

Thermal Area Law for Lattice Bosons

Marius Lemm and Oliver Siebert

Department of Mathematics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

A physical system is said to satisfy a thermal area law if the mutual information between two adjacent regions in the Gibbs state is controlled by the area of their boundary. Lattice bosons have recently gained significant interest because they can be precisely tuned in experiments and bosonic codes can be employed in quantum error correction to circumvent classical no-go theorems. However, the proofs of many basic information-theoretic inequalities such as the thermal area law break down for bosons because their interactions are unbounded. Here, we rigorously derive a thermal area law for a class of bosonic Hamiltonians in any dimension which includes the paradigmatic Bose-Hubbard model. The main idea to go beyond bounded interactions is to introduce a quasi-free reference state with artificially decreased chemical potential by means of a double Peierls-Bogoliubov estimate.

1 Introduction

In quantum many-body systems with translation-invariant short-ranged interactions the entanglement entropy of the ground state typically satisfies an *area law* – meaning that it is bounded by a constant times the boundary surface area of A (as opposed to the trivial bound which would entail the volume of A). The area law captures our physical intuition that correlations are concentrated on short distances and therefore only occur across the boundary cut. It is extremely useful in practice as it severely restricts the admissible many-body states for approximating ground states (i.e., quantum matter) and can thus serve to overcome the notorious *curse of dimensionality* through the famous density matrix renormalization group (DMRG) numerical algorithm [1]–[4]. The connection is clearest for 1D lattice systems, where a state satisfies an area law if and only if it is representable as a matrix product state (MPS) with fixed bond dimension independent of the system size [5], [6]. For detailed reviews also covering the higher-dimensional situation, see [7], [8].

Area laws for the entanglement entropy as described above have their origins in the holographic principle in the context of quantum gravity [9] and

Marius Lemm: marius.lemm@uni-tuebingen.de
 Oliver Siebert: oliver.siebert@uni-tuebingen.de

have been numerically observed in a large number of many-body systems. They have been derived for gapped 1D spin systems [10]–[14], for 1D quantum states with finite correlation lengths [15], [16], gapped harmonic lattice systems [17]–[20], ground states in the same gapped phase as others obeying an area law [21], [22], models whose Hamiltonian spectra satisfy related conditions [23], [24], certain frustration-free spin systems [25], tree-graph systems [26], models exhibiting local topological order [27] and high-dimensional systems under additional assumptions such as frustration-freeness [23], [24], [28]–[31]. There has also been recent progress for certain long-range interactions [32], [33]. A general statement in higher dimensions remains elusive and this problem is known as the *area law conjecture*.

The analog of the area law for Gibbs states is called the thermal area law. Gibbs states are important for fundamental reasons and their efficient simulability via tensor networks hinges on thermal area laws [34]–[36]. For Gibbs states, the total correlations between two regions A and B are quantified by their *mutual information* [34], [37], [38]

$$I(A : B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}),$$

where S denotes the von Neumann entropy, ρ_{AB} the Gibbs state of the full system, and ρ_A, ρ_B the reduced density matrices corresponding to A and B , respectively. At zero temperature, $I(A : B)$ reduces to twice the entanglement entropy. An area law at positive temperature was derived in a seminal work of Wolf et. al [39] who proved for local and bounded interactions that

$$I(A : B) \leq C\beta |\partial_{AB}|$$

with ∂_{AB} being the boundary region between A and B , and whenever A and B are disjoint and together make up the entire lattice. Very recently, the β -scaling result was improved to $\beta^{2/3}$ [34] which matters for the experimentally relevant regime of low temperatures ($\beta \rightarrow \infty$). This dependence is not far from optimal, since Gottesman and Hastings found a 1D model for which the scaling of the mutual information is at least $\beta^{1/5}$ for large β [40]. Moreover, a generalization to various Rényi generalizations of the mutual information was given in [35] and this has important applications to simulating and approximating Gibbs states [36]. Further results of thermal area laws were established for free fermions [41], for the entanglement negativity (instead of the mutual information) [42],

as a result of rapid mixing for dissipative quantum lattice systems [43], [44] (with a logarithmic correction) and numerically for some spin chains showing a $\log \beta$ -dependence [45]. A current account of thermal area laws and related phenomena is given in [38]. There has also been recent progress in the experimental verification of area laws for both the entanglement entropy and the mutual information at positive temperature by means of ultra-cold atom simulators [46].

Thermal area laws provide us with universal properties of Gibbs states independent of the system size. They are especially valuable for lower temperatures, while at high temperatures many analytic properties are available, e.g. exponential decay of correlations [47]–[52], the large deviation principle [53]–[55] or the approximate quantum Markov property [56], [57]. Such characterizations are important for the computation of Gibbs states, in general an NP-hard problem [58], [59], which in turn is fundamental in novel applications such as quantum machine learning [60], [61], semidefinite programming solvers [62], [63] or the imaginary-time evolution in the framework of near-term quantum devices [64]–[70].

In particular, area laws can be used for the approximation of Gibbs state by matrix product operators (MPO) and their higher-dimensional analogs [34], [36], [38], [71]. In special cases like one-dimensional quantum spin systems they gave rise to concrete algorithms for the efficient approximation by MPO, where the temperature behavior in the area law determines the maximal bond dimension [34]. Such algorithms also proved to be useful for the representation of Gibbs states as a convex combination of MPS [72], or for the approximation of ground states under a low-energy-density assumption typically observed for gapped systems. It is generally believed that the scaling of the mutual information with β in the low temperature regime is related to the computational complexity of the ground space of the models [38]. Another direct way to use a thermal area law is to note that controlling the mutual information automatically controls all standard correlation functions, see [39] and Appendix A.3 below.

A critical limitation of the existing results is that they only hold for *bounded* interactions and bounded local Hilbert space dimension. This is naturally the case for quantum spin systems and lattice fermions. However, for lattice *bosons* as described, e.g., by the paradigmatic Bose-Hubbard Hamiltonian, the interactions are *unbounded* and the standard arguments fail.

There has recently been a surge of interest in bosonic lattice systems and related models for three main reasons: (i) The Hamiltonians can be experimentally fine-tuned for cold atoms in optical lattices [73], which makes them promising platform for quantum simulation and quantum engineering, see also [74]. (ii) Bosonic encoding can be used in quantum

information processing which can provide multiple advantages over finite-dimensional discrete-variable (DV) codes [75], [76]. (iii) In many cases the standard techniques of quantum information theory fail (including the derivations of the thermal area law) because of the unbounded interactions.

Area laws for non-interacting bosons were considered in [19], [20], [77], but the case of interacting bosons, including the paradigmatic Bose-Hubbard model proved elusive to rigorous analysis. A partly numerical investigation was given in [78] with a focus on the phase transition from Mott insulator to superfluid by analogy with other symmetry breaking transitions [79]–[81]. Recently, Abrahamsen et al. rigorously proved an area law for gapped ground states of 1D bosonic lattice Hamiltonians in [82] by using a truncation of the local Hilbert spaces and a quantum number tail bound from [83]. Their work only concerns the zero temperature case and leaves open the positive temperature case.

In this work we rigorously derive the first thermal area law for a broad class of bosonic Hamiltonians in any dimension including the paradigmatic Bose-Hubbard model. In a nutshell, our result states that under natural assumptions on the bosonic lattice gases (e.g., short-ranged hopping), we again have the bound

$$I(A : B) \leq C\beta |\partial_{AB}|$$

for all $\beta \geq 1$. The precise result is Theorem 2 below. The β -scaling is the same as that found by [39] and our proof uses the same basic idea as a starting point, namely to use the Gibbs variational principle to bound the mutual information by a difference of boundary energy expectations (Lemma 1). However, the unbounded interactions then pose technical difficulties which we overcome by introducing a quasi-free reference state with artificially decreased chemical potential by means of a double Peierls-Bogoliubov estimate. This reduces us to computations with quasi-free states that can be completed with Wick’s rule. Further details are explained below and in the appendix.

2 Setup for infinite-dimensional Hilbert spaces

A technical point in the description of many-boson systems is that the local Hilbert spaces are infinite-dimensional since the particle number is unbounded. For this reason, we include this short preliminary section in which we recall the elegant approach to thermal area laws via the Gibbs variational principle by Wolf et al. [39] and note that it adapts straightforwardly to the infinite-dimensional situation. These abstract results are then utilized for the Bose-Hubbard model in the following section.

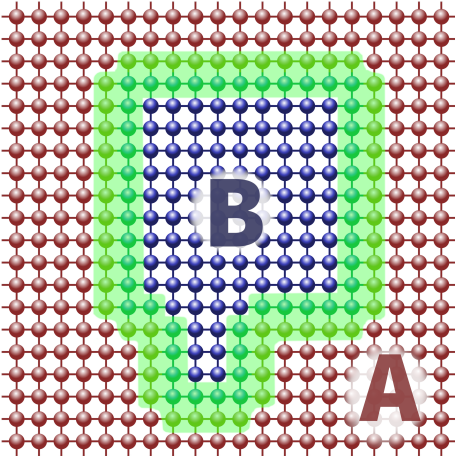


Figure 1: Periodic box for $d = 2$ and $L = 20$ decomposed into two regions A and B . The green region shows the boundary region ∂_{AB} . The bonds connecting A and B make up the boundary Hamiltonian H_{∂} .

Let $\mathfrak{h}$ be the local Hilbert space for one site, Λ a finite set and $A, B \subseteq \Lambda$ such that $A \cap B = \emptyset$ and $A \sqcup B = \Lambda$. We set

$$\mathcal{H}_A = \bigotimes_{x \in A} \mathfrak{h}, \quad \mathcal{H}_B = \bigotimes_{x \in B} \mathfrak{h}, \quad \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B.$$

We suppose that the Hamiltonian can be decomposed as

$$H_{AB} = H_A \otimes \mathbb{1} + \mathbb{1} \otimes H_B + H_{\partial} \quad (1)$$

For details about operator domains, which are relevant because our operators are unbounded, see Appendix A.1. Let $\mathcal{T}_1^+(\mathcal{H})$ denote the set of all density matrices on $\mathcal{H}$. Then we define the free energy as

$$F_{AB}^{\beta} = \inf_{\rho \in \mathcal{T}_1^+(\mathcal{H}_{AB})} \mathcal{F}^{\beta}(\rho),$$

where

$$\mathcal{F}^{\beta}(\rho) = \text{tr}(H_{AB}\rho) - \frac{S(\rho)}{\beta}, \quad S(\rho) = -\text{tr}(\rho \ln \rho).$$

The Gibbs state

$$\rho_{AB} = \frac{e^{-\beta H_{AB}}}{Z_{AB}}, \quad Z_{AB} = \text{tr} e^{-\beta H_{AB}},$$

minimizes the free energy, i.e., $F_{AB}^{\beta} = \mathcal{F}^{\beta}(\rho_{AB})$. (See Proposition 4 for a proof of this in the infinite-dimensional setting.) We reduce to the A , respectively B subsystem by taking partial traces of the Gibbs state

$$\rho_A = \text{tr}_{\mathcal{H}_B}(\rho_{AB}), \quad \rho_B = \text{tr}_{\mathcal{H}_A}(\rho_{AB}).$$

The general bound from [39] straightforwardly extends to the infinite-dimensional setting as follows.

Lemma 1 (Boundary energy controls mutual informat.)

Let $\beta > 0$ and suppose that $\text{tr} e^{-\beta H_{AB}} < \infty$. Then

$$I(A : B) \leq \beta \text{tr}(H_{\partial}(\rho_A \otimes \rho_B - \rho_{AB})).$$

Proof. We start from

$$\mathcal{F}^{\beta}(\rho_{AB}) = F_{AB}^{\beta} \leq \mathcal{F}^{\beta}(\rho_A \otimes \rho_B).$$

Using $S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B)$, we obtain

$$I(A : B) \leq \beta \text{tr}(H_{AB}(\rho_A \otimes \rho_B - \rho_{AB}))$$

and the right-hand side equals $\beta \text{tr}(H_{\partial}(\rho_A \otimes \rho_B - \rho_{AB}))$ by basic properties of the partial trace. $\square$

3 Main Result

Now we consider the Bose-Hubbard model in the framework of the previous section. Let $\Lambda \equiv \Lambda_L$ denote a box of side length L in the d -dimensional lattice with periodic boundary conditions. For $x, y \in \Lambda_L$ we write $x \sim y$ if x and y are nearest neighbors in the periodized lattice. At each site lives a bosonic particle described by the local Hilbert space $\mathfrak{h} = \ell^2(\mathbb{N})$.

The total Hilbert space $\mathcal{H}_{AB} = \bigotimes_{x \in \Lambda_L} \mathfrak{h}$ is isomorphic to the Fock space $\mathfrak{F}(\ell^2(\Lambda_L))$. On it, we consider the Bose-Hubbard Hamiltonian

$$H_{AB} = -J \sum_{x \sim y} a_x^{\dagger} a_y + \frac{U}{2} \sum_{x \in \Lambda_L} n_x(n_x - 1) - \mu \mathcal{N}, \quad (2)$$

where $J \in \mathbb{R}$ represents the strength of the kinetic nearest-neighbor hopping, $U > 0$ the strength of the on-site repulsion and $\mu \in \mathbb{R}$ the chemical potential, and $\mathcal{N} = \sum_{x \in \Lambda_L} n_x$ is the total number operator. The Hamiltonian is self-adjoint on a suitable domain $\mathcal{D}(H_{AB})$; see e.g., [84] and Appendix A.1.

We are now ready to state the main result. We decompose the box into two regions A and B with boundary region

$$\begin{aligned} \partial_{AB} = & \{x \in A : \exists y \in B : x \sim y\} \\ & \cup \{y \in B : \exists x \in A : x \sim y\} \end{aligned}$$

as shown in Figure 1.

Theorem 2 (Main result: thermal area law)

For all $\beta, U, \mu > 0$, we have

$$I(A : B) \leq c(J, U, \mu) \max\{1, \beta\} |\partial_{AB}|$$

A few remarks are in order: (i) The repulsiveness assumption $U > 0$ is necessary as it ensures stability of the system. (ii) The assumption that $\mu > 0$ is standard, cf. the usual phase diagram in Figure 13(a) in [73]. Indeed, note that if one would take μ sufficiently

negative, then the system becomes effectively devoid of particles in the grand-canonical setting. (iii) The constant $c(J, U, \mu)$ can be made explicit from (11). (iv) The maximum $\max\{1, \beta\}$ means that the bound behaves as β for low temperatures in accordance with [39]. We recall that some growth in β is strongly expected without any gap assumption [40]. For high temperature $\beta < 1$, we find a temperature independent lower bound which matches the classical situation [39]. (v) As explained in [39], a bound on the mutual information implies a bound for the correlation of any pair of bounded observables and the same is true in the bosonic setting, see Appendix A.3.

We close the presentation by discussing several extensions of the result which can be obtained from the same methods. The proof can be extended to Hamiltonians of the form

$$H = H_0 + W,$$

with

$$\begin{aligned} H_0 &= \sum_{k=1}^M \sum_{l=1}^k \sum_{\substack{\{x_1, \dots, x_l, \\ y_1, \dots, y_l\} \subset \Lambda_L}} \sum_{\nu_1 + \dots + \nu_l = k} J_{x_1 \dots x_l y_1 \dots y_l}^{\nu_1 \dots \nu_l} \\ &\quad \times (a_{x_1}^\dagger)^{\nu_1} \dots (a_{x_l}^\dagger)^{\nu_l} a_{y_1}^{\nu_1} \dots a_{y_l}^{\nu_l}, \\ W &= \sum_x f(n_x), \end{aligned} \quad (3)$$

where $M \in \mathbb{N}$, $f \geq 0$ is a polynomially bounded function, growing faster than x^M , and $J_{x_1 \dots x_l y_1 \dots y_l}^{\nu_1 \dots \nu_l}$ is uniformly bounded and finite-range. Moreover, the proof also works if we add to the original Hamiltonian density-density interactions of the form

$$\tilde{H} = \sum_{x, y} J_{xy} n_x n_y,$$

provided that U is sufficiently large, and J_{xy} is uniformly bounded and finite-range. Furthermore, instead of finite-range interactions, we can consider hopping terms decaying at infinity fast enough, e.g., $-\sum_{x, y} J_{xy} a_x^\dagger a_y$ for $J_{xy} \geq 0$, $x \in \mathbb{Z}^d$, satisfying $J_{xy} \leq (1 + |x - y|)^{-\alpha}$ for sufficiently large $\alpha > d$.

Finally, the underlying lattice structure can be easily modified as well, though, the constant will be less explicit since it depends on the spectrum of the graph Laplacian. In summary, the thermal area law can be proved for an entire class of bosonic lattice gases in any dimension.

The translation-invariance of the underlying lattice is in fact necessary in our current proof. Dropping this assumption would require to control the number of bosons potentially accumulating on the boundaries of the whole system, see also the proof of Proposition 5. It is an interesting open problem to remove the translation-invariance assumption. Furthermore, as we control the H_0 term with the on-site interaction W , we also need the rather strong decay assumption

on J_{xy} . Therefore, an interesting problem is to develop an alternative approach allowing for long-range interactions with α arbitrary close to d .

4 Sketch of proof of Theorem 2

The detailed proof of Theorem 2 is given in Appendix B. Here we give a sketch of the main ideas.

We decompose the Hamiltonian as

$$H_{AB} = H_0 + W + (\mu - 2dJ)\mathcal{N}$$

where $H_0 = -J \sum_{x \sim y} a_x^\dagger a_y + 2dJ\mathcal{N}$ is the shifted kinetic term and $W = \frac{U}{2} \sum_{x \in X} n_x(n_x - 1)$ is the on-site interaction.

To use Lemma 1, we again decompose the Hamiltonian as $H_{AB} = H_A + H_B + H_\partial$ where we define the subsystem Hamiltonians with open boundary conditions along the cut. More precisely, for $X \in \{A, B\}$, we set

$$H_X = -J \sum_{\substack{x \sim y, \\ x, y \in X}} a_x^\dagger a_y + \frac{U}{2} \sum_{x \in X} n_x(n_x - 1) - \mu \sum_{x \in X} n_x$$

$$\text{and } H_\partial = -J \sum_{x \in A, y \in B} (a_x^\dagger a_y + a_y^\dagger a_x).$$

Notice that the boundary Hamiltonian H_∂ contains at most $d|\partial_{AB}|$ many summands, so the right-hand side of Lemma 1 seems to exhibit the desired scaling in L and β . The main challenge is that the hopping terms $a_x^\dagger a_y + a_y^\dagger a_x$ between A and B are unbounded in contrast to the cases of spin systems or lattice fermions.

Our first idea is that since expectations with respect to the full Gibbs state are rather difficult to handle, we aim for the expectation in a quasifree state which can be computed via Wick's rule. To this end, we want to remove the W term in $e^{-\beta H_{AB}}$. The technical tool to rigorously implement such a shift in the operator exponent will be a double application of the Peierls-Bogoliubov inequality [85, (2.14)], which has a long history in the study of quantum many-body systems and quantum information theory. Applying it twice, we obtain

$$\frac{\text{tr}(Pe^K)}{\text{tr}(e^K)} \leq \frac{\text{tr}(Pe^{K+P})}{\text{tr}(e^{K+P})}. \quad (4)$$

We use this bound with $K = -\beta H_{AB}$ and $P = \beta(W - (\mu + \gamma - 2dJ)\mathcal{N})$ so that the new effective Hamiltonian is

$$K + P = -\beta(H_0 + (\gamma + 2dJ)\mathcal{N})$$

and $e^{-\beta(H_0 + (\gamma + 2dJ)\mathcal{N})}$ is a trace-class quasifree state, so that expectations can be calculated via Wick's rule. Here we introduced a parameter $\gamma > 0$ large enough in order to make $e^{-\beta(H_0 + (\gamma + 2dJ)\mathcal{N})}$ normalizable. This can be interpreted as an *artificial decrease of the chemical potential* which is introduced to stabilize the system by balancing the loss of the repulsion

W from the exponential. (Indeed, note that without help from γ , we would get $e^{-\beta(H_0-(\mu+2dJ)\mathcal{N})}$ which has infinite trace for $\mu > -2dJ$.)

The final expression that we arrive at via (4) can then be evaluated using Wick's theorem. Subsequently, by means of the corresponding one-particle density operator, we obtain rather explicit expressions which amount to a Riemann sum of the density of Planck's law. This density decays for large β in an integrable way. In particular, we see that the resulting expression as well as the error terms are bounded for $\beta \geq 1$ and Theorem 2 follows. For the details, see Appendix B.

For the discussed generalizations (3), one has to bound H_0 by W and then remove the generalized hopping term H_0 instead of W in the exponent by means of the Peierls-Bogoliubov argument. In the end, one obtains a trace just involving number operators, which can be easily computed as well.

5 Conclusions

We presented a rigorous proof for a thermal area law for the Bose-Hubbard model and related bosonic lattice gases. This result closes a gap in the recently growing literature about the quantum information theory of lattice bosons and provides a positive-temperature counterpart to the area law for gapped bosonic ground states (in 1D) [82].

The idea of the proof is based on the general idea in [39] together with a Peierls-Bogoliubov argument which artificially decreases the chemical potential in order to get a trace-class free reference state. The method is highly robust and extends to many other bosonic lattice gases and any lattice dimension.

Natural follow-up problems include the approximability of bosonic thermal states by generalized matrix product operators in the spirit of [71]. This is related to area laws for the generalized Rényi entropy [6], so it would be interesting to extend the present results to some Rényi generalizations of the mutual information (as in [35]), see also [40]. Furthermore, in light of recent progress of Lieb-Robinson bounds for bosons [84], [86]–[91] one could explore the applicability of such bounds and their imaginary time counterparts in the context of thermal area laws, see also [34], [44] for connections between imaginary time Lieb-Robinson bounds and thermal area laws.

On the one hand, our result is of fundamental nature in the quantum information theory of lattice systems. On the other hand, it paves the way for future information-theoretic studies of lattice bosons such as the ones described above. The goal is to unlock the full potential of these experimentally finely tunable systems for modern applications such as quantum machine learning [60], [61] and semidefinite programming solvers [62], [63].

Acknowledgments

The authors are grateful to Álvaro Alhambra and Ángela Capel Cuevas for useful comments on a draft version of the manuscript.

References

- [1] S. R. White, “Density-matrix algorithms for quantum renormalization groups,” *Phys. Rev. B*, vol. 48, no. 14, p. 10345, 1993.
- [2] F. Verstraete and J. I. Cirac, “Renormalization algorithms for quantum-many body systems in two and higher dimensions,” *arXiv:cond-mat/0407066*, 2004.
- [3] U. Schollwöck, “The density-matrix renormalization group: A short introduction,” *Philos. Trans. Royal Soc. A*, vol. 369, no. 1946, pp. 2643–2661, 2011.
- [4] E. M. Stoudenmire and S. R. White, “Studying two-dimensional systems with the density matrix renormalization group,” *Annu. Rev. Condens. Matter Phys.*, vol. 3, no. 1, pp. 111–128, 2012.
- [5] A. M. Dalzell and F. G. Brandão, “Locally accurate MPS approximations for ground states of one-dimensional gapped local Hamiltonians,” *Quantum*, vol. 3, p. 187, 2019.
- [6] F. Verstraete and J. I. Cirac, “Matrix product states represent ground states faithfully,” *Phys. Rev. B*, vol. 73, no. 9, p. 094423, 2006.
- [7] J. Eisert, M. Cramer, and M. B. Plenio, “Colloquium: Area laws for the entanglement entropy,” *Rev. Mod. Phys.*, vol. 82, no. 1, p. 277, 2010.
- [8] Y. Ge and J. Eisert, “Area laws and efficient descriptions of quantum many-body states,” *New J. Phys.*, vol. 18, no. 8, p. 083026, 2016.
- [9] R. Bousso, “The holographic principle,” *Rev. Mod. Phys.*, vol. 74, no. 3, p. 825, 2002.
- [10] M. B. Hastings, “An area law for one-dimensional quantum systems,” *J. Stat. Mech. Theory Exp.*, vol. 2007, no. 08, P08024, 2007.
- [11] I. Arad, Z. Landau, and U. Vazirani, “Improved one-dimensional area law for frustration-free systems,” *Phys. Rev. B*, vol. 85, no. 19, p. 195145, 2012.
- [12] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani, “An area law and sub-exponential algorithm for 1D systems,” 2013.
- [13] I. Arad, Z. Landau, U. Vazirani, and T. Vidick, “Rigorous RG algorithms and area laws for low energy eigenstates in 1D,” *Commun. Math. Phys.*, vol. 356, no. 1, pp. 65–105, 2017.

- [14] Y. Huang, “Area law in one dimension: Degenerate ground states and Renyi entanglement entropy,” *arXiv:1403.0327*, 2014.
- [15] F. G. Brandão and M. Horodecki, “An area law for entanglement from exponential decay of correlations,” *Nat. Phys.*, vol. 9, no. 11, pp. 721–726, 2013.
- [16] J. Cho, “Realistic area-law bound on entanglement from exponentially decaying correlations,” *Phys. Rev. X*, vol. 8, no. 3, p. 031 009, 2018.
- [17] K. Audenaert, J. Eisert, M. Plenio, and R. Werner, “Entanglement properties of the harmonic chain,” *Phys. Rev. A*, vol. 66, no. 4, p. 042 327, 2002.
- [18] M. B. Plenio, J. Eisert, J. Dreissig, and M. Cramer, “Entropy, entanglement, and area: Analytical results for harmonic lattice systems,” *Phys. Rev. Lett.*, vol. 94, no. 6, p. 060 503, 2005.
- [19] M. Cramer and J. Eisert, “Correlations, spectral gap and entanglement in harmonic quantum systems on generic lattices,” *New J. Phys.*, vol. 8, no. 5, p. 71, 2006.
- [20] M. Cramer, J. Eisert, M. B. Plenio, and J. Dreissig, “Entanglement-area law for general bosonic harmonic lattice systems,” *Phys. Rev. A*, vol. 73, no. 1, p. 012 309, 2006.
- [21] K. Van Acoleyen, M. Mariën, and F. Verstraete, “Entanglement rates and area laws,” *Phys. Rev. Lett.*, vol. 111, no. 17, p. 170 501, 2013.
- [22] M. Mariën, K. M. Audenaert, K. Van Acoleyen, and F. Verstraete, “Entanglement rates and the stability of the area law for the entanglement entropy,” *Commun. Math. Phys.*, vol. 346, no. 1, pp. 35–73, 2016.
- [23] M. B. Hastings, “Entropy and entanglement in quantum ground states,” *Phys. Rev. B*, vol. 76, no. 3, p. 035 114, 2007.
- [24] L. Masanes, “Area law for the entropy of low-energy states,” *Phys. Rev. A*, vol. 80, no. 5, p. 052 104, 2009.
- [25] N. de Beaudrap, M. Ohliger, T. Osborne, and J. Eisert, “Solving frustration-free spin systems,” *Phys. Rev. Lett.*, vol. 105, no. 6, p. 060 504, 2010.
- [26] N. Abrahamsen, “A polynomial-time algorithm for ground states of spin trees,” *arXiv:1907.04862*, 2019.
- [27] S. Michalakakis, “Stability of the area law for the entropy of entanglement,” *arXiv:1206.6900*, 2012.
- [28] F. G. Brandao and M. Cramer, “Entanglement area law from specific heat capacity,” *Phys. Rev. B*, vol. 92, no. 11, p. 115 134, 2015.
- [29] J. Cho, “Sufficient condition for entanglement area laws in thermodynamically gapped spin systems,” *Phys. Rev. Lett.*, vol. 113, no. 19, p. 197 204, 2014.
- [30] A. Anshu, I. Arad, and D. Gosset, “Entanglement subvolume law for 2D frustration-free spin systems,” in *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing*, 2020, pp. 868–874.
- [31] A. Anshu, I. Arad, and D. Gosset, “An area law for 2d frustration-free spin systems,” in *Proceedings of the 54th Annual ACM SIGACT Symposium on Theory of Computing*, 2022, pp. 12–18.
- [32] Z.-X. Gong, M. Foss-Feig, F. G. S. L. Brandão, and A. V. Gorshkov, “Entanglement area laws for long-range interacting systems,” *Phys. Rev. Lett.*, vol. 119, p. 050 501, 5 Jul. 2017.
- [33] T. Kuwahara and K. Saito, “Area law of non-critical ground states in 1D long-range interacting systems,” *Nat. Commun.*, vol. 11, no. 1, pp. 1–7, 2020.
- [34] T. Kuwahara, Á. M. Alhambra, and A. Anshu, “Improved thermal area law and quasilinear time algorithm for quantum Gibbs states,” *Phys. Rev. X*, vol. 11, no. 1, p. 011 047, 2021.
- [35] S. O. Scalet, Á. M. Alhambra, G. Styliaris, and J. I. Cirac, “Computable Rényi mutual information: Area laws and correlations,” *Quantum*, vol. 5, p. 541, Sep. 2021.
- [36] Á. M. Alhambra and J. I. Cirac, “Locally accurate tensor networks for thermal states and time evolution,” *PRX Quantum*, vol. 2, p. 040 331, 4 Nov. 2021.
- [37] M. A. Nielsen and I. Chuang, *Quantum computation and quantum information*, 2002.
- [38] Á. M. Alhambra, “Quantum many-body systems in thermal equilibrium,” *arXiv:2204.08349*, 2022.
- [39] M. M. Wolf, F. Verstraete, M. B. Hastings, and J. I. Cirac, “Area laws in quantum systems: Mutual information and correlations,” *Phys. Rev. Lett.*, vol. 100, no. 7, p. 070 502, 2008.
- [40] D. Gottesman and M. B. Hastings, “Entanglement versus gap for one-dimensional spin systems,” *New J. Phys.*, vol. 12, no. 2, p. 025 002, 2010.
- [41] H. Bernigau, M. J. Kastoryano, and J. Eisert, “Mutual information area laws for thermal free fermions,” *J. Stat. Mech: Theory Exp.*, vol. 2015, no. 2, P02008, Feb. 2015.

- [42] N. E. Sherman, T. Devakul, M. B. Hastings, and R. R. Singh, “Nonzero-temperature entanglement negativity of quantum spin models: Area law, linked cluster expansions, and sudden death,” *Phys. Rev. E*, vol. 93, no. 2, p. 022 128, 2016.
- [43] M. J. Kastoryano and J. Eisert, “Rapid mixing implies exponential decay of correlations,” *J. Math. Phys.*, vol. 54, no. 10, p. 102 201, 2013.
- [44] F. G. Brandao, T. S. Cubitt, A. Lucia, *et al.*, “Area law for fixed points of rapidly mixing dissipative quantum systems,” *J. Math. Phys.*, vol. 56, no. 10, p. 102 202, 2015.
- [45] M. Žnidarič, T. Prosen, and I. Pižorn, “Complexity of thermal states in quantum spin chains,” *Phys. Rev. A*, vol. 78, no. 2, p. 022 103, 2008.
- [46] M. Tajik, I. Kukuljan, S. Sotiriadis, *et al.*, “Verification of the area law of mutual information in a quantum field simulator,” *Nat. Phys.*, pp. 1–5, 2023.
- [47] H. Araki, “Gibbs states of a one dimensional quantum lattice,” *Commun. Math. Phys.*, vol. 14, no. 2, pp. 120–157, 1969.
- [48] L. Gross, “Decay of correlations in classical lattice models at high temperature,” *Commun. Math. Phys.*, vol. 68, no. 1, pp. 9–27, 1979.
- [49] Y. M. Park and H. J. Yoo, “Uniqueness and clustering properties of gibbs states for classical and quantum unbounded spin systems,” *J. Stat. Phys.*, vol. 80, no. 1, pp. 223–271, 1995.
- [50] D. Ueltschi, “Cluster expansions and correlation functions,” *Moscow Math. J.*, vol. 4, no. 2, pp. 511–522, 2004.
- [51] M. Kliesch, C. Gogolin, M. Kastoryano, *et al.*, “Locality of temperature,” *Phys. Rev. X*, vol. 4, no. 3, p. 031 019, 2014.
- [52] J. Fröhlich and D. Ueltschi, “Some properties of correlations of quantum lattice systems in thermal equilibrium,” *J. Math. Phys.*, vol. 56, no. 5, p. 053 302, 2015.
- [53] M. Lenci and L. Rey-Bellet, “Large deviations in quantum lattice systems: One-phase region,” *J. Stat. Phys.*, vol. 119, no. 3, pp. 715–746, 2005.
- [54] K. Netočný and F. Redig, “Large deviations for quantum spin systems,” *J. Stat. Phys.*, vol. 117, no. 3, pp. 521–547, 2004.
- [55] T. Kuwahara and K. Saito, “Gaussian concentration bound and ensemble equivalence in generic quantum many-body systems including long-range interactions,” *Ann. Phys.*, vol. 421, p. 168 278, 2020.
- [56] K. Kato and F. G. Brandao, “Quantum approximate markov chains are thermal,” *Commun. Math. Phys.*, vol. 370, no. 1, pp. 117–149, 2019.
- [57] T. Kuwahara, K. Kato, and F. G. Brandao, “Clustering of conditional mutual information for quantum gibbs states above a threshold temperature,” *Phys. Rev. Lett.*, vol. 124, no. 22, p. 220 601, 2020.
- [58] F. Barahona, “On the computational complexity of ising spin glass models,” *J. Phys. A: Math. Gen.*, vol. 15, no. 10, p. 3241, 1982.
- [59] L. A. Goldberg and M. Jerrum, “A complexity classification of spin systems with an external field,” *Proc. Natl. Acad. Sci. U.S.A.*, vol. 112, no. 43, pp. 13 161–13 166, 2015.
- [60] M. H. Amin, E. Andriyash, J. Rolfe, *et al.*, “Quantum Boltzmann machine,” *Phys. Rev. X*, vol. 8, no. 2, p. 021 050, 2018.
- [61] A. Anshu, S. Arunachalam, T. Kuwahara, and M. Soleimanifar, “Sample-efficient learning of interacting quantum systems,” *Nat. Phys.*, vol. 17, no. 8, pp. 931–935, 2021.
- [62] F. G. Brandao and K. M. Svore, “Quantum speed-ups for solving semidefinite programs,” in *2017 IEEE 58th Annual Symposium on Foundations of Computer Science (FOCS)*, IEEE, 2017, pp. 415–426.
- [63] J. Van Apeldoorn, A. Gilyén, S. Gribling, and R. de Wolf, “Quantum SDP-solvers: Better upper and lower bounds,” *Quantum*, vol. 4, p. 230, 2020.
- [64] M. Motta, C. Sun, A. T. Tan, *et al.*, “Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution,” *Nat. Phys.*, vol. 16, no. 2, pp. 205–210, 2020.
- [65] H. Lamm and S. Lawrence, “Simulation of nonequilibrium dynamics on a quantum computer,” *Phys. Rev. Lett.*, vol. 121, no. 17, p. 170 501, 2018.
- [66] M. J. Beach, R. G. Melko, T. Grover, and T. H. Hsieh, “Making trotters sprint: A variational imaginary time ansatz for quantum many-body systems,” *Phys. Rev. B*, vol. 100, no. 9, p. 094 434, 2019.
- [67] X. Yuan, S. Endo, Q. Zhao, *et al.*, “Theory of variational quantum simulation,” *Quantum*, vol. 3, p. 191, 2019.
- [68] S. McArdle, T. Jones, S. Endo, *et al.*, “Variational ansatz-based quantum simulation of imaginary time evolution,” *Npj Quantum Inf.*, vol. 5, no. 1, pp. 1–6, 2019.
- [69] K. Yeter-Aydeniz, R. C. Pooser, and G. Siopsis, “Practical quantum computation of chemical and nuclear energy levels using quantum imaginary time evolution and lanczos algorithms,” *Npj Quantum Inf.*, vol. 6, no. 1, pp. 1–8, 2020.

- [70] P. J. Love, “Cooling with imaginary time,” *Nat. Phys.*, vol. 16, no. 2, pp. 130–131, 2020.
- [71] J. Guth Jarkovský, A. Molnár, N. Schuch, and J. I. Cirac, “Efficient description of many-body systems with matrix product density operators,” *PRX Quantum*, vol. 1, p. 010304, 1 Sep. 2020.
- [72] M. Berta, F. G. S. L. Brandão, J. Haegeman, *et al.*, “Thermal states as convex combinations of matrix product states,” *Phys. Rev. B*, vol. 98, p. 235154, 23 Dec. 2018.
- [73] I. Bloch, J. Dalibard, and W. Zwerger, “Many-body physics with ultracold gases,” *Rev. Mod. Phys.*, vol. 80, no. 3, p. 885, 2008.
- [74] A. M. Childs, D. Gosset, and Z. Webb, “The Bose-Hubbard model is QMA-complete,” in *International Colloquium on Automata, Languages, and Programming*, Springer, 2014, pp. 308–319.
- [75] V. V. Albert, “Bosonic coding: Introduction and use cases,” *arXiv:2211.05714*, 2022.
- [76] S. M. Girvin, “Introduction to quantum error correction and fault tolerance,” *SciPost Phys. Lect. Notes*, p. 70, 2023.
- [77] M. Cramer, J. Eisert, and M. Plenio, “Statistics dependence of the entanglement entropy,” *Phys. Rev. Lett.*, vol. 98, no. 22, p. 220603, 2007.
- [78] V. Alba, M. Haque, and A. M. Läuchli, “Entanglement spectrum of the two-dimensional Bose-Hubbard model,” *Phys. Rev. Lett.*, vol. 110, no. 26, p. 260403, 2013.
- [79] M. A. Metlitski and T. Grover, “Entanglement entropy of systems with spontaneously broken continuous symmetry,” *arXiv:1112.5166*, 2011.
- [80] A. B. Kallin, M. B. Hastings, R. G. Melko, and R. R. Singh, “Anomalies in the entanglement properties of the square-lattice Heisenberg model,” *Phys. Rev. B*, vol. 84, no. 16, p. 165134, 2011.
- [81] H. F. Song, N. Laflorencie, S. Rachel, and K. Le Hur, “Entanglement entropy of the two-dimensional Heisenberg antiferromagnet,” *Phys. Rev. B*, vol. 83, no. 22, p. 224410, 2011.
- [82] N. Abrahamsen, Y. Su, Y. Tong, and N. Wiebe, “Entanglement area law for 1D gauge theories and bosonic systems,” *arXiv:2203.16012*, 2022.
- [83] Y. Tong, V. V. Albert, J. R. McClean, *et al.*, “Provably accurate simulation of gauge theories and bosonic systems,” *Quantum*, vol. 6, p. 816, 2022.
- [84] J. Faupin, M. Lemm, and I. M. Sigal, “Maximal speed for macroscopic particle transport in the Bose-Hubbard model,” *Phys. Rev. Lett.*, vol. 128, no. 15, p. 150602, 2022.
- [85] E. Carlen, “Trace inequalities and quantum entropy: An introductory course,” in *Entropy and the quantum*, ser. Contemp. Math. Vol. 529, Amer. Math. Soc., Providence, RI, 2010, pp. 73–140.
- [86] N. Schuch, S. K. Harrison, T. J. Osborne, and J. Eisert, “Information propagation for interacting-particle systems,” *Phys. Rev. A*, vol. 84, no. 3, p. 032309, 2011.
- [87] Z. Wang and K. R. Hazzard, “Tightening the Lieb-Robinson bound in locally interacting systems,” *PRX Quantum*, vol. 1, no. 1, p. 010303, 2020.
- [88] T. Kuwahara and K. Saito, “Lieb-Robinson bound and almost-linear light cone in interacting boson systems,” *Phys. Rev. Lett.*, vol. 127, no. 7, p. 070403, 2021.
- [89] J. Faupin, M. Lemm, and I. M. Sigal, “On Lieb-Robinson bounds for the Bose-Hubbard model,” *Commun. Math. Phys.*, vol. 394, no. 3, pp. 1011–1037, 2022.
- [90] C. Yin and A. Lucas, “Finite speed of quantum information in models of interacting bosons at finite density,” *Phys. Rev. X*, vol. 12, no. 2, p. 021039, 2022.
- [91] T. Kuwahara, T. Van Vu, and K. Saito, “Optimal light cone and digital quantum simulation of interacting bosons,” *arXiv:2206.14736*, 2022.
- [92] M. B. Ruskai, “Inequalities for traces on von neumann algebras,” *Commun. Math. Phys.*, vol. 26, no. 4, pp. 280–289, 1972.
- [93] D. Ruelle, *Statistical Mechanics: Rigorous Results*. New York: W.A. Benjamin, 1969.
- [94] O. Bratteli and D. Robinson, *Operator Algebras and Quantum Statistical Mechanics: Equilibrium States. Models in Quantum Statistical Mechanics* (Theoretical and Mathematical Physics). Springer Berlin Heidelberg, 2003.
- [95] M. Ohya and D. Petz, *Quantum entropy and its use*. Springer Science & Business Media, 2004.
- [96] G. Lindblad, “Completely positive maps and entropy inequalities,” *Commun. Math. Phys.*, vol. 40, no. 2, pp. 147–151, 1975.

A Preliminaries

A.1 Operator domains

For the general setup, we require the following statements about operator domains. We assume that H_A and H_B are densely defined symmetric operators on $\mathcal{D}(A)$ and $\mathcal{D}(B)$, respectively and the boundary Hamiltonian is defined on H_∂ on $\mathcal{D}(A) \otimes \mathcal{D}(B)$. We assume that H_{AB} is essentially self-adjoint on $\mathcal{D}(A) \otimes \mathcal{D}(B)$ which is then the appropriate domain for the equality

$$H_{AB} = H_A \otimes \mathbb{1} + \mathbb{1} \otimes H_B + H_\partial \quad (5)$$

Concerning the Bose-Hubbard model, in the total Fock space $\mathfrak{F}(\ell^2(\Lambda_L))$, we consider the dense domain

$$\mathfrak{F}_{\text{fin}}(\ell^2(\Lambda_L)) = \{\psi \in \mathfrak{F}(\ell^2(\Lambda_L)) : \exists n_0 \in \mathbb{N} : \forall n \geq n_0 : \psi_n = 0\}.$$

The operator H_{AB} is self-adjoint on the largest domain $\mathcal{D}(H_{AB})$, where it can be defined, cf. [84]. It then follows from $[H_{AB}, \mathcal{N}] = 0$ that H_{AB} is indeed essentially self-adjoint on $\mathfrak{F}_{\text{fin}}(\ell^2(\Lambda_L))$. Moreover, for subsystems $X \in \{A, B\}$, we always set $\mathcal{D}(X) = \mathfrak{F}_{\text{fin}}(\mathcal{H}_X)$. The above properties can then be verified.

A.2 Trace inequalities in infinite dimensions

Lemma 3 (Peierls-Bogoliubov inequality)

Let $\mathcal{N} \geq 0$ be self-adjoint operator with purely discrete spectrum, let $\Pi_N := \mathbb{1}_{\mathcal{N} \leq N}$, $N \in \mathbb{N}$ and assume that $\Pi_N \mathcal{H}$ is finite-dimensional for all $N \in \mathbb{N}$. Let $(\mathcal{D}(K), K)$ be a self-adjoint and $(\mathcal{D}(P), P)$ be a symmetric operator such that $[K, \mathcal{N}] = 0$, $[P, \mathcal{N}] = 0$, $K + P$ is self-adjoint, and e^K , Pe^K , e^{K+P} are all trace-class. Then we have

$$\frac{\text{tr}(Pe^K)}{\text{tr}(e^K)} \leq \log \left(\frac{\text{tr}(e^{K+P})}{\text{tr}(e^K)} \right), \quad (6)$$

In particular, if Pe^{K+P} is trace-class as well, we obtain (4), i.e.,

$$\frac{\text{tr}(Pe^K)}{\text{tr}(e^K)} \leq \frac{\text{tr}(Pe^{K+P})}{\text{tr}(e^{K+P})}. \quad (7)$$

Proof of Lemma 3. The inequality (6) is well-known for matrices, see for example [85, (2.14)] (or more generally if P is bounded [92]). Therefore, we have

$$\frac{\text{tr}(Pe^K \Pi_N)}{\text{tr}(e^K \Pi_N)} \leq \log \left(\frac{\text{tr}(e^{K+P} \Pi_N)}{\text{tr}(e^K \Pi_N)} \right),$$

where $\Pi_N = \mathbb{1}_{\mathcal{N} \leq N}$. Taking the limit $N \rightarrow \infty$ yields the desired result. Finally, (4) follows from (6) by means of

$$\log \left(\frac{\text{tr}(e^{K+P})}{\text{tr}(e^K)} \right) = -\log \left(\frac{\text{tr}(e^K)}{\text{tr}(e^{K+P})} \right) \leq \frac{\text{tr}(Pe^{K+P})}{\text{tr}(e^{K+P})}.$$

This proves Lemma 3. □

Proposition 4 (Gibbs variational principle)

Let $(H, \mathcal{D}(H))$ be a self-adjoint operator such that $\text{tr} e^{-\beta H} < \infty$ for all $\beta > 0$. Let $\mathcal{F}^\beta(\rho) := \left(\text{tr}(H\rho) - \frac{S(\rho)}{\beta} \right)$. Then

$$\inf_{\rho \in \mathcal{T}_1^+(\mathcal{H})} \mathcal{F}^\beta(\rho) = \mathcal{F}^\beta(\rho_H),$$

where $\rho_H = e^{-\beta H} / \text{tr} e^{-\beta H}$.

Proof of Proposition 4. We have

$$\text{tr}(K \ln K - K \ln P) \geq \text{tr}(K - P)$$

for all positive self-adjoint trace class operators K, P [93, Prop. 2.5.3]. This yields [94, Section 5.3.1]

$$\mathcal{F}^\beta(\rho) = \beta^{-1} \text{tr}(\rho \ln \rho - \rho \ln \rho_H) - \beta^{-1} \ln \text{tr} e^{-\beta H} \geq -\beta^{-1} \ln \text{tr} e^{-\beta H} = \mathcal{F}^\beta(\rho_H). \quad \square$$

A.3 Truncated correlations bound

Let M_A, M_B be two bounded self-adjoint operators on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. We denote their truncated correlation function as

$$\mathcal{C}(A, B) = \text{tr}(M_A \otimes M_B \rho_{AB}) - \text{tr}(M_A \rho_A) \text{tr}(M_B \rho_B).$$

For all $\beta, U, \mu > 0$, we have

$$\frac{\mathcal{C}(A, B)^2}{2 \|M_A\|^2 \|M_B\|^2} \leq 2c(J, U, \mu) \max\{1, \beta\} |\partial_{AB}|, \quad (8)$$

with the same constant as in Theorem 2. This follows from the quantum Pinsker inequality $I(A : B) \geq \frac{1}{2} \|\rho_{AB} - \rho_A \otimes \rho_B\|_1^2$ and $\|X\|_1 \geq \text{tr}(XY)/\|Y\|$. We mention that the standard proof of the quantum Pinsker inequality, cf. [95, Theorem 1.15] extends to infinite dimensions since the data processing inequality holds for trace-class operators [96].

Note however that (8) is trivial unless $|\partial_{AB}|$ stays bounded in the infinite-volume limit, e.g. if A or B are kept at fixed size, as its left-hand side is always bounded by one. Therefore, in order to find more regimes where this is useful, it is an interesting open question if our main estimate in Theorem 2 can be improved for $\beta \rightarrow 0$, as it is the case for spin systems [34], [39].

B Proof of Theorem 2

To begin, we notice that we may assume without loss of generality that $J > 0$. Indeed, if $J = 0$, the Gibbs state is a product state (Mott insulator) and the claim is trivial and if $J < 0$ we can employ the unitary transformation $a_x \rightarrow -a_x$ at every second lattice site to reduce to the case $J > 0$.

B.1 Step 1: Controlling boundary energy by particle number

In this section, we prove the following bound

Proposition 5

We have

$$I(A : B) \leq \frac{4d |\partial_{AB}|}{L^d} \beta J \text{tr}(\mathcal{N} \rho_{AB}).$$

Proof of Proposition 5. Using Lemma 1 and the operator Cauchy-Schwarz inequality $\pm(a_x^\dagger a_y + a_y^\dagger a_x) \leq n_x + n_y$ we get

$$I(A : B) \leq \beta J \sum_{\substack{x \sim y, \\ x \in A, y \in B}} \text{tr}((n_x + n_y)(\rho_A \otimes \rho_B + \rho_{AB})).$$

Since, for $x \in A$, $\text{tr}(n_x \rho_A \otimes \rho_B) = \text{tr}(n_x \rho_A) = \text{tr}(n_x \rho_{AB})$ and similarly for n_y and ρ_B , we obtain

$$I(A : B) \leq 2\beta J \sum_{\substack{x \sim y, \\ x \in A, y \in B}} \text{tr}((n_x + n_y) \rho_{AB}). \quad (9)$$

Observe that H_{AB} is translation-invariant, i.e., for all $x \in \Lambda_L$,

$$\mathcal{T}_x^* H_{AB} \mathcal{T}_x = H_{AB},$$

where $\mathcal{T}_x$ denotes the unitary translation operator by x , $(\mathcal{T}_x \psi)(y) = \psi(y + x \bmod L)$. This implies $\mathcal{T}_x^* \rho_{AB} \mathcal{T}_x = \rho_{AB}$ and therefore, $\text{tr}(n_x \rho_{AB}) = \text{tr}(n_y \rho_{AB})$ for all x, y . The summation in (9) is over $|\partial_{AB}|$ many terms, so

$$\sum_{x \sim y, x \in A, y \in B} \text{tr}((n_x + n_y) \rho_{AB}) \leq 2d |\partial_{AB}| \text{tr}(n_{x_0} \rho_{AB}) = 2d |\partial_{AB}| \frac{\text{tr}(\mathcal{N} \rho_{AB})}{L^d},$$

where $x_0 \in \Lambda$ is some arbitrary element. This proves Proposition 5. $\square$

B.2 Step 2: Removing the interaction from the exponential

In the following we write $\langle P \rangle_K := \text{tr}(Pe^{-K})/\text{tr}(e^{-K})$ for operators K and P and we will also drop the subscript AB and write $H = H_{AB}$.

Proposition 6

Let $C_0 = \frac{1}{4} \frac{U}{\gamma + \mu}$. For all $\gamma > 0$, we have

$$\langle \mathcal{N} \rangle_{\beta H} \leq 2 \left(\frac{C_0}{U/2} \langle W - (\mu + \gamma - 2dJ)\mathcal{N} \rangle_{\beta(H_0 + \gamma\mathcal{N})} + \frac{C_0}{4} (1 + C_0^{-1})^2 L^d \right).$$

Proof of Proposition 6. Let $C > 0$. We have $n \leq Cn(n-1) + \frac{C}{4}(1+C^{-1})^2$ for all $n \in \mathbb{N}$. Thus, we obtain

$$\langle \mathcal{N} \rangle_{\beta H} = \left\langle \sum_{x \in \Lambda_L} n_x \right\rangle_{\beta H} \leq \sum_{x \in \Lambda_L} \left\langle Cn_x(n_x - 1) + \frac{C}{4}(1 + C^{-1})^2 \right\rangle_{\beta H} = \frac{C}{U/2} \langle W \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d.$$

This leads to

$$\begin{aligned} \langle \mathcal{N} \rangle_{\beta H} \left(1 - \frac{C}{U/2} (\mu + \gamma) \right) &\leq \frac{C}{U/2} \langle W - (\mu + \gamma)\mathcal{N} \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d \\ &\leq \frac{C}{U/2} \langle W - (\mu + \gamma - 2dJ)\mathcal{N} \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d. \end{aligned}$$

We now apply twice the Peierls-Bogoliubov inequality, i.e., (4) in Lemma 3 with $P = \beta(W - (\mu + \gamma - 2dJ)\mathcal{N})$ and $K = -\beta H$, and get

$$\langle W - (\mu + \gamma - 2dJ)\mathcal{N} \rangle_{\beta H} \leq \langle W - (\mu + \gamma - 2dJ)\mathcal{N} \rangle_{\beta(H_0 + \gamma\mathcal{N})}.$$

Using this in the previous bound and setting $C = C_0$ yields the desired estimate. This proves Proposition 6. $\square$

B.3 Step 3: Calculation for quasi-free states

The estimate of the on-site interaction in the free reference states leads to an estimate of the particle number on a specific site via the one-particle density matrix. Here we get a Riemann sum of the density function of Planck's law.

We set

$$f(\gamma, \beta, J) := \int_{[0, \frac{1}{2}]^d} \left(e^{4J\beta \sum_{j=1}^d \sin^2(\pi x_j) + \beta\gamma} - 1 \right)^{-1} dx,$$

and denote the error terms by

$$\begin{aligned} \epsilon_1 &= \frac{(L+1)^d}{L^d} - 1, \\ \epsilon_2 &= \frac{(e^{\beta\gamma} - 1)^{-1}}{L^d} ((L+2)^d - (L+1)^d). \end{aligned}$$

We shall use the following two lemmas.

Lemma 7

For all $\gamma > 0$ and $x \in \Lambda_L$,

$$\langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma\mathcal{N})} \leq 2^d (1 + \epsilon_1) f(\gamma, \beta, J) + \epsilon_2.$$

Lemma 8

For all $\gamma > 0$,

$$f(\gamma, \beta, J) \leq \frac{1}{2^d} \frac{1}{\beta\gamma}.$$

We postpone the proofs of these lemmas for now and show how they imply the main result.

Proof of Theorem 2. Wick's theorem for quasi-free states [94, p.40 and Prop. 5.2.28] yields

$$\langle n_x(n_x - 1) \rangle_{\beta(H_0 + \gamma\mathcal{N})} = \langle (a_x^\dagger a_x)^2 \rangle_{\beta(H_0 + \gamma\mathcal{N})} = 2 \langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma\mathcal{N})}^2.$$

By Lemma 7,

$$\langle W \rangle_{\beta(H_0 + \gamma\mathcal{N})} = 2L^d \langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma\mathcal{N})}^2 \leq 2^{2d+2} L^d (1 + \epsilon_1)^2 f(\gamma, \beta, J)^2 + 4L^d \epsilon_2^2.$$

Using this and $\langle -(\mu + \gamma - 2dJ)\mathcal{N} \rangle_{\beta(H_0 + \gamma\mathcal{N})} \leq 0$ in the upper bound of Proposition 6, we obtain that for all $\gamma > 2dJ - \mu$,

$$\langle \mathcal{N} \rangle_{\beta H} \leq 2L^d \left(\frac{C_0}{U/2} (2^{2d+2} (1 + \epsilon_1)^2 f(\gamma, \beta, J)^2 + 4\epsilon_2^2) + \frac{C_0}{4} (1 + C_0^{-1})^2 \right).$$

Next we use that $f(\gamma, \beta, J) \leq \frac{1}{2^d} \frac{e^{-\alpha\beta\gamma}}{(1-\alpha)\beta\gamma}$ for all $\alpha \in (0, 1)$, cf. Lemma 8. The upper bound for $\langle \mathcal{N} \rangle_{\beta H}$ then becomes

$$2L^d \left(\frac{1}{2} \frac{1}{\gamma + \mu} \left(4(1 + \epsilon_1)^2 \frac{1}{\beta^2 \gamma^2} + 4\epsilon_2^2 \right) + \frac{1}{16} \frac{U}{\gamma + \mu} + \frac{\gamma + \mu}{U} + \frac{1}{2} \right).$$

Estimating $1 + \epsilon_1 \leq 2^d$ and $\epsilon_2 \leq 3^d (e^{\beta\gamma} - 1)^{-1}$ and choosing $\gamma = \max\{1/\beta, 2dJ + 1\}$ (such that $\beta\gamma \geq 1$), we arrive at the bound

$$\begin{aligned} \langle \mathcal{N} \rangle_{\beta H} &\leq 2L^d \left(\frac{1}{2(2dJ + 1 + \mu)} \left(4 \cdot 4^d + 4 \cdot 3^{2d} (e - 1)^{-2} \right) + \frac{1}{16} \frac{U}{2dJ + 1 + \mu} + \frac{\max\{1/\beta, 2dJ + 1\} + \mu}{U} + \frac{1}{2} \right) \\ &\leq \frac{L^d}{8} \max \left\{ \frac{1}{\beta}, 1 \right\} c(J, U, \mu), \end{aligned} \quad (10)$$

with

$$c(J, U, \mu) := 16dJ \left(\frac{4^d + 4 \cdot 3^{2d} (e - 1)^{-2}}{2(2dJ + 1 + \mu)} + \frac{1}{16} \frac{U}{2dJ + 1 + \mu} + \frac{2dJ + 1 + \mu}{U} + \frac{1}{2} \right), \quad (11)$$

and where the last step (10) follows from distinguishing the cases $\beta \gtrless 1$. Finally, we conclude the proof with Proposition 5. $\square$

Remark 9. Notice that the error terms ϵ_1 and ϵ_2 converge to zero as $L \rightarrow \infty$. It is of separate interest whether the remaining term $2^d f(\gamma, \beta, J)$ actually captures the correct asymptotic behavior of $\langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma\mathcal{N})}$, cf. Lemma 7.

B.4 Laplace eigenvalues and eigenvectors for periodic boundary conditions

The proofs proof of Lemma 7 requires information on the spectral theory of the one-body graph Laplacian, for which introduce notation here.

Consider the discrete Laplacian $-\Delta \geq 0$ on the chain $\{0, 1, \dots, L\}$, $L \in \mathbb{N}$, with periodic boundary conditions, i.e., assume that the nodes 0 and L are identified such that every vector on $\ell^2(\{0, 1, \dots, L\})$ satisfies $v(0) = v(L)$. So it suffices to use vectors $v \in \ell^2(\{1, \dots, L\})$.

The L eigenvalues λ_i and eigenvectors v_i , $i = 1, \dots, L$ of $-\Delta$ in this situation are given by

$$\begin{aligned} \lambda_{2k+1} &= 4 \sin^2 \left(\frac{k\pi}{L} \right), \quad k = 0, \dots, \left\lfloor \frac{L-1}{2} \right\rfloor, \\ \lambda_{2k} &= 4 \sin^2 \left(\frac{k\pi}{L} \right), \quad k = 1, \dots, \left\lfloor \frac{L}{2} \right\rfloor, \end{aligned}$$

and

$$\begin{aligned} v_1(i) &= L^{-1/2}, \\ v_L(i) &= L^{-1/2} (-1)^i \text{ if } L \text{ even}, \\ v_{2k+1}(i) &= \sqrt{2/L} \cos \left(\frac{\pi k}{L} (2i - 1) \right), \quad k = 1, \dots, \left\lfloor \frac{L-1}{2} \right\rfloor, \\ v_{2k}(i) &= \sqrt{2/L} \sin \left(\frac{\pi k}{L} (2i - 1) \right), \quad k = 1, \dots, \left\lfloor \frac{L-1}{2} \right\rfloor. \end{aligned}$$

B.5 Proofs of Lemmas 7 and 8

In this section, we give the still outstanding proofs of Lemmas 7 and 8.

Proof of Lemma 7. Let $x_0 = (1, \dots, 1) \in \Lambda_L$. By the formula for the one-particle density matrix, cf. e.g. [94, Prop. 5.2.28] and by translation-invariance we find

$$\begin{aligned} \langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma \mathcal{N})} &= \langle \delta_x, e^{-\beta \gamma} e^{-\beta(-J\Delta)} (\mathbb{1} - e^{-\beta \gamma} e^{-\beta(-J\Delta)})^{-1} \delta_x \rangle \\ &= \langle \delta_{x_0}, (e^{\beta(-J\Delta + \gamma)} - \mathbb{1})^{-1} \delta_{x_0} \rangle \\ &= \sum_{i_1, \dots, i_d=1}^L (e^{\beta(J \sum_{j=1}^d \lambda_{i_j} + \gamma)} - 1)^{-1} \prod_{j=1}^d |v_{i_j}(1)|^2. \end{aligned}$$

Let $\ell = \lceil \frac{L}{2} \rceil$. Then we have for any $c > 0$

$$\begin{aligned} \sum_{i=1}^L (e^{\beta(J\lambda_i + c)} - 1)^{-1} |v_i(1)|^2 &= \frac{1}{L} (e^{\beta c} - 1)^{-1} + \sum_{i=1}^{\ell} (e^{\beta(J\lambda_{2i} + c)} - 1)^{-1} \left(|v_{2i}(1)|^2 + \mathbb{1}_{L=2\ell+1} |v_{2i+1}(1)|^2 \right) \\ &\leq \frac{1}{L} (e^{\beta c} - 1)^{-1} + \frac{2}{L} \sum_{i=1}^{\ell} (e^{\beta(J\lambda_{2i} + c)} - 1)^{-1}. \end{aligned} \quad (12)$$

Then, by induction over d and using (12) for the induction step, we find as an upper bound

$$\langle a_x^\dagger a_x \rangle_{\beta(H_0 + \gamma \mathcal{N})} \leq \frac{1}{L^d} \sum_{k=0}^d \binom{d}{k} 2^k \sum_{i_1, \dots, i_k=1}^{\ell} (e^{\beta(J \sum_{j=1}^k \lambda_{2i_j} + \gamma)} - 1)^{-1}, \quad (13)$$

where the sum over the $i_1, \dots, i_k$ is defined to be one if $k = 0$. This can be proven like the binomial theorem, more precisely,

$$\begin{aligned} \sum_{i_1, \dots, i_{d+1}=1}^L (e^{\beta(J \sum_{j=1}^{d+1} \lambda_{i_j} + \gamma)} - 1)^{-1} \prod_{j=1}^{d+1} |v_{i_j}(1)|^2 \\ \leq \frac{1}{L^d} \sum_{k=0}^d \binom{d}{k} 2^k \sum_{i_1, \dots, i_k=1}^{\ell} \sum_{i_{d+1}=1}^L (e^{\beta(J \sum_{j=1}^k \lambda_{2i_j} + \lambda_{i_{d+1}} + \gamma)} - 1)^{-1} |v_{i_{d+1}}(1)|^2 \\ \leq \frac{1}{L^{d+1}} \sum_{k=0}^d \binom{d}{k} 2^k \sum_{i_1, \dots, i_k=1}^{\ell} \left((e^{\beta(J \sum_{j=1}^k \lambda_{2i_j} + \gamma)} - 1)^{-1} + 2 \sum_{i_{d+1}=1}^{\ell} (e^{\beta(J \sum_{j=1}^{k+1} \lambda_{2i_j} + \gamma)} - 1)^{-1} \right) \\ = \frac{1}{L^{d+1}} \sum_{k=0}^{d+1} \binom{d+1}{k} 2^k \sum_{i_1, \dots, i_k=1}^{\ell} (e^{\beta(J \sum_{j=1}^k \lambda_{2i_j} + \gamma)} - 1)^{-1}, \end{aligned}$$

where we use the induction hypothesis in the first step and (12) for the second step. With $2\ell - 1 \leq L$ the first terms for $k = 0, \dots, d-1$ in (13) can be estimated by

$$\frac{(e^{\beta \gamma} - 1)^{-1}}{L^d} \sum_{k=0}^{d-1} \binom{d}{k} (2\ell)^k \leq \frac{(e^{\beta \gamma} - 1)^{-1}}{L^d} \sum_{k=0}^{d-1} \binom{d}{k} (L+1)^k = \frac{(e^{\beta \gamma} - 1)^{-1}}{L^d} ((L+2)^d - (L+1)^d) = \epsilon_2.$$

The term for $k = d$ in (13) represents a Riemann sum of a function, decreasing in each argument, which is evaluated at the minimal points of the hypercubes $[(i_1 - 1)\pi/2, i_1\pi/2] \times \dots \times [(i_d - 1)\pi/2, i_d\pi/2]$, i.e.,

$$\begin{aligned} \frac{2^d}{L^d} \sum_{i_1, \dots, i_d=1}^{\ell} (e^{\beta(J \sum_{j=1}^d \lambda_{2i_j} + \gamma)} - 1)^{-1} \\ = \frac{(2\ell)^d}{L^d \ell^d} \sum_{i_1, \dots, i_d=1}^{\ell} (e^{\beta(4J \sum_{j=1}^d \sin^2(i_j \pi / L) + \gamma)} - 1)^{-1} \\ \leq \frac{(L+1)^d}{L^d \ell^d} \sum_{i_1, \dots, i_d=1}^{\ell} (e^{\beta(4J \sum_{j=1}^d \sin^2(i_j \pi / (2\ell)) + \gamma)} - 1)^{-1} \end{aligned}$$

$$\begin{aligned}
&\leq \frac{(L+1)^d}{L^d} \int_{[0,1]^d} (e^{\beta(4J \sum_{j=1}^d \sin^2(x_j \pi/2) + \gamma)} - 1)^{-1} dx \\
&= 2^d \frac{(L+1)^d}{L^d} f(\gamma, \beta, J).
\end{aligned}$$

□

Proof of Lemma 8. We have for any $\alpha \in (0, 1)$,

$$\begin{aligned}
&\int_{[0, \frac{1}{2}]^d} (e^{4J\beta \sum_{j=1}^d \sin^2(\pi x_j) + \beta\gamma} - 1)^{-1} dx \\
&= e^{-\alpha\beta\gamma} \int_{[0, \frac{1}{2}]^d} (e^{4J\beta \sum_{j=1}^d \sin^2(\pi x_j) + (1-\alpha)\beta\gamma} - e^{-\alpha\beta\gamma})^{-1} dx \\
&\leq e^{-\alpha\beta\gamma} \int_{[0, \frac{1}{2}]^d} (e^{4J\beta \sum_{j=1}^d \sin^2(\pi x_j) + (1-\alpha)\beta\gamma} - 1)^{-1} dx \\
&\leq e^{-\alpha\beta\gamma} \int_{[0, \frac{1}{2}]^d} ((1-\alpha)\beta\gamma)^{-1} dx = \frac{1}{2^d} \frac{e^{-\alpha\beta\gamma}}{(1-\alpha)\beta\gamma}.
\end{aligned}$$

Then taking $\alpha \rightarrow 0$ proves Lemma 8.

□