A Multi-Dimensional Lieb–Schultz–Mattis Theorem

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A MULTI-DIMENSIONAL LIEB-SCHULTZ-MATTIS THEOREM

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Abstract. For a large class of finite-range quantum spin models with half-integer spins, we prove that uniqueness of the ground state implies the existence of a low-lying excited state. For systems of linear size $L$, of arbitrary finite dimension, we obtain an upper bound on the excitation energy (i.e., the gap above the ground state) of the form $(C \log L)/L$. This result can be regarded as a multi-dimensional Lieb-Schultz-Mattis theorem [7] and provides a rigorous proof of the main result in [4].

1. Introduction and main result

1.1. Introduction. Ground state properties of Heisenberg-type antiferromagnets on a variety of lattices are of great interest in condensed matter physics and material science. Antiferromagnetic Heisenberg models are directly relevant for the low-temperature behavior of many materials, most notably the cuprates that exhibit high-$T_c$ superconductivity [9].

There are several general types of ground states that are known, or expected, to occur in specific models: a disordered ground state or spin liquid, critical correlations (power law decay), dimerization (spin-Peierls states), columnar phases, incommensurate phases, and Néel order. More exotic phenomena such as chiral symmetry breaking have also been considered [14, 15].

Which behavior occurs in a given model depends on the lattice, in particular the dimension and whether or not the lattice is bipartite, on the type of spin (integer versus half-integer) and of course also on the interactions. In this paper we are considering a class of half-integral spin models (or models where the magnitude of at least some of the spins is half-integral). Our aim is to prove a generalization of the Lieb-Schultz-Mattis Theorem [7]. Such a generalization was presented by Hastings in [4] and a substantial part of our proof is based on his work. Our main contribution is to provide what we hope is a more transparent argument which in addition is mathematically rigorous.

The well known theorem by Lieb and Mattis [6] implies, among other things, that the ground state of the Heisenberg antiferromagnet on a bipartite lattice with isomorphic sublattices, is non-degenerate. For one-dimensional and quasi-one-dimensional systems of even length and with half-integral spin Affleck and Lieb [1], generalizing the original result by Lieb, Schultz, and Mattis [7], proved that the gap in the spectrum above the ground state is bounded above by $constant/L$. A vanishing gap can be expected to lead to a gapless continuous spectrum above the ground state in the thermodynamic limit. Such an excitation spectrum is generically associated with power-law (as opposed to exponential) decay of correlations. Aizenman and Nachtergaele proved for the spin-1/2 antiferromagnetic chain that if translation invariance is not broken (in particular, when the ground state is unique), the
spin-spin correlation function can decay no faster than $1/r^3$ [2]. In other words, uniqueness of the ground state implies slow (power-law) decay of correlations. Recently, it was proved rigorously that a non-vanishing spectral gap implies exponential decay of correlations [13, 5]. Therefore, non-exponential decay of correlations implies the absence of a gap. In particular, the result by Aizenman and Nachtergaele implies the absence of a gap in the infinite spin-1/2 antiferromagnetic chain if the translation invariance is not broken, e.g., if the ground state is unique. This result can be generalized to an interesting class of antiferromagnetic chains of half-integer spins [10]. The Lieb-Schultz-Mattis Theorem has also been extended to fermion systems on the lattice [18, 17]. All these results are for one-dimensional systems. The bulk of the applications of the spin-1/2 Heisenberg antiferromagnet are in two-dimensional physics and therefore, the rigorous proof we provide here, based in part on ideas of Hastings [4], should be of considerable interest as it is applicable to higher-dimensional models.

The most common argument employed to bound a spectral gap from above uses the variational principle. Often, the variational state is a perturbation of the ground state. The proofs in [7] and [1] are of this kind. However, since the ground state is not known, and no assumptions are made about it except for its uniqueness, these proofs are not a variational calculation in the usual sense. The variational states are defined by acting with suitable local operators $A$ on the (unknown) ground state. In order to obtain a useful bound on the energy of the first excited state one then has to estimate the effect of $A$ using the few properties of the ground state one assumes, such as its uniqueness and symmetries. Furthermore, one must show that the variational state has a sufficiently large component in the orthogonal complement of the ground state. We carry this out for finite systems of size $L$. It is interesting to note that the energy estimate we obtain will itself contain the spectral gap of the finite system in such a way that assuming a large gap leads to an upper bound less than the assumed gap. From this contradiction one can conclude an upper bound on the finite-volume gaps.

Our results apply to a rather general class of models, which we will define precisely in the next section. The application of our general result to spin-1/2 Hamiltonians with translation invariant (or periodic) isotropic finite-range spin-spin interactions on a $d$-dimensional lattice is easy to state. First, let $A_L = [1, L] \times V_L$ with $L$ even and with periodic boundary conditions in the 1-direction, i.e., in the direction that is of even size. It will be important that the number of spins in $V_L$, $|V_L|$, is odd, and satisfies $|V_L| \leq cL^{d-1}$, for some $d \geq 1$ and a suitable constant $c$. Assuming that the ground state of the model on $A_L$ has a unique ground state, we prove that the spectral gap $\gamma_L$ satisfies the bound

$$\gamma_L \leq C \log \frac{L}{L},$$

where $C$ depends on $d$ and the specifics of the interaction, but not on $L$.

Because of the presence of the factor $\log L$, the bound (1.1) applied to one-dimensional models does not fully recover the original Lieb-Schultz-Mattis Theorem in [7] or the bound proved by Affleck and Lieb in [1]. This indicates that in general our bound is not optimal. Our proof uses in an essential way Lieb-Robinson bounds [8, 13, 5], as does Hastings’ argument in [4], and the appearance of the factor $\log L$ seems to be an inevitable consequence of this.

1.2. Setup and main result. The arguments we develop below can be applied to a rather general class of quantum spin Hamiltonians defined on a large variety of lattices. We believe
it is useful to present them in a suitably general framework which applies to many interesting models. Attempting to be as general as possible, however, would lead us into a morass of impenetrable notation. Therefore, we have limited the discussion of further generalizations to some brief comments in Section 1.4.

We assume that the Hamiltonians describe interactions between spins that are situated at the points of some underlying set $\Lambda$. For simplicity, one may think of $\Lambda = \mathbb{Z}^d$, but we need only assume that the set $\Lambda$ has one direction of translational invariance, which we will refer to as the 1-direction. We assume that there is an increasing sequence of sets $\{\Lambda_L\}_{L=1}^{\infty}$ which exhaust $\Lambda$ of the form $\Lambda_L = [1, L] \times V_L$ where $|V_L| \leq cL^{d-1}$ for some $d \geq 1$. Here each $x \in \Lambda_L$ can be written as $x = (n, v)$ where $n \in \{1, 2, \ldots, L\}$ and $v \in V_L$, and we will denote by $(n, V_L)$ the set of all $x \in \Lambda_L$ of the form $x = (n, v)$ for some $v \in V_L$.

Estimates on the decay of correlations in the ground state and Lieb-Robinson bounds on the dynamics will play an important role in the proof of the main result. Both are expressed of a connected graph and easily verify that (1.3) holds with

$$F_1 \text{ and } F_2 \text{ are restrictive conditions only when } \Lambda \text{ is infinite, however, for finite } \Lambda, \text{ the constants } \|F\| \text{ and } C(F) \text{ will be useful in our estimates. It is also important to note that for any given set } \Lambda \text{ and function } F \text{ that satisfies } F_1 \text{ and } F_2 \text{ above, we can define a one-parameter family of functions, } F_\lambda, \lambda \geq 0, \text{ by}$$

$$F_\lambda(x) := e^{-\lambda x} F(x),$$

and easily verify that $F_1$ and $F_2$ hold for $F_\lambda$, with $\|F_\lambda\| \leq \|F\|$ and $C(F) \leq C(F)$.

As a concrete example, take $\Lambda = \mathbb{Z}^d$ and $d(x, y) = |x - y|$. In this case, one may take the function $F(x) = (1 + x)^{-d-\varepsilon}$ for any $\varepsilon > 0$. Clearly, (1.2) is satisfied, and a short calculation demonstrates that (1.3) holds with

$$C(F) \leq 2^{d+\varepsilon+1} \sum_{n \in \mathbb{Z}^d} \frac{1}{(1 + |n|)^{d+\varepsilon}}.$$
An interaction for the system is a map $\Phi$ from the finite subsets of $\Lambda$ to $\mathcal{A}$ such that for each finite $X \subset \Lambda$, $\Phi(X)^* = \Phi(X) \in \mathcal{A}_X$. For given $\Lambda$ and $F$, and any $\lambda \geq 0$, let $\mathcal{B}_\lambda(\Lambda)$ be the set of interactions that satisfy

$$
\|\Phi\|_\lambda := \sup_{x,y \in \Lambda} \sum_{X \ni x,y} \frac{\|\Phi(X)\|}{F_\lambda(d(x,y))} < \infty.
$$

All interactions considered in this paper are assumed to belong to $\mathcal{B}_\lambda(\Lambda)$ for some choice of $F$ and $\lambda > 0$. The constant $\|\Phi\|_\lambda$ will show up in many estimates. The finite volume Hamiltonians are defined in terms of the interaction $\Phi$ in the usual way by

$$
H_L = \sum_{X \subset \Lambda_L} \Phi(X) + \text{boundary terms}.
$$

We will always assume periodic boundary conditions in the 1-direction and free boundary conditions (i.e., no additional boundary terms) in the other directions.

The condition that $\|\Phi\|_\lambda$ is finite is sufficient to guarantee the existence of the dynamics in the thermodynamic limit as a one-parameter group of automorphisms on $\mathcal{A}$. In particular this means that the limits

$$
\alpha_t^\Phi(A) := \lim_{L \to \infty} \alpha_t^{\Phi,L}(A) := \lim_{L \to \infty} e^{itH_L}Ae^{-itH_L}
$$

exist in norm for all $t \in \mathbb{R}$, and all observables $A \in \mathcal{A}_X$, for any finite $X \subset \Lambda$. We will often suppress the $L$ or $\Phi$ dependence in the notation $\alpha_t^{\Phi,L}$. See [3, 16, 11] for more details.

Next, we turn to a set of conditions that more specifically describe the class of models to which the Lieb-Schultz-Mattis Theorem may be applied.

**Condition LSM1:** We assume that the interaction is translation invariant in at least one direction, which we will take to be the 1-direction. This means

$$
\Phi(X + e_1) = \tau_1(\Phi(X)),
$$

where, for any $X \subset \Lambda$, $X + e_1$ is translation of all points in $X$ by one unit in the 1-direction.

We will consider finite systems with Hamiltonians $H_L$ defined with periodic boundary conditions in the 1-direction. For convenience of the presentation we will assume free boundary conditions in the other directions but this is not crucial. Assuming periodic boundary conditions, we can implement the translation invariance for finite systems by a unitary $T \in \mathcal{A}_{\Lambda_L}$ such that $\Phi(X + e_1) = T^*\Phi(X)T$, for all $X \subset \Lambda_L$. Here $T$ depends on $L$, but we suppress this dependence in the notation.

**Condition LSM2:** The interactions are assumed to be of finite range in the 1-direction, i.e., there exists $R > 0$ (the range), such that if $X \subset \Lambda$ and $X \ni x_i = (n_i, v_i)$ for $i = 1, 2$ with $|n_1 - n_2| \geq R$, then $\Phi(X) = 0$.

**Condition LSM3:** We assume rotation invariance about one axis. More precisely, we assume that there is a hermitian matrix in every $\mathcal{A}_{\{x\}}, x \in \Lambda$, which we will denote by $S^3_x$, with eigenvalues that are either all integer or all half-integer (i.e. belonging to $\mathbb{Z} + \frac{1}{2}$). We also require that $\tau_m(S^3_x) = S^3_{x+me_1}$. Define, for $\theta \in \mathbb{R}$, the unitary $U(\theta) \in \mathcal{A}_{\Lambda_L}$ by

$$
U(\theta) = \bigotimes_{x \in \Lambda_L} e^{i\theta S^3_x}.
$$

The interaction is taken to be rotation invariant in the sense that for each finite $X \subset \Lambda$

$$
U^*(\theta)\Phi(X)U(\theta) = \Phi(X) \text{ for all } \theta \in \mathbb{R}.
$$
**Condition LSM4:** We assume that the $S^3_x$ are uniformly bounded: there exists $S$ such that $\|S^3_x\| \leq S$, for all $x \in \Lambda$. The following condition, which we call **odd parity**, is crucial: define the parity of $x$, $p_x$ to be 0 if the eigenvalues of $S^3_x$ are integers, and $p_x = 1/2$ if they are half-integers. We assume that $\sum_{v \in V_L} p(n,v) \in \mathbb{Z} + 1/2$, for all $n \in \mathbb{Z}$. The simplest and most important case where this is satisfied is when we have a spin 1/2 at each site, and $|V_L|$ is odd.

**Condition LSM5:** The ground state of $H_L$ is assumed non-degenerate. This implies it is an eigenvector of the translation $T$ and rotations $U(\theta)$. We assume that 1 is the corresponding eigenvalue in each case.

**Condition LSM6:** We assume that there are orthonormal bases of the Hilbert spaces $\mathcal{H}_{\Lambda_L}$ with respect to which $S^3_x$ and $\Phi(X)$ are real, for all $x \in \Lambda_L, X \subset \Lambda_L$.

We will also use the following quantities:

\begin{equation}
\|\Phi\|_1 := \sup_{x \in \Lambda} \sum_{X \ni x} \|\Phi(X)\| < \infty,
\end{equation}

and

\begin{equation}
\|\Phi\|_2 := \sup_{x \in \Lambda} \sum_{X \ni x} |X| \sum_{x' \in X} \|S^3_{x'}, \Phi(X)\| < \infty.
\end{equation}

It is not hard to show that the conditions F1 and F2 are sufficient to imply that $\|\Phi\|_1$ and $\|\Phi\|_2$ are finite.

We can now state our main result.

**Theorem 1.1.** Let $\gamma_L$ be the spectral gap, i.e., the difference between the lowest and next-lowest eigenvalue of the Hamiltonian $H_L$ of a model satisfying conditions F1, F2, and LSM1-6. Then, there exists a constant $C$, depending only on properties of $\Lambda$ (such as the dimension), the constants $\|F\|$ and $C(F)$, and the interaction ($\|\Phi\|_\lambda$, for some $\lambda > 0$, $\|\Phi\|_1$, and $\|\Phi\|_2$), such that

\begin{equation}
\gamma_L \leq C \frac{\log L}{L}.
\end{equation}

**1.3. Structure of the proof.** The simplest way to present the proof is as a proof by contradiction. Under the assumption that there exists a sufficiently large constant $C > 0$, such that $\gamma_L$ exceeds $(C \log L)/L$ for large $L$, we will construct a state orthogonal to the ground state with an energy difference that is boundable by a quantity that is strictly less than the assumed gap for sufficiently large $L$. Thus, the proof is in essence a variational argument. The variational state is constructed as a perturbation of the ground state, as the solution of the evolution equation proposed by Hastings [4] with the ground state as initial condition (see Section 2 for this equation). The important idea is that this evolution will lead to a state which resembles the ground state of the Hamiltonian with twisted rather than periodic boundary conditions (see Section 2.1 for the definition of the twists), at least in part of the system, say the left half. In the right half the ground state will be left essentially unperturbed. This state is defined in Section 2.

After the variational state has been defined, there are two main steps in the proof: estimating its excitation energy and verifying that it is “sufficiently orthogonal” to the ground state. In general, one may also have to consider the normalization of the variational state, but in our case the evolution equation defining it will be manifestly norm preserving. Hence, this is not an issue for our proof.
The main difficulty is that under the general assumptions we have made, no explicit information about the ground state is available. Its uniqueness, translation, and rotation invariance are the only properties we can use. In combination with the general assumptions on the interactions and the assumption on the magnitude of the spectral gap above the ground state, however, one can obtain an upper bound on the decay of correlations of the ground state in the 1-direction. The recently proved Lieb-Robinson bounds \[13, 5, 11\] will be essential to show that the effects of the perturbations we define in the left half of the system remain essentially localized there. This allows us to compare the energy of the variational state with the ground state energy of a Hamiltonian, \( H_{\theta_{-\theta}} \) introduced in (2.4), which, instead of twisted boundary conditions, has two twists that cancel each other. The twisted Hamiltonian is unitarily equivalent to the original one and therefore has the same ground state energy. We work out this argument in Section 3. The result is

\[
|\langle \psi_1, H_L \psi_1 \rangle - E_0| \leq C \nu L e^{-\gamma_L L},
\]

where \( \psi_1 \) is the normalized variational state we construct, and \( E_0 \) is the ground state energy. The dependence of both quantities on \( L \) is suppressed in the notation. \( \nu, C \) and \( c \) are positive constants that only depend on properties of the lattice and the interactions.

For the orthogonality, our strategy is to show that \( \psi_1 \) is almost an eigenvector of the translation \( T \) with eigenvalue \(-1\). Since the ground state \( \psi_0 \) is an eigenvector of \( T \) with eigenvalue \( 1 \), by assumption, this shows that \( \psi_1 \) is nearly orthogonal to \( \psi_0 \). Concretely, in Section 4 we obtain a bound on their inner product of the following form:

\[
|\langle \psi_1, \psi_0 \rangle| \leq C' \nu' L e^{-c' \gamma_L L},
\]

where \( \nu', C' \) and \( c' \) are positive constants similar to \( \nu, C \) and \( c \).

The proof of Theorem 1.1 then easily follows: if one assume \( \gamma_L \geq (C \log L)/L \), with sufficiently large constant \( C \), one obtains a contradiction for \( L \) large enough.

To help the reader see the forest through the trees we have tried to streamline the estimates in Sections 3 and 4 by collecting some results of a more technical nature in Section 5.

1.4. Generalizations. One can envision several generalizations of Theorem 1.1. An obvious one is to remove the condition that the interaction is strictly finite range in the 1-direction. It is not hard to see that the arguments given in the following sections can be extended to long-range interactions with sufficiently fast decay.

One may wonder whether the assumption that \( L \) is even is essential. It is used in the proof of near orthogonality of the variational state, which is based on investigating the behavior under translations of the state: the variational state is close to an eigenvector with eigenvalue \(-1\) of the translation operator \( T \), whereas the ground state has eigenvalue \( 1 \). Our proof of this fact assumes that the ground state is an eigenvector of the rotations with eigenvalue \( 1 \). For \( L \) odd, our assumptions preclude the existence of such an eigenvector. However, it seems plausible that for odd \( L \) a slight modification of our proof will work to show that the ground state and the variational excited state have opposite eigenvalues for translations.

The main applications we think of are to SU(2)-invariant Hamiltonians with antiferromagnetic interactions. Affleck and Lieb [1] pointed out that their proof easily extends to a class of models with SU(N) symmetry. There are no obstructions to generalizing our arguments to such models with SU(N) symmetry given by suitable representations.

It may also be of interest to consider different topologies of the underlying lattice and/or the twistings. Instead of cylindrical systems with periodic boundary conditions which can
be deformed by a twist, one could apply a similar strategy to systems defined on a ball or a sphere. We do not explore such possibilities here.

2. Construction of the variational state

2.1. Twisted Hamiltonians. The main motivation behind the construction of the variational excited state is that it should resemble the ground state of the model with twisted (as opposed to periodic) boundary conditions. Therefore, we first describe some elementary properties of a family of perturbations of the Hamiltonian, which we will call twisted Hamiltonians for reasons that will become obvious.

Given an interaction $\Phi$ which satisfies the general assumptions outlined in Section 1.2, we will now define a two parameter family of “twisted Hamiltonians” to analyze. These Hamiltonians will be defined on a finite volume $\Lambda_L = [1, L] \times V_L$ for some $L > 4R$ where $R > 0$ is the range of $\Phi$ in the 1-direction. Recall that each point $x \in \Lambda_L$ can be written as $x = (n, v)$ where $n \in \{1, 2, \ldots, L\}$ and $v \in V_L$, and we will denote by $(n, V_L) = \{x \in \Lambda_L : x = (n, v)\}$ for some $v \in V_L$. For any $\theta \in \mathbb{R}$ and $n \in \{1, 2, \ldots, L\}$, denote by $U_n(\theta)$ the unitary rotation about the third axis by an angle $\theta$ at the sites $x \in (n, V_L)$, compare with (1.10). For $m \in \{1, 2, \ldots, L - 1\}$, we will denote by $V_m(\theta)$ the unitary given by

\begin{equation}
V_m(\theta) = \bigotimes_{m < n \leq L} U_n(\theta).
\end{equation}

The “twisted Hamiltonian” are defined to be perturbations of the initial Hamiltonian

\begin{equation}
H_L = \sum_{X \subset \Lambda_L} \Phi(X).
\end{equation}

The $L$-dependence will often be dropped from the notation and periodic boundary conditions in the 1-direction have been assumed. The perturbations have the following form:

\begin{equation}
H_\theta(m) := \sum_{X \subset \Lambda_L} V_m(\theta)^* \Phi(X) V_m(\theta) - \Phi(X).
\end{equation}

Clearly, if $X \subset \bigcup_{m < n \leq L} (n, V_L)$ or $X \subset \bigcup_{1 \leq n < m} (n, V_L)$, then $V_m(\theta)^* \Phi(X) V_m(\theta) - \Phi(X)$ will vanish by rotation invariance of the interaction, and therefore only those interactions across the column $(m, V_L)$ contribute in (2.3). For $\theta, \theta' \in \mathbb{R}$ and $m \in \{1, 2, \ldots, L/2 - 1\}$ fixed, we define

\begin{equation}
H_{\theta, \theta'} := H + H_\theta(m) + H_{\theta'}(m + L/2),
\end{equation}

to be a doubly twisted Hamiltonian. With $m$ fixed, we regard $\Lambda_L$ as the disjoint union of two sets

\begin{equation}
\Lambda_L = \Lambda_L^{(W)} \cup \Lambda_L^{(S)},
\end{equation}

where $\Lambda_L^{(W)}$ consists of two windows, one about each column at which a twist has been applied; namely

\begin{equation}
\Lambda_L^{(W)} := \Lambda_L^{(W)}(m) \cup \Lambda_L^{(W)}(m + L/2) \quad \text{and} \quad \Lambda_L^{(W)}(y) := \bigcup_{|n - y| \leq \frac{L}{4} - R} (n, V_L),
\end{equation}

for $y \in \{m, m + L/2\}$. Moreover, $\Lambda_L^{(S)}$ comprises the remaining strips in $\Lambda_L$. Here we regard $\Lambda_L$ as having periodic boundary conditions, with respect to the 1-direction, in which $L + 1$
identified with 1. Given this decomposition of the underlying space, the twisted Hamiltonian can be written as

\[ H_{\theta,\theta'} = H_{\theta,\theta'}^{(W)} + H^{(S)}, \]

where

\[ H^{(S)} = \sum_{X \subseteq \Lambda, X \cap \Lambda^{(S)} \neq \emptyset} \Phi(X), \]

and \( H_{\theta,\theta'}^{(W)} \) denotes the remaining terms in \( H_{\theta,\theta'} \), which, due to (2.8), are supported strictly within the windows.

There are a variety of useful symmetries the Hamiltonians \( H_{\theta,\theta'} \), introduced in (2.4), possess. With \( m^2 f_1, 2, \ldots, L = b \) fixed as above, one may define

\[ W(\phi) := \bigotimes_{m < n \leq m + L/2} U_n(-\phi), \]

for any real \( \phi \). It is easy to check that for any angles \( \theta, \theta', \phi, \phi' \in \mathbb{R} \), one has that

\[ W^*(\phi) H_{\theta,\theta'} W(\phi) = H_{\theta-\phi,\theta'+\phi}, \]

due to the (term by term) rotation invariance of the interactions. Given this relation, it is clear that along the path \( \theta' = -\theta \) the twisted Hamiltonian is unitarily equivalent to the untwisted Hamiltonian, i.e.,

\[ W(\theta)^* H_{\theta,-\theta} W(\theta) = H_{0,0} = H. \]

Since the untwisted Hamiltonian is translation invariant (in the 1-direction), we have that \( T^* H T = H \), where \( T \) is the unit translation in the 1-direction. Thus,

\[ T^* W(\theta)^* H_{\theta,-\theta} W(\theta) T = W(\theta)^* H_{\theta,-\theta} W(\theta), \]

i.e.,

\[ H_{\theta,-\theta} = T_{\theta,-\theta} H_{\theta,-\theta} T_{\theta,-\theta}, \]

where we denote by

\[ T_{\theta,-\theta} := W(\theta) T W(\theta)^* \]

the twisted translation. Clearly, \( T^* W(\theta) T = U_m(\theta) U_{m+L/2}(-\theta) W(\theta) \), and therefore, we may write

\[ T_{\theta,-\theta} = T U_m(\theta) U_{m+L/2}(-\theta). \]

If we denote by \( \psi_0 \) the (unique) ground state of \( H \), i.e., \( H \psi_0 = E_0 \psi_0 \), then \( T \psi_0 = \psi_0 \) as \( H \) is translation invariant. Moreover, using the unitary equivalence (2.11), we see that the ground state of the twisted Hamiltonian \( H_{\theta,-\theta} \) satisfies \( H_{\theta,-\theta} \psi_0(\theta, -\theta) = E_0(\theta, -\theta) \psi_0(\theta, -\theta) \) with \( E_0(\theta, -\theta) = E_0 \) and \( \psi_0(\theta, -\theta) = W(\theta) \psi_0 \). Although the twisted ground state \( \psi_0(\theta, -\theta) \) is not translation invariant, it does satisfy invariance with respect to the twisted translations, i.e., \( T_{\theta,-\theta} \psi_0(\theta, -\theta) = \psi_0(\theta, -\theta) \). As a consequence, we have the following simple but important property of \( E_0 \).

Lemma 2.1. The partial derivatives of \( E_0 \) vanish on the line \( \theta' = -\theta \):

\[ \partial_1 E_0(\theta, -\theta) = \partial_2 E_0(\theta, -\theta) = 0. \]
Proof. First, we note that $E_0$ is differentiable in its two variables by the non-degeneracy condition LSM5, extended to all $\theta$ by unitary equivalence. For $\psi, \phi \in \mathbb{R}$, let $\mathcal{E}(\psi, \phi) = E_0(\psi - \phi, \psi + \phi)$ denote the ground state energy of $H_{\psi - \phi, \psi + \phi}$. Due to the unitary equivalence eq. (2.10), $\mathcal{E}$ depends only on $\psi$. Hence, $\partial_\psi \mathcal{E}(\psi, \phi) = 0$, for all $\psi, \phi$. Under the additional assumption that the interactions $\Phi(X)$ are real (LSM6), we have that $\prod_{\theta, \theta'} = H_{-\theta, -\theta'}$, and therefore $\mathcal{E}(\psi, 0) = \mathcal{E}(-\psi, 0)$. Hence, $\mathcal{E}$ is an even function of $\psi$ and $\partial_\psi \mathcal{E}(\psi, \phi)|_{\psi=0} = 0$. Using these properties and the fact that the partial derivatives of $E_0$ are linear combinations of the partial derivatives of $\mathcal{E}$, we find that both partial derivatives of $E_0$ vanish on the line $\theta' = -\theta$. □

2.2. The variational state. Our aim is to construct a state that resembles the ground state of $H_{\theta, \theta}$ in a region surrounding those spins that were twisted by an angle of $\theta$, while it otherwise resembles the ground state of $H = H_{0, 0}$. To motivate our method of constructing such a state, we consider a parameter dependent self-adjoint operator $H(\theta)$ with a non-degenerate ground state satisfying $H(\theta)\psi_0(\theta) = E_0(\theta)\psi_0(\theta)$, and assume that $\partial_\theta E_0(\theta_0) = 0$. Then, a formal calculation shows that

$$
\partial_\theta \psi_0(\theta_0) = - [H(\theta_0) - E_0(\theta_0)]^{-1} \partial_\theta H(\theta_0) \psi_0(\theta_0).
$$

For any vector $\psi$, this leads to

$$
\langle \psi, \partial_\theta \psi_0(\theta_0) \rangle = - \int_{E_0(\theta_0)}^{\infty} \frac{1}{E - E_0(\theta_0)} \, d \langle \psi, P^\theta_E \partial_\theta H(\theta_0) \psi_0(\theta_0) \rangle
$$

$$
= - \int_{E_0(\theta_0)}^{\infty} \int_0^\infty e^{-(E - E_0(\theta_0))t} \, dt \, d \langle \psi, P^\theta_E \partial_\theta H(\theta_0) \psi_0(\theta_0) \rangle
$$

$$
= - \int_0^\infty \langle \psi, \alpha^\theta_t (\partial_\theta H(\theta_0)) \psi_0(\theta_0) \rangle \, dt,
$$

where $\alpha^\theta_t$ is the imaginary time-evolution corresponding to the Hamiltonian $H(\theta_0)$. Motivated by this calculation, we introduce the family of operators $B(A, H)$, where $H$ is a Hamiltonian for which the dynamics $\{\alpha_t, \ t \in \mathbb{R}\}$ exists as a strongly continuous group of $*$-automorphisms and $A$ is any local observable, defined by

$$
B(A, H) = - \int_0^\infty \alpha_t(A) \, dt,
$$

where $\alpha_t$ is the imaginary time evolution. For unbounded Hamiltonians $H$, it may not be obvious that $B(A, H)$ can be defined on a dense domain. However, if $\psi$ is a ground state corresponding to the Hamiltonian $H$, then $B(A, H)\psi$ exists. Moreover, from (2.17), we conclude that

$$
\partial_\theta \psi_0(\theta_0) = B(A(\theta_0), H(\theta_0)) \psi_0(\theta_0),
$$

where $A(\theta_0) = \partial_\theta H(\theta_0)$. Similarly, in the density matrix formalism, for

$$
\rho_0(\theta) := |\psi_0(\theta)\rangle \langle \psi_0(\theta)|,
$$

equation (2.19) implies that

$$
\partial_\theta \rho_0(\theta_0) = B(A(\theta_0), H(\theta_0)) \rho_0(\theta_0) + \rho_0(\theta_0) B(A(\theta_0), H(\theta_0))^*.
$$

We will define the proposed excited state $\psi$ as the solution of a differential equation analogous to (2.19). First, we need to introduce some further notation. Let $H$ be a Hamiltonian.
for which the dynamics \(\{\alpha_t\}\) exists; finite volume is sufficient. For any \(a > 0, t \in \mathbb{R} \setminus \{0\}\), and local observable \(A \in \mathcal{A}\), we may define

\[
A_a(it, H) := \frac{1}{2\pi i} e^{-at^2} \int_{-\infty}^{\infty} \alpha_s(A) e^{-as^2} \frac{ds}{s - it}.
\]

In addition, for \(T > 0\) the quantity

\[
B_{a,T}(A, H) := -\int_0^T A_a(it, H) - A_a(it, H)^* dt,
\]

will play a crucial role. In Lemma 5.12 of Section 5, we will show that when projected onto the ground state of a gapped Hamiltonians \(H\), the quantity \(B_{a,T}(A, H)\) well approximates \(B(A, H)\) for a judicious choice of parameters \(a\) and \(T\); we note that the observable \(A\) must also satisfy a constraint. With this in mind, consider the solution of the differential equation

\[
\partial_\theta \psi_{a,T}(\theta) = B_{a,T}(\tilde{A}_\theta, H_{\theta,-\theta}) \psi_{a,T}(\theta),
\]

subject to the boundary condition \(\psi_{a,T}(0) = \psi_0\). Here we have taken a specific local observable; namely \(\tilde{A}_\theta := \partial_\theta H_{\theta,0}\). Note that \(B_{a,T}(\tilde{A}_\theta, H_{\theta,-\theta})\) is anti-hermitian, and hence any \(\psi_{a,T}(\theta)\) solving (2.24) will have constant norm.

To be explicit, the proposed state \(\psi_{a,T}(\theta)\) differs from the actual ground state \(\psi_0(\theta, -\theta)\), of the rotated Hamiltonian \(H_{\theta, -\theta}\), in three essential ways. Compare (2.18) in the case that \(A = \partial_\theta H_{\theta,0}\) and \(H = H_{\theta,0}\) with (2.23) given that \(A = \partial_\theta H_{\theta,0}\) and \(H = H_{\theta,0}\).

i) We have introduced a cut-off at \(T < \infty\).

ii) We have approximated the imaginary-time evolution of an observable \(A\), \(\alpha_{it}(A)\), by \(A_a(it, H) - A_a(it, H)^*\).

iii) We have replaced the observable \(A_\theta = \partial_\theta H_{\theta,0}\) with \(\tilde{A}_\theta = \partial_\theta H_{\theta,0}\).

3. Energy estimates

3.1. Estimates on the states. In this subsection we prove a technical lemma which estimates, uniformly in \(\theta\), the norm difference between the ground state of \(H_{\theta,0}\) and the proposed state in the left half of the system, more precisely in the window centered around the location, \((m, V_L)\) where the \(\theta\)-twist occurs. Since the restrictions of the states to the half-systems are described by density matrices, it is natural to use the trace norm for this estimate. Recall that for any bounded operator \(A\) on a Hilbert space \(\mathcal{H}\), the trace norm is defined by

\[
\|A\|_1 = \text{Tr} \sqrt{A^* A},
\]

assuming this quantity is finite. Using the polar decomposition for bounded linear operators, it is easy to see that, alternatively,

\[
\|A\|_1 = \sup_{B \in \mathcal{B}(\mathcal{H}), \|B\| = 1} |\text{Tr} AB|,
\]

Recall that the density matrix corresponding to the ground state of the \(H_{\theta,0}\) Hamiltonian satisfies the evolution equation

\[
\partial_\theta \rho_0(\theta, -\theta) = B(\theta) \rho_0(\theta, -\theta) + \rho_0(\theta, -\theta) B(\theta)^*,
\]
where here and in the remainder of this section we use the notation $B(\theta) := B(A_\theta, H_{\theta,-\theta})$ and the operator $B$ is as defined in (2.18) with observable $A_\theta = \partial_\theta H_{\theta,-\theta}$. On the other hand, we evolve the proposed state according to

\begin{equation}
\partial_\theta \rho_{a,T}(\theta) = [B_{a,T}(\theta), \rho_{a,T}(\theta)],
\end{equation}

where, in analogy with (3.3), we have used the shorthand $B_{a,T}(\theta) := B_{a,T}(\tilde{A}_\theta, H_{\theta,-\theta})$ for the operator defined by (2.23) with observable $\tilde{A}_\theta = \partial_\theta H_{\theta,0}$. In contrast to (3.3), a commutator appears in (3.4) as the operator $B_{a,T}(\theta)$ is anti-hermitian. Given a gap of size $\gamma = \gamma L > 0$ above the ground state of the $H_L = H_{0,0}$ Hamiltonian, we will be able to estimate the difference in these two states by first taking a partial trace onto a region that excludes those sites which have been twisted by the angle $\theta$. We will denote by $\Tr_{m^c}[\cdot]$ the trace over the Hilbert space corresponding to $\Lambda_L^{(S)} \cup \Lambda_L^{(W)}(m + L/2)$. Our estimates show that the operator $\partial_\theta \Tr_{m^c}[\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)]$ has small trace norm, which implies a bound on the difference $\Tr_{m^c}[\rho_{a,T}(\theta) - \Tr_{m^c}[\rho_0(\theta, -\theta)]$. We prove

\begin{lemma}
Let $\Phi$ be an interaction satisfying the assumptions set aside above. If $\gamma > 0$ is sufficiently small with $\gamma L \geq 1$, then there exists constants $C > 0$ and $k > 0$ for which

\begin{equation}
\|\Tr_{m^c}[\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)]\|_1 \leq C L^2 d e^{-k\gamma L},
\end{equation}

along the path where $a = \frac{\gamma}{T}$ and $T = \frac{L}{2}$. Here $C$ and $k$ depend only on the interaction $\Phi$.

\begin{proof}
The proof of Lemma 3.1 follows by deriving a uniform bound on the $\theta$-derivatives of the differences of these density matrices. Specifically, the bound is in trace norm, and the uniformity is with respect to $\theta \in [0, 2\pi]$. In what follows, we will denote by $B_{a,T}^{(W)}(\theta)$ the operator defined by $B_{a,T} \left(\tilde{A}_\theta, H_{\theta,-\theta}^{(W)}\right)$ where the quantity $B_{a,T}$ is defined in (2.23), the observable $\tilde{A}_\theta = \partial_\theta H_{\theta,0}$, and the Hamiltonian $H_{\theta,-\theta}^{(W)}$ is the full Hamiltonian restricted to the windows, see (2.7).

Using (3.3) and (3.4), one may easily verify that

\begin{equation}
\partial_\theta \Tr_{m^c}[\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)] = \Tr_{m^c}\left([B_{a,T}^{(W)}(\theta), \rho_{a,T}(\theta) - \rho_0(\theta, -\theta)]\right) + \sum_{i=1}^{3} r_i(\theta),
\end{equation}

where the three remainder terms are given by

\begin{equation}
r_1(\theta) := \Tr_{m^c}\left([B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta), \rho_{a,T}(\theta)]\right),
\end{equation}

\begin{equation}
r_2(\theta) := \Tr_{m^c}\left([B_{a,T}^{(W)}(\theta), \rho_0(\theta, -\theta)] - \partial_\theta \rho_0(\theta, -\theta)\right),
\end{equation}

and

\begin{equation}
r_3(\theta) := \Tr_{m^c}[\partial_\theta \rho_0(\theta, -\theta) - \partial_\theta \rho_0(\theta, -\theta)].
\end{equation}

As $\tilde{A}_\theta = \partial_\theta H_{\theta,0}$ is supported near $(m, V_L)$ and $H_{\theta,-\theta}^{(W)}$ contains only those interaction terms over sets $X \subset \Lambda_L^{(W)}$, it is clear that $B_{a,T}^{(W)}(\theta) \in \mathcal{A}(m)$, which we use to denote the algebra of local observables $\mathcal{A}(m) = \mathcal{A}_X$ with $X = \Lambda_L^{(W)}(m)$. Therefore,

\begin{equation}
\Tr_{m^c}\left([B_{a,T}^{(W)}(\theta), \rho_{a,T}(\theta) - \rho_0(\theta, -\theta)]\right) = [B_{a,T}(\theta), \Tr_{m^c}[\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)]].
\end{equation}
Since $B_{a,T}^{(W)}(\theta)$ is anti-hermitian, we may apply norm preservation, i.e. Theorem 5.15, to (3.6) and conclude that

\begin{equation}
\| \text{Tr}_{m^c} [\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)] \|_1 \leq \sum_{i=1}^{3} \int_0^\theta \| r_i(\theta') \|_1 d\theta'.
\end{equation}

We need only bound the trace norms of the remainder terms $r_i(\theta)$.

As $\rho_{a,T}(\theta)$ is a density matrix, in particular non-negative with a normalized trace, one has that

\begin{equation}
\| r_1(\theta) \|_1 \leq 2 \| B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \|.
\end{equation}

Given the Lieb-Robinson bound from Lemma 5.3, we may estimate the right hand side above using Lemma 5.6; see also Remark 5.7. Choosing $a = \gamma/L$ and $T = L/2$, one finds that

\begin{equation}
\| r_1(\theta) \|_1 \leq C_1 L^{2d} e^{-C_2 \gamma L},
\end{equation}

for sufficiently small $\gamma$. Here the constants $C_1$ and $C_2$ depend only on the interaction $\Phi$; specifically, not on $L$ or $\gamma$.

To estimate $r_2(\theta)$, we note that as in (3.3),

\begin{equation}
\partial_t \rho_0(\theta, -\theta) = B_1(\theta) \rho_0(\theta, -\theta) + \rho_0(\theta, -\theta) B_1(\theta)^*,
\end{equation}

where $B_1(\theta) := B(A_1(\theta), H_{\theta,-\theta})$ and $A_1(\theta) := \partial_1 H_{\theta,-\theta} = \tilde{A}_\theta$. Here we have used that $\partial_1 E_0(\theta, -\theta) = 0$, see Lemma 2.1. A simple norm estimate yields that

\begin{equation}
\| r_2(\theta) \|_1 \leq 2 \left\| \left( B_{a,T}^{(W)}(\theta) - B_1(\theta) \right) P_0^\theta \right\| 
\end{equation}

\begin{equation}
\leq 2 \left\| B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \right\| + 2 \left\| \left( B_{a,T}(\theta) - B_1(\theta) \right) P_0^\theta \right\|,
\end{equation}

where $P_0^\theta$ is the projection onto the ground state $\psi_0(\theta, -\theta)$. The first term on the right hand side of (3.15) is identical to the estimate we got for the first remainder, while the second may be bounded explicitly in terms of the gap $\gamma$ as is done in Lemma 5.12; see also Remark 5.13. With the same choice of parameters as above, one has that

\begin{equation}
\| r_2(\theta) \|_1 \leq C_3 L^{2d} e^{-C_4 \gamma L},
\end{equation}

again, for sufficiently small $\gamma$. As above, the constants $C_3$ and $C_4$ depend only on the interaction.

Clearly, $r_3(\theta) = \text{Tr}_{m^c} [\partial_2 \rho_0(\theta, -\theta)]$. This term we bound by setting $A_2(\theta) := \partial_2 H_{\theta,-\theta}$ and deriving the analogue of (3.14) for $\partial_2 \rho_0(\theta, -\theta)$, using that $\partial_2 E_0(\theta, -\theta) = 0$ as well. Hence,\n
\begin{equation}
\| r_3(\theta) \|_1 = \sup_{\|O\| = 1} \| \text{Tr} \left[ O \left( B_2(\theta) \rho_0(\theta, -\theta) + \rho_0(\theta, -\theta) B_2(\theta)^* \right) \right] \|
\end{equation}

\begin{equation}
\leq 2 \sup_{\|O\| = 1} \int_0^\infty \| \psi_0(\theta, -\theta), O \alpha(t) (A_2(\theta)) \psi_0(\theta, -\theta) \| dt,
\end{equation}

where the observables $O$ are arbitrary elements of $A(m)$, the algebra of local observables $A_X$ with $X = L^{(W)}_L(m)$, as introduced above. Integrals of this type are bounded using Lemma 5.9; see also Remark 5.10. Since the observables we are considering have a distance of at least $L/4$, we may estimate

\begin{equation}
\| r_3(\theta) \|_1 \leq C_5 L^{d+1} e^{-C_6 \gamma L},
\end{equation}
for sufficiently small $\gamma$ and $\gamma L \geq 1$.

Combining the results found in (3.13), (3.16), and (3.18) we arrive at the desired estimate (3.5). $\square$

### 3.2. Bound on the energy

Given Lemma 3.1, we can prove the energy estimate which facilitates our argument. Recall that we are analyzing a two parameter family of Hamiltonians which satisfy

\[
(3.19) \quad H_{\theta,-\theta} = H_{\theta}^{(W)} + H^{(S)} \quad \text{and} \quad W(\theta)^* H_{\theta,-\theta} W(\theta) = H.
\]

For what follows, it will be useful to further subdivide the Hamiltonian as

\[
(3.20) \quad H_{\theta,-\theta}^{(W)} = H_{\theta}^{(W)}(m) + H_{\theta}^{(W)}(m + L/2),
\]

where $H_{\theta}^{(W)}(m)$ contains all those interaction terms in $H_{\theta,-\theta}^{(W)}$ with support in $\Lambda_{L}^{(W)}(m)$ and similarly, $H_{\theta}^{(W)}(m + L/2)$ contains all those interaction terms in $H_{\theta,-\theta}^{(W)}$ with support in $\Lambda_{L}^{(W)}(m + L/2)$. For any state $\psi$, one may calculate

\[
E_\theta(\psi) := \langle \psi, H_{\theta,0} \psi \rangle = \langle \psi, H_{\theta}^{(W)}(m) \psi \rangle + \langle \psi, \left( H_0^{(W)}(m + L/2) + H^{(S)} \right) \psi \rangle
\]

\[
= \langle \psi_0(\theta,-\theta), H_{\theta}^{(W)}(m) \psi_0(\theta,-\theta) \rangle + \langle \psi_0, \left( H_0^{(W)}(m + L/2) + H^{(S)} \right) \psi_0 \rangle
\]

\[
+ R_1(\theta) + R_2(\theta),
\]

where the remainder terms are given by

\[
(3.22) \quad R_1(\theta) := \langle \psi, H_{\theta}^{(W)}(m) \psi \rangle - \langle \psi_0(\theta,-\theta), H_{\theta}^{(W)}(m) \psi_0(\theta,-\theta) \rangle,
\]

\[
(3.23) \quad R_2(\theta) := \langle \psi, \left( H_0^{(W)}(m + L/2) + H^{(S)} \right) \psi \rangle - \langle \psi_0, \left( H_0^{(W)}(m + L/2) + H^{(S)} \right) \psi_0 \rangle,
\]

and $\psi_0$ is the ground state of $H = H_{0,0}$. Clearly then, we have the bound

\[
(3.24) \quad |E_\theta(\psi) - E_0| \leq |R_1(\theta)| + |R_2(\theta)|,
\]

for any state $\psi$. Inserting our proposed state $\psi_{a,T}(\theta)$ and rewriting the remainders in density matrix formalism, we find that

\[
(3.25) \quad R_1(\theta) = \text{Tr} \left[ (\rho_{a,T}(\theta) - \rho_0(\theta,-\theta)) H_{\theta}^{(W)}(m) \right]
\]

\[
= \text{Tr}_m \left[ \text{Tr}_{m'} [\rho_{a,T}(\theta) - \rho_0(\theta,-\theta)] H_{\theta}^{(W)}(m) \right],
\]

where the partial traces are as defined in the previous section. From this we easily conclude that

\[
(3.26) \quad |R_1(\theta)| \leq \|H_{\theta}^{(W)}(m)\| \|\text{Tr}_{m'} [\rho_{a,T}(\theta) - \rho_0(\theta,-\theta)]\|_1
\]

\[
\leq C L^{2d+1} e^{-k \gamma L},
\]

where we have used Lemma 3.1 for the final inequality above.

For the second remainder,

\[
(3.27) \quad R_2(\theta) = \text{Tr} \left[ (\rho_{a,T}(\theta) - \rho_0(0,0)) \left( H_0^{(W)}(m + L/2) + H^{(S)} \right) \right],
\]
we observe that the only $\theta$ dependence is in the density matrix corresponding to the proposed state. Using the evolution equation, we find that

$$ R_2(\theta) = \text{Tr} \left( [B_{a,T}(\theta), \rho_{a,T}(\theta)] \left( H_W^0(m + L/2) + H(S) \right) \right) $$

$$ = - \text{Tr} \left( [B_{a,T}(\theta), (H_W^0(m + L/2) + H(S))] \rho_{a,T}(\theta) \right). $$

The first term above is easy to estimate. Recall that the quantity $B_{a,T}(\theta)$ is supported in $\Lambda^W_L(m)$, whereas $H_W^0(m + L/2)$ has support in $\Lambda^W_L(m + L/2)$. Thus

$$ \left[ B_{a,T}(\theta), H_W^0(m + L/2) \right] = \left[ B_{a,T}(\theta) - B_{a,T}^W(\theta), H_W^0(m + L/2) \right], $$

and moreover,

$$ \left| \text{Tr} \left( [B_{a,T}(\theta) - B_{a,T}^W(\theta), H_W^0(m + L/2)] \rho_{a,T}(\theta) \right) \right| \leq 2 \left\| H_W^0(m + L/2) \right\| \left\| B_{a,T}(\theta) - B_{a,T}^W(\theta) \right\| \leq \tilde{C} L^{2d+1} e^{-\kappa \gamma L}. $$

The second term may be similarly estimated. Let $\tilde{H}_\theta^W$ be defined as in (2.7), excepting that the windows are slightly smaller: of size $\frac{L}{2} - 2R$. Then $[\tilde{H}_\theta^W(\theta), H(S)] = 0$, and the argument above applies. We have bounded $R_2(\theta)$.

4. Orthogonality

4.1. Observations concerning the twisted ground state. To see that the constructed state is orthogonal to the ground state, we will first investigate the twisted ground state. Recall that in Section 2.1, we saw that the twisted ground state is invariant with respect to the twisted translations; i.e., $T_{\theta,-\theta} \psi_0(\theta, -\theta) = \psi_0(\theta, -\theta)$. In this case, one easily sees that

$$ \partial_\theta [T_{\theta,-\theta} \psi_0(\theta, -\theta) - \psi_0(\theta, -\theta)] = 0. $$

One may rewrite this derivative in the form of an operator acting on $\psi_0(\theta, -\theta)$, i.e., (4.1) is equivalent to

$$ D(\theta) \psi_0(\theta, -\theta) = 0, $$

where $D(\theta)$ is given by

$$ D(\theta) = \partial_\theta T_{\theta,-\theta} T_{\theta,-\theta}^* + T_{\theta,-\theta} B(\theta) T_{\theta,-\theta}^* - B(\theta). $$

Here we have used the evolution equation (2.19), see also (3.3), with the operator $B(\theta) = B(\theta, H_{\theta,-\theta})$ and observable $A_{\theta} = \partial_\theta H_{\theta,-\theta}$ as in the previous section. Using (2.14), it is easy to see that

$$ \partial_\theta T_{\theta,-\theta} T_{\theta,-\theta}^* = i \sum_{v \in V_L} S_3^3(m+1,v) - i \sum_{v \in V_L} S_3^3(m+L/2+1,v). $$

It is useful to write $D(\theta) = D_{m+1}(\theta) - D_{m+L/2+1}(\theta)$ where

$$ D_{m+1}(\theta) = i \sum_{v \in V_L} S_3^3(m+1,v) + T_{\theta,-\theta} B_1(\theta) T_{\theta,-\theta}^* - B_1(\theta), $$

and

$$ D_{m+L/2+1}(\theta) = i \sum_{v \in V_L} S_3^3(m+L/2+1,v) + T_{\theta,-\theta} B_2(\theta) T_{\theta,-\theta}^* - B_2(\theta), $$
and for \(i = 1, 2\), we have set \(B_i(\theta) = B(A_i(\theta), H_{\theta, -\theta})\) with \(A_i(\theta) = \partial_i H_{\theta, -\theta}\), again, as in the previous section. Denoting by \(\langle A \rangle_\theta = \langle \psi_0(\theta, -\theta), A\psi_0(\theta, -\theta) \rangle\) the twisted ground state expectation of the local observable \(A\), we have demonstrated in Lemma 2.1 that \(\langle A_i(\theta) \rangle_\theta = \partial_i E_0(\theta, -\theta) = 0\) for \(i = 1, 2\). From this, we conclude that

\[
\langle T_{\theta, -\theta} B_i(\theta) T_{\theta, -\theta}^* \rangle_\theta = \langle B_i(\theta) \rangle_\theta = \langle A_i(\theta) \rangle_\theta = 0,
\]

for \(i = 1, 2\). Moreover, for any \(x \in \{m + 1, m + L/2 + 1\}\), we have that

\[
\langle D_x(\theta) \rangle_\theta = 0 \quad \text{as} \quad \left\langle \sum_{v \in V_L} S^3_{(x,v)} \right\rangle_\theta = \left( \sum_{v \in V_L} S^3_{(x,v)} \right)_0 = 0.
\]

For the last equality, we used that \(\psi_0(\theta, -\theta) = W(\theta)\psi_0\), \(W(\theta)\) commutes with the third component of the spins, rotation invariance implies that the total spin is zero, and translation invariance in the 1-direction.

Since \(D(\theta)\psi_0(\theta, -\theta) = 0\), we have that \(D_{m+1}(\theta)\psi_0(\theta, -\theta) = D_{m+1}(\theta)\psi_0(\theta, -\theta)\) from which it is clear that

\[
0 = \langle D(\theta)^* D(\theta) \rangle_\theta = 2\langle D_{m+1}(\theta)^* D_{m+1}(\theta) \rangle_\theta - 2\langle D_{m+1}(\theta)^* D_{m+1}(\theta) \rangle_\theta.
\]

Our goal is to prove that the first term on the right hand side above is exponentially small. We do so by showing that the second is. Observe that

\[
\langle D_{m+1}(\theta)^* D_{m+1}(\theta) \rangle_\theta = -\sum_{v,v' \in V_L} \langle S^3_{(m+1,v)} S^3_{(m+1,v')} \rangle_0
\]

\[
+ i \sum_{v \in V_L} \int_0^\infty \left\langle \left( S^3_{(m,v)} - S^3_{(m,v+1)} \right) \alpha_{iv}(A_2(\theta)) \right\rangle_\theta dt
\]

\[
+ \int_0^\infty \int_0^\infty \left\langle \alpha_{iv}(A_1(\theta))^* \left( \alpha_{iv}(A_2(\theta)) - \alpha_{iv}(T_{\theta, -\theta}^* A_2(\theta) T_{\theta, -\theta}) \right) \right\rangle_\theta ds dt
\]

\[
+ i \sum_{v' \in V_L} \int_0^\infty \left\langle \alpha_{iv}(A_1(\theta))^* \left( S^3_{(m+1+v',v')} - S^3_{(m+1,v')} \right) \right\rangle_\theta dt
\]

\[
+ \int_0^\infty \int_0^\infty \left\langle \alpha_{iv}(A_1(\theta))^* \left( \alpha_{iv}(A_2(\theta)) - \alpha_{iv}(T_{\theta, -\theta} A_2(\theta) T_{\theta, -\theta}^*) \right) \right\rangle_\theta ds dt.
\]

That each of these terms is small follows from our decay of correlations results, Lemma 5.9; see also Remark 5.10. Applying this lemma yields a bound of the type

\[
\langle D_{m+1}(\theta)^* D_{m+1}(\theta) \rangle_\theta \leq C L^{\max(2(d-1),4)} e^{-k\gamma L}.
\]

4.2. Orthogonality of the excited state. We now prove that the proposed excited state, evaluated at \(\theta = 2\pi\), is orthogonal to the ground state. Recall that \(T_\psi_0 = \psi_0\) and \(T_{2\pi, 0} = -T\).

From this we see that

\[
\langle \psi_{a,T}(2\pi), \psi_0 \rangle = \langle T_{2\pi, 0}^* \psi_{a,T}(2\pi), T_\psi_0 \rangle + \langle (I - T_{2\pi, 0}) \psi_{a,T}(2\pi), \psi_0 \rangle,
\]

which leads to the estimate

\[
|\langle \psi_{a,T}(2\pi), \psi_0 \rangle| \leq \frac{1}{2} \| (T_{2\pi, 0} - I) \psi_{a,T}(2\pi) \|.
\]

The remainder of this section will be used to prove that

\[
\| \partial_\theta [T_{\theta, 0} \psi_{a,T}(\theta) - \psi_{a,T}(\theta)] \|
\]
is uniformly small for $\theta \in [0, 2\pi]$.

A short calculation, using (2.24), shows that this derivative may be written as the sum of two terms:

\begin{align*}
\partial_{\theta} [T_{\theta,0} \psi_{a,T}(\theta) - \psi_{a,T}(\theta)] &= C_{a,T}(\theta) \left[ T_{\theta,0} \psi_{a,T}(\theta) - \psi_{a,T}(\theta) \right] + D_{a,T}(\theta) \psi_{a,T}(\theta),
\end{align*}

where

\begin{align*}
C_{a,T}(\theta) &= \partial_{\theta} T_{\theta,0} T_{\theta,0}^* + T_{\theta,0} B_{a,T}(\theta) T_{\theta,0}^*,
\end{align*}

and

\begin{align*}
D_{a,T}(\theta) &= \partial_{\theta} T_{\theta,0} T_{\theta,0}^* + T_{\theta,0} B_{a,T}(\theta) T_{\theta,0}^*, - B_{a,T}(\theta),
\end{align*}

are both anti-Hermitian operators. Here, as in the previous section, $B_{a,T}(\theta) = B_{a,T}(\hat{A}_{\theta}, H_{\theta,-\theta})$ and the observable $\tilde{A}_{\theta} = \partial_{\theta} H_{\theta,0} = A_1(\theta)$. The first term on the right hand side of (4.14) is norm-preserving, and therefore, we need only bound the norm of the second by Theorem 5.15.

The norm of the second term appearing in (4.14) may be written as

\begin{align*}
\| D_{a,T}(\theta) \psi_{a,T}(\theta) \|^2 &= \text{Tr} [D_{a,T}(\theta)^* D_{a,T}(\theta) \rho_{a,T}(\theta)] \\
&= \text{Tr} [D_{a,T}(\theta)^* D_{a,T}(\theta) \rho_0(\theta, -\theta)] \\
&+ \text{Tr} [D_{a,T}(\theta)^* D_{a,T}(\theta) (\rho_{a,T}(\theta) - \rho_0(\theta, -\theta))].
\end{align*}

The first term above is estimated by observing that

\begin{align*}
\| D_{a,T}(\theta) \psi_{0}(\theta, -\theta) \| &\leq \| D_{m+1}(\theta) \psi_{0}(\theta, -\theta) \| + \| (D_{a,T}(\theta) - D_{m+1}(\theta)) \psi_{0}(\theta, -\theta) \|
\end{align*}

where $D_{m+1}(\theta)$ is as introduced in the previous subsection. Clearly,

\begin{align*}
\| D_{m+1}(\theta) \psi_{0}(\theta, -\theta) \|^2 &= \langle D_{m+1}(\theta)^* D_{m+1}(\theta) \rangle_{\theta},
\end{align*}

which can be bounded using (4.10). Moreover, one easily sees that

\begin{align*}
D_{a,T}(\theta) - D_{m+1}(\theta) &= T_{\theta,-\theta} (B_{a,T}(\theta) - B_1(\theta)) T_{\theta,-\theta}^* \\
&+ T_{\theta,0} \left( B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \right) T_{\theta,0}^* \\
&- T_{\theta,-\theta} \left( B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \right) T_{\theta,-\theta}^* \\
&+ B_1(\theta) - B_{a,T}(\theta),
\end{align*}

from which it is clear that

\begin{align*}
\| (D_{a,T}(\theta) - D_{m+1}(\theta)) \psi_{0}(\theta, -\theta) \| &\leq 2 \| B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \| \\
&+ 2 \| (B_{a,T}(\theta) - B_1(\theta)) P_{0}^{\theta} \|.
\end{align*}

To bound the final term on the right hand side of (4.17), we insert and remove

\begin{align*}
D_{a,T}^{(W)}(\theta) &= \partial_{\theta} T_{\theta,0} T_{\theta,0}^* + T_{\theta,0} B_{a,T}^{(W)}(\theta) T_{\theta,0}^*, - B_{a,T}^{(W)}(\theta).
\end{align*}

Clearly,

\begin{align*}
\text{Tr} [D_{a,T}(\theta)^* D_{a,T}(\theta) (\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)) = \text{Tr} \left[ D_{a,T}^{(W)}(\theta) (\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)) \right]
\end{align*}

\begin{align*}
&+ \text{Tr} \left[ (D_{a,T}(\theta)^* D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta)^* D_{a,T}^{(W)}(\theta)) (\rho_{a,T}(\theta) - \rho_0(\theta, -\theta)) \right].
\end{align*}
The first term above may be estimated by

\begin{equation}
\left| \text{Tr}_m \left[ D_{a,T}^{(W)}(\theta) D_{a,T}^{(W)}(\theta) \right] \text{Tr}_m \left[ \rho_{a,T}(\theta) - \rho_0(\theta, -\theta) \right] \right|
\leq \left\| D_{a,T}^{(W)}(\theta) D_{a,T}^{(W)}(\theta) \right\| \left\| \text{Tr}_m \left[ \rho_{a,T}(\theta) - \rho_0(\theta, -\theta) \right] \right\|_1
\leq Ca^{-1} L^{4d-2} e^{-k\gamma L},
\end{equation}

where for the final inequality above we used Lemma 3.1 and Proposition 5.4.

For the second term, we rewrite the difference as

\begin{equation}
D_{a,T}(\theta)^* D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta)^* D_{a,T}^{(W)}(\theta)
= \left( D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta) \right)^* D_{a,T}(\theta) + D_{a,T}(\theta)^* \left( D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta) \right),
\end{equation}

and apply the norm estimate

\begin{equation}
\left\| D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta) \right\| \leq 2 \left\| B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \right\|.
\end{equation}

We find that

\begin{equation}
\text{Tr} \left[ \left( D_{a,T}(\theta)^* D_{a,T}(\theta) - D_{a,T}^{(W)}(\theta)^* D_{a,T}^{(W)}(\theta) \right) \left( \rho_{a,T}(\theta) - \rho_0(\theta, -\theta) \right) \right] \leq 4 \left\| B_{a,T}(\theta) - B_{a,T}^{(W)}(\theta) \right\| \left( \| D_{a,T}(\theta) \| + \| D_{a,T}^{(W)}(\theta) \| \right).
\end{equation}

We have proven the orthogonality result.

5. Auxiliary results

In this section, we collect a number of auxiliary results, technical estimates as well as a few lemmas of a more general nature, which are needed for the proofs in Sections 3 and 4. For a review of these and other results on quantum spin systems see [12].

In Section 5.1 below, we first recall the Lieb-Robinson bounds which are used to demonstrate quasi-locality of the dynamics associated to general quantum spin systems, see Theorem 5.1. Then, we observe in Proposition 5.2 that these Lieb-Robinson bounds may be used to compare the dynamics of a Hamiltonian defined on a given system with the dynamics of the same Hamiltonian restricted to a subsystem. Next, we provide in Lemma 5.3 an explicit bound which applies to the specific type of interactions we consider in this work.

In Section 5.2, we introduce the operators $B_{a,T}(A, H)$ which play a prominent role in our argument. We first discuss a few of their basic properties, and then use Proposition 5.2 to estimate the difference that arises in defining the operator with the full Hamiltonian as opposed to the Hamiltonian restricted to a subsystems; this is the content of Lemma 5.6. Lastly, we remark on exactly how this estimate will be used in the main text.

Next, in Section 5.3 we review the Exponential Clustering Theorem, which we use to prove a technical estimate (Lemma 5.9). Also in this section we prove that, for gapped systems, $B_{a,T}(A, H)$ well approximates the imaginary time evolution when projected onto the ground state.

Lastly, we formulate a statement concerning solutions of certain simple differential equations in Section 5.4.
5.1. Lieb-Robinson bounds. Throughout this section, we adopt the same general framework for quantum spin models that was described in Section 1.2, including Conditions F1 and F2 and the assumption that \( \| \Phi \|_\lambda < +\infty \) for some \( \lambda > 0 \) (see (1.6) for the definition of the norm \( \| \cdot \|_\lambda \)).

We will use the following version of the Lieb-Robinson bound [11], which is a variant of the Lieb-Robinson result proven in [13, 5].

**Theorem 5.1 (Lieb-Robinson Bound).** Let \( \lambda \geq 0 \) and take \( \Phi \in B_\lambda (\Lambda) \). For any pair of local observables \( A \in A_X \) and \( B \in A_Y \) with \( X, Y \subseteq \Lambda \), one may estimate

\[
\| [\alpha_t(A), B] \| \leq 2 \frac{\| A \| \| B \|}{C_\lambda} \sum_{x \in X} \sum_{y \in Y} F_\lambda (d(x, y)),
\]

for any \( t \in \mathbb{R} \). Here \( \{ \alpha_t \} \) is the dynamics generated by \( \Phi \), and one may take

\[
g_\lambda (t) = \begin{cases} 
( e^{2 \| \Phi \|_\lambda |t|} - 1 ) & \text{if } d(X, Y) > 0, \\
\frac{e^{2 \| \Phi \|_\lambda |t|}}{2} & \text{otherwise}.
\end{cases}
\]

Our proof of the Lieb-Schultz-Mattis theorem relies heavily on comparing the time evolution corresponding to the full Hamiltonian to that of the Hamiltonian restricted to a subsystem. The errors that result from such a comparison can be estimated in terms of a specific commutator to which the Lieb-Robinson bounds readily apply.

**Proposition 5.2.** Let \( \lambda \geq 0 \) and write \( \Phi_0 \in B_\lambda (\Lambda) \) as \( \Phi_0 = \Phi_1 + \Phi_2 \). For any local observable \( A \in A_X \) and \( t \in \mathbb{R} \), denote by \( \alpha_t^{(0)}(A) \) and \( \alpha_t^{(1)}(A) \), for \( i = 0, 1, 2 \), the time evolution and Hamiltonian corresponding to each \( \Phi_i \), respectively. One has

\[
\| \alpha_t^{(0)}(A) - \alpha_t^{(1)}(A) \| \leq \int_0^{|t|} \| [H_2, \alpha_s^{(1)}(A)] \| \, ds.
\]

**Proof.** Define the function \( f : \mathbb{R} \to A \) by

\[
f(t) := \alpha_t^{(0)}(A) - \alpha_t^{(1)}(A).
\]

A simple calculation shows that \( f \) satisfies the following differential equation:

\[
f'(t) = i \left( H_0 - H_1, \alpha_t^{(1)}(A) \right) + i \left[ H_0, f(t) \right],
\]

subject to the boundary condition \( f(0) = 0 \). As this is a first order equation, the solution can be found explicitly:

\[
f(t) = \alpha_t^{(0)} \left( \int_0^t \alpha_{-s}^{(0)} \left( i \left[ H_2, \alpha_s^{(1)}(A) \right] \right) \, ds \right).
\]

Using expression (5.6) and the automorphism property of \( \alpha_t^{(0)} \), it is clear that

\[
\| f(t) \| \leq \int_0^{|t|} \| [H_2, \alpha_s^{(1)}(A)] \| \, ds,
\]

as claimed. \( \square \)

To estimate the norm of the commutator appearing in Proposition 5.2, specifically in the bound (5.3), it is useful to specialize the general Lieb-Robinson bounds described above to the exact context we encounter in the present work. For example, we will be interested in specific Hamiltonians, those defined in Section 2 as \( H_{a,b,r} \), and particular observables, such
as $A_1 := \partial_\theta H_{\theta, \theta'}$ and $A_2 := \partial_\theta H_{\theta, \theta'}$. Let $\alpha_t$ be the time evolution corresponding to the $H_{\theta, \theta'}$ Hamiltonian, and let $\alpha_t^{(W)}$ denote the dynamics associated with the Hamiltonian $H_{\theta, \theta'}^{(W)}$ which is defined in (2.7). We use the following estimates several times.

**Lemma 5.3.** Let $\Phi \in B_\lambda(\Lambda)$, then

$$
\max_{i=1,2} \left\| \left[ H^{(S)}, \alpha_t^{(W)}(A_i) \right] \right\| \leq c_1 L^{2(d-1)} e^{c_3 |t| - c_3 L},
$$

where the coefficients $c_1$, $c_2$, and $c_3$ depend only on the properties of the underlying set $\Lambda$ and the interaction $\Phi$; not $L$.

**Proof.** We will estimate the above commutator in the case that the observable is $A_1$; an analogous result holds for $A_2$. Recall that in (2.8) we wrote $H^{(S)}$ as a sum of interaction terms. Similarly, if one denotes by $P_m(\theta; Y) := V_m(\theta)^* \Phi(Y) V_m(\theta) - \Phi(Y)$, then $A_1$ may be written as

$$
A_1 = \sum_{\substack{Y \subseteq \Lambda_L \setminus P_m(\theta; Y) \neq 0 \\text{ s.t.}}} \partial_\theta [V_m(\theta)^* \Phi(Y) V_m(\theta)] = -i \sum_{\substack{Y \subseteq \Lambda_L \setminus P_m(\theta; Y) \neq 0 \\text{ s.t.}}} \sum_{y \in Y} V_m(\theta)^* [S^3_{y}, \Phi(Y)] V_m(\theta),
$$

where $Y_+$ is the set of sites $y \in Y$ strictly to the right of $m$. Inserting both of these expressions into the right hand side of (5.8) and applying the triangle inequality, it is clear that we must bound many terms of the form

$$
\left\| \left[ \Phi(X), \alpha_t^{(W)} \left( V_m(\theta)^* [S^3_{y}, \Phi(Y)] V_m(\theta) \right) \right] \right\|.
$$

Term by term, we apply the Lieb-Robinson bound provided by Theorem 5.1, and use that the distance between the supports of $X$ and $Y$ is linear in $L$; concretely for any $x \in X$ and $y \in Y$, $d(x, y) \geq d(X, Y) \geq \frac{L}{4} - 3R$. We find that each term described by (5.10) satisfies an upper bound of the form

$$
C \| \Phi(X) \| |Y| \| [S^3_{y}, \Phi(Y)] \| e^{-\lambda L/4},
$$

where $C$ may be taken as

$$
C = \frac{2\| F \|}{C_\lambda(F)} e^{2C_\lambda(F) \| \Phi \| |t| + 3\lambda R}.
$$

We need only count the number of terms. The combinatorics of the sums may be naively estimated as follows:

$$
\sum_{\substack{X \subseteq \Lambda_L \setminus \Lambda_L^{(S)} \neq 0 \\text{ s.t.}}} \leq \sum_{n = \frac{L}{4} - R - 1}^{\frac{L}{4} + R - 1} \sum_{\substack{v \in V_L \setminus \exists (m + n, v) \\text{ s.t.}}} + \sum_{n = \frac{L}{4} + R - 1}^\infty \sum_{v \in V_L \setminus \exists (m + n, v)},
$$

and

$$
\sum_{\substack{Y \subseteq \Lambda_L \setminus \Lambda_L^{(S)} \neq 0 \\text{ s.t.}}} \sum_{y \in Y} \leq \sum_{n = m - R}^{m + R} \sum_{v \in V_L \setminus \exists (n, v)} \sum_{y \in Y}
$$

Putting everything together, we have obtained that

$$
\left\| \left[ H^{(S)}, \alpha_t^{(W)}(A_1) \right] \right\| \leq 2C \| \Phi \| \|1\| \| \Phi \| \|2\| (2R + 1) (2R - 1) e^{-\lambda L},
$$
which proves the claim. Recall,
\begin{equation}
|||\Phi|||_1 := \sup_{x \in \Lambda} \sum_{X \ni x} ||\Phi(X)||
\end{equation}
and
\begin{equation}
|||\Phi|||_2 := \sup_{x \in \Lambda} \sum_{X \ni x} |X| \sum_{x' \in X} ||[S_{X'}^3, \Phi(X)]||.
\end{equation}

\[ \square \]

5.2. Approximation of the imaginary time evolution. In our proof of the Lieb-Schultz-Mattis Theorem, we require estimates on the imaginary time dynamics of certain observables. For this reason, we introduce an explicit approximation of the imaginary time evolution in this subsection. Let $\lambda \geq 0$ and $\Phi \in \mathcal{B}_\lambda(\Lambda)$ be an interaction on $\mathcal{A}$. Denote by $\alpha_t$, for $t \in \mathbb{R}$, the (real-time) dynamics associated to $\Phi$. For any local observable $A \in \mathcal{A}_X$, $a > 0$, $M > 0$, and $t \neq 0$, define
\begin{equation}
A_{a,M}(it, \Phi) := \frac{e^{-at^2}}{2\pi i} \int_{-M}^{M} \alpha_s(A) \frac{e^{-as^2}}{s - it} ds,
\end{equation}
and set $A_a(it; \Phi) := \lim_{M \to \infty} A_{a,M}(it; \Phi)$. In addition, the operator
\begin{equation}
B_{a,T}(A, \Phi) := -\int_0^T A_a(it, \Phi) - A_a(it, \Phi)^* dt,
\end{equation}
will be useful in many of our arguments. We note that in the main text the operator $B_{a,T}(A, \Phi)$ is defined with respect to the Hamiltonian $H$ rather than the interaction $\Phi$. Due to the $L$-dependent boundary terms and twists, we found this more convenient. For this more general context, in which the set $\Lambda$ may not be finite, we find it more appropriate to describe these operators in terms of their interactions $\Phi$. We begin with some basic properties.

**Proposition 5.4** (Shanti’s Bound). Let $\Phi \in \mathcal{B}_\lambda(\Lambda)$, $A \in \mathcal{A}$, $a > 0$, and $T > 0$. The operator $B_{a,T}(A, \Phi)$ is anti-hermitian and bounded. In particular,
\begin{equation}
||B_{a,T}(A, \Phi)|| \leq \frac{||A||}{2} \sqrt{\frac{\pi}{a}}.
\end{equation}

**Proof.** That $B_{a,T}(A, \Phi)$ is anti-hermitian follows immediately from (5.19). Combining (5.18) and (5.19), one finds that
\begin{equation}
B_{a,T}(A, \Phi) = \frac{i}{\pi} \int_0^T \int_{-\infty}^{\infty} e^{-a(s^2 + t^2)} \alpha_s(A) \frac{s}{s^2 + t^2} ds dt,
\end{equation}
from which (5.20) easily follows as
\begin{equation}
||B_{a,t}(A, \Phi)|| \leq \frac{||A||}{\pi} \int_{-\infty}^{\infty} e^{-as^2} \left|\int_0^T \frac{1}{s^2 + t^2} dt\right| ds \leq \frac{||A||}{2} \sqrt{\frac{\pi}{a}}.
\end{equation}
\[ \square \]

In situations where the local observable $A$ and the interaction $\Phi$ are fixed, we will often write $A_a(it)$ and $B_{a,T}$ to simplify notation. The following estimate is a simple consequence of (5.18).
Proposition 5.5. Let $\Phi \in B_\Lambda(\Lambda)$ and $A \in A_X$. One has that
\begin{equation}
\left\| \int_0^T A_a(it) - A_{a,M}(it) \, dt \right\| \leq \frac{T}{2M} \frac{\|A\|}{\sqrt{\pi a}} e^{-aM^2}.
\end{equation}

Proof. For any $t \neq 0$,
\begin{equation}
A_a(it) - A_{a,M}(it) = \frac{e^{-at^2}}{2\pi i} \int_{|s|>M} \alpha_s(A) \frac{e^{-as^2}}{s-it} \, ds,
\end{equation}
and therefore, one has the pointwise estimate
\begin{equation}
\|A_a(it) - A_{a,M}(it)\| \leq e^{-at^2} \frac{\|A\|}{2\pi M} e^{-aM^2} \sqrt{\frac{\pi}{a}}.
\end{equation}
Upon integration, (5.23) readily follows. \qed

We will now prove an analogue of Proposition 5.2 for the quantities $B_{a,T}(A, \Phi)$ introduced in (5.19). The estimate provided below is made explicit in terms of an a priori input, an assumed form of the Lieb-Robinson bound, see (5.26) below.

Lemma 5.6. Let $\Phi_0 \in B_\Lambda(\Lambda)$ and write $\Phi_0 = \Phi_1 + \Phi_2$. For any local observable $A \in A_X$ and $t \in \mathbb{R}$, denote by $\alpha_t^{(i)}(A)$ and $H_i$, for $i = 0, 1, 2$, the time evolution and Hamiltonian corresponding to each $\Phi_i$, respectively. Assume that for each local observable $A$, there exists constants $c_i > 0$, $i = 1, 2, 3$, with
\begin{equation}
\left\| [H_2, \alpha_t^{(i)}(A)] \right\| \leq c_1 e^{c_2|t|} - c_3,
\end{equation}
for all $t \in \mathbb{R}$. Then, the following estimate holds
\begin{equation}
\|B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1)\| \leq \frac{2T}{M} e^{-aM^2} \left( \frac{\|A\|}{\sqrt{\pi a}} + \frac{c_1M^2}{\pi} \right),
\end{equation}
where $M$ may be choosen as the positive solution of
\begin{equation}
aM^2 + c_2M - c_3 = 0.
\end{equation}

Proof. One may write
\begin{equation}
B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1) = -\int_0^T A_a(it, \Phi_0) - A_a(it, \Phi_1) \, dt
+ \int_0^T A_a(it, \Phi_0)^* - A_a(it, \Phi_1)^* \, dt,
\end{equation}
and therefore
\begin{equation}
\|B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1)\| \leq 2 \left\| \int_0^T A_a(it, \Phi_0) - A_a(it, \Phi_1) \, dt \right\|.
\end{equation}
Moreover, the integrand may be expressed as
\begin{equation}
A_a(it, \Phi_0) - A_a(it, \Phi_1) = A_a(it, \Phi_0) - A_{a,M}(it, \Phi_0) +
A_{a,M}(it, \Phi_0) - A_{a,M}(it, \Phi_1) + A_{a,M}(it, \Phi_1) - A_a(it, \Phi_1),
\end{equation}
and for $j = 0, 1$, the bounds
\begin{equation}
\left\| \int_0^T A_a(it, \Phi_j) - A_{a,M}(it, \Phi_j) \, dt \right\| \leq \frac{T}{2M} \frac{\|A\|}{\sqrt{\pi a}} e^{-aM^2},
\end{equation}
follow immediately from Proposition 5.5. From this we conclude that for any $M > 0$,
\[
\| B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1) \| \leq 2 \left\| \int_0^T A_{a,M}(it, \Phi_0) - A_{a,M}(it, \Phi_1) \, dt \right\| + \frac{2T}{M} \frac{\| A \|}{\sqrt{\pi a}} e^{-aM^2}.
\]

(5.33)

Clearly, the pointwise estimate
\[
\| A_{a,M}(it, \Phi_0) - A_{a,M}(it, \Phi_1) \| \leq \frac{e^{-aT^2}}{2\pi} \int_{-M}^M \frac{\| \alpha_s^{(0)}(A) - \alpha_s^{(1)}(A) \|}{|s|} e^{-as^2} \, ds,
\]

follows directly from (5.18). By Proposition 5.2, we have that
\[
\| \alpha_s^{(0)}(A) - \alpha_s^{(1)}(A) \| \leq \int_0^{|s|} \| [H_2, \alpha_s^{(1)}(A)] \| \, dx,
\]

and by assumption (5.26), the integrand satisfies a uniform bound for $|s| \leq M$. The implication is that for all $|s| \leq M$,
\[
\frac{\| \alpha_s^{(0)}(A) - \alpha_s^{(1)}(A) \|}{|s|} \leq c_1 e^{c_2M - c_3}.
\]

(5.36)

Putting everything together, we obtain that
\[
\| B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1) \| \leq \frac{2T}{M} \frac{\| A \|}{\sqrt{\pi a}} e^{-aM^2} + \frac{c_1 e^{c_2M - c_3}}{\pi} \int_0^T \int_{-M}^M e^{-a(t^2 + s^2)} \, dsdt.
\]

(5.37)

As $M$ here was arbitrary, we choose it as the (positive) solution of the following quadratic equation $aM^2 + c_2M - c_3 = 0$. In this case,
\[
\| B_{a,T}(A, \Phi_0) - B_{a,T}(A, \Phi_1) \| \leq \frac{2T}{M} \frac{\| A \|}{\sqrt{\pi a}} + \frac{c_1 M^2}{\pi}
\]

(5.38)

as claimed. \hfill \Box

Remark 5.7. In the main text of the paper, we will often use Lemma 5.6 with a specific parametrization. The typical setting assumes that the full Hamiltonian $H_0$ depends on a length scale $L$ and has a gap $\gamma = \gamma(L) > 0$ above the ground state energy. Let $A$ be a local observable with $\| A \| \leq L^d$ for which one may prove a Lieb-Robinson estimate of the form (5.26) with $c_1 = cL^{2(d-1)}$, $c_2 = \tilde{c}$, and $c_3 = c' L$, where $c, \tilde{c},$ and $c'$ depend only on the interaction. In this case, we will choose the parametrization $aL = \gamma$ and $2T = L$. With this choice, the positive solution $M$ of (5.28) may be written as $M = kL$ with $0 < k_1 \leq k \leq k_2 < \infty$ for $\gamma$ sufficiently small; $4\gamma c' \leq 1$ will do. Under these assumptions, the estimate (5.27) takes the more simple form:
\[
\| B_{a,T}(A; \Phi_0) - B_{a,T}(A; \Phi_1) \| \leq C L^d e^{-k_2^2 \gamma L}.
\]

(5.39)
5.3. Estimates for gapped systems. The second crucial estimate in this section, Lemma 5.12 below, demonstrates that if a system is gapped, then the operators $B_{a,T}$ and $B_a$, defined in (2.18) and (2.23) respectively, remain exponentially close, when projected onto the ground state.

In this section, we will consider Hamiltonians $H$, of the type introduced in section 5.1, with an additional feature: a gap above the ground state energy. To state the gap condition precisely, we consider a representation of the system on a Hilbert space $\mathcal{H}$. This means that there is a representation $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$, and a self-adjoint operator $H$ on $\mathcal{H}$ such that

$$\pi(\alpha_t(A)) = e^{itH}\pi(A)e^{-itH},$$

for all $t \in \mathbb{R}$ and $A \in \mathcal{A}$. For the results which follow, we will assume that $H \geq 0$ and that $\Omega \in \mathcal{H}$ is a normalized ground state, i.e., a vector state for which $H\Omega = 0$ and $\|\Omega\| = 1$. We say that the system has a spectral gap in this representation if there exists $\delta > 0$ such that $\sigma(H) \cap (0, \delta) = \emptyset$, where $\sigma(H)$ is the spectrum of the operator $H$. In that case, the spectral gap, $\gamma$, is defined to be

$$\gamma = \sup\{\delta > 0 \mid \sigma(H) \cap (0, \delta) = \emptyset\}.$$  

Let $P_0$ denote the orthogonal projection onto $\ker H$. From now on, we will work in this representation and simply write $A$ instead of $\pi(A)$.

The following result concerning exponential clustering was proven in [13].

**Theorem 5.8 (Exponential Clustering).** Fix $\lambda > 0$. Let $\Phi \in \mathcal{B}_\lambda(\Lambda)$ be an interaction for which the corresponding self-adjoint Hamiltonian has a representation $H \geq 0$ with a normalized ground state vector $\Omega$, i.e., $H\Omega = 0$ and $\|\Omega\| = 1$. If $H$ has a spectral gap of size $\gamma > 0$ above the ground state energy, then there exist $\mu > 0$ such that for any local observables $A$ with $A \in \mathcal{A}_X$, $B \in \mathcal{A}_Y$, $d := \text{dist}(X, Y) > 0$, and $P_0B\Omega = P_0B^*\Omega = 0$, where $P_0$ is the projection onto the ground state, the estimate

$$\langle \Omega, A\alpha_t(B)\Omega \rangle \leq C(A, B) e^{-\mu d} \left(1 + \frac{\|C\|_\lambda C + \gamma}{\sqrt{\pi\mu d}}\right),$$

holds for all $t : 0 \leq t(4\|\Phi\|_\lambda C_\lambda + \gamma) \leq 2\lambda d$. Here, one may choose

$$C(A, B) = \|A\| \|B\| \left(1 + \frac{2}{\pi C_\lambda} \sum_{x \in X} \sum_{y \in Y} F(d(x, y)) + \frac{1}{\sqrt{\pi\mu d}}\right)$$

and

$$\mu = \frac{\lambda \gamma}{4\|\Phi\|_\lambda C_\lambda + \gamma}.$$  

The above result easily leads to estimates on integrals of these ground state expectations. We state two such bounds in the next lemma, as they will arise in the proof of our main result.

**Lemma 5.9.** Under the assumptions of Theorem 5.8, we may also prove,

$$\int_0^\infty |\langle \Omega, A\alpha_{it}(B)\Omega \rangle| dt \leq \left(2\mu d C(A, B) + \|A\| \|B\| e^{\mu d}\right) \frac{e^{-\mu d}}{\gamma}.$$
and
\begin{equation}
\int_0^\infty \int_0^\infty \left| \langle \Omega, A^{\alpha_i(s+t)}(B)\Omega \rangle \right| \, ds \, dt \leq \left[ (\mu d)^2 C(A, B) + \|A\| \|B\| \left( 2\mu d + e^{-\mu d} \right) \right] e^{-\frac{\mu d}{\gamma^2}}.
\end{equation}

Proof. Define $T$ by the equation $\gamma T = 2\mu d$. We have that
\begin{equation}
\int_0^T \left| \langle \Omega, A^{\alpha_i}(B)\Omega \rangle \right| \, dt \leq C(A, B) T e^{-\mu d},
\end{equation}
and also
\begin{equation}
\int_T^\infty \left| \langle \Omega, A^{\alpha_i}(B)\Omega \rangle \right| \, dt \leq \frac{\|A\| \|B\|}{\gamma} e^{-\gamma T}.
\end{equation}
Combining these two bounds, we arrive at (5.44). Similarly, one may estimate
\begin{equation}
\int_0^{T/2} \int_0^{T/2} \left| \langle \Omega, A^{\alpha_i(s+t)}(B)\Omega \rangle \right| \, ds \, dt \leq \frac{C(A, B) T^2}{4} e^{-\mu d},
\end{equation}
\begin{equation}
\int_{T/2}^\infty \int_0^{T/2} \left| \langle \Omega, A^{\alpha_i(s+t)}(B)\Omega \rangle \right| \, ds \, dt \leq \frac{\|A\| \|B\| T}{2\gamma} e^{-\mu d},
\end{equation}
and finally,
\begin{equation}
\int_{T/2}^\infty \int_{T/2}^\infty \left| \langle \Omega, A^{\alpha_i(s+t)}(B)\Omega \rangle \right| \, ds \, dt \leq \frac{\|A\| \|B\|}{\gamma^2} e^{-\gamma T}.
\end{equation}

$\square$

**Remark 5.10.** We continue with the discussion we began in Remark 5.7. Let $A$ and $B$ be local observables whose supports have a distance proportional to $L$, and assume that $B$ is of the form $\partial_i H_{0,y}$. Because of Lemma 2.1 and the Feynman-Hellman Theorem this form of $B$ guarantees that $P_0 B \Omega = P_0 B^* \Omega = 0$. If the gap $0 < \gamma \leq 1/2$, then $0 < c_1 \gamma L \leq \mu d \leq c_2 \gamma L < \infty$. In this case,
\begin{equation}
\int_0^\infty \left| \langle \Omega, A^{\alpha_i}(B)\Omega \rangle \right| \, dt \leq C L^2 \|A\| \|B\| \min \{ |X|, |Y| \} e^{-c_1 \gamma L},
\end{equation}
and
\begin{equation}
\int_0^\infty \int_0^\infty \left| \langle \Omega, A^{\alpha_i(s+t)}(B)\Omega \rangle \right| \, ds \, dt \leq C L^4 \|A\| \|B\| \min \{ |X|, |Y| \} e^{-c_1 \gamma L},
\end{equation}
hold if $\gamma L \geq 1$.

For the next lemma we will need the following basic estimate involving the decay of certain Fourier transforms.

**Proposition 5.11.** Let $a > 0$ and $T > 0$ be given. Define a function $F_{a,T} : \mathbb{R} \to \mathbb{C}$ by
\begin{equation}
F_{a,T}(E) := \frac{1}{2\pi i} \int_0^T e^{-at^2} \int_{-\infty}^\infty e^{-iEs} e^{-as^2} \frac{ds \, dt}{s - it}.
\end{equation}
For all $E \in \mathbb{R}$, $F_{a,T}(E) \geq 0$ and the estimate
\begin{equation}
F_{a,T}(E) \leq \frac{T}{2} e^{-\frac{E^2}{4a}},
\end{equation}
is valid for $E \geq 0$. In the parameter range, $E \geq 2aT > 0$, one may also show that

\begin{equation}
(5.55) \quad \int_0^T e^{-Et} \, dt - F_{a,T}(-E) \leq \frac{T}{2} e^{-\frac{E^2}{4a}}.
\end{equation}

Proof. One may easily verify that for any $t > 0$,

\begin{equation}
(5.56) \quad \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-itE} e^{-as^2}}{s - it} \, ds = \frac{1}{2\sqrt{\pi a}} \int_0^\infty e^{-tw} e^{-\frac{(w+E)^2}{4a}} \, dw,
\end{equation}

for all $E \in \mathbb{R}$, see e.g. Lemma 1 in [13]. This implies the first claim. Evaluating the Gaussian integral yields

\begin{equation}
(5.57) \quad \frac{1}{2\sqrt{\pi a}} \int_0^\infty e^{-tw} e^{-\frac{(w+E)^2}{4a}} \, dw \leq \frac{1}{2} e^{-\frac{E^2}{4a}},
\end{equation}

in the case that $E \geq 0$, from which (5.54) is clear.

To obtain (5.55), we first recall that the Fourier transform of a Gaussian is a Gaussian, i.e., for all $z \in \mathbb{C}$,

\begin{equation}
(5.58) \quad e^{-\frac{z^2}{2}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} e^{-ixz} \, dx,
\end{equation}

and therefore, by rescaling $z \mapsto -\sqrt{2a}z$, multiplying through by $e^{iEz}$ (for $E \in \mathbb{R}$), and changing variables $w = \sqrt{2a}x + E$, we have that

\begin{equation}
(5.59) \quad e^{iEz} e^{-az^2} = \frac{1}{2\sqrt{\pi a}} \int_{-\infty}^{\infty} e^{iwz} e^{-\frac{(w+E)^2}{4a}} \, dw,
\end{equation}

for all $z \in \mathbb{C}$.

Now, by direct substitution into (5.56), we have that

\begin{equation}
(5.60) \quad F_{a,T}(-E) = \frac{1}{2\sqrt{\pi a}} \int_0^T e^{-at^2} \int_0^\infty e^{-tw} e^{-\frac{(w+E)^2}{4a}} \, dw.
\end{equation}

Applying (5.59), with the special choice of $z = it$, one sees that

\begin{equation}
(5.61) \quad \int_0^T e^{-Et} \, dt - F_{a,T}(-E) = \frac{1}{2\sqrt{\pi a}} \int_0^T e^{-at^2} \int_{-\infty}^{\infty} e^{-tw} e^{-\frac{(w+E)^2}{4a}} \, dw.
\end{equation}

Since $w < 0$ and $t > 0$, the integrand above

\begin{equation}
(5.62) \quad e^{-tw} e^{-\frac{(w+E)^2}{4a}} = e^{-\frac{E^2}{4a}} e^{-\frac{(E-2at)w}{2a}} e^{-\frac{w^2}{4a}}
\end{equation}

satisfies a trivial bound when $E \geq 2aT$. For these values of $E$, (5.55) holds. □

We may now prove the main estimate for gapped systems.

Lemma 5.12. Let $H \geq 0$ be a self-adjoint operator with a normalized ground state vector $\Omega$, i.e. $H\Omega = 0$ and $\|\Omega\| = 1$. Let $P_0$ denote the projection onto this ground state. Suppose $H$ has a gap $\gamma > 0$ above the ground state energy, then for any observable $A$ with $A^* = e^{i\phi} A$ (for $\phi \in [0,2\pi)$) and $P_0AP_0 = 0$, one has that

\begin{equation}
(5.63) \quad \| (B_{a,T} - B) P_0 \| \leq \left( T e^{-\frac{\gamma^2}{4a}} + \frac{e^{-\gamma T}}{\gamma} \right) \|AP_0\|,
\end{equation}

if $2aT \leq \gamma$. 

Proof. One may rewrite the difference in these operators as
\[
(B_{u,T} - B) P_0 = \int_0^T (\alpha_{it}(A) - A_{a}(it)) \, dt \, P_0
\]
(5.64)
\[
+ \int_T^\infty \alpha_{it}(A) \, dt \, P_0 + \int_0^T A_{a}(it)^* \, dt \, P_0.
\]
Each of these terms may be bounded in norm.

For any vectors \(f\) and \(g\), one may calculate
\[
\int_T^\infty \langle f, \alpha_{it}(A) g \rangle \, dt = \int_T^\infty \langle f, e^{-itH} A P_0 g \rangle \, dt
\]
(5.65)
\[
= \int_T^\infty \int_\gamma e^{-itE} \, d\langle f, P_E A P_0 g \rangle \, dt,
\]
where we have used the spectral theorem to rewrite the time evolution and the fact that \(P_0 P_0 = 0\). Clearly, for \(E \geq \gamma > 0\), one has that
\[
\int_T^\infty e^{-itE} \, dt \leq \frac{e^{-\gamma T}}{\gamma},
\]
(5.66)
and therefore,
\[
\left\| \int_T^\infty \alpha_{it}(A) \, dt \, P_0 \right\| \leq \frac{e^{-\gamma T}}{\gamma} \|AP_0\|.
\]
(5.67)
Likewise, one may similarly calculate
\[
\int_0^T \langle A_{a}(it) f, P_0 g \rangle \, dt = - \int_0^T \frac{e^{-at^2}}{2\pi i} \int_{-\infty}^\infty \langle \alpha_s(A) f, P_0 g \rangle \frac{e^{-as^2}}{s + it} \, ds \, dt
\]
(5.68)
\[
= e^{i\phi} \int_\gamma \int_0^\infty F_{a,T}(E) \, d\langle f, P_E A P_0 g \rangle,
\]
using that \(A^* = e^{i\phi} A\) and introducing \(F_{a,T}(E) = \overline{F_{a,T}(E)}\) as in (5.53) of Proposition 5.11 above. The estimate
\[
\left\| \int_0^T A_{a}(it)^* \, dt \, P_0 \right\| \leq \frac{T}{2} e^{-\frac{\gamma^2}{8}} \|AP_0\|,
\]
(5.69)
readily follows from (5.54) of Propostion 5.11 and the fact that \(0 < \gamma \leq E\).

Lastly, an analogous calculation shows that
\[
\int_0^T \langle f, [\alpha_{it}(A) - A_{a}(it)] P_0 g \rangle \, dt =
\]
(5.70)
\[
\int_\gamma \left[ \int_0^T e^{-Et} \, dt - F_{a,T}(-E) \right] \, d\langle f, P_E A P_0 g \rangle.
\]
Thus, for \(2aT \leq \gamma\), we may apply (5.55) of Proposition 5.11 and establish the bound
\[
\left\| \int_0^T [\alpha_{it}(A) - A_{a}(it)] \, dt \, P_0 \right\| \leq \frac{T}{2} e^{-\frac{\gamma^2}{8}} \|AP_0\|.
\]
(5.71)
Compiling our estimates, we have proven that: if $2aT \leq \gamma$, then
\begin{equation}
\| (B_{a,T} - B) P_0 \| \leq \left( Te^{-\frac{a^2}{4}} + \frac{e^{-\gamma T}}{\gamma} \right) \| AP_0 \|,
\end{equation}
as claimed. □

**Remark 5.13.** Again, with the parametrization described in Remark 5.7, this estimate yields that
\begin{equation}
\| (B_{a,T} - B) P_0 \| \leq C L e^{-\frac{a}{4}} \| AP_0 \|,
\end{equation}
if $\gamma L \geq 1$.

5.4. **Norm preserving flows.** In this section, we collect some basic facts about the solutions of first order, inhomogeneous differential equations.

**Definition 5.14.** Let $\mathcal{B}$ be a Banach space. For each $\theta \in \mathbb{R}$, let $A(\theta) : \mathcal{B} \to \mathcal{B}$ be a bounded linear operator, and denote by $X(\theta)$ the solution of the differential equation
\begin{equation}
\partial_\theta X(\theta) = A(\theta) X(\theta)
\end{equation}
with boundary condition $X(0) = X_0 \in \mathcal{B}$. We say that the family of operators $A(\theta)$ is norm-preserving if the corresponding flow is isometric, i.e., for every $X_0 \in \mathcal{B}$, the mapping $\gamma_0 : \mathcal{B} \to \mathcal{B}$ which associates $X_0 \to X(\theta)$, i.e., $\gamma_0(X_0) = X(\theta)$, satisfies
\begin{equation}
\| \gamma_0(X_0) \| = \| X_0 \| \quad \text{for all } \theta \in \mathbb{R}.
\end{equation}

Two typical examples are the case where $\mathcal{B}$ is a Hilbert space and $A(\theta)$ is anti-hermitian and the case where $\mathcal{B}$ is a Banach space of linear operators on a Hilbert space with a spectral norm (such as a $p$-norm with $p \in [1, +\infty]$), and where $A(\theta)$ is a symmetric derivation (e.g., $i$ times the commutator with a self-adjoint operator).

**Theorem 5.15.** Let $A(\theta)$, for $\theta \in \mathbb{R}$, be a family of norm preserving operators in some Banach space $\mathcal{B}$. For any bounded measurable function $B : \mathbb{R} \to \mathcal{B}$, the solution of
\begin{equation}
\partial_\theta Y(\theta) = A(\theta) Y(\theta) + B(\theta),
\end{equation}
with boundary condition $Y(0) = Y_0$, satisfies the bound
\begin{equation}
\| Y(\theta) - \gamma_\theta(Y_0) \| \leq \int_0^\theta \| B(\theta') \| d\theta'.
\end{equation}

**Proof.** For any $\theta \in \mathbb{R}$, let $X(\theta)$ be the solution of
\begin{equation}
\partial_\theta X(\theta) = A(\theta) X(\theta)
\end{equation}
with boundary condition $X(0) = X_0$, and let $\gamma_\theta$ be the linear mapping which takes $X_0$ to $X(\theta)$. By variation of constants, the solution of the inhomogeneous equation (5.76) may be expressed as
\begin{equation}
Y(\theta) = \gamma_\theta \left( Y_0 + \int_0^\theta (\gamma_s)^{-1} (B(s)) \, ds \right).
\end{equation}
The estimate (5.77) follows from (5.79) as $A(\theta)$ is norm preserving. □

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