamiltonian to witness large errors in the output parameters. The following Lemma achieves this and furthermore singles out one coefficient, which is needed to achieve bounds uniformly.

Lemma 5.4.5 (Local identifiability of Hamiltonian terms)**.** *Suppose $\ell \geq 1+\mathfrak{d}$. For each Hamiltonian coefficient λ_α, there are k-$(1+\mathfrak{d})$-$\mathfrak{G}$-supported operators a_1, a_2, a_3, a_4 with $\|a_i\| \leq e^{\mathcal{O}_{k,\mathfrak{d}}(\beta)}$ and*

$$|\lambda_\alpha - \lambda'_\alpha| = \left|\sum_{i=1}^{4} \langle a_i|\, \boldsymbol{H} - \boldsymbol{H}'\, |a_i\rangle\right|.$$

Proof. Recall from [Bak+23, Lemma 9.8] that there are a', b such that $\|a\| = \|b\| = 1$, $\mathrm{supp}(a') = \mathrm{supp}(b) = \mathrm{supp}(E_\alpha)$[5] and

$$\left|\frac{1}{2}\,\mathrm{tr}([h - h', b]a')\right| = |\lambda_\alpha - \lambda'_\alpha|$$

[5]The statement of the Lemma in the reference is slightly weaker, but the argument of the proof directly yields this stronger constraint on the supports.

by denoting by $\overline{\rho}$ the marginal of the Gibbs state ω on the union of supports of $[h-h',b]$ and a', by $D_{\overline{\rho}}$ the dimension of this support, and defining $a = a'(\overline{\rho}D_{\overline{\rho}})^{-1}$ we have

$$|\lambda_\alpha - \lambda'_a| = \left|\frac{1}{2}\operatorname{tr}([h-h',b]a\overline{\rho}D_{\overline{\rho}})\right| \tag{5.75}$$

$$= \frac{1}{2}|\omega([h-h',b]a)| \tag{5.76}$$

$$= \frac{1}{2}|\langle a|H-H'|b\rangle| \tag{5.77}$$

$$= \frac{1}{2}|\langle a|\,\boldsymbol{H}-\boldsymbol{H}'\,|b\rangle|, \tag{5.78}$$

where the last line is because $\ell \geq 1+\mathfrak{d}$. Then by the "no small local marginals" result [Bak+23, Corollary 2.14] or concretely the formulation in terms of density matrices [FFS23, Lemma 3.8], we have $\|a\| \leq \exp(\mathcal{O}_{k,\mathfrak{d}}(\beta))$. Note that a and b are both supported on the union of $\operatorname{supp}(E_\alpha)$ and all $\operatorname{supp}(E_{\alpha'})$ intersecting with $\operatorname{supp}(E_\alpha)$. In particular, any linear combination of a and b is k-($\mathfrak{d}$ +1)-$\mathfrak{G}$-supported.

Applying the polarization identity to (5.78) gives

$$|\lambda_\alpha - \lambda'_\alpha| = \frac{1}{2}\,|\langle a|\,\boldsymbol{H}-\boldsymbol{H}'\,|b\rangle| \tag{5.79}$$

$$= \left|\frac{1}{8}\sum_{n=1}^{4}\langle a+i^n b|\,\boldsymbol{H}-\boldsymbol{H}'\,|a+i^n b\rangle\right|. \tag{5.80}$$

□

The hermiticity of the GNS-Hamiltonian is equivalent to a stationary condition of the state (see Lemma 5.4.1). As part of our constraint system we enforce approximate hermiticity for its measured version. The following Lemma leverages this constraint to prove that h' approximately commutes with h and with $\rho^{1/2}$.

Lemma 5.4.6. *Suppose $\ell \geq 3$ and suppose $h' = \sum_{\alpha=1}^m \lambda'_\alpha E_\alpha$ satisfies $\|\,\boldsymbol{H}' - (\boldsymbol{H}')^\dagger\| \leq \mu$. Then we have*

$$\|H|h'\rangle\|_{gns} \leq m\beta\mu \tag{5.81}$$

$$\|\Delta^{1/2}|h'\rangle - |h'\rangle\|_{gns} \leq \frac{1}{2}(m\beta)^{1/2}\mu. \tag{5.82}$$

Proof. It is easy to check that for k-ℓ-$\mathfrak{G}$-local operators a, b we have

$$|\langle a|H' - H'^{\dagger}|b\rangle| = |\langle a|\, \boldsymbol{H'} - (\boldsymbol{H'})^{\dagger}|b\rangle| \tag{5.83}$$

$$\leq \mu \||a\rangle\|_{gns} \||b\rangle\|_{gns}. \tag{5.84}$$

Since $\ell \geq 3$, setting $|a\rangle = |1\rangle$ and $|b\rangle = |[h, h']\rangle = H|h'\rangle$ we have

$$|\langle 1|H'H|h'\rangle| = |\langle 1|(H' - H'^{\dagger})H|h'\rangle| \tag{5.85}$$

$$\leq \mu \|H|h'\rangle\|_{gns} \tag{5.86}$$

since $H'|1\rangle = 0$. An elementary calculation using the fact that $\omega([h, a]) = 0$ for all $a \in \mathcal{B}(\mathcal{H})$ shows that $\langle 1|H'H|h'\rangle = 2\langle h'|H|h'\rangle$ and so

$$\langle h'|H|h'\rangle \leq \frac{1}{2}\mu \|H|h'\rangle\|_{gns}. \tag{5.87}$$

Using the above inequality with Lemma 5.4.2 and using the fact that $\|h\| \leq m\beta$, we have

$$\|H|h'\rangle\|_{gns}^2 = \langle h'|H^2|h'\rangle \tag{5.88}$$

$$\leq 2m\beta \langle h'|H|h'\rangle \tag{5.89}$$

$$\leq m\beta\mu \|H|h'\rangle\|_{gns}, \tag{5.90}$$

which proves (5.81). For (5.82), using $\Delta = e^{-H}$ we write

$$\|\Delta^{1/2}|h'\rangle - |h'\rangle\|_{gns}^2 = \langle h'|(e^{-H/2} - 1)^2|h'\rangle. \tag{5.91}$$

For any $x \in \mathbb{R}$ we have

$$(e^{x/2} - 1)^2 = \left(\frac{\tanh(x/4)}{x}\right) x(e^x - 1) \leq \frac{x(e^x - 1)}{4} \tag{5.92}$$

replacing x with $-H$ using the functional calculus we may continue (5.91) as follows:

$$\|\Delta^{1/2}|h'\rangle - |h'\rangle\|_{gns}^2 \leq \frac{1}{4}\langle h'|H(1 - e^{-H})|h'\rangle \tag{5.93}$$

$$= \frac{1}{4}\left(\langle h'|H|h'\rangle - \langle h'|H\Delta|h'\rangle\right) \tag{5.94}$$

$$= \frac{1}{4}\left(\langle h'|H|h'\rangle - \langle h'|[h, h']^*\rangle\right) \tag{5.95}$$

$$= \frac{1}{2}\langle h'|H|h'\rangle \tag{5.96}$$

$$\leq \frac{1}{4} m\beta\mu^2. \tag{5.97}$$

□

Lemma 5.4.7. *Suppose $\ell \geq 3$, and let h' be a Hamiltonian with $\| \boldsymbol{H}' - (\boldsymbol{H}')^\dagger \| \leq \mu$ for some $\mu > 0$. Suppose a is an operator such that $\|\rho a \rho^{-1}\| \leq \mathcal{D} \|a\|$ for some $\mathcal{D} > 0$. Then*

$$| \langle a| \, JH'J + H' \, |a\rangle \, | \leq \frac{1}{2} \|a\|^2 (\mathcal{D} + 1)(m\beta)^{1/2}\mu. \tag{5.98}$$

Proof. It is easy to check that $SH'S = -H'$. Indeed, for any $a \in \mathcal{B}(\mathcal{H})$ we have

$$SHS|a\rangle = |[h, a^*]^*\rangle = -|[h, a]\rangle. \tag{5.99}$$

Therefore,

$$\begin{aligned} \langle a| \, JH'J \, |a\rangle &= \langle a| \, \Delta^{1/2} SH'S \Delta^{-1/2} \, |a\rangle \\ &= - \langle a| \, \Delta^{1/2} H' \Delta^{-1/2} \, |a\rangle \end{aligned}$$

and so it suffices to bound the magnitude of $\langle a|\Delta^{1/2}H'\Delta^{-1/2} - H'|a\rangle$. Writing this quantity in terms of operators on the physical Hilbert space and using the identities $\Delta^{1/2}|a\rangle = |\rho^{1/2} a \rho^{-1/2}\rangle$, $\omega(ab) = \omega(b(\rho a \rho^{-1})) = \omega((\rho^{-1} b \rho)a)$, and $\omega(\rho^{-1/2} a \rho^{1/2}) = \omega(a)$, we have

$$\langle a|\Delta^{1/2}H'\Delta^{-1/2} - H'|a\rangle = \omega((\rho^{1/2} a \rho^{-1/2})^* [h', \rho^{-1/2} a \rho^{1/2}]) - \omega(a^*[h', a]) \tag{5.100}$$

$$= \omega(\rho^{-1/2} a^* \rho^{1/2} h' \rho^{-1/2} a \rho^{1/2}) - \omega(\rho^{-1/2} a^* a \rho^{1/2} h') - \omega(a^*[h', a]) \tag{5.101}$$

$$= \omega(\rho^{-1} a \rho a^* \rho^{1/2} h' \rho^{-1/2}) - \omega(\rho^{-1/2} a^* a \rho^{1/2} h') - \omega(\rho^{-1} a \rho a^* h') + \omega(a^* a h') \tag{5.102}$$

$$= \omega((\rho^{-1} a \rho a^* - a^* a)(\rho^{1/2} h' \rho^{-1/2} - h')) \tag{5.103}$$

$$= \langle a \rho a^* \rho^{-1} - a^* a | \rho^{1/2} h' \rho^{-1/2} - h' \rangle. \tag{5.104}$$

By the Cauchy-Schwartz inequality and Lemma 5.4.6 we get

$$\begin{aligned} |\langle a|\Delta^{1/2}H'\Delta^{-1/2} - H'|a\rangle| &\leq \frac{1}{2}(m\beta)^{1/2}\mu \| |a \rho a^* \rho^{-1} - a^* a\rangle \|_{gns} && (5.105) \\ &\leq \frac{1}{2}(m\beta)^{1/2}\mu \left(\|a \rho a^* \rho^{-1}\| + \|a^* a\| \| \right) && (5.106) \\ &\leq \frac{1}{2}\|a\|^2 (\mathcal{D} + 1)(m\beta)^{1/2}\mu. && (5.107) \end{aligned}$$

□

Lemma 5.4.8. *Suppose h is commuting as in Definition 5.2.2. Then for any k-ℓ'-$\mathfrak{G}$-supported operator a we have*

$$\|\rho a\rho^{-1}\| \leq e^{2\mathcal{C}\beta(1+\mathfrak{d})\ell'}\|a\|. \tag{5.108}$$

Proof. Since a is k-ℓ'-$\mathfrak{G}$-supported there is a set $L \subset \{1,\ldots,m\}$ with $|L| = \ell'$ such that $\mathrm{supp}(a) \subset \bigcup_{\alpha\in L}\mathrm{supp}(E_\alpha)$. Let $\tilde{L}$ be the set of $\alpha \in \{1,\ldots,m\}$ for which there is an $\alpha' \in L$ with $\mathrm{supp}(E_\alpha)\cap\mathrm{supp}(E_{\alpha'}) \neq \varnothing\}$. Then $|\tilde{L}| \leq (1+\mathfrak{d})\ell'$. Let $\tilde{h} = \sum_{\alpha\in\tilde{L}}\nu_\alpha F_\alpha$. Then $\|\tilde{h}\| \leq \mathcal{C}\beta(\mathfrak{d}+1)\ell'$ and so

$$\|\rho a\rho^{-1}\| = \|e^{-\tilde{h}}ae^{\tilde{h}}\| \tag{5.109}$$

$$\leq \|a\|e^{2\mathcal{C}\beta(\mathfrak{d}+1)\ell'}. \tag{5.110}$$

□

The following Lemma relates Δ and J to their local counterparts in a strong way. It is based on the commuting Hamiltonian assumption, exploiting the fact that the complex time-evolution operator of commuting Hamiltonians maps local observables to strictly local observables.

Lemma 5.4.9. *Suppose h is commuting.*

1. *For any $\ell' > 0$, any k-ℓ'-$\mathfrak{G}$-supported operator a, and any nonnegative integer p, the operator $\Delta^p|a\rangle$ is k-$(1+\mathfrak{d})\ell'$-$\mathfrak{G}$-supported.*

2. *For any $\ell' \leq \ell/(1+\mathfrak{d})$, any k-ℓ'-$\mathfrak{G}$-supported a, and any nonnegative integer p we have*

$$\Delta^p|a\rangle = \boldsymbol{\Delta}^p|a\rangle. \tag{5.111}$$

3. *For any $\ell' \leq \ell/(1+\mathfrak{d})$ and any k-ℓ'-$\mathfrak{G}$-supported a we have*

$$\Delta^{1/2}|a\rangle = \boldsymbol{\Delta}^{1/2}|a\rangle \tag{5.112}$$

$$J|a\rangle = \boldsymbol{J}\,|a\rangle. \tag{5.113}$$

Proof. 1.
We have to consider the operator

$$e^{-ph}ae^{ph}.$$

We can define the set A of indices such that $[F_\alpha, a] = 0$ for all $\alpha \in A$ such that

$$
\begin{aligned}
e^{-ph} a e^{ph} &= e^{-p\sum_{\alpha\in A^c}\nu_\alpha F_\alpha} a e^{-p\sum_{\alpha\in A}\nu_\alpha F_\alpha} e^{p\sum_{\alpha\in A}\nu_\alpha F_\alpha} e^{p\sum_{\alpha\in A^c}\nu_\alpha F_\alpha} \\
&= e^{-p\sum_{\alpha\in A^c}\nu_\alpha F_\alpha} a e^{p\sum_{\alpha\in A^c}\nu_\alpha F_\alpha}.
\end{aligned}
$$

By the definition of k-ℓ'-$\mathfrak{G}$-locality, the operator a is supported on $\bigcup_{\alpha\in S} E_\alpha$ for some connected S with $|S| \leq \ell'$. Since all terms F_α for $\alpha \in A^c$ have overlapping support with $\mathrm{supp}(a)$, all terms in the above equation have support in $\bigcup\{\mathrm{supp}(E_\alpha) | \exists \alpha' \text{ s.t. } \mathrm{supp}(E_\alpha) \cap \mathrm{supp}(E_{\alpha'}) \neq \emptyset\}$, which is the union of at most $(1+\mathfrak{d})\cdot \ell'$ connected supports and thereby k-$(1+\mathfrak{d})\ell'$-$\mathfrak{G}$-local.

2.

The case $p = 0$ is trivial and we prove the cases $p > 0$ by induction. Write $Q : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ for the orthogonal (in the GNS inner product) projection onto $\mathrm{span}\{P_1, \ldots, P_r\} \subset \mathcal{B}(\mathcal{H})$. Notice that for any ℓ-supported operator $b \in \mathcal{B}(\mathcal{H})$ we have $Q|b\rangle = |b\rangle$. The induction then follows from

$$
\begin{aligned}
\boldsymbol{\Delta}^{p+1}|a\rangle &= Q\Delta Q \boldsymbol{\Delta}^p |a\rangle && (5.114)\\
&= Q\Delta Q \Delta^p |a\rangle && (5.115)\\
&= Q\Delta^{p+1}|a\rangle && (5.116)\\
&= \Delta^{p+1}|a\rangle. && (5.117)
\end{aligned}
$$

The second line is by the inductive hypothesis, and the third and fourth lines are by part 1.

3.

Let $x_0 = \max\{\|\Delta\|, \|\boldsymbol{\Delta}\|\}$ and $x^{1/2} = \sum_{k=0}^\infty a_k (x_0 - x)^k$ be the Taylor series for the square root. By part 2, we have

$$
\begin{aligned}
\Delta^{1/2}|a\rangle &= \sum_{k=0}^{\infty} a_k (x_0 - \Delta)^k |a\rangle && (5.118)\\
&= \sum_{k=0}^{\infty} a_k (x_0 - \boldsymbol{\Delta})^k |a\rangle && (5.119)\\
&= \boldsymbol{\Delta}^{1/2}|a\rangle. && (5.120)
\end{aligned}
$$

The second statement then follows from $\boldsymbol{J} = \boldsymbol{\Delta}^{1/2}\, \boldsymbol{S}$. □

Corollary 5.4.1. *Suppose $\ell \geq 3$ and that h is commuting. Let h' be a Hamiltonian with $\|\, \boldsymbol{H'} - \boldsymbol{H'}^\dagger \,\| \leq \mu$ for some $\mu \geq 0$. Let a be k-ℓ'-$\mathfrak{G}$-supported for some $\ell' \leq (\ell-1)/(1+\mathfrak{d})$. Then,*

$$
|\,\langle a|\, \boldsymbol{J}\, \boldsymbol{H'}\, \boldsymbol{J} + \boldsymbol{H'}\, |a\rangle\,| \leq \frac{1}{2}\|a\|^2 (e^{2\mathcal{C}\beta(\mathfrak{d}+1)\ell'} + 1)(m\beta)^{1/2}\mu. \qquad (5.121)
$$

Proof. Note that by Lemma 5.4.9, $\boldsymbol{J}\,|a\rangle$ is k-$\ell'(1+\mathfrak{d})$-$\mathfrak{G}$-supported. Using that H increases the locality by one and Lemmas 5.4.7 and 5.4.8, we have

$$\begin{aligned}|\langle a|\,\boldsymbol{J}\,\boldsymbol{H}'\,\boldsymbol{J}+\boldsymbol{H}'|a\rangle &= |\langle a|\,\boldsymbol{J}\,H'\,\boldsymbol{J}+H'|a\rangle & (5.122)\\ &= |\langle a|JH'J+H'|a\rangle & (5.123)\\ &\leq \frac{1}{2}\|a\|^2(e^{2\mathcal{C}\beta(\mathfrak{d}+1)\ell'}+1)(m\beta)^{1/2}\mu. & (5.124)\end{aligned}$$

□

Proposition 5.4.1. *Suppose for some* $\mu_1,\mu_2\geq 0$ *that* h' *satisfies*

$$\log(\boldsymbol{\Delta})+\sum_\alpha \lambda'_\alpha(\boldsymbol{H}_\alpha+\boldsymbol{H}_\alpha^\dagger)/2\geq -\mu_1 \tag{5.125}$$

$$\pm i\sum_\alpha \lambda'_\alpha(\boldsymbol{H}_\alpha-\boldsymbol{H}_\alpha^\dagger)/2\leq \mu_2 \tag{5.126}$$

and let $a\in\mathcal{B}(\mathcal{H})$ *be an operator with*

$$\langle a|\,\boldsymbol{H}+\boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J}\,|a\rangle=0 \tag{5.127}$$

$$\mathrm{Re}\,(\langle a|\,\boldsymbol{H}'+\boldsymbol{J}\,\boldsymbol{H}'\,\boldsymbol{J}\,|a\rangle)\leq\delta\|a\|^2 \tag{5.128}$$

for some $\delta\geq 0$*. Then*

$$|\langle a|\,\boldsymbol{H}'-\boldsymbol{H}\,|a\rangle|\leq(\mu_1+\mu_2+\delta)\|a\|^2. \tag{5.129}$$

Proof. Let $\boldsymbol{H}'_\pm := (\boldsymbol{H}'\pm\boldsymbol{H}'^\dagger)/2$, $\boldsymbol{H}_\pm := (\boldsymbol{H}\pm\boldsymbol{H}^\dagger)/2$. Applying antisymmetry of $\log\boldsymbol{\Delta}$ under conjugation by $\boldsymbol{J}$, $\boldsymbol{J}=\boldsymbol{J}^\dagger$, and $\boldsymbol{J}^2=1$ to (5.125) we get

$$\log\boldsymbol{\Delta}+\boldsymbol{H}'_+\geq-\mu_1 \tag{5.130}$$

$$-\log\boldsymbol{\Delta}+\boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}\geq-\mu_1. \tag{5.131}$$

At the same time, by Theorem 5.2.1, we have $\boldsymbol{H}_+=\boldsymbol{H}$ and

$$\log\boldsymbol{\Delta}+\boldsymbol{H}\geq 0 \tag{5.132}$$

$$-\log\boldsymbol{\Delta}+\boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J}\geq 0. \tag{5.133}$$

Using (5.131) and (5.132) we have

$$\begin{aligned}\boldsymbol{H}'_+-\boldsymbol{H} &\leq \boldsymbol{H}'_++\log\boldsymbol{\Delta} & (5.134)\\ &= \boldsymbol{H}'_++\boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}-\boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}+\log\boldsymbol{\Delta} & (5.135)\\ &\leq \boldsymbol{H}'_++\boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}+\mu_1. & (5.136)\end{aligned}$$

On the other hand, using (5.130) and (5.133) we have

$$\boldsymbol{H}'_+ - \boldsymbol{H} \geq -\log \boldsymbol{\Delta} - \mu - \boldsymbol{H} \tag{5.137}$$

$$= -\log \boldsymbol{\Delta} - \mu_1 - \boldsymbol{H} - \boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J} + \boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J} \tag{5.138}$$

$$\geq -\mu_1 - (\boldsymbol{H} + \boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J}). \tag{5.139}$$

Thus, for any operator a we have

$$-\mu_1\langle a|a\rangle - \langle a|\,\boldsymbol{H} + \boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J}\,|a\rangle \leq \langle a|\,\boldsymbol{H}'_+ - \boldsymbol{H}\,|a\rangle \leq \langle a|\,\boldsymbol{H}'_+ + \boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}\,|a\rangle + \mu_1\langle a|a\rangle. \tag{5.140}$$

Since $\langle a|\,\boldsymbol{H}'_+ + \boldsymbol{J}\,\boldsymbol{H}'_+\,\boldsymbol{J}\,|a\rangle = \mathrm{Re}(\langle a|\,\boldsymbol{H}' + \boldsymbol{J}\,\boldsymbol{H}'\,\boldsymbol{J}\,|a\rangle)$, if a further satisfies (5.127) and (5.128) then we get

$$|\,\mathrm{Re}(\langle a|\,\boldsymbol{H}' - \boldsymbol{H}\,|a\rangle)| = |\langle a|\,\boldsymbol{H}'_+ - \boldsymbol{H}\,|a\rangle| \tag{5.141}$$

$$\leq \mu_1\langle a|a\rangle + \delta|a\|^2 \tag{5.142}$$

$$\leq (\mu_1 + \delta)\|a\|^2. \tag{5.143}$$

On the other hand

$$|\,\mathrm{Im}(\langle a|\,\boldsymbol{H}' - \boldsymbol{H}\,|a\rangle)| = |\langle a|\,\boldsymbol{H}'_-\,|a\rangle| \leq \|a\|^2\mu_2, \tag{5.144}$$

and putting this bound together with the previous one proves the Proposition.

□

We are now ready to prove Theorem 5.2.4, which we restate for convenience:

Theorem (A priori convergence in the commuting case)**.** *Suppose h is commuting and that $\{P_1, \ldots, P_r\} = \mathcal{P}_{k,\ell}$ for $\ell = \max(3, 1 + (1+\mathfrak{d})^2)$. There is an error threshold*

$$\tau = m^{-6} e^{-\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} \tag{5.145}$$

(where $\mathcal{C}$ is the constant from Definition 5.2.2) such that if $\epsilon_0 \leq \tau$ then for any $\lambda' \in \mathbb{R}^m$ satisfying

$$\log\left(\tilde{\boldsymbol{\Delta}}\right) + \sum_{\alpha=1}^{m} \lambda'_\alpha(\tilde{\boldsymbol{H}}_\alpha + \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \succeq -\mu_1, \tag{5.146}$$

$$\pm i \sum_{\alpha=1}^{m} \lambda'_\alpha(\tilde{\boldsymbol{H}}_\alpha - \tilde{\boldsymbol{H}}_\alpha^\dagger)/2 \preceq \mu_2, \tag{5.147}$$

we have

$$\sup_{\alpha=1,\ldots m} |\lambda'_\alpha - \lambda_\alpha| \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)}\left(\mu_1 + m^{1/2}\mu_2\right) + \varepsilon_0/\tau. \tag{5.148}$$

Proof. Suppose $\lambda' \in \mathbb{R}^m$ satisfies (5.146) and (5.147). By Theorem 5.2.3, there are constants $\mathcal{D}, \mathcal{E} \geq 0$ depending only on k and $\mathfrak{d}$ such that setting

$$\sigma := m^{-2} e^{-\mathcal{D}\beta - \mathcal{E}} \tag{5.149}$$

and assuming $\varepsilon_0 \leq \sigma$, we have $K \leq 1/\sigma = e^{\mathcal{O}_{k,\mathfrak{d}}(\beta)}$. Applying the continuity bounds in Proposition 5.3.1 to (5.146) gives

$$\log(\boldsymbol{\Delta}) + \sum_\alpha \lambda'_\alpha (\boldsymbol{H}_\alpha + \boldsymbol{H}_\alpha^\dagger)/2 \succeq -\mu_1 - (2K^3 + 3m\beta' K^2)\varepsilon_0 \tag{5.150}$$

$$\succeq -\mu_1 - e^{3\mathcal{D}\beta + 3\mathcal{E}} \left(2m^6 + 3m^5\beta'\right) \varepsilon_0, \tag{5.151}$$

where $\beta' = \max_{\alpha=1,\ldots m} |\lambda'_\alpha|$. Doing so to (5.147) gives

$$\pm i \sum_\alpha \lambda'_\alpha (\boldsymbol{H}_\alpha - \boldsymbol{H}_\alpha^\dagger)/2 \preceq \mu_2 + 3m\beta' K^2 \varepsilon_0 \tag{5.152}$$

$$\preceq \mu_2 + 3m^5 \beta' e^{2\mathcal{D}\beta + 2\mathcal{E}} \varepsilon_0. \tag{5.153}$$

Let a be any $(k, 1+\mathfrak{d})$-$\mathfrak{G}$-local operator. By Lemma 5.4.9 we have $\langle a | \boldsymbol{H} + \boldsymbol{J}\,\boldsymbol{H}\,\boldsymbol{J} | a \rangle = \langle a | J + JHJ | a \rangle = 0$. Applying this fact, together with the bound from Corollary 5.4.1 and the inequalities (5.151) and (5.153), to Proposition 5.4.1, we have

$$|\langle a | \boldsymbol{H} - \boldsymbol{H}' | a \rangle| \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} (\mu_1 + m^{1/2}\mu_2 + (m^6 + m^{5.5}\beta')\varepsilon_0), \tag{5.154}$$

and so by Lemma 5.4.5 we get

$$\max_{\alpha=1,\ldots,m} |\lambda'_\alpha - \lambda_\alpha| \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} (\mu_1 + m^{1/2}\mu_2 + (m^6 + m^{5.5}\beta')\varepsilon_0). \tag{5.155}$$

The locality constraint $\ell = 1 + (1+\mathfrak{d})^2$ follows from combining the choices in Lemma 5.4.5, Lemma 5.4.9, and Corollary 5.4.1, which are $\ell \geq 3$, $\mathfrak{d} + 1 = \ell' \leq \ell/(1+\mathfrak{d})$ and $\mathfrak{d} + 1 = \ell' \leq (\ell - 1)/(1+\mathfrak{d})$, respectively. This is essentially the result we need but contains a parameter β'. While it is possible to simply set explicit bounds on the parameter domain during the optimization to bound β', we show in the following that this is not needed. The previous expression can be summarized as

$$\max_{\alpha=1,\ldots,m} |\lambda'_\alpha - \lambda_\alpha| \leq \gamma + \varepsilon_0/\tau + \delta\beta'\varepsilon_0 \tag{5.156}$$

by defining constants that can be chosen to satisfy

$$\gamma \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} (\mu_1 + m^{1/2}\mu_2) \tag{5.157}$$

$$1/\tau \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} m^6 \tag{5.158}$$

$$\delta \leq e^{\mathcal{O}_{k,\mathfrak{d},\mathcal{C}}(\beta)} m^{5.5}. \tag{5.159}$$

We can upper bound β' as

$$\beta' \leq \beta + \max_{\alpha=1,\ldots,m} |\lambda'_\alpha - \lambda_\alpha| \leq \beta + \gamma + \varepsilon_0/\tau + \delta\beta'\varepsilon_0 \tag{5.160}$$

so by requiring $\varepsilon_0 \leq 1/2\delta$ we have

$$\beta' \leq 2(\beta + \gamma + \varepsilon_0/\tau). \tag{5.161}$$

Plugging the bound for β' back into the error estimates we obtain

$$\max_{\alpha=1,\ldots,m} |\lambda'_\alpha - \lambda_\alpha| \leq 2\gamma + 2\varepsilon_0/\tau + \delta\beta\varepsilon_0. \tag{5.162}$$

The proof follows from recalling the conditions $\varepsilon_0 \leq \sigma$ and $\varepsilon_0 \leq 1/2\delta$ and collecting the worst case estimates of all constants above.

□

5.5 Antilinear operators

Let $\mathcal{K}$ be a finite-dimensional complex Hilbert space. A map $T : \mathcal{K} \to \mathcal{K}$ is called *antilinear* if it is linear over $\mathbb{R}$ and satisfies $T(\lambda v) = \overline{\lambda} T v$ for every $v \in \mathcal{K}$ and $\lambda \in \mathbb{C}$. Equivalently, $\mathcal{K}$ can be viewed as a real vector space (of double the dimension) and T is a $\mathbb{R}$-linear operator on this real vector space that anticommutes with the $\mathbb{R}$-linear operator $v \mapsto \sqrt{-1}v$. The composition of a linear operator with an antilinear operator (in either order) is antilinear, and the composition of two antilinear operators is linear. If T is antilinear then its adjoint is defined by the relation:

$$\langle u|T^\dagger v\rangle = \overline{\langle Tu|v\rangle} \quad \text{for all } u, v \in \mathcal{K}. \tag{5.163}$$

Note the complex conjugation, which is absent from the definition for complex-linear operators. An antilinear operator U is called *anti-unitary* if $U^\dagger U = 1$. One defines the polar decomposition of an antilinear operator T in a way analogous to linear operators: the operators U and P form a polar decomposition of T iff U is anti-unitary, $P \succeq 0$ is linear, and $T = UP$. If T is invertible then U and P are uniquely defined as $P := \sqrt{T^\dagger T}$ and $U = TP^{-1}$.

We call an operator T an *involution* if $T^2 = 1$. The following is a structure theorem for the the polar decomposition of an antilinear involution:

Lemma 5.5.1. *Let $S : \mathcal{K} \to \mathcal{K}$ be an antilinear involution on $\mathcal{K}$. Define $\Delta := S^\dagger S$ and $J := S\Delta^{-1/2}$ so that $S = J\Delta^{1/2}$ is the polar decomposition of S. Then we have*

1. *$S\log\Delta S = -\log\Delta$ and $S\Delta^p S = \Delta^{-p}$ for any $p \in \mathbb{R}$.*

2. *$J = \Delta^{1/2}S$ and $J^\dagger = J$ and $J^2 = 1$.*

3. *$J\log\Delta J = -\log\Delta$ and $J\Delta^p J = \Delta^{-p}$ for any $p \in \mathbb{R}$.*

Proof. 1. Since $S^2 = (S^\dagger)^2 = 1$, we have $S\Delta S\Delta = SS^\dagger SSS^\dagger S = 1$, and so $S\Delta S = \Delta^{-1}$. From here we can write

$$\begin{aligned} e^{-\log\Delta} &= \Delta^{-1} \\ &= S\Delta S \\ &= S\sum_{k\geq 0}\frac{\log\Delta^k}{k!}S \\ &= \sum_{k\geq 0}\frac{(S\log\Delta S)^k}{k!} \\ &= e^{S\log\Delta S}, \end{aligned}$$

and so $S\log\Delta S = -\log\Delta$. Finally, we have

$$\begin{aligned} S\Delta^p S &= S\sum_{k\geq 0}\frac{(p\log\Delta)^k}{k!}S \\ &= \sum_{k\geq 0}\frac{(-p\log\Delta)^k}{k!} \\ &= \Delta^{-p}. \end{aligned}$$

2. The first two statements follow from

$$\begin{aligned} J^\dagger &= \Delta^{-1/2}S^\dagger \\ &= \Delta^{-1/2}S^\dagger SS \\ &= \Delta^{1/2}S \\ &= S\Delta^{-1/2} \\ &= J, \end{aligned}$$

where the second-last line follows from part 1 with $p = 1/2$. The third statement follows from

$$J^2 = (S\Delta^{-1/2})(\Delta^{1/2}S) = 1.$$

3. The first statement follows from $J\log\Delta J = S\Delta^{-1/2}\log\Delta\Delta^{1/2}S = S\log\Delta S = -\log\Delta$ and the second follows from a similar argument. $\square$

References

[Ans+] Anurag Anshu et al. *Efficient learning of commuting hamiltonians on lattices*. URL: https://anuraganshu.seas.harvard.edu/files/anshu/files/learning_commuting_hamiltonian.pdf.

[Ans+21] Anurag Anshu et al. "Sample-efficient learning of interacting quantum systems". In: *Nature Physics* 17.8 (May 2021), pp. 931–935. ISSN: 1745-2481. DOI: 10.1038/s41567-021-01232-0. URL: http://dx.doi.org/10.1038/s41567-021-01232-0.

[Ara+77] Huzihiro Araki et al. "Extension of KMS states and chemical potential". In: *Communications in Mathematical Physics* 53.2 (June 1977), pp. 97–134. ISSN: 1432-0916. DOI: 10.1007/bf01609126. URL: http://dx.doi.org/10.1007/BF01609126.

[Art24] Adam Artymowicz. *Efficient Hamiltonian learning from Gibbs states*. 2024. DOI: 10.48550/ARXIV.2403.18061. URL: https://arxiv.org/abs/2403.18061.

[AS77] Huzihiro Araki and Geoffrey L Sewell. "KMS conditions and local thermodynamical stability of quantum lattice systems". In: *Communications in Mathematical Physics* 52 (1977), pp. 103–109.

[Bak+23] Ainesh Bakshi et al. *Learning quantum Hamiltonians at any temperature in polynomial time*. 2023. DOI: 10.48550/ARXIV.2310.02243. URL: https://arxiv.org/abs/2310.02243.

[BAL19] Eyal Bairey, Itai Arad, and Netanel H Lindner. "Learning a local Hamiltonian from local measurements". In: *Physical review letters* 122.2 (2019), p. 020504.

[Bha97] Rajendra Bhatia. *Matrix analysis*. Vol. 169. Springer Science & Business Media, 1997.

[BR87] Ola Bratteli and Derek W. Robinson. *Operator algebras and quantum statistical mechanics. 1. C^*- and W^*-algebras, symmetry groups, decomposition of states.* 2nd ed. Texts and Monographs in Physics. Springer-Verlag, New York, 1987.

[Che+23] Chi-Fang Chen et al. "Quantum thermal state preparation". In: *arXiv preprint arXiv:2303.18224* (2023).

[CW87] J. S. Cohen and M. Winnink. "Stable thermodynamic states". In: *Journal of Mathematical Physics* 28.6 (June 1987), pp. 1394–1397. ISSN: 1089-7658. DOI: 10.1063/1.527493. URL: http://dx.doi.org/10.1063/1.527493.

[Dal+22] Marcello Dalmonte et al. "Entanglement Hamiltonians: From Field Theory to Lattice Models and Experiments". In: *Annalen der*

Physik 534.11 (Aug. 2022). ISSN: 1521-3889. DOI: 10.1002/andp.202200064. URL: http://dx.doi.org/10.1002/andp.202200064.

[EHF19] Tim J Evans, Robin Harper, and Steven T Flammia. "Scalable bayesian hamiltonian learning". In: *arXiv preprint arXiv:1912.07636* (2019).

[FFS23] Hamza Fawzi, Omar Fawzi, and Samuel O. Scalet. *Certified algorithms for equilibrium states of local quantum Hamiltonians*. 2023. arXiv: 2311.18706 [quant-ph]. URL: https://arxiv.org/abs/2311.18706.

[GCC22] Andi Gu, Lukasz Cincio, and Patrick J Coles. "Practical black box Hamiltonian learning". In: *arXiv preprint arXiv:2206.15464* (2022).

[HHW67] R. Haag, N. M. Hugenholtz, and M. Winnink. "On the equilibrium states in quantum statistical mechanics". In: *Communications in Mathematical Physics* 5.3 (June 1967), pp. 215–236. ISSN: 1432-0916. DOI: 10.1007/bf01646342. URL: http://dx.doi.org/10.1007/BF01646342.

[HKT24] Jeongwan Haah, Robin Kothari, and Ewin Tang. "Learning quantum Hamiltonians from high-temperature Gibbs states and real-time evolutions". In: *Nature Physics* 20.6 (Mar. 2024), pp. 1027–1031. ISSN: 1745-2481. DOI: 10.1038/s41567-023-02376-x. URL: http://dx.doi.org/10.1038/s41567-023-02376-x.

[Kok+21] Christian Kokail et al. "Entanglement Hamiltonian tomography in quantum simulation". In: *Nature Physics* 17.8 (2021), pp. 936–942.

[Kuw24] Tomotaka Kuwahara. *Clustering of conditional mutual information and quantum Markov structure at arbitrary temperatures*. 2024. arXiv: 2407.05835 [quant-ph]. URL: https://arxiv.org/abs/2407.05835.

[Lif+21] Yotam Y Lifshitz et al. "Practical Quantum State Tomography for Gibbs states". In: *arXiv preprint arXiv:2112.10418* (2021).

[Nar24] Shyam Narayanan. *Improved algorithms for learning quantum Hamiltonians, via flat polynomials*. arXiv:2407.04540 [quant-ph]. July 2024. URL: http://arxiv.org/abs/2407.04540 (visited on 07/08/2024).

[Sch92] Bernhard A. Schmitt. "Perturbation bounds for matrix square roots and pythagorean sums". In: *Linear Algebra and its Applications* 174 (1992), pp. 215–227. ISSN: 0024-3795. DOI: https://doi.org/10.1016/0024-3795(92)90052-C. URL: https://www.sciencedirect.com/science/article/pii/002437959290052C.

[Sew77] Geoffrey L. Sewell. "KMS conditions and local thermodynamical stability of quantum lattice systems. II". In: *Communications in Mathematical Physics* 55.1 (Feb. 1977), pp. 53–61. ISSN: 1432-0916. DOI: 10.1007/bf01613149. URL: http://dx.doi.org/10.1007/BF01613149.

[Sti+24] Daniel Stilck França et al. "Efficient and robust estimation of many-qubit Hamiltonians". In: *Nature Communications* 15.1 (2024), p. 311.

[Tem+11] Kristan Temme et al. "Quantum metropolis sampling". In: *Nature* 471.7336 (2011), pp. 87–90.

[Wan+17] Jianwei Wang et al. "Experimental quantum Hamiltonian learning". In: *Nature Physics* 13.6 (2017), pp. 551–555.

[Wie+14] Nathan Wiebe et al. "Hamiltonian learning and certification using quantum resources". In: *Physical review letters* 112.19 (2014), p. 190501.

[WRL18] Xueda Wen, Shinsei Ryu, and Andreas W W Ludwig. "Entanglement Hamiltonian evolution during thermalization in conformal field theory". In: *Journal of Statistical Mechanics: Theory and Experiment* 2018.11 (Nov. 2018), p. 113103. ISSN: 1742-5468. DOI: 10.1088/1742-5468/aae84e. URL: http://dx.doi.org/10.1088/1742-5468/aae84e.