Thermal Area Law for the Bose-Hubbard Model

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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. Thermal area laws have been derived for systems with bounded local interactions such as quantum spin systems. However, for lattice bosons these arguments break down because the interactions are unbounded. 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.

Entanglement is central to the foundations of quantum mechanics and has received increasing attention in recent years due to the rise of quantum information theory and quantum computing. It can be quantified and compared by associating suitable entropy functionals to subsystems. A prime example is the so-called entanglement entropy of a region A, defined as the von Neumann entropy of the reduced density matrix on A which is obtained by taking the partial trace over the complement of A.

It is expected that in typical systems with translation-invariant short-ranged interactions the entanglement entropy of the ground state 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] and its higher-dimensional extensions [2–4]. 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 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 [28, 29, 30, 31]. There has also been recent progress for certain long-range interactions [32]. A general statement in higher dimensions remains elusive and this problem is known as the area law conjecture.

Since realistic physical systems are never precisely at zero temperature, it is important for applications, e.g., for designing quantum memory, to understand the analog of the area law at positive temperature. At positive temperature, the ground states are replaced by thermal Gibbs states and the entanglement between regions A and B is quantified by their mutual information

\[ I(A : B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \]

At zero temperature, \( I(A : B) \) reduces to the entanglement entropy. An area law at positive temperature was derived in a seminal work of Wolf et. al [33] who proved for local and bounded interactions that

\[ I(A : B) \leq C \beta |\partial A|. \]

A key difference to the temperature zero case is that the proof does not require a spectral gap. Very recently, the \( \beta \)-scaling result was improved to \( \beta^{2/3} \) [34] which matters for the experimentally relevant regime of low temperatures (\( \beta \to \infty \)). 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 \( \beta \) [35]. Moreover, a generalization to various Rényi generalizations of the mutual information was given in [36]. Further results of thermal area laws were established for free fermions [37], for the entanglement negativity (instead of the mutual information) [38] as a result of rapid mixing for dissipative quantum lattice systems [39, 40] (with a logarithmic correction) and numerically for some spin chains showing a log \( \beta \)-dependence [41]. A current account of thermal area laws and related phenomena is given in [42].

The applications of thermal area laws mirror those of their ground state counterparts. In particular, a thermal area law can be used for the important problem of approximating the Gibbs state by matrix product operators (MPO)—mixed-state cousins of the standard matrix.
product states—and their higher-dimensional analogs \[34, 42, 44\]. It is generally believed that the scaling of the mutual information with $\beta$ in the low temperature regime is related to the computational complexity of the ground space of the models \[42\]. Another way to use a thermal area law is to note that controlling the mutual information automatically controls all standard correlation functions. More precisely, the mutual information upper bounds all truncated correlations

$$\text{tr}(M_A \otimes M_B \rho_{AB}) - \text{tr}(M_A \rho_A) \text{tr}(M_B \rho_B)$$

between arbitrary bounded observables $M_A$ and $M_B$; see \[34\] and Corollary 3 below.

One limitation of the existing results is that they only hold for bounded interactions. 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. We recall that bosonic lattice gases can be experimentally realized and fine-tuned using cold atoms in optical lattices and thus provide a promising platform for quantum engineering \[45\].

Area laws for non-interacting bosons were considered in \[19, 20, 46\], but the case of interacting bosons, including the paradigmatic Bose-Hubbard model proved elusive to rigorous analysis. A partly numerical investigation was given in \[47\] with a focus on the phase transition from Mott insulator to superfluid by analogy with other symmetry breaking transitions \[48–50\].

Then, in a remarkable recent work, Abrahamsen et al. rigorously proved an area law for gapped ground states of 1D bosonic lattice Hamiltonians in \[51\] by using a truncation of the local Hilbert spaces and a quantum number tail bound from \[52\]. Their work only concerns the zero temperature case and leaves open the positive temperature case.

Given all this background, it is a fundamental and rather timely question whether a thermal area law holds for interacting bosonic lattice gases. In this work, we answer this question in the affirmative for a broad class of interacting bosonic lattice gases.

That is, 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

$$I(A : B) \leq C\beta |\partial A|$$

for all $\beta \geq 1$. The precise result is Theorem 2 below. The $\beta$-scaling is the same as that found by \[33\] 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 Supplemental Material \[54\].

An immediate application of the result is a general bound on correlation functions of Gibbs states, cf. Corollary 3. Further physical applications, e.g., to the approximability of bosonic Gibbs states in the spirit of \[34, 42\] are postponed to future work.

**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. \[33\] 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.

Let $\mathfrak{h}$ be the local Hilbert space for one site, $\Lambda$ a finite set and $A, B \subseteq \Lambda$ such that $A \cap B = \emptyset$ and $A \cup B = \Lambda$. 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 (cf. Figure 1)

$$H_{AB} = H_A \otimes 1 + 1 \otimes H_B + H_\beta$$

We define the free energy as

$$F_{AB}^\beta = \inf_{\rho \in T_1^+(\mathcal{H}_{AB})} \mathcal{F}^\beta(\rho),$$

Figure 1. Periodic box decomposed into two regions $A$ and $B$. The bonds connecting $A$ and $B$ make up the boundary Hamiltonian $H_\beta$. 
where
\[ F^β(\rho) = \text{tr}(H_{AB}\rho) - \frac{S(\rho)}{β}, \quad S(\rho) = -\text{tr}(\rho \ln \rho). \]
The Gibbs state
\[ \rho_{AB} = \frac{e^{-βH_{AB}}}{Z_{AB}}, \quad Z_{AB} = \text{tr} e^{-βH_{AB}}, \]
minimizes the free energy, i.e., \( F^β(\rho_{AB}) = F^β(\rho) \).
(See Proposition 5 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
\[ \rho_A = \text{tr}_{H_B}(\rho_{AB}), \quad \rho_B = \text{tr}_{H_A}(\rho_{AB}). \]
The general bound from \([33]\) straightforwardly extends to the infinite-dimensional setting as follows.

**Lemma 1** (Boundary energy controls mutual informat.) Let \( β > 0 \) and suppose that \( \text{tr} e^{-βH_{AB}} < \infty \). Then
\[ I(A : B) ≤ β \text{tr}(H_{AB}(\rho_A \otimes \rho_B - \rho_{AB})). \]
**Proof.** We start from
\[ F^β(\rho_{AB}) = F^β(\rho) ≤ F^β(\rho_A \otimes \rho_B). \]
Using \( S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B) \), we obtain
\[ I(A : B) ≤ β \text{tr}(H_{AB}(\rho_A \otimes \rho_B - \rho_{AB})) \]
and the right-hand side equals \( β \text{tr}(H_{AB}(\rho_A \otimes \rho_B - \rho_{AB})) \) by basic properties of the partial trace. \( \square \)

**MAIN RESULT**

Now we consider the Bose-Hubbard model in the framework of the previous section. Let \( Λ \equiv Λ_L \) denote a box of side length \( L \) in the \( d \)-dimensional lattice with periodic boundary conditions. For \( x, y \in Λ_L \) 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 \( ℓ(\mathbb{N}) \).

The total Hilbert space \( H_{AB} = \bigotimes_{x \in Λ_L} ℓ(\mathbb{N}) \) is isomorphic to the Fock space \( ℬ(ℓ^2(Λ_L)) \). On it, we consider the Bose-Hubbard Hamiltonian
\[ H_{AB} = -J \sum_{x \sim y} a_x^† a_y + \frac{U}{2} \sum_{x \in Λ_L} n_x(n_x - 1) - µN, \quad (2) \]
where \( J \in \mathbb{R} \) represents the strength of the kinetic nearest-neighbor hopping, \( U > 0 \) the strength of the on-site repulsion and \( µ \in \mathbb{R} \) the chemical potential, and \( N = \sum_{x \in Λ_L} n_x \) is the total number operator. The Hamiltonian is self-adjoint on a suitable domain \( D(H_{AB}) \); see e.g., \([33, 43]\).

We are now ready to state the main result. We decompose the box into two regions \( A \) and \( B \) as shown in Figure 4. We write \( L_A \in \{1, \ldots, L\} \) for the width of region \( A \).

**Theorem 2** (Main result: thermal area law)
For all \( β, U, µ > 0 \), we have
\[ I(A : B) ≤ c(J, U, µ) \max \{1, β\} L^{d-1}. \]
Since \( L^{d-1} \) is the size of the boundary between \( A \) and \( B \), this proves the thermal area law.

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 \( µ > 0 \) is standard, cf. the usual phase diagram in Figure 13(a) in \([45]\). 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 \( c(J, U, µ) \) can be made explicit from \([35]\). (iv) The maximum \( \max \{1, β\} \) means that the bound behaves as \( β \) for low temperatures in accordance with \([33]\). We recall that some growth in \( β \) is strongly expected without any gap assumption \([35]\). For high temperature \( β < 1 \), we find a temperature independent lower bound which matches the classical situation \([33]\).

As explained in \([33]\), 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. Let \( M_A, M_B \) be two bounded self-adjoint operators on \( H_A \) and \( H_B \), respectively. We denote their truncated correlation function as
\[ C(A, B) = \text{tr}(M_A \otimes M_B \rho_{AB}) - \text{tr}(M_A \rho_A) \text{tr}(M_B \rho_B). \]

**Corollary 3** (Control on truncated correlations)
For all \( β, U, µ > 0 \), we have
\[ \frac{C(A, B)^2}{2 \|M_A\|^2 \|M_B\|^2} ≤ 2c(J, U, µ) \max \{1, β\} L^{d-1}, \]
with the same constant as in Theorem 2.

**Proof of Corollary** This follows from the quantum Pinsker inequality \( I(A : B) ≥ \frac{1}{2} \|\rho_{AB} - \rho_A \otimes \rho_B\|^2 \) and \( \|X\|_1 ≥ \text{tr}(XY)/\|Y\| \). We mention that the standard proof of the quantum Pinsker inequality, cf. \([35]\) Theorem 1.15) extends to infinite dimensions since the data processing inequality holds for trace-class operators \([56]\). \( \square \)

We close the presentation by discussing several extensions of the result which can be obtained from the same methods. First, the proof extends to on-site interaction terms \( ∑_x f(n_x) \) for any function \( f \geq 0 \) which is polynomially bounded and grows at least linearly at infinity. Second, it is possible to replace the nearest-neighbor hopping term \( -J \sum_{x \sim y} a_x^† a_y \) by a more general hopping which is translation-invariant and sufficiently decaying at infinity. More precisely, one could consider \( -\sum_{x,y} J_{x-y} a_x^† a_y \) for \( J_x ≥ 0, x \in \mathbb{Z}^d \), satisfying \( J_{x-y} ≤ (1 + |x-y|^{-\alpha}) \) for sufficiently large \( α > d \). Third, 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.

**SKETCH OF PROOF OF THEOREM 2**

The detailed proof of Theorem 2 is given in the supplemental material [54]. Here we give a sketch of the main ideas.

We decompose the Hamiltonian as

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

where \( H_0 = -J \sum_{x,y} a_x^\dagger a_y + 2dJN \) 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 \( H_{AB} = H_A + H_B + H_0 \) where we define the subsystem Hamiltonians with open boundary conditions along the cut. More precisely, for \( X \in \{A,B\} \), we set

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

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

Notice that the boundary Hamiltonian \( H_\partial \) contains \( L^{d-1} \) terms, so the right-hand side of Lemma 1 seems to exhibit the desired scaling in \( L \) and \( \beta \). The main challenge is that the hopping terms \( a_x^\dagger a_y + a_y^\dagger a_x \) between \( A \) and \( B \) regions 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 [57], which has a long history in the study of quantum many-body systems and quantum information theory. Applying it twice, we obtain

\[ \frac{\text{tr}(Te^S)}{\text{tr}(e^S)} \leq \frac{\text{tr}(Te^{S+T})}{\text{tr}(e^{S+T})}. \tag{3} \]

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

\[ S + T = -\beta(H_0 + (\gamma + 2dJ)N) \]

and \( e^{-\beta(H_0+(\gamma+2dJ)N)} \) 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 \( e^{-\beta(H_0+(\gamma+2dJ)N)} \) 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 \( \gamma \), we would get \( e^{-\beta(H_0-\mu+2dJ)N} \) which has infinite trace for \( \mu > -2dJ \).)

The final expression that we arrive at via (3) 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 \( \beta \) 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 [54].

**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 literature which so far contained thermal area laws for bounded interactions (quantum spin systems and lattice fermions) [33,34] and a recent proof of an area law for 1D gapped bosonic ground states [51].

The result holds in arbitrary lattice dimension and general parameter values, which means that it covers all the phases of the Bose-Hubbard model (superfluid and Mott insulator). For low temperatures \( (\beta \geq 1) \) the constant in front of the area grows linearly in \( \beta \).

The idea of the proof is based on the general idea in [35] 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 robust and extends to many other bosonic lattice gases.

Natural follow-up problems include the approximability of bosonic thermal states by matrix product operators in the spirit of [44]. 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 [30]).

Another natural problem is to refine the \( \beta \)-dependence in the constant of the area law for low temperatures. For example one could ask if it is possible to use the ideas of [24] to obtain a bound proportional to \( \beta^{2/3} \), or to find lower bounds on the exponent of \( \beta \) by identifying a bosonic analog of [35].

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Supplemental Material:
The Thermal Area Law for the Bose-Hubbard model

PRELIMINARIES

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 $D(A)$ and $D(B)$, respectively and the boundary Hamiltonian is defined on $H_B$ on $D(A) \otimes D(B)$. We assume that $H_{AB}$ is essentially self-adjoint on $D(A) \otimes D(B)$ which is then the appropriate domain for the equality

$$H_{AB} = H_A \otimes 1 + 1 \otimes H_B + H_\partial$$

(S1)

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 $D(H_{AB})$, where it can be defined, cf. \[53\]. It then follows from $[H_{AB},N] = 0$ 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 $D(X) = \mathfrak{F}_{\text{fin}}(H_X)$. The above properties can then be verified.

Trace inequalities in infinite dimensions

**Lemma 4** (Peierls-Bogoliubov inequality) 
Let $\mathcal{N} \geq 0$ be self-adjoint operator with purely discrete spectrum, let $P_N := 1_{\mathcal{N} \leq N}$, $N \in \mathbb{N}$ and assume that $P_N H$ is finite-dimensional for all $N \in \mathbb{N}$. Let $(D(S),S)$ be a self-adjoint and $(D(T),T)$ be a symmetric operator such that $[S,\mathcal{N}] = 0$ and $[T,\mathcal{N}] = 0$, and assume that $S + T$ is self-adjoint. Then we have

$$\frac{\text{tr}(Te^S)}{\text{tr}(e^S)} \leq \log \left( \frac{\text{tr}(e^{S+T})}{\text{tr}(e^S)} \right),$$

provided that all traces exist. In particular, we obtain \[3\], i.e.,

$$\frac{\text{tr}(Te^S)}{\text{tr}(e^S)} \leq \frac{\text{tr}(Te^{S+T})}{\text{tr}(e^{S+T})}.$$  

(S3)

**Proof of Lemma 4** The inequality \[S2\] is well-known for matrices, see for example \[58\] (2.14) \(or more generally if \(T\) is bounded \[59\]). Therefore, we have

$$\frac{\text{tr}(Te^S P_N)}{\text{tr}(e^S P_N)} \leq \log \left( \frac{\text{tr}(e^{S+T} P_N)}{\text{tr}(e^S P_N)} \right),$$

where $P_N = 1_{\mathcal{N} \leq N}$. Taking the limit $N \to \infty$ yields the desired result. Finally, \[S3\] follows from \[S2\] by means of

$$\log \left( \frac{\text{tr}(e^{S+T})}{\text{tr}(e^S)} \right) = - \log \left( \frac{\text{tr}(e^S)}{\text{tr}(e^{S+T})} \right) \leq \frac{\text{tr}(Te^{S+T})}{\text{tr}(e^{S+T})}.$$  

This proves Lemma 4. \qed

**Proposition 5** (Gibbs variational principle) 
Let $(H,D(H))$ 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

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

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

Proof of Proposition 5. We have
\[ \text{tr}(S \ln S - S \ln T) \geq \text{tr}(S - T) \]
for all positive self-adjoint trace class operators \( S, T \) \cite{60}. This yields \cite{61, Section 5.3.1}
\[ F^\beta(\rho) = \beta^{-1} \text{tr}(\rho \ln \rho - \rho \ln \rho_H) - \beta^{-1} \ln \text{tr} e^{-\beta H} \geq -\beta^{-1} \ln \text{tr} e^{-\beta H} = F^\beta(\rho_H). \]

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 \( J > 0 \).

Step 1: Controlling boundary energy by particle number

In this section, we prove the following bound

Proposition 6

We have
\[ I(A : B) \leq \frac{8}{L} \beta J \text{tr}(N \rho_{AB}). \]

Proof of Proposition 6 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
\[ I(A : B) \leq \beta J \sum_{x \sim y, x \in A, y \in B} \text{tr}((n_x + n_y)(\rho_A \otimes \rho_B + \rho_{AB})). \]

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 \( \rho_B \), we obtain
\[ I(A : B) \leq 2\beta J \sum_{x \sim y, x \in A, y \in B} \text{tr}((n_x + n_y)\rho_{AB}). \]

Observe that \( H_{AB} \) is translation-invariant, i.e., for all \( x \in \Lambda_L \),
\[ T_x^* H_{AB} T_x = H_{AB}, \]
where \( T_x \) denotes the unitary translation operator by \( x \), \( (T_x \psi)(y) = \psi(y + x \mod L) \). This implies \( T_x^* \rho_{AB} T_x = \rho_{AB} \) and therefore, \( \text{tr}(n_x \rho_{AB}) = \text{tr}(n_y \rho_{AB}) \) for all \( x, y \). The summation in (S4) is over \( 2L^{d-1} \) terms, so
\[ \sum_{x \sim y, x \in A, y \in B} \text{tr}((n_x + n_y)\rho_{AB}) = 4L^{d-1} \text{tr}(n_{x_0} \rho_{AB}) = 4L^{d-1} \frac{\text{tr}(N \rho_{AB})}{L^d}, \]
where \( x_0 \in \Lambda \) is some arbitrary element. This proves Proposition 6.

Step 2: Removing the interaction from the exponential

In the following we write \( \langle T \rangle_S := \text{tr}(T e^{-S}) / \text{tr}(e^{-S}) \) for operators \( S \) and \( T \) and we will also drop the subscript \( AB \) and write \( H = H_{AB} \).
Proposition 7
Let \( C_0 = \frac{1}{4} \frac{U}{\gamma + \mu} \). For all \( \gamma > 0 \), we have
\[
\langle N \rangle_{\beta H} \leq 2 \left( \frac{C_0}{U/2} \langle W - (\mu + \gamma - 2dJ)N \rangle_{\beta(H_0+\gamma N)} + \frac{C_0}{4} (1 + C_0^{-1})^2 L^d \right).
\]

Proof of Proposition 7
Let \( C > 0 \). We have \( n \leq C n(1 + \frac{C}{4} (1 + C^{-1})^2) \) for all \( n \in \mathbb{N} \). Thus, we obtain
\[
\langle N \rangle_{\beta H} = \left\langle \sum_{x \in \Lambda_L} n_x \right\rangle \leq \sum_{x \in \Lambda_L} \left\langle C n_x(n_x - 1) + \frac{C}{4} (1 + C^{-1})^2 \right\rangle_{\beta H} = \frac{C}{U/2} \langle W \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d.
\]
This leads to
\[
\langle N \rangle_{\beta H} \left( 1 - \frac{C}{U/2} (\mu + \gamma) \right) \leq \frac{C}{U/2} \langle W - (\mu + \gamma)N \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d
\]
\[
\leq \frac{C}{U/2} \langle W - (\mu + \gamma - 2dJ)N \rangle_{\beta H} + \frac{C}{4} (1 + C^{-1})^2 L^d.
\]
In the upper bound of Proposition 7 we apply twice the Peierls-Bogoliubov inequality, i.e., (3) in Lemma 4 with \( T = \beta(W - (\mu + \gamma - 2dJ)N) \) and \( S = -\beta H \), and get
\[
\langle W - (\mu + \gamma - 2dJ)N \rangle_{\beta H} \leq \langle W - (\mu + \gamma - 2dJ)N \rangle_{\beta(H_0+\gamma N)}.
\]
Using this in the previous bound and setting \( C = C_0 \) yields the desired estimate. This proves Proposition 7.

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
\[
f(\gamma, \beta, J) := \int_{[0, \frac{1}{2}]} \left( e^{4J\beta \sum_{j=1}^{d} \sin(\pi x_j) + \beta \gamma} - 1 \right)^{-1} dx,
\]
and denote the error terms by
\[
\epsilon_1 = \frac{(L + 1)^d}{L^d} - 1,
\]
\[
\epsilon_2 = \frac{(e^{\beta \gamma} - 1)^{-1} (2(2L + 1))^{d-1}}{2L - 1}.
\]
We shall use the following two lemmas.

Lemma 8
For all \( \gamma > 0 \) and \( x \in \Lambda_L \),
\[
\langle a_x^\dagger a_x \rangle_{\beta(H_0+\gamma N)} \leq 2^d (1 + \epsilon_1) f(\gamma, \beta, J) + \epsilon_2.
\]

Lemma 9
For all \( \gamma > 0 \) and \( \alpha \in (0, 1) \),
\[
f(\gamma, \beta, J) \leq \frac{1}{2^d (1 - \alpha) \beta \gamma}.
\]
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 [61] yields

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

By Lemma 8

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

Using this and \( -(\mu + \gamma - 2dJ)N \) \( \in \beta(H_0 + \gamma N) \leq 0 \) in the upper bound of Proposition 7, we obtain that for all \( \gamma > 2dJ - \mu \),

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

Next we use that \( f(\gamma, \beta, J) \leq \frac{1}{2\pi} \left( \frac{e^{-a\beta\gamma}}{1 - \alpha^2 \beta^2 \gamma^2} \right) \) for all \( \alpha \in (0, 1) \), cf. Lemma 9. The upper bound for \( \langle N \rangle_{\beta H} \) then becomes

\[ 2L^d \left( \frac{1}{2(\gamma + \mu)} \left( 16 \frac{e^{-2a\beta\gamma}}{(1 - \alpha^2 \beta^2 \gamma^2)} + 4 \cdot 6^{(d-1)}(e^{2\beta\gamma} - 1)^{-2} \right) + \frac{1}{16} \frac{U}{\gamma + \mu} + \frac{1}{2} \right). \]

Estimating \( \epsilon_1 \leq 1 \) and \( \epsilon_2 \leq 6^{d-1}(e^{2\beta\gamma} - 1)^{-1} \), we arrive at the bound

\[ 2L^d \left( \frac{1}{2(\gamma + \mu)} \left( 16 \frac{e^{-2a\beta\gamma}}{(1 - \alpha^2 \beta^2 \gamma^2)} + 4 \cdot 6^{(d-1)}(e^{2\beta\gamma} - 1)^{-2} \right) + \frac{1}{16} \frac{U}{\gamma + \mu} + \frac{1}{2} \right). \]

Finally, choosing \( \gamma = \max\{1/\beta, 2dJ + 1\} \) (such that \( \beta \gamma \geq 1 \), considering the limit \( \alpha \to 0 \) and in view of Proposition 6, the theorem holds with

\[ c(J, U, \mu) = 16J \left( \frac{16 + 4 \cdot 6^{(d-1)}(e - 1)^{-2}}{2(2dJ + 1 + \mu)} + \frac{1}{16} \frac{U}{2dJ + 1 + \mu} + \frac{2dJ + 1 + \mu}{U} + \frac{1}{2} \right). \]  

Distinguishing the cases for \( \beta \) completes the proof of Theorem 2. \( \square \)

**Laplace eigenvalues and eigenvectors for periodic boundary conditions**

The proofs proof of Lemma 8 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 \( \{0, 1, \ldots, L\} \), \( L \in \mathbb{N} \), with periodic boundary conditions, i.e., assume that the nodes 0 and \( L \) are connected and every vector on \( \ell^2(\{0, 1, \ldots, L\}) \) satisfies \( v(0) = v(L) \). So it suffices to use vectors \( v \in \ell^2(\{0, 1, \ldots, L\}) \).

The \( L \) eigenvalues \( \lambda_i \) and eigenvectors \( v_i \), \( i = 1, \ldots, L \), of \(-\Delta\) in this situation are given by

\[ \lambda_{2k+1} = 4 \sin^2 \left( \frac{k\pi}{L} \right), \quad k = 0, \ldots, \left\lfloor \frac{L - 1}{2} \right\rfloor, \]

\[ \lambda_{2k} = 4 \sin^2 \left( \frac{k\pi}{L} \right), \quad k = 1, \ldots, \left\lfloor \frac{L}{2} \right\rfloor, \]

and

\[ v_1(i) = L^{-1/2}, \]

\[ v_L(i) = L^{-1/2} (-1)^i \text{ if } L \text{ even}, \]

\[ v_{2k+1}(i) = \sqrt{2/L} \cos \left( \frac{\pi k}{L} (2i - 1) \right), \quad k = 1, \ldots, \left\lfloor \frac{L - 1}{2} \right\rfloor, \]

\[ v_{2k}(i) = \sqrt{2/L} \sin \left( \frac{\pi k}{L} (2i - 1) \right), \quad k = 1, \ldots, \left\lfloor \frac{L - 1}{2} \right\rfloor. \]
Proofs of Lemmas 8 and 9

In this section, we give the still outstanding proofs of Lemmas 8 and 9.

Proof of Lemma 8. Let $x_0 = (1, \ldots, 1) \in A_L$. By the formula for the one-particle density matrix, cf. e.g. [11] Prop. 5.2.28] and by translation-invariance we find

$$
\begin{align*}
\langle a_c^+ a_x \rangle_{\beta(H_0+\gamma N)} &= \langle \delta_x, e^{-\beta \gamma} e^{-\beta(-J \Delta)} (1 - e^{-\beta \gamma} e^{-\beta(-J \Delta)})^{-1} \delta_x \rangle \\
&= \langle \delta_{x_0}, (e^{\beta(-J \Delta + \gamma)} - 1)^{-1} \delta_{x_0} \rangle \\
&= \sum_{i_1, \ldots, i_d = 1}^L (e^{\beta(J \sum_{j=1}^d \lambda_{ij} + \gamma)} - 1)^{-1} \prod_{j=1}^d |v_{ij}(1)|^2.
\end{align*}
$$

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

$$
\sum_{i = 1}^L (e^{\beta(J_{i,1} + c)} - 1)^{-1} |v_i|^2 = \frac{1}{L} (e^{bc} - 1)^{-1} + \sum_{i = 1}^L (e^{\beta(J_{i,1} + c)} - 1)^{-1} \left( |v_{2i}(1)|^2 + 1 \right)
\leq \frac{1}{L} (e^{bc} - 1)^{-1} + 2 \sum_{i = 1}^\ell (e^{\beta(J_{i,1} + c)} - 1)^{-1}.
$$

Then, by induction over $d$ we find as an upper bound

$$
\begin{align*}
\langle a_c^+ a_x \rangle_{\beta(H_0+\gamma N)} &\leq \frac{1}{L^d} (e^{\beta \gamma} - 1)^{-1} + \frac{1}{L^d} \sum_{k=0}^{d-1} \frac{4^k}{L^d} \sum_{i_1, \ldots, i_d = 1}^\ell (e^{\beta(J \sum_{j=1}^d \lambda_{ij} + \gamma)} - 1)^{-1} \\
&\quad + \frac{2^d}{L^d} \sum_{i_1, \ldots, i_d = 1}^\ell (e^{\beta(J \sum_{j=1}^d \lambda_{ij} + \gamma)} - 1)^{-1}.
\end{align*}
$$

(S6)

Using $2\ell - 1 \leq L \leq 2\ell$ the terms in (S6) can be estimated by

$$
\frac{(e^{\beta \gamma} - 1)^{-1}}{L^d} \sum_{k=0}^{d-1} (4\ell)^k = \frac{(e^{\beta \gamma} - 1)^{-1}}{L^d} (4\ell)^d - 1 \leq \epsilon_2.
$$

The last term (S7) represents a Riemann sum of a function, decreasing in each argument, which is evaluated at the minimal points of the hypercubes $[(i_1 - 1)\pi/2, i_1 \pi/2] \times \ldots \times [(i_d - 1)\pi/2, i_d \pi/2]$, i.e.,

$$
\begin{align*}
\sum_{i_1, \ldots, i_d = 1}^\ell &\left( e^{\beta(J \sum_{j=1}^d \lambda_{ij} + \gamma)} - 1 \right)^{-1} \\
&= \frac{(2\ell)^d}{L^d} \sum_{i_1, \ldots, i_d = 1}^\ell \left( e^{\beta(J \sum_{j=1}^d \sin^2(i_j \pi/L) + \gamma)} - 1 \right)^{-1} \\
&\leq \frac{(L+1)^d}{L^d} \sum_{i_1, \ldots, i_d = 1}^\ell \left( e^{\beta(J \sum_{j=1}^d \sin^2(i_j \pi/(2\ell)) + \gamma)} - 1 \right)^{-1} \\
&\leq \frac{(L+1)^d}{L^d} \int_{[0,1]^d} \left( e^{\beta(J \sum_{j=1}^d \sin^2(x_j \pi/2) + \gamma)} - 1 \right)^{-1} dx \\
&= 2^d \frac{(L+1)^d}{L^d} f(\gamma, \beta, J).
\end{align*}
$$

Proof of Lemma 9. We have

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

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

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

\[ \leq e^{-\alpha \beta \gamma} \int_{[0, \frac{1}{2}]^d} ((1 - \alpha) \beta \gamma)^{-1} dx = \frac{1}{2^d} \frac{e^{-\alpha \beta \gamma}}{(1 - \alpha) \beta \gamma} . \]

This proves Lemma 9