Localization theory for propagation of quantum information

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Abstract

In this thesis, we propose a generic framework of localization theory for the propagation of information in non-relativistic quantum mechanics. Specifically, for a large class of quantum dynamics that are known to lack strict light cones, we prove the existence of effective light cones, obtain explicit upper bounds on the maximal propagation speed of quantum information, and derive long-time decay estimates for the probability leakage away from the effective light cones. Our method, geometric in nature, is based on monotonicity estimates and adiabatic approximations using certain observables that identify the spacetime localization property of evolving states. Applications of our framework include energy-dependent effective light cones for continuous Markovian open quantum systems and Lieb-Robinson-type bounds for long-range interacting bosonic many-body quantum systems.

Resumé

I denne afhandling præsenterer vi en generisk teoretisk ramme af lokaliseringsteori for udbredelse af information i ikke-relativistisk kvantemekanik. Mere konkret, for en større klasse af kvantedynamik som er kendt for mangel på stringente lyskegler, beviser vi eksistensen af effektive lyskegler, finder eksplicitte øvre grænser på den maksimale udbredelsesfart på kvanteinformation og udleder langtids-henfaldsestimater for sandsynlighedslækagen væk fra de effektive lyskegler. Vores metode, som er geometrisk anlagt, er baseret på monotonicitetsestimater og adiabatiske approksimationer ved hjælp af visse observabler som identificerer rumtids-lokaliseringsegenskaben for udbredende tilstande. Anvendelser af vores teoretisk ramme inkluderer energiafhængige lyskegler for kontinuerte, markoviske åbne kvantesystemer, og Lieb-Robinson-type grænser for vekselvirkende bosoniske mange-legeme kvantesystemer med lang rækkevidde.

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List of publications

This thesis is based on the following papers, to which all authors have made equal contributions:

1. Sigal, I. M. and Zhang, Jingxuan. On propagation of information in quantum many-body systems. Preprint (2022). `https://arxiv.org/abs/2212.14472` (Chapter 1 and Paper B).
2. Sigal, I. M. and Zhang, Jingxuan. Propagation of information in long-range quantum systems. Preprint (2023). `https://arxiv.org/abs/2303.06506` (Chapter 1 and Paper B). This paper is a short announcement for Item 1 above.
3. Breteaux, S., Faupin, J., Lemm, M., Ouyang, D., Sigal, I. M., and Zhang, Jingxuan. Light cones for open quantum systems. Preprint (2023). `https://arxiv.org/abs/2303.08921` (Chapter 1 and Paper A).

The Author (Jingxuan Zhang) has also (co-)authored the following papers, which are not included in this thesis:

1. Zhang, Jingxuan. Adiabatic approximation for the motion of Ginzburg-Landau vortex filaments. Commun. Math. Phys. **389**, 1061–1085 (2022).
2. Zhang, Jingxuan. A generic framework of adiabatic approximation for nonlinear evolutions. Lett. Math. Phys. **112**, 31 (2022).
3. Zhang, Jingxuan. Adiabatic theory for the area-constrained Willmore flow. J. Math. Phys. **63**, 041503 (2022).
4. Zhang, Jingxuan. Asymptotic stability of generic singularities of the mean curvature flow. Preprint (2021). `https://arxiv.org/abs/2111.10111`
5. Zhang, Jingxuan. A generic framework of adiabatic approximation for nonlinear evolutions II. Preprint (2022). `https://arxiv.org/abs/2203.11053`
6. Ercolani, N. M., Sigal, I. M. and Zhang, Jingxuan. Ginzburg-Landau equations on non-compact Riemann surfaces. Preprint (2022). `https://arxiv.org/abs/2203.14179`

Contents

Chapter 1

Introduction

1.1 Context and basic problem

The question of *locality* versus *nonlocality* is a fundamental issue of physics. It underlies both classical and quantum theory of fields, which originated from attempts to dispel the nonlocal concept of action at a distance. Einstein's theory of relativity further stipulates that information propagates at a definite velocity in any reference frame. Thus, one naturally expects that in any realistic physical model, the state at each fixed spacetime depends only on information of the system within a finite spacetime region, usually known as the *causal* or *light cone*.

As a manifestation of such light-cone localization, we consider a dynamical system with information initially localized in a non-empty region

$$X \subset \mathbb{R}^d, \quad d \geq 1,$$

described by an evolving family of states supported in X at time $t = 0$. If the system has local interactions, then one expects that due to the principle of locality, information of the system should propagate with finite speed in the ambiance space $\mathbb{R}^d$. Consequently, the evolving states should be supported, at each time $t > 0$, inside the light cone

$$X_{ct} := \left\{x \in \mathbb{R}^d : \mathrm{dist}_X(x) \leq ct\right\}, \quad \mathrm{dist}_X(x) := \inf_{y\in X} |y - x|\,,$$

for some fixed and finite $c > 0$ independent of the initial state and region X.

This is indeed the case in classical and relativistic quantum physics. As for the corresponding mathematical models, the finite speed of propagation is perhaps the most salient feature of solutions to the wave equations and, in general, evolution equations arising from classical and quantum field theory. However, it is more delicate to establish a maximal speed for the propagation of information in non-relativistic quantum mechanics, because the dispersive structure of the governing evolution equations generally leads to an apparent lack of locality in the restrictive sense above.

Suppose one defines, as usual, the maximal propagation speed as the infimum of all c's such that states initially supported in $X \subset \mathbb{R}^d$ at time $t = 0$ remains supported in X_{ct} for all times $t > 0$. Then, even for the simplest example of a free particle evolving according to the Schrödinger equation $i\partial_t\psi = -\Delta\psi$, infinite speed of propagation can be observed by examining the Fourier transform of the solution and using the superlinear growth of the dispersion relation.[1] This general idea also leads to infinite speed of propagation, with the usual definition above, for typical 1-body quantum evolutions described by a large class of dispersive equations [7, 77].

[1] Following [7], we consider a sufficiently regular solution ψ_t to $i\partial_t\psi_t = -\partial_{xx}\psi_t$ on $\mathbb{R}$ with compactly supported initial state ψ. The Fourier transform of ψ_t is given by $\hat{\psi}_t(k) = \hat{\psi}(k)e^{-ik^2t}$, whose analytic extension satisfies $\hat{\psi}_t(k + ih) = \hat{\psi}(k+ih)e^{-i(k+ih)^2t}$, and so $\lim_{|k|\to\infty} \log|\hat{\psi}_t(k+ih)|\,|k|^{-1} \gtrsim |ht|$. Consequently, by the Paley–Wiener theorem, ψ_t cannot be compactly supported for $t > 0$.

In the corresponding physical models, the evolution of states is described by wave functions ψ_t, $t \geq 0$ solving the initial value problem associated to a Schrödinger equation in a suitable Hilbert space $\mathfrak{h}$. For any vector $\psi \in \mathfrak{h}$ and subset $X \subset \mathbb{R}^d$, we denote by

$$X^c := \mathbb{R}^d \setminus X$$

the complement of X, and

$$\mathrm{Prob}(\psi \in X) := \langle \psi, \mathbf{1}_X \psi \rangle_{\mathfrak{h}}$$

the probability of finding the particle in X. Suppose we have a localized initial state, ψ, with $\mathrm{Prob}(\psi \in X^c) = 0$. Then the consideration from the last paragraph shows that in general, we have $\mathrm{Prob}(\psi_t \in Y) > 0$ for any $t > 0$ and test domain $Y \subset \mathbb{R}^d$, regardless of the distance between Y and the region X of initial localization.[2]

For quantum evolutions described by time-dependent Schrödinger equations with Hamiltonians $H = -\Delta + V$, where the potential V is sufficiently regular, one approach to recover an appropriate sense of locality is to introduce an energy cutoff adapted to the spectrum of H on the initial state, and then show that the probability of finding the (microlocalized) state in the classically forbidden region vanishes asymptotically in time. Thus, localization properties of evolving states are reformulated in terms of propagation estimates for certain time-dependent observables identifying the spacetime support of states at time t, and finite speed of propagation is established in terms of the resulting propagation estimates.

More precisely, V. Enss proved in his seminal works [23, 24] that if a particle with unit mass is initially localized in a ball X at $t = 0$ and has energy below $c^2/2$, then the probability, $p(t)$, of finding the particle at time $t > 0$ in the classically forbidden region $X^c_{ct} \equiv \mathbb{R}^d \setminus X_{ct}$ vanishes as a L^1 function, i.e., $\int p(t)\,dt < \infty$. This way one obtains *effective light cones*, viz., regions outside of which the probability of finding the particle vanishes asymptotically in time. Notice that the effective light cones obtained this way are energy-dependent, in agreement with the physical intuition that a particle should move at a speed proportional to the square root of its energy.

The result of Enss was subsequently improved in [67, 70] and, more recently, [2], to Schrödinger equations with time-dependent Hamiltonians. Such propagation properties have played crucial roles in scattering theory, leading to important breakthroughs in the study of asymptotic completeness of N-body problems by Enss [25,26], Skibsted [71,72], and Sigal-Soffer [63–66], among many others. For reviews of the development in scattering theory along this line, see [43,44].

For quantum many-body systems, due to their intrinsic complexity, the localization properties are even more relevant for practical understanding. Similarly as above, scattering states in interacting particle systems cannot remain compactly supported in a nontrivial time interval, even with only local (i.e. finite-range) interactions present. To remedy this apparent lack of locality in the strictest sense, Lieb and Robinson discovered some 50 years ago a notion of *approximate locality* for quantum spin systems [49] (or *quasi-locality*, using the terminology from [58]). The celebrated Lieb-Robinson bound implies the existence of effective light cones for spin systems with finite-range interactions, by providing explicit and time-decaying upper bounds on the commutators of localized observables with disjoint spacetime supports.

Starting with Lieb-Robinson's seminal work [49] and motivated by M. B. Hastings' extension, using the Lieb-Robinson bound, of the Lieb-Schultz-Mattis theorem in condensed matter physics to higher dimensions [37], the search of *approximate locality* in non-relativistic quantum mechanics has become an increasingly active research area in mathematical physics. Attesting to the rapid development in this field, we mention that within the past 15 years, Lieb-Robinson-type bounds have been obtained for general finite-range lattice systems [62], XY chains [19, 20], long-range fermionic lattice systems [22,31,32,51,76], harmonic and anharmonic lattice systems [56,59], continuous fermionic systems [33], and the Bose-Hubbard model with unbounded finite-range interactions [28,29,48], just to name a few.

The approximate locality has proved to be a powerful tool for analyzing the evolution of states and observables in interacting particle systems. It has been demonstrated that Lieb-Robinson-type bounds

[2] One could argue that physically, a more relevant definition of localized state is by requiring ψ to decay exponentially away from X. But this could still fail for scattering solutions to Schrödinger equations with long-range (i.e., polynomially decaying) potentials, for which typical localized initial states generate solutions with only polynomially decaying probability tails [2].

impose direct constraints on state transport [27,28], error in quantum simulation algorithms [75,76], equilibration in condensed matter physics [34], existence of dynamics in the thermodynamic limit [52,53,55], and scrambling time for the dispersal of local information [15,47,60]. Further applications of the approximate locality in the study of quantum many-body systems include, among many others, the exponential clustering theorems in gapped ground states [40,54] and quantum messaging, correlation creation, scaling and area laws for the entanglement entropy, and belief propagation in quantum information theory [8,9,21,38,39]. We refer the interested readers to [46,57,58] for more detailed reviews of recent developments along this line.

In this thesis, we propose a generic framework that provides effective light cones and other approximate locality results for a large class of quantum evolutions. Our method is based on the analysis of the monotonicity properties of certain adiabatic observables that identify the spacetime localization property of evolving states. This method originated from the classical works of Sigal and Soffer's [63–67] in scattering theory, where the authors proved that for general time-dependent Schrödinger equations, evolving states admit effective light cones that spread out in space at a finite rate. The results of the seminal works [64,67] were improved in [2,41,70] and extended to non-relativistic QED in [6] and, most recently, to condensed matter physics in [28,29].

To fix ideas, let $\mathfrak{h}$ be a complex Hilbert space with inner product $\langle\cdot,\,\cdot\rangle$. We consider a quantum system described by a Hamiltonian (i.e., self-adjoint operator), H, with a dense domain $\mathcal{D}\subset\mathfrak{h}$.[3] The evolution of a state, $\psi\in\mathcal{D}$, is governed by the Schrödinger equation $i\partial_t\psi_t = H\psi_t$ with initial condition $\psi_t|_{t=0}=\psi$. The basic problem we study in this thesis is twofold:

- (Effective light cones.) Show that, *up to asymptotically vanishing probability leakage*, a compactly supported state ψ is *essentially localized* in a light cone. In symbols, we seek $c>0$ such that for all non-empty subsets $X\subset\mathbb{R}^d$ and initial states ψ with $\operatorname{supp}\psi\subset X$,
$$\lim_{t\to\infty}\operatorname{Prob}(\psi_t\in X_{ct}^{\mathrm{c}})=0,\tag{P1}$$
where, recall, $X_{ct}=\left\{x\in\mathbb{R}^d:\operatorname{dist}_X(x)\le ct\right\}$, $X_{ct}^{\mathrm{c}}=\mathbb{R}^d\setminus X_{ct}$, and $\operatorname{Prob}(\psi_t\in X_{ct}^{\mathrm{c}})=\left\langle\psi,\,\mathbf{1}_{X_{ct}^{\mathrm{c}}}\psi\right\rangle$. Then determine long-time decay estimates for the probability leakage in the l.h.s. of (P1).
- (Maximal velocity bound.) Derive explicit upper bounds on the maximal propagation speed of the effective light cone. In symbols, we seek explicit constants $\kappa>0$ such that
$$\inf\left\{c>0: c\text{ satisfies (P1)}\right\}\le\kappa.\tag{P2}$$

In the next section, we illustrate our methodology to tackle the problem above for abstract quantum dynamics.

1.2 Methodology

In a nutshell, the approach proposed in this thesis, pioneered in [2, 6, 28, 29, 41, 67, 70], is based on differential inequalities for certain propagation-identifying observables and commutator expansions. It is convenient for our purpose to consider the 'Heisenberg picture' and study, for a fixed state $\psi\in\mathcal{D}$, the evolution of a family of observables (i.e., bounded operators), $A(t)$, $t\ge 0$. To this end, we define the Heisenberg derivative
$$D_HA(t):=\frac{\partial}{\partial t}A(t)+i[H,A(t)],\tag{1.2.1}$$
and consider the evolution of observables, A, dual to the Schrödinger equation $i\partial_t\psi_t=H\psi_t$, w.r.t. the coupling $(A,\psi)\mapsto\langle\psi,\,A\psi\rangle$, given by
$$A\mapsto\alpha_t(A)\text{ with }\langle\psi,\,\alpha_t(A)\psi\rangle=\langle\psi_t,\,A\psi_t\rangle\,.\tag{1.2.2}$$
In the remainder of this section, we break our tasks (P1)–(P2) into a modular paradigm.

[3] In what follows, one could also take $H=H(t)$ to be a time-dependent Hamiltonian with a common dense domain $\mathcal{D}$ for all times, or a many-body Hamiltonian acting on a Fock space over $\mathfrak{h}$.

1.2.1 ASTLOs

Fix a test light-cone slope $c > 0$. In the Heisenberg picture, (P1) is equivalent to

$$\text{s-lim}_{t\to\infty} \mathbf{1}_X \alpha_t(\mathbf{1}_{X^c_{ct}})\mathbf{1}_X = 0, \tag{1.2.3}$$

where, recall, $\mathbf{1}_S$ denotes the characteristic function of $S \subset \mathbb{R}^d$. Our goal is to establish long-time decay estimates on the evolution $\alpha_t(A(t))$ for suitable time-dependent observables, $A(t)$, which are designed to control the l.h.s. of (1.2.3) for large t.

Let $s > 0$ be a large adiabatic parameter and ϕ a densely defined self-adjoint operator on $\mathfrak{h}$. For times $0 \le t < s$ and smooth cutoff functions χ in a suitable class $\mathcal{X} \subset C^\infty \cap L^\infty(\mathbb{R}, \mathbb{R}_{\ge 0})$ (see Figure 1.1 below), we define the *adiabatic spacetime localization observables* (following the terminology of [28, 29]), or *ASTLOs*, as

$$\mathcal{A}_s(t,\chi) := \chi\left(\frac{\phi - ct}{s}\right). \tag{ASTLO}$$

Note that $\mathcal{A}_s(\cdot)$ is an operator-valued function defined by functional calculus of the self-adjoint operator $s^{-1}(\phi - ct)$.

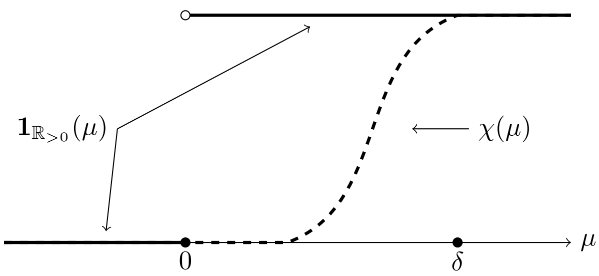

Figure 1.1: A typical function $\chi \in \mathcal{X}$ compared with the characteristic function of $\mathbb{R}_{>0}$. Here $\delta > 0$ is a parameter entering the definition of $\mathcal{X}$ through (RME) below. In essence, χ is a smoothed-out version of $\mathbf{1}_{\mathbb{R}>0}$ with derivative supported in $(0, \delta)$.

The precise definition of the class $\mathcal{X}$ is given in (3.0.2).

We say that $\mathcal{A}_s(t,\chi)$ is adiabatic since, for a test light-cone slope $c = O(1)$ and a large adiabatic parameter $s \gg 1$, the velocity

$$\partial_t \mathcal{A}_s(t,\chi) = -cs^{-1}\mathcal{A}_s(t,\chi') = O(s^{-1})$$

varies at a slow scale. To see that $\mathcal{A}_s(t,\chi)$ identifies the spacetime localization property of states, let $\phi(x) := \text{dist}_X(x) \equiv d_X$ for some $X \subset \mathbb{R}^d$. Then $\mathcal{A}_s(t,\chi) \equiv \chi\left(\frac{d_X - ct}{s}\right)$ is localized away from the light cone $X_{ct} = \{d_X(x) \le ct\}$ (see Figure 1.2).

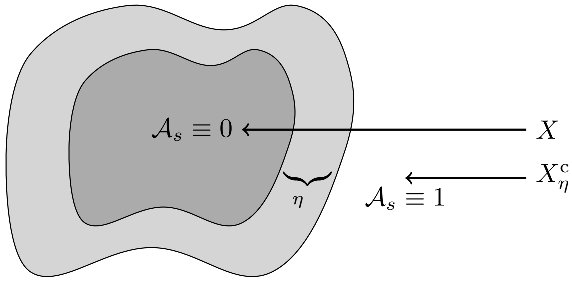

Figure 1.2: Schematic diagram demonstrating the localization property of $\mathcal{A}_s(t,\chi)$ for $\phi = d_X$. Here $\eta = \delta s + ct > ct$ where δ is as in Figure 1.1. In essence, $\mathcal{A}_s(t,\chi)$ is a smoothed-out version of the characteristic function on X^c_η.

Geometrically, from Figs. 1.1–1.2, we see that with the choice $\phi = d_X$ in (ASTLO), $\mathcal{A}_s(t,\chi)$ identifies the probability leakage outside the light cone of X in the sense that, for $\eta > ct$,

$$\mathcal{A}_s(0,\chi) \le \mathbf{1}_{X^c}, \quad \mathbf{1}_{X^c_\eta} \le \mathcal{A}_s(t,\chi). \tag{1.2.4}$$

For functions χ in appropriate classes, relations (1.2.4) are formulated with details and proved in Proposition 3.3.

In view of (1.2.3), we note that since the evolution α_t is positive-preserving, decay estimates for $\alpha_t(A_s(t,\chi))$ along t give control of $\alpha_t(\mathbf{1}_{X^c_\eta})$ through relation (1.2.4).

1.2.2 Monotonicity estimates

Our goal now is to derive decay estimates for $\alpha_t(\mathcal{A}_s(t,\chi))$. As a starting point, we assume that $\mathcal{A}_s$ satisfies the following differential identity w.r.t. some autonomous *reference Hamiltonian* H_0 on $\mathcal{D}(H_0)$: for all s, t,

$$\partial_t \alpha_t(\mathcal{A}_s(t,\chi)) = \alpha_t(D_{H_0}\mathcal{A}_s(t,\chi)), \tag{H}$$

where D_{H_0} is the Heisenberg derivative (1.2.1) with H_0 in place of H. Note that if we take H_0 to be the system Hamiltonian H, then (H) follows immediately from definitions (1.2.1)–(1.2.2), since $\partial_t(\alpha_t(A(t))) = \alpha_t(D_H(A(t)))$ on $\mathcal{D}$ for any differentiable family of bounded operators $A(t)$. But in general, we do not need to take $H_0 = H$ in (H). See discussions in Section 1.4 and concrete examples in Section 4.

Our main technical assumption is given in terms of the commutators of the reference Hamiltonian H_0 from identity (H) and the self-adjoint operator ϕ entering the definition (ASTLO). For some $n \ge 1$, we require that the multiple commutators $\mathrm{ad}^p_\phi(H_0)$, $p = 1,\dots,n+1$, extend to bounded operators on $\mathfrak{h}$[4] and satisfy, for some $\kappa_1,\dots,\kappa_{n+1} > 0$,

$$\left\|\mathrm{ad}^p_\phi(H_0)\right\| \le \kappa_p \qquad (p = 1,\dots,n+1). \tag{A}$$

In particular, condition (A) with $p = 1$ implies that identity (H) extends to all of $\mathfrak{h}$.

Let

$$\kappa \equiv \kappa_1, \tag{1.2.5}$$

so that $\kappa = \|i[H_0,\phi]\|$, the norm of the 'group velocity operator'. Then we have:

Theorem 1.1 (Recursive monotonicity estimate for $\mathcal{A}_s(t,\chi)$)**.** *Suppose the evolution α_t satisfies identity* (H)*, and condition* (A) *holds for some $n \ge 1$. Then, for any $c > \kappa$ and $\chi \in \mathcal{X}$, there exists $C > 0$, $\xi \in \mathcal{X}$ such that for $\delta := c - \kappa > 0$ and all s, t:*

$$\partial_t \alpha_t(\mathcal{A}_s(t,\chi)) \le -\delta s^{-1}\alpha_t(\mathcal{A}_s(t,\chi')) + Cs^{-2}\alpha_t(\mathcal{A}_s(t,\xi')) + Cs^{-(n+1)}. \tag{RME}$$

This theorem is proved in Section 3.1.

The differential inequality (RME) is 'recursive monotone' because the second, remainder term on the r.h.s. is of the same form as the leading, negative term. Notice that (RME) (more precisely, the proof of it) is the only place where information of the evolution α_t is used. The only property we require of the underlying evolution is the differential identity (H), which establishes a relation between the operators $\partial_t\alpha_t(\mathcal{A}_s)$ and the reference Heisenberg derivative $D_{H_0}\mathcal{A}_s = \partial_t\mathcal{A}_s + i[H_0,\mathcal{A}_s]$. Using this relation and the commutator bounds in the main technical assumption (A), we can derive an expansion formula for $i[H_0,\mathcal{A}_s]$ in terms of the bounded multiple commutators entering (A). Combining this expansion with the explicit form of $\partial_t\mathcal{A}_s$ then yields (RME).

Through (RME), we control the growth of $\mathcal{A}_s(t,\chi)$ by the following:

[4] We define $\mathrm{ad}^p_\phi(A)$ on $\mathcal{D}(A)\cap\mathcal{D}(\phi)$ (as quadratic forms) iteratively as $\mathrm{ad}^0_\phi(A) = A$ and $\mathrm{ad}^{p+1}_\phi(A) = [\mathrm{ad}^p_\phi(A),\phi]$.

Theorem 1.2 (Approximate monotonicity of $\mathcal{A}_s(t,\chi)$)**.** *Suppose* (RME) *holds for $n \geq 1$. Then, for any $c > \kappa$ and $\chi \in \mathcal{X}$, there exists $C > 0$, $\xi \in \mathcal{X}$ such that for all $s \geq 1$, $t \geq 0$:*

$$\alpha_t\left(\mathcal{A}_s(t,\chi)\right) \leq \mathcal{A}_s(0,\chi) + s^{-1}\mathcal{A}_s(0,\xi) + Cts^{-(n+1)}. \tag{ME}$$

This theorem is proved in Section 3.2.

Estimate (ME) shows that the expectation of $\mathcal{A}_s(t,\chi)$ is bounded by a time-decaying envelope for large $s \gg 1$ and all $0 \leq t < s$. To see this, we evaluate the expectation of both side of (ME) on a state $\psi \in \mathcal{D}$ and use the duality $\langle \psi,\, \alpha_t(A)\psi\rangle = \langle \psi_t,\, A\psi_t\rangle$ (see (1.2.2)). Thus we find

$$\langle \psi_t,\, \mathcal{A}_s(t,\chi)\psi_t\rangle \leq \langle \psi,\, \mathcal{A}_s(0,\chi)\psi\rangle + s^{-1}\langle \psi,\, \mathcal{A}_s(0,\xi)\psi\rangle + Cts^{-(n+1)}\left\|\psi\right\|^2, \tag{1.2.6}$$

see Figure 1.3 below.

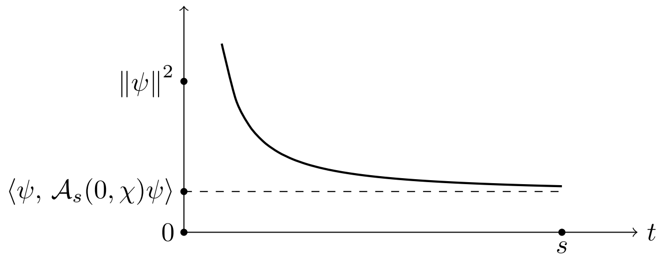

Figure 1.3: Schematic diagram illustrating the monotone envelop on the r.h.s. of (1.2.6).

Estimate (ME) is derived from bootstrapping (RME), roughly as follows. First, we integrate (RME) and drop certain non-negative terms to find

$$\delta s^{-1}\int_0^t \alpha_t\left(\mathcal{A}_s(t,\chi')\right) \leq \mathcal{A}_s(0,\chi) + Cs^{-2}\int_0^t \alpha_t\left(\mathcal{A}_s\left(t,\xi'\right)\right) + Cts^{-(n+1)}, \tag{1.2.7}$$

$$\alpha_t\left(\mathcal{A}_s(t,\chi)\right) \leq \mathcal{A}_s(0,\chi) + Cs^{-2}\int_0^t \alpha_t\left(\mathcal{A}_s\left(t,\xi'\right)\right) + Cts^{-(n+1)}. \tag{1.2.8}$$

Since the l.h.s. term in (1.2.7) is of the same form as the second term on the r.h.s., we can apply the same estimate to the latter, while introducing another cutoff function η in the same class $\mathcal{X}$ as χ and ξ.

Next, we iterate this procedure n times on (1.2.7) until no integral is present in the r.h.s. to obtain

$$\int_0^t \alpha_t\left(\mathcal{A}_s(t,\chi')\right) \leq C\left(s\mathcal{A}_s(0,\chi) + \mathcal{A}_s(0,\xi) + \cdots + s^{-(n-2)}\mathcal{A}_s(0,\eta) + ts^{-n}\right), \tag{1.2.9}$$

for n cutoff functions $\xi,\ldots,\eta \in \mathcal{X}$. Lastly, we apply (1.2.9) to bound the integral in the r.h.s. of (1.2.8). This, together with some additional algebraic properties of the ASTLOs, yields (ME). See Section 3.2 for detailed derivations.

1.2.3 Approximate locality

Suppose, for the moment, that both χ and ξ are sharp cutoff functions supported in $(0,\infty)$. Then, for $s \geq 1$ and $0 \leq t < s$, estimate (1.2.6) implies

$$\left\langle \psi_t,\, P_{\{\phi > ct\}}\psi_t\right\rangle \leq 2\left\langle \psi,\, P_{\{\phi>0\}}\psi\right\rangle + Ct^{-n}\left\|\psi\right\|^2,$$

where the operator $P_{\{\phi>a\}}$, identifying the localized part in the spectral subspace $\{\phi > a\}$, is given by

$$P_{\{\phi>a\}} := \theta(\phi - a), \quad \theta(\mu) := \mathbf{1}_{\mathbb{R}>0}(\mu). \tag{1.2.10}$$

If, moreover, the initial state ψ is supported within the spectral subspace $\{\phi \leq 0\}$, then the leading term above vanishes and we obtain an $O(t^{-n})$ estimate on the probability leakage outside the 'spectral light cone' $\{\phi \leq ct\}$. This can be made rigorous using the geometric properties of $\mathcal{A}_s(t,\chi)$ (c.f. Figure 1.1 and (1.2.4)) as follows:

Theorem 1.3 (Approximate locality of states)**.** *Suppose* (ME) *holds for* $n \geq 1$*. Then, for any* $c > \kappa$*, there exists* $C > 0$ *such that the following holds for all* $t \geq 1$*:*

$$\alpha_t\left(P_{\{\phi>ct\}}\right) \leq C\left(P_{\{\phi>0\}} + t^{-n}\right). \tag{1.2.11}$$

This theorem is proved in Section 3.3. Notice that the statement of (1.2.11) does not involve the ASTLOs.

In particular, with the choice $\phi(x) = d_X(x)$ for $X \subset \mathbb{R}^d$ in (ASTLO), we derive from estimates (1.2.11) the following effective light-cone localization:

$$\left\langle \psi_t,\, P_{\{d_X(x)>ct\}}\psi_t \right\rangle \leq Ct^{-n}\left\|\psi\right\|^2 \text{ for initial state } \psi \text{ with } \operatorname{supp}\psi \subset X. \tag{LC}$$

By definition, $P_{\{d_X(x)>ct\}} \equiv \mathbf{1}_{X_{ct}^c}$. Hence, the l.h.s. of (LC) coincides with the probability leakage outside the line cone as in (P1). This shows that (P1) holds with the test light-cone slope c, with probability leakage of the order $O(t^{-n})$. Moreover, since (LC) holds for all $c > \kappa$, we conclude that

$$\inf\left\{c > 0 : c \text{ satisfies (LC)}\right\} \leq \kappa. \tag{1.2.12}$$

This, together with (1.2.11), shows that κ from (1.2.5) is a desired maximal velocity bound as in (P2). Thus we have completed the tasks set out in (P1)–(P2).

1.3 Comments on the methodology

We are interested in the localization theory of general quantum evolutions in the sense of (P1)–(P2). We have proposed a modular paradigm that accomplishes this goal, as long as the underlying evolution satisfies (H) with a reference Hamiltonian that satisfies (A). In fact, we have achieved more: It is evident from the previous section that the same paradigm yields general localization property of evolving states w.r.t. the spectral decomposition of the self-adjoint operator ϕ entering (ASTLO) and establishes the generalized locality estimate (1.2.11) in terms of the 'spectral light cone' $\{\phi \leq ct\}$.

Our method is based on the connection between monotonicity estimates of certain time-dependent observables (the ASTLOs) and the propagation properties of states (solutions to the Schrödinger equation). In hindsight, this general philosophy is prevalent in the analysis of dissipative equations, especially in the context of geometric flows. For exmaple, it is curious to compare the role played by the (expectations of) ASTLOs to that by Huisken's F-functional [42] and Colding-Minicozzi's entropy [16] in the analysis of the mean curvature flow. In these contexts, the equations of interest all lacks strict localization theory. Nonetheless, one could recover approximate locality (or *pseudolocality* by the geometers, see e.g. [14]) theorems for the evolving states (manifolds in the geometric context), which are rather difficult to control directly, based on monotonicity estimates of appropriate quantities.

Our method is geometric in nature, as it traces back to the line of works by Enss, Hunziker, Sigal, Skibsted, Soffer and others, who have laid out the foundation of the geometric method for scattering theory of the Schrödinger operators (see [43, 44] for reviews). Indeed, the asymptotic localization theory of general quantum evolutions (1.2.1)–(1.2.2), which we consider here, bears an intrinsic similarity to the scattering theory of the standard Schödinger operators. Both problems concern with the semiclassical behaviour of particles for large time. Notice however that the parameter $s > 0$ in (ASTLO), essentially a semiclassical parameter, does not come with the model (1.2.1)–(1.2.2), but is imposed by the problem directly. In essence, as we are interested in the long-time behaviour of states, we can choose $s = O(t)$ for large t. The precise choice of s is given in (3.3.2).

1.4 Extensions

A main technical advantage of our localization theory based on the analysis of ASTLOs lies in its flexibility. Whereas strictly monotone quantities along a given evolution equation are rare to find, the approximately monotone ASTLOs are rather easy to engineer. One reason is that the underlying evolution does not enter directly into our analysis, but only through assumption (A) on a reference Hamiltonian and differential identity (H) for the evolution.

For example, consider a system Hamiltonian of the form $H = H_0 + V$, where H_0 with $\mathcal{D}(H_0) = \mathcal{D}$ satisfies (A) and $[V, \phi] = 0$ on $\mathcal{D}$ (e.g., when V and ϕ are both multiplication operators). Then the multiple commutator between ϕ and H satisfy $\mathrm{ad}^p_H(\phi) = \mathrm{ad}^p_{H_0}(\phi)$ for all p. Thus $D_H\mathcal{A}_s = D_{H_0}\mathcal{A}_s$, where D_* is the Heisenberg derivative defined in (1.2.1). Therefore the ASTLOs satisfy the differential identity (H) with the reference Hamiltonian H_0. Since the evolution only enters our analysis through (RME) and the latter depends only on (A) and (H), we conclude that (RME) and all subsequent modular theorems hold. See Section 4 for more details.

Moreover, since the system Hamiltonian does not enter directly into the main technical assumption (A), but only through its commutators with ϕ in (ASTLO), we can derive conditional localization properties when the commutator assumption (A) fails for the obvious choice of ϕ. Consider the case $H_0 = -\Delta$ acting on $\mathbb{R}^d$. Let d_X be a smoothed distance function to a smooth bounded domain X. The obvious choice $\bar{\phi} = d_X$ does not satisfies (A), since $[-\Delta, d_X] = -\Delta d_X - 2\nabla d_X \cdot \nabla$ is unbounded. However, with an energy cutoff $g = g_E(H_0)$, where $E \in \sigma(H_0)$ and g_E is a smooth cutoff function supported in $\mathbb{R}_{\le E}$, one can check that, with the microlocalized position operator $\phi = g d_X g$, the (microlocal) group velocity $i[H_0, \phi]$ (together with higher commutators) is bounded. Using this microlocalized version of ϕ in (ASTLO) and running the paradigm above, we obtain energy-dependent effective light cones for $H_0 = -\Delta$. See [10] for concrete results of this nature, with applications to Markovian open quantum systems.

Lastly, since our method is based on monotonicity estimate in the form of differential inequalities, we can reduce localization theory for quantum many-body problems to the corresponding 1-body problems. Consider an abstract second quantization map, $\mathrm{d}\Gamma$, mapping 1-body observables A acting on $\mathfrak{h}$ to many-body observables $\hat{A}$ acting on a Fock space $\mathcal{F}$ over $\mathfrak{h}$. We assume the map $\mathrm{d}\Gamma$ is positive-preserving, i.e., for any self-adjoint 1-body operators A, B,

$$A \le B \implies \hat{A} \le \hat{B}, \tag{1.4.1}$$

and, with $\hat{\alpha}_t$ denoting the many-body evolution of observables on $\mathcal{F}$,

$$\mathrm{d}\Gamma(\alpha_t(A)) = \hat{\alpha}_t(\hat{A}). \tag{1.4.2}$$

Then, applying $\mathrm{d}\Gamma$ on both sides of (ME) yields the many-body approximate monotonicity estimate

$$\hat{\alpha}_t\left(\hat{\mathcal{A}}_s(t,\chi)\right) \le \hat{\mathcal{A}}_s(0,\chi) + C(s^{-1}\hat{\mathcal{A}}_s(0,\xi) + ts^{-(n+1)}N), \tag{1.4.3}$$

where $N = \mathrm{d}\Gamma(\mathbf{1})$ is the number operator. This allows one to derive approximate locality theorems for many-body states and observables without knowing the detailed structure of the underlying Fock space $\mathcal{F}$. See [68] for related results with detailed proofs based on this technique for quantum many-body systems.

1.5 Organization of the thesis

We have given a brief overview of the machinery behind our method and illustrated its main technical advantages. The remainder of this thesis is devoted to detaild proofs and various applications of the general framework to concrete quantum dynamical systems for which strict light cones are absent.

In Chapter 2, we present some technical estimates that are needed to establish certain key expansion formulae. Using these, in Chapter 3, we prove our main results, Theorems 1.1–1.3.

In Chapter 4, we illustrate the application of our framework to certain continuous nonlocal Schrödinger equations. The model under consideration there has a favourable property that it satisfies (A) with ϕ given by the distance function. This should be viewed as a toy model since the Laplacian $H_0 = -\Delta$ does not enjoy this property, as we have discussed above.

In Paper A (Ref. [10]), we study a more realistic nonlocal continuous quantum dynamical system, in which the particle interacts with the rest of the world (i.e., open quantum system). Here suitable energy cutoff is introduced to remedy the failure of (A) with $\phi = d_X$ and $H_0 = -\Delta$.

In Paper B (Ref. [68, 69]), we give applications of our localization theory to general discrete quantum many-body dynamical systems, including those with unbounded and long-range (i.e., power-law) interactions. We give physically relevant applications of our approximate locality theory, which leads to Lieb-Robinson-type bounds for general quantum many-body systems (including long-range interacting bosons).

Chapter 2

Preliminaries

2.1 Remainder estimates

In this section and the next one, we present some estimates and commutator expansions, first derived in [67] and then improved in [44, 70] etc. Below, we adapt some of the arguments from [44] and results from [10].

Throughout this section we fix an integer $\nu \geq 0$. For integers $p \geq 0$ and smooth functions $f \in C^{\nu+2}(\mathbb{R})$, we define a weighted norm

$$\mathcal{N}(f,p) := \sum_{m=0}^{\nu+2} \int_{\mathbb{R}} \langle x\rangle^{m-p-1} \left| f^{(m)}(x) \right| dx. \tag{2.1.1}$$

Note that

$$p \leq p' \implies \mathcal{N}(f,p') \leq \mathcal{N}(f,p), \tag{2.1.2}$$

and we have the following property:

Lemma 2.1. *Let $p \geq 0$ be an integer. Suppose $f \in C^{\nu+2}(\mathbb{R})$ and there exist C_0, $\rho > 0$ such that for $m = 0, \ldots, \nu+2$,*

$$\left\| \langle x\rangle^{m-p+\rho} f^{(m)}(x) \right\|_{L^\infty} \leq C_0. \tag{2.1.3}$$

Then there exists $C > 0$ depending only on ρ, C_0, ν such that

$$\mathcal{N}(f,p) \leq C. \tag{2.1.4}$$

Proof. We have

$$\begin{aligned} \mathcal{N}(f,p) \leq & \sum_{m=0}^{\nu+2} \left\| \langle x\rangle^{m-p+\rho} f^{(m)}(x) \right\| \int_{\mathbb{R}} \langle x\rangle^{-1-\rho} dx \\ \leq & (\nu+3) C_0 \int_{\mathbb{R}} \langle x\rangle^{-1-\rho} dx, \end{aligned}$$

and the integral converges for $\rho > 0$. □

Write $z = x + iy \in \mathbb{C}$ and $\partial_{\bar{z}} = \partial_x + i\partial_y$. In what follows, as in [44, eq.(B.5)], for $f \in C^{\nu+2}(\mathbb{R})$, we take $\tilde{f}(z)$ to be an almost analytic extension of f defined by

$$\tilde{f}(z) := \eta\left(\frac{y}{\langle x\rangle}\right) \sum_{k=0}^{\nu+1} f^{(k)}(x) \frac{(iy)^k}{k!}, \tag{2.1.5}$$

where $\eta \in C_c^\infty(\mathbb{R})$ is a cutoff function with $\eta(\mu) \equiv 1$ for $|\mu| \le 1$, $\eta(\mu) \equiv 0$ for $|\mu| \ge 2$, and $|\eta'(\mu)| \le 1$ for all μ. This $\widetilde{f}(z)$ induces a measure on $\mathbb{C}$ as

$$d\widetilde{f}(z) := -\frac{1}{2\pi}\partial_{\bar{z}}\widetilde{f}(z)dx\,dy. \tag{2.1.6}$$

In the remainder of this section, we derive integral estimate for various functions against the measure (2.1.6).

The next result is obtained by adapting the argument in [44, Lem. B.1]:

Lemma 2.2 (Remainder estimate)**.** *Let $0 \le p \le \nu$. Let $f \in C^{\nu+2}(\mathbb{R})$ satisfy* (2.1.4)*. Then the extension $\widetilde{f}$ from* (2.1.5) *satisfies the following estimate for some $C = C(f,\nu,p) > 0$:*

$$\int \left|d\widetilde{f}(z)\right| |\mathrm{Im}(z)|^{-(p+1)} \le C. \tag{2.1.7}$$

Proof. Differentiating formula (2.1.5), we obtain the estimate

$$\left|\partial_{\bar{z}}\widetilde{f}(z)\right| \le \eta\left(\frac{y}{\langle x\rangle}\right)\frac{|y|^{\nu+1}}{(\nu+1)!}\left|f^{(\nu+2)}(x)\right| + \sum_{k=0}^{\nu+1}\rho\left(\frac{y}{\langle x\rangle}\right)\frac{|y|^k}{k!}\left|\frac{1}{\langle x\rangle}f^{(k)}(x)\right|, \tag{2.1.8}$$

where

$$\rho(\mu) := |\eta'(\mu)|\langle \mu\rangle \tag{2.1.9}$$

is supported on $1 < |\mu| < 2$.

For each fixed x, we define

$$G(x) := p.v.\int |\partial_{\bar{z}}f(z)|\,|y|^{-(p+1)}\,dy \tag{2.1.10}$$

by integrating (2.1.8) against $|y|^{-(p+1)}$. Using that $\eta(y/\langle x\rangle) \equiv 0$ for $|y| > \langle x\rangle$ and $\rho(y/\langle x\rangle) \equiv 0$ for $|y| \le \langle x\rangle$ or $|y| \ge 2\langle x\rangle$, we find

$$G(x) \le \int_{|y|\le\langle x\rangle}\frac{|y|^{\nu-p}}{(\nu+1)!}\eta\left(\frac{y}{\langle x\rangle}\right)dy\left|f^{(\nu+2)}(x)\right| \tag{2.1.11}$$

$$+\sum_{k=0}^{\nu+1}\int_{\langle x\rangle<|y|<2\langle x\rangle}\rho\left(\frac{y}{\langle x\rangle}\right)\frac{|y|^{k-p-1}}{k!}dy\left|\frac{1}{\langle x\rangle}f^{(k)}(x)\right|. \tag{2.1.12}$$

Since $0 \le \eta(\mu) \le 1$ and $\nu \ge p$, the integral in line (2.1.11) converges and can be bounded as

$$\int_{|y|\le\langle x\rangle}\frac{|y|^{\nu-p}}{(p+1)!}\eta\left(\frac{y}{\langle x\rangle}\right)dy\left|f^{(p+2)}(x)\right| \le \frac{2\langle x\rangle^{\nu-p+1}}{(p+1)!}\left|f^{(p+2)}(x)\right|. \tag{2.1.13}$$

To bound line (2.1.12), we use that $\rho(y/\langle x\rangle) < \sqrt{5}$ and $|y|^{k-p-1} \le \langle x\rangle^{k-p-1}$ for $\langle x\rangle < |y| < 2\langle x\rangle$, $0 \le k \le p+1$ (see (2.1.9)). Thus each integral in line (2.1.12) can be bounded as

$$\sum_{k=0}^{\nu+1}\int_{\langle x\rangle<|y|<2\langle x\rangle}\rho\left(\frac{y}{\langle x\rangle}\right)\frac{|y|^{k-p-1}}{k!}dy\left|\frac{1}{\langle x\rangle}f^{(k)}(x)\right|$$

$$\le\sum_{k=0}^{p+1}\frac{4\sqrt{5}\langle x\rangle^{k-p-1}}{k!}\left|f^{(k)}(x)\right| + \sum_{k=p+1}^{\nu+1}\frac{\sqrt{5}\cdot 2^{k-p+1}\langle x\rangle^{k-p-1}}{k!}\left|f^{(k)}(x)\right|. \tag{2.1.14}$$

Combining (2.1.13)–(2.1.14) in (2.1.12), we conclude that

$$|G(x)| \le CF(x), \quad F(x) := \sum_{m=0}^{\nu+2}\langle x\rangle^{m-p-1}\left|f^{(m)}(x)\right|. \tag{2.1.15}$$

Let $G_\lambda(x) := \mathbf{1}_{[-\lambda,\lambda]}G(x)$ with $\lambda > 0$. Then $G_\lambda \in L^1$ and $|G_\lambda(x)| \le CF(x)$ for any λ. By assumption (2.1.4) and definition(2.1.1), we have $\|F\|_{L^1} = \mathcal{N}(f,p) < \infty$ and so $F \in L^1$. Therefore, sending $\lambda \to \infty$ and using the dominated convergence theorem yields $G \in L^1$ with

$$\|G\|_{L^1} \le C\,\|F\|_{L^1}\,. \tag{2.1.16}$$

Recalling definition (2.1.10), we find $(2\pi)^{-1}\|G\|_{L^1}$ =l.h.s. of (2.1.7). Thus we conclude (2.1.7) from (2.1.16). □

2.2 Commutator expansions

In this section, we take $\widetilde{f}(z)$, $d\widetilde{f}(z)$ to be as in (2.1.5)–(2.1.6).

We frequently use the following result, taken from [44, Lems. B.2]:

Lemma 2.3. *Let $f \in C^{\nu+2}(\mathbb{R})$ satisfy (2.1.4) for some $p \ge 0$. Then for any self-adjoint operator A on $\mathfrak{h}$,*

$$\frac{1}{p!}f^{(p)}(A) = \int_{\mathbb{C}} d\widetilde{f}(z)(z-A)^{-(p+1)}, \tag{2.2.1}$$

where the integral converges absolutely in operator norm and is uniformly bounded in A.

Remark 1. Condition (2.1.4) ensures that $f^{(p)}$ is bounded independent of A and the remainder estimate in Lemma 2.2 ensures the norm convergence of the r.h.s. of (2.2.1).

We call equation (2.2.1) the *Helffer-Sjöstrand (HS) representation.* The HS representation (2.2.1), together with the remainder estimate (2.1.7), implies the following commutator expansion:

Lemma 2.4. *Let $n \ge 1$. Let $f \in C^{n+3}(\mathbb{R})$ satisfy (2.1.4) with $p = 1$. Let A be an operator on $\mathfrak{h}$. Let ϕ be a densely defined self-adjoint operator on $\mathfrak{h}$. Let $f_s := f(s^{-1}(\phi-\alpha))$ for some fixed α and all $s > 0$.*

Suppose

$$B_k := \mathrm{ad}_\phi^k(A) \in \mathcal{B}(\mathfrak{h}) \quad (1 \le k \le n+1). \tag{2.2.2}$$

Then $[A, f_s] \in \mathcal{B}(\mathfrak{h})$, and we have the expansion

$$[A,f_s] = \sum_{k=1}^{n}(-1)^k\frac{s^{-k}}{k!}B_k f_s^{(k)} + (-1)^{n+1}s^{-(n+1)}\mathrm{Rem}_{\mathrm{left}}(s) \tag{2.2.3}$$

$$= \sum_{k=1}^{n}\frac{s^{-k}}{k!}f_s^{(k)}B_k + s^{-(n+1)}\mathrm{Rem}_{\mathrm{right}}(s), \tag{2.2.4}$$

where the remainders are defined by these relations and given explicitly by (2.2.12)–(2.2.13).

Moreover, there exists $c > 0$ depending only on n and $\mathcal{N}(f, n+1)$, such that

$$\|\mathrm{Rem}_{\mathrm{left}}(s)\|_{\mathrm{op}} + \|\mathrm{Rem}_{\mathrm{right}}(s)\|_{\mathrm{op}} \le c\,\|B_{n+1}\|\,, \tag{2.2.5}$$

Remark 2. Note that f needs not to be bounded. By (2.1.3), it suffices for f to have strictly sublinear growth.

Proof of Lemma 2.4. Within this proof we write $R = (z - x_s)^{-1}$ with $x_s = s^{-1}(\phi - \alpha)$.

Since R is bounded, it follows that

$$\big[A, R\big] = s^{-1}R\,\mathrm{ad}_\phi(A)R \tag{2.2.6}$$

holds in the sense of quadratic forms on $\mathcal{D}(A)$. Since $\mathrm{ad}_\phi(A)$ is bounded by assumption, the r.h.s. of (2.2.6) is bounded and so $[A, R]$ extends to an bounded operator on $\mathfrak{h}$. Using (2.2.6), we proceed by commuting successively the commutators $B_k := \mathrm{ad}_\phi^k(A)$ to left and right, respectively.Iteratively, we obtain

$$\begin{aligned}
&[A,R]\\
=&\sum_{k=1}^{n}(-1)^k s^{-k}B_kR^{k+1}+(-1)^{n+1}s^{-(n+1)}RB_{n+1}R^{n+1} \qquad (2.2.7)\\
=&\sum_{k=1}^{n}s^{-k}R^{k+1}B_k+s^{-(n+1)}R^{n+1}B_{n+1}R, \qquad (2.2.8)
\end{aligned}$$

which hold on all of $\mathfrak{h}$ since B_k's are bounded operators by assumption (2.2.2).

Let $\eta^\lambda \in C_c^\infty(\mathbb{R})$, $\lambda > 0$ be cutoff functions with $\eta^\lambda(x) \equiv 1$ for $|x| \le \lambda$, $\eta(x) \equiv 0$ for $|\mu| \ge \lambda + 1$, and $\left\|\eta^\lambda\right\|_{C^{n+3}} \le C$ for all λ. Set $f^\lambda := \eta^\lambda f$. Since $f^\lambda \in C_c^{n+3}$, it satisfies (2.1.4) for all $p \ge 0$. (Note that f itself, a priori, does not satisfy (2.1.4) with $p = 0$.) Thus the HS representation 2.2.1 holds with $p = 0$ and so

$$[A, f_s^\lambda] = \int d\widetilde{f^\lambda}(z)\big[A,R\big], \qquad (2.2.9)$$

which holds a priori on $\mathcal{D}(A)$. Plugging expansions (2.2.7)–(2.2.8) into (2.2.9) yields

$$\begin{aligned}
&[A,f_s^\lambda]\\
=&\sum_{k=1}^{n}(-1)^k\frac{s^{-k}}{k!}B_k\int d\widetilde{f^\lambda}(z)R^{k+1}+(-1)^{n+1}s^{-(n+1)}\mathrm{Rem}_{\text{left}}^\lambda(s), \qquad (2.2.10)\\
=&\sum_{k=1}^{n}\frac{s^{-k}}{k!}\int d\widetilde{f^\lambda}(z)R^{k+1}B_k+s^{-(n+1)}\mathrm{Rem}_{\text{right}}^\lambda(s), \qquad (2.2.11)
\end{aligned}$$

where

$$\mathrm{Rem}_{\text{left}}^\lambda(s)=\int d\widetilde{f^\lambda}(z)RB_{n+1}R^{(n+1)}, \qquad (2.2.12)$$

$$\mathrm{Rem}_{\text{right}}^\lambda(s)=\int d\widetilde{f^\lambda}(z)R^{(n+1)}B_{n+1}R. \qquad (2.2.13)$$

Since the operator B_{n+1} is bounded independent of λ, z, and $\|R\| \le |\mathrm{Im}(z)|^{-1}$, we have

$$\begin{aligned}
&\left\|\mathrm{Rem}_{\text{left}}^\lambda(s)\right\|_{\text{op}}+\left\|\mathrm{Rem}_{\text{right}}^\lambda(s)\right\|_{\text{op}}\\
\le&2\|B_{n+1}\|\int|d\widetilde{f^\lambda}(z)|R^{n+2}\\
\le&2\|B_{n+1}\|\int|d\widetilde{f^\lambda}(z)||\mathrm{Im}(z)|^{-(n+2)}. \qquad (2.2.14)
\end{aligned}$$

Similarly we could bound the sums in (2.2.10)–(2.2.11). Thus we see $[A, f_s^\lambda]$ extends to a bounded operator on $\mathfrak{h}$ for each λ.

By (2.1.2) and the assumption $\mathcal{N}(f, 1) \le C$, f satisfies condition (2.1.4) with $p = 1, \dots, n+1$. Hence, sending $\lambda \to \infty$ in (2.2.10)–(2.2.13) and using (2.2.1) for $p = 1, \dots, n$ and remainder estimate (2.1.7) for $p = n + 1$, we conclude that $[A, f_s] \in \mathcal{B}(\mathfrak{h})$ and expansions (2.2.4) and estimate (2.2.5) hold. □

Chapter 3

Proofs of Theorems 1.1–1.3

To begin with, we make precise the definition of (ASTLO).

Fix a real number $c > \kappa$ with κ from (1.2.5), together with a densely defined self-adjoint operator ϕ. For each $s > 0$, we define a class of observables by functional calculus:

$$\begin{array}{rccl} \mathcal{A}_s & : & \mathbb{R}_{\geq 0} \times L^\infty(\mathbb{R}) & \longrightarrow & \mathcal{B}(\mathfrak{h}) \\ & & (t, \chi) & \longmapsto & \chi\left(\frac{\phi - ct}{s}\right) \end{array} . \tag{3.0.1}$$

For a parameter $0 < \delta < 1$, we define a class $\mathcal{X} \equiv \mathcal{X}_\delta$ as follows:

$$\mathcal{X} := \left\{ \chi \in C^\infty(\mathbb{R}, \mathbb{R}_{\geq 0}) \left| \begin{array}{l} \operatorname{supp} \chi \subset (0, \infty),\ \chi' \geq 0, \\ \sqrt{\chi'} \in C_c^\infty,\ \operatorname{supp} \chi' \subset (0, \delta) \end{array} \right. \right\}. \tag{3.0.2}$$

Then, for all s, t, the operator $\mathcal{A}_s(t, \chi)$, $\chi \in \mathcal{X}$ is bounded and non-negative definite, with $\|\mathcal{A}_s(t, \chi)\| \leq \|\chi\|_{L^\infty}$. Typical examples of functions in $\mathcal{X}$ are suitably smoothed characteristic functions of $\mathbb{R}_{\geq 0}$. Here we note two properties of the space $\mathcal{X}$, which can be readily verified:

(X1) If $\xi(x) = \int_0^x w^2(y)\, dy$ for some $w \in C_c^\infty$ with $\operatorname{supp} w \subset (0, \delta)$, then $\xi \in \mathcal{X}$.

(X2) For any ξ_1, $\xi_2 \in \mathcal{X}$ and $c \geq 0$, there exists $\xi \in \mathcal{X}$ with $\xi \geq \xi_1 + c\xi_2$.

3.1 Proof of Theorem 1.1

Let $\vec{\kappa} := (\kappa_1, \ldots, \kappa_{n+1})$ as in (A). The main result of this section is the following differential operator inequality:

Theorem 3.1. *Suppose the assumption of Theorem 1.1 holds. Then, for all $c > \kappa$, $\chi \in \mathcal{X}$ and Lipschitz ϕ, there exists a constant $C = C(n, \vec{\kappa}, \operatorname{Lip}(\phi), \chi) > 0$ and $\xi_k = \xi_k(\chi) \in \mathcal{X}$, $k = 2, \ldots, n$ (dropped if $n = 1$) such that for all $t \geq 0$, $s > 0$,*

$$\begin{aligned} &\partial_t \alpha_t \left(\mathcal{A}_s(t, \chi)\right) \\ &\leq -\delta s^{-1} \alpha_t \left(\mathcal{A}_s(t, \chi')\right) + \sum_{k=2}^{n} s^{-k} \alpha_t \left(\mathcal{A}_s\left(t, \xi_k'\right)\right) + C s^{-(n+1)}, \end{aligned} \tag{3.1.1}$$

where α_t is the Heisenberg evolution given by (1.2.2) *and $\delta := c - \kappa$.*

This theorem is proved at the end of this section. Estimate (3.1.1), together with property (X2) and the relation $\mathcal{A}_s(t, \chi_1) + \mathcal{A}_s(t, \chi_2) = \mathcal{A}_s(t, \chi_1 + \chi_2)$, implies Theorem 1.1. In the remainder of this section, we write $H \equiv H_0$ in (H) and

$$DA(t) = \frac{\partial}{\partial t} A(t) + i[H, A(t)], \tag{3.1.2}$$

so that (H) becomes

$$\partial_t \alpha_t(A(t)) = \alpha_t(DA(t)). \tag{3.1.3}$$

Remark 3. Identity (3.1.3) plays a crucial role in our analysis, and it is precisely in (3.1.3) that the Hamiltonian structure of (4.1.1) is used. Indeed, for a heat-type equation $\partial_t u = -Hu$ with self-adjoint H, we have, instead of (3.1.3),

$$\partial_t \alpha_t(A(t)) = \partial_t A(t) - \{H, A\},$$

where the brace denotes the anti-commutator. The change $[\cdot,\cdot] \to \{\cdot,\cdot\}$ renders key expansion formulae below unavailable.

We first prove the following lemma:

Lemma 3.2. *Suppose the assumption of Theorem 1.1 holds. Then there exist* $\xi_k = \xi_k(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) \in \mathcal{X}$, $k = 2, \dots, n$ *(dropped if* $n = 1$*), together with a constant* $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$*, such that as bounded self-adjoint operators on* $\mathfrak{h}$*,*

$$\begin{aligned} &i[H, \mathcal{A}_s(t,\chi)] \\ \le& s^{-1}\kappa \mathcal{A}_s(t,\chi') + \sum_{k=2}^{n} s^{-k} \mathcal{A}_s(t, \xi_k') + Cs^{-(n+1)} \quad (t \ge 0, s > 0). \end{aligned} \tag{3.1.4}$$

(The sum in the r.h.s. is dropped if $n = 1$*.)*

Proof. Within this proof, we fix t and write $\mathcal{A}_s(\chi) \equiv \mathcal{A}_s(t,\chi)$. Also, we set $B_k \equiv \pm i\, \mathrm{ad}_\phi^k(H)$ for $k = 1, ..., n+1$. (The sign is irrelevant for our argument.)

1. By condition (A), there exists $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi)) > 0$, such that

$$\|B_k\| \le C, \quad k = 1, \dots, n+1. \tag{3.1.5}$$

This, together with the definition of $\mathcal{X}$ (see (3.0.2)), implies that the hypotheses of Lemma 2.4 are satisfied for $\chi \in \mathcal{X}$. We apply this lemma to $\mathcal{A}_s(\chi)$ by adding commutator expansion (2.2.4) to its adjoint and dividing the result by two. This way we obtain

$$i[H, \mathcal{A}_s(\chi)] = \mathrm{I} + \mathrm{II} + \mathrm{III}, \tag{3.1.6}$$

$$\mathrm{I} = \frac{1}{2} s^{-1} \left(\mathcal{A}_s(\chi') B_k + B_k^* \mathcal{A}_s(\chi') \right), \tag{3.1.7}$$

$$\mathrm{II} = \frac{1}{2} \sum_{k=2}^{n} \frac{s^{-k}}{k!} \left(\mathcal{A}_s(\chi^{(k)}) B_k + B_k^* \mathcal{A}_s(\chi^{(k)}) \right), \tag{3.1.8}$$

$$\mathrm{III} = \frac{1}{2} s^{-(n+1)} \left(R_{n+1} + R_{n+1}^* \right), \tag{3.1.9}$$

where the term II is dropped for $n = 1$ and, by (3.1.5) and the remainder estimate (2.2.5),

$$\|R_{n+1}\| \le C, \tag{3.1.10}$$

for some $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$.

2. We first bound the term I in line (3.1.7). Let $u := \sqrt{\chi'}$, which is well defined and lies in $C_c^\infty(\mathbb{R})$ by (3.0.2). Thus, by (3.1.5), expansion (2.2.4) holds for u. This expansion, together with the fact that

$\mathrm{ad}_\phi^l(B_k) = B_{k+l}$, implies

$$
\begin{aligned}
&\mathcal{A}_s(\chi')B_k + B_k^*\mathcal{A}_s(\chi')\\
&= \mathcal{A}_s(u)^2 B_1 + B_1\mathcal{A}_s(u)^2\\
&= 2\mathcal{A}_s(u)B_1\mathcal{A}_s(u) + \mathcal{A}_s(u)[\mathcal{A}_s(u), B_1] + [B_1, \mathcal{A}_s(u)]\mathcal{A}_s(u)\\
&= 2\mathcal{A}_s(u)B_1\mathcal{A}_s(u)\\
&\quad + \sum_{l=1}^{n-1} \frac{s^{-l}}{l!}\left(\mathcal{A}_s(u)B_{1+l}\mathcal{A}_s(u^{(l)}) + \mathcal{A}_s(u^{(l)})B_{1+l}^*\mathcal{A}_s(u)\right) && (3.1.11)\\
&\quad + s^{-n}(\mathcal{A}_s(u)\mathrm{Rem}_1 + \mathrm{Rem}_1^*\mathcal{A}_s(u)), && (3.1.12)
\end{aligned}
$$

where line (3.1.11) is dropped for $n = 1$ and, by the remainder estimate (2.2.5),

$$\|\mathrm{Rem}_1\| \le C, \tag{3.1.13}$$

for some $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$.

We will bound the terms in (3.1.11)–(3.1.12) using the operator estimate

$$\pm(P^*Q + Q^*P) \le P^*P + Q^*Q. \tag{3.1.14}$$

For the terms in line (3.1.11), we use (3.1.14) with

$$P = \mathcal{A}_s(u), \quad Q := B_{1+l}\mathcal{A}_s(u^{(l)}), \quad l = 1, \dots, n-1, \tag{3.1.15}$$

yielding

$$
\begin{aligned}
&s^{-l}(\mathcal{A}_s(u)B_{1+l}\mathcal{A}_s(u^{(l)}) + \mathcal{A}_s(u^{(l)})B_{1+l}^*\mathcal{A}_s(u))\\
\le& s^{-l}\left(\mathcal{A}_s(u)^2 + \|B_{1+l}\|^2(\mathcal{A}_s(u^{(l)}))^2\right). && (3.1.16)
\end{aligned}
$$

For the remainder terms in (3.1.12), we apply (3.1.14) with

$$P = \mathcal{A}_s(u), \quad Q = \mathrm{Rem}_1, \tag{3.1.17}$$

to obtain

$$s^{-n}(\mathcal{A}_s(u)\mathrm{Rem}_1 + \mathrm{Rem}_1^*\mathcal{A}_s(u)) \le s^{-n}\left(\mathcal{A}_s(u)^2 + \|\mathrm{Rem}_1\|^2\right). \tag{3.1.18}$$

Combining (3.1.16) and (3.1.18) in (3.1.7) yields

$$
\begin{aligned}
\mathrm{I} \le& s^{-1}\mathcal{A}_s(u)B_1\mathcal{A}_s(u) && (3.1.19)\\
&+ \frac{1}{2}\sum_{l=1}^{n-1}\frac{s^{-(l+1)}}{l!}\left(\mathcal{A}_s(u)^2 + \|B_{1+l}\|^2(\mathcal{A}_s(u^{(l)}))^2\right) + \frac{1}{2}s^{-(n+1)}\|\mathrm{Rem}_1\|^2.
\end{aligned}
$$

This bound the term I (3.1.7).

3. For $n \ge 2$, the term II in line (3.1.8) is bounded similarly as in Step 2. For $k = 2, ..., n$, we take $\theta^k \in C_c^\infty(\mathbb{R})$ with

$$\mathrm{supp}\,\theta^k \subset (0, \delta), \quad \theta^k \equiv 1 \text{ on } \mathrm{supp}\,\chi^{(k)}. \tag{3.1.20}$$

We claim that for some bounded operator $\mathrm{Rem}_k = O(1)$,

$$
\begin{aligned}
&s^{-k}\left(\mathcal{A}_s(\chi^{(k)})B_k + B_k^*\mathcal{A}_s(\chi^{(k)})\right)\\
=& s^{-k}\left(\mathcal{A}_s(\chi^{(k)})B_k\mathcal{A}_s(\theta^k) + \mathcal{A}_s(\theta^k)B_k^*\mathcal{A}_s(\chi^{(k)})\right) + s^{-(n+1)}\mathrm{Rem}_k. && (3.1.21)
\end{aligned}
$$

For this, it suffices to show that

$$\mathcal{A}_s(\chi^{(k)})B_k = \mathcal{A}_s(\chi^{(k)})B_k\mathcal{A}_s(\theta^k) + s^{-(n+1-k)}\mathrm{Rem}_k. \tag{3.1.22}$$

Using relation (3.1.20), commutator expansion (2.2.4), and the fact that $\mathrm{ad}_\phi^l(B_k) = B_{k+l}$, we have

$$\begin{aligned}
&\mathcal{A}_s(\chi^{(k)})B_k \\
&= \mathcal{A}_s(\chi^{(k)})\mathcal{A}_s(\theta^k)B_k \\
&= \mathcal{A}_s(\chi^{(k)})B_k\mathcal{A}_s(\theta^k) + \mathcal{A}_s(\chi^{(k)})[\mathcal{A}_s(\theta^k), B_k] \\
&= \mathcal{A}_s(\chi^{(k)})B_k\mathcal{A}_s(\theta^k) \\
&\quad + \sum_{l=1}^{n-k} \frac{s^{-l}}{l!}\mathcal{A}_s(\chi^{(k)})\mathcal{A}_s((\theta^k)^{(l)})B_{k+l} + s^{-(n+1-k)}\mathcal{A}_s(\chi^{(k)})\mathrm{Rem}_k,
\end{aligned} \tag{3.1.23}$$

where the l-sum is dropped for $k = n$ and

$$\mathrm{Rem}_k \le C, \quad k = 2, \dots, n, \tag{3.1.24}$$

for some $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$.

Since $\theta^k \equiv 1$ on $\mathrm{supp}(\chi^{(k)})$, we have $\mathrm{supp}((\theta^k)^{(l)}) \cap \mathrm{supp}(\chi^{(k)}) = \emptyset$ for all $l \ge 1$ and so in line (3.1.23),

$$\mathcal{A}_s(\chi^{(k)})\mathcal{A}_s((\theta^k)^{(l)})B_{k+l} = 0, \quad l = 1, \dots n-k.$$

Estimate (3.1.22) follows from here. Thus we conclude claim (3.1.21).

Now, we apply estimate (3.1.14) on the first term on the r.h.s. of (3.1.21) with

$$P = \mathcal{A}_s(\chi^{(k)}), \quad Q = B_k\mathcal{A}_s(\theta^k), \tag{3.1.25}$$

and then sum over k to obtain

$$\mathrm{II} \le \frac{1}{2}\sum_{k=1}^{n-1} \frac{s^{-k}}{k!}\left((\mathcal{A}_s(\chi^{(k)}))^2 + \|B_k\|^2(\mathcal{A}_s(\theta^k))^2\right) + \frac{1}{2}s^{-(n+1)}\|\mathrm{Rem}_k\|^2. \tag{3.1.26}$$

This bounds the term II in line (3.1.8).

4. Plugging (3.1.19), (3.1.26) back to (3.1.6) and using bounds (3.1.5), (3.1.10), (3.1.13), and (3.1.24), we find that for some $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$,

$$\begin{aligned}
&i[H, \mathcal{A}_s(\chi)] \le s^{-1}\mathcal{A}_s(u)B_1\mathcal{A}_s(u) \\
&+ C\sum_{k=2}^{n} s^{-k}\left(\mathcal{A}_s(u)^2 + (\mathcal{A}_s(u^{(k-1)}))^2 + \mathcal{A}_s(\chi^{(k)}))^2 + (\mathcal{A}_s(\theta^k))^2\right) + Cs^{-(n+1)}.
\end{aligned} \tag{3.1.27}$$

Now, for $k = 2, \dots, n$, we choose, with C, u, θ^k from (3.1.27),

$$\begin{aligned}
w_k &\in C_c^\infty, \quad \mathrm{supp}\, w_k \subset (0, \delta), \\
w_k^2 &\ge C\left(u^2 + (u^{(k-1)})^2 + (\chi^{(k)})^2 + (\theta^k)^2\right),
\end{aligned} \tag{3.1.28}$$

which is possible since the r.h.s. of (3.1.28) is supported in $(0, \delta)$ by construction. Then the function

$$\xi_k(x) := \int_0^x w_k^2(y)\, dy \tag{3.1.29}$$

lies in $\mathcal{X}$ by identity (X1). Thus, by (3.1.27), the desired estimate (3.1.4) holds with the choice of ξ_k from (3.1.29). This completes the proof of Lemma 3.2. □

Proof of Theorem 3.1. To prove estimate (3.1.1), we first apply the differential identity (3.1.3) with $A(t) = \mathcal{A}_s(t, \chi)$ for each s, χ. This yields

$$\partial_t\alpha_t(\mathcal{A}_s(t, \chi)) = \alpha_t(\partial_t\mathcal{A}_s(t, \chi)) + \alpha_t(i[H, \mathcal{A}_s(t, \chi)]). \tag{3.1.30}$$

By definition (3.0.1), we find

$$\partial_t \mathcal{A}_s(t,\chi) = -s^{-1}c\,\mathcal{A}_s(t,\chi'). \tag{3.1.31}$$

By estimate (3.1.4), we find

$$i[H, \mathcal{A}_s(t,\chi)] \le s^{-1}\kappa \mathcal{A}_s(t,\chi') + \sum_{k=2}^{n} s^{-k}\mathcal{A}_s(t,\xi_k') + Cs^{-(n+1)}, \tag{3.1.32}$$

where $C = C(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) > 0$, and the second term in the r.h.s. is dropped for $n = 1$. Plugging (3.1.31) and (3.1.32) back to (3.1.30) and using the positive-preserving property of evolution α_t yields (3.1.1). □

3.2 Proof of Theorem 1.2

Within this proof, all constants $C > 0$ depend only on n, χ, $\mathrm{Lip}(\phi)$, $\vec{\kappa}$, and $\delta = c - \kappa$. For simplicity, we write

$$\bar{A}_s(t,\chi) := \alpha_t(\mathcal{A}_s(t,\chi)). \tag{3.2.1}$$

Note that $\bar{A}_s(0,\chi) \equiv A_s(0,\chi)$.

To begin with, we claim the following holds: There exist $\tilde{\xi}_k \in \mathcal{X}$, $2 \le k \le n$ (dropped for $n = 1$), depending only on $n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi$, such that for all $t \ge 0\,, s > 0$,

$$\int_0^t \bar{A}_s(r,\chi')dr \le C\left(s\mathcal{A}_s(0,\chi) + \sum_{k=2}^{n} s^{-k+2}\mathcal{A}_s(0,\tilde{\xi}_k) + ts^{-n}\right), \tag{3.2.2}$$

where the sum is dropped if $n = 1$.

To prove (3.2.2), we bootstrap the recursive monotonicity estimate (3.1.1). For each fixed s, integrating formula (3.1.3) with $A(t) \equiv \mathcal{A}_s(t,\chi)$ in t gives

$$\bar{\mathcal{A}}_s(t,\chi) - \int_0^t \partial_r \bar{\mathcal{A}}_s(r,\chi)\,dr = \mathcal{A}_s(0,\chi). \tag{3.2.3}$$

We apply inequality (3.1.1) to the second term on the l.h.s. of (3.2.3) to obtain, after transposing the leading term,

$$\begin{aligned}&\bar{\mathcal{A}}_s(t,\chi) + s^{-1}\delta \int_0^t \bar{\mathcal{A}}_s(r,\chi')\,dr \\ \le&\mathcal{A}_s(0,\chi) + \sum_{k=2}^{n} s^{-k}\int_0^t \bar{\mathcal{A}}_s(r,\xi_k')\,dr + Cts^{-(n+1)},\end{aligned} \tag{3.2.4}$$

where $\delta = c - \kappa$, $\xi_k = \xi_k(n, \vec{\kappa}, \mathrm{Lip}(\phi), \chi) \in \mathcal{X}$, and the second term in the r.h.s. is dropped for $n = 1$.

Since $s\,,\delta > 0$, estimate (3.2.4) implies, after dropping $\bar{\mathcal{A}}_s(t,\chi)$ on the l.h.s., which is non-negative-definite due to the positive-preserving property of evolution (4.2.2), and multiplying both sides by $s\delta^{-1} > 0$, that

$$\int_0^t \bar{\mathcal{A}}_s(r,\chi')\,dr \le \frac{1}{\delta}\left(s\mathcal{A}_s(0,\chi) + \sum_{k=2}^{n} s^{-k+1}\int_0^t \bar{\mathcal{A}}_s(r,\xi_k')\,dr + Cts^{-n}\right), \tag{3.2.5}$$

where the second term in the r.h.s. is dropped for $n = 1$.

If $n = 1$, then (3.2.5) gives (3.2.2). If $n \ge 2$, we proceed to apply (3.2.5) to the term $\int_0^t \bar{\mathcal{A}}_s(r,\xi_2')\,dr$ up to $(n-1)$-th order to get

$$\int_0^t \bar{\mathcal{A}}_s(r,\xi_2')\,dr \le \frac{1}{\delta}\left(s\mathcal{A}_s(0,\xi_2) + \sum_{k=2}^{n-1} s^{-k+1}\int_0^t \bar{\mathcal{A}}_s(r,\eta_k')\,dr + Cts^{-(n-1)}\right), \tag{3.2.6}$$

where $C = C(n, \vec{\kappa}, c, \mathrm{Lip}(\phi), \xi_2) > 0$ and

$$\eta_k = \eta_k(\xi^2) = \eta_k(\chi) \in \mathcal{X}, \quad k = 2, \dots, n-1.$$

Plugging (3.2.6) back to (3.2.5), we find

$$\begin{aligned}&\int_0^t \bar{\mathcal{A}}_s(r, \chi')\, dr \\ \leq &\frac{1}{\delta}\left(s\mathcal{A}_s(0,\chi) + \frac{1}{\delta}\mathcal{A}_s(0,\xi_2) + \sum_{k=3}^n s^{-k+1}\int_0^t \bar{\mathcal{A}}_s(r, \rho_k')\, dr + \left(1+\frac{1}{\delta}\right) Cts^{-n}\right),\end{aligned} \tag{3.2.7}$$

where the third term in the r.h.s. is dropped for $n = 2$ and the functions $\rho_k \in \mathcal{X}$, $\rho_k \geq \xi_k + \frac{1}{\delta}\eta_k$ for $k = 3, \dots, n$ (see (X2)). Bootstrapping this procedure, we arrive at (3.2.2).

Now we use (3.2.2) to derive the desire estimate (ME).

Dropping the second term in the l.h.s. of (3.2.4), which is non-negative since $\delta > 0$ and $\bar{\mathcal{A}}_s(r, \chi') \geq 0$ for all r, we obtain

$$\bar{\mathcal{A}}_s(t,\chi) \leq \mathcal{A}_s(0,\chi) + \sum_{k=2}^n s^{-k}\int_0^t \bar{\mathcal{A}}_s(r, \xi_k')\, dr + Cts^{-(n+1)}, \tag{3.2.8}$$

where the second term is dropped for $n = 1$ (in which case we are done). If $n \geq 2$, then for each $k = 2, \dots, n$, we apply estimate (3.2.2) to the k-th summand in the second term in the r.h.s. of (3.2.8), with remainder expanded to $(n-k+1)$-th order. This way we obtain

$$\bar{\mathcal{A}}_s(t,\chi) \leq \mathcal{A}_s(0,\chi) + C\left(\sum_{k=2}^n\sum_{l=2}^{n-k} s^{-(k-1)}\mathcal{A}_s(0,\tilde{\xi}_k) + s^{-(l+k-2)}\mathcal{A}_s(0,\tilde{\xi}_{k,l})\right) + Cts^{-(n+1)}. \tag{3.2.9}$$

where the k-sum is dropped for $n = 1$, the l-sum is dropped if $n-k \leq 1$, and C, $\tilde{\xi}_{k,l}$ are chosen according to (3.2.2).

Since $s \geq 1$, using property (X2), we can choose $\xi \in \mathcal{X}$ such that for C, $\tilde{\xi}_k$, $\tilde{\xi}_{k,l}$ as in (3.2.9),

$$\xi \geq C\left(\sum_{k=2}^n\sum_{l=2}^{n-k} s^{-(k-2)}\mathcal{A}_s(0,\tilde{\xi}_k) + s^{-(l+k-3)}\mathcal{A}_s(0,\tilde{\xi}_{k,l})\right). \tag{3.2.10}$$

With this choice of ξ, we conclude the desired estimate, (ME), from (3.2.9). This completes the proof of Theorem 1.2. □

3.3 Proof of Theorem 1.3

Recall that ϕ is a densely defined self-adjoint operator on $\mathfrak{h}$ and $P_{\{\phi>a\}}$ denotes the spectral cutoff operator defined in (1.2.10). We first prove the following proposition:

Proposition 3.3. *Let δ, $c' > 0$. For functions $f(t) > c't$ and $\eta \in C^1(\mathbb{R}, \mathbb{R}_{\geq 0}) \cap L^\infty(\mathbb{R})$ with*

$$\eta \not\equiv 0, \quad \operatorname{supp}\eta \subset (0,\infty), \quad \operatorname{supp}\eta' \subset (0,\delta), \tag{3.3.1}$$

let

$$s := \delta^{-1}(f(t) - c't), \quad \mathcal{A}(t,\eta) := \eta(s^{-1}(\phi - c't)). \tag{3.3.2}$$

Then the following estimates hold (c.f. (1.2.4)):

$$\|\eta\|_{L^\infty}^{-1}\mathcal{A}(0,\eta) \leq P_{\{\phi>0\}}, \tag{3.3.3}$$

$$P_{\{\phi>f(t)\}} \leq \|\eta\|_{L^\infty}^{-1}\mathcal{A}(t,\eta). \tag{3.3.4}$$

Proof. First, by (3.3.1), we have $\operatorname{supp}\eta\left(\frac{\cdot}{s}\right) \subset (0,\infty)$ for $s > 0$. This implies

$$\|\eta\|_{L^\infty}^{-1}\,\mathcal{A}(0,\eta) \equiv \|\eta\|_{L^\infty}^{-1}\,\eta\,(\phi/s) \leq \theta(\phi) \equiv P_{\{\phi>0\}}, \tag{3.3.5}$$

where $\theta : \mathbb{R} \to \mathbb{R}$ is the characteristic function of $\mathbb{R}_{>0}$ (see Figure 3.1). Thus (3.3.3) follows.

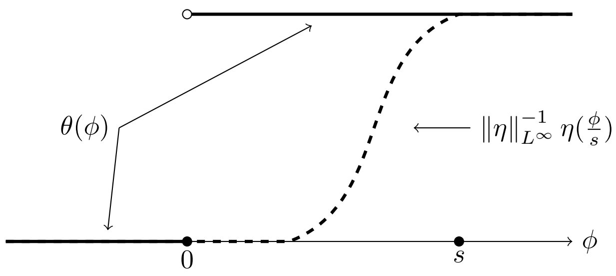

Figure 3.1: Schematic diagram illustrating (3.3.5)

Next, again by (3.3.1), we have $\|\eta\|_{L^\infty}^{-1}\,\eta(\mu) \equiv 1$ for $\mu > \delta$ and so, by definition (3.3.2),

$$\|\eta\|_{L^\infty}^{-1}\,\mathcal{A}(t,\eta) \equiv \|\eta\|_{L^\infty}^{-1}\,\eta\left(\delta\frac{\phi - c't}{f(t) - c't}\right) \equiv \mathbf{1}, \tag{3.3.6}$$

on the subspace $\operatorname{Ran} P_{\{\phi>f(t)\}}$. Since $P_{\{\phi>f(t)\}} \equiv \theta(\phi - f(t))$, estimate (3.3.6) implies

$$\|\eta\|_{L^\infty}^{-1}\,\mathcal{A}(t,\eta) \geq \theta(\phi - f(t)), \tag{3.3.7}$$

see Figure 3.2. Thus (3.3.4) follows.

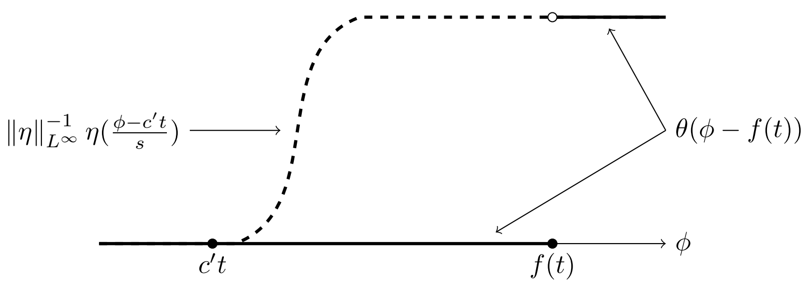

Figure 3.2: Schematic diagram illustrating (3.3.7).

This completes the proof of Proposition 3.3. □

We now use Proposition 3.3 and Theorem 1.2 to prove Theorem 1.3.

First, for $c > \kappa$ as in the statement of Theorem 1.3, we set

$$\delta := \frac{1}{3}(c - \kappa) > 0, \quad c' := \kappa + \delta. \tag{3.3.8}$$

Fix $\chi \in \mathcal{X}_\delta$ (see (3.0.2)). We apply Theorem 1.2 with $c' > \kappa$ to get a constant $C > 0$ and a function $\xi \in \mathcal{X}$ such that

$$\alpha_t\left(\mathcal{A}_s(t,\chi)\right) \leq \mathcal{A}_s(0,\chi) + s^{-1}\mathcal{A}_s(0,\xi) + Cts^{-(n+1)}. \tag{3.3.9}$$

Next, we apply Proposition 3.3 with

$$f(t) := ct > c't, \quad s := \delta^{-1}(c - c')t > t, \tag{3.3.10}$$

where the inequalities are ensured by the choice (3.3.8). The function χ clearly satisfies condition (3.3.1). If the function $\xi \not\equiv 0$ in (3.3.9), then ξ also satisfy (3.3.1). (If $\xi \equiv 0$ then we drop the second term in the r.h.s. of (3.3.9)). Hence, applying (3.3.3)–(3.3.4) with $\eta = \chi, \xi$ and $\mathcal{A} \equiv \mathcal{A}_s$ as in (3.3.2), we conclude the desired estimate, (1.2.11), from estimate (3.3.9).

This completes the proof of Theorem 1.3. $\square$

Chapter 4

Applications to nonlocal Hamiltonians

In this chapter, we illustrate the general localization theory laid out in Chapter 1 by analyzing a model of nonlocal quantum evolutions.

4.1 Setup

We consider the following nonlocal non-autonomous Schrödinger equation:

$$i\partial_t u = H(t)u. \tag{4.1.1}$$

Here $u = u(\cdot, t)$, $t \in \mathbb{R}$ is a path of functions in the Hilbert space $\mathfrak{h} := L^2(\mathbb{R}^d, \mathbb{C})$, $d \geq 1$. The Hamiltonian $H(t) = H_0 + V(t)$ consists of a nonlocal part

$$H_0[u](x) = \int_{y \in \mathbb{R}^d} (u(x) - u(y))K(x, y), \tag{4.1.2}$$

for some symmetric integral kernel K with $K(y, x) = \overline{K(x, y)}$, together with a time-dependent potential $V(t)$. As a standing assumption, we assume that H_0 is self-adjoint on a dense domain $\mathcal{D} \equiv \mathcal{D}(H_0) \subset \mathfrak{h}$ and $V(t)$ is bounded for all t. This way $H(t)$ is self-adjoint on $\mathcal{D}$ and, by elementary perturbation theory, admits bounded propagator $U(t, s)$ with $t, s \in \mathbb{R}$.

Our main technical assumption for (4.1.2) is the following: For some integer $n \geq 1$, the first to $(n + 1)$-th moments of K are all finite. Precisely, we assume

$$\sup_{1 \leq p \leq n+1} \sup_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} |K(x, y)| \, |x - y|^p \leq \kappa < \infty \tag{4.1.3}$$

for some $\kappa > 0$.

Condition (4.1.3) stipulates the long-range interaction in H_0 decays as power-law. Such condition arises naturally and is widely used in the study of interacting quantum dynamical systems, see e.g. [28, 29, 74, 76]. We note that condition (4.1.3) unfortunately excludes the fractional Laplacians, which are of the form (4.1.4) with $J(x) = |x|^{-(d+2s)}$, $0 < s < 1$, due to insufficient decay at infinity.

An important class of operators satisfying (4.1.2) are the nonlocal diffusion operators

$$H_0 = 1 - J*, \tag{4.1.4}$$

where J is a non-negative radial function with profile satisfying

$$\sup_{1 \leq p \leq n+1} \int_0^\infty r^{p+d-1} J(r) \, dr < \infty. \tag{4.1.5}$$

Typical examples are $J(x) = (1 + |x|^2)^{-a/2}$ with $a > d + n + 1$. By interpolation, we can also handle mild singularity at 0 such as $J(x) = O(|x|^{-b})$ with $b < d + 1$.

Evolution equations involving nonlocal operators of the form (4.1.2), subject to similar conditions as (4.1.5), have received much research attention in recent years. In particular, using the mean value property, one can view the usual Laplacian as an infinitesimal version of (4.1.4) with

$$J_\epsilon(x) = \frac{1}{\epsilon^2 |B_\epsilon(0)|} \chi(B_\epsilon(0))(x)$$

and $\epsilon \to 0+$ [61].

For recent results concerning evolution equations involving (4.1.4) subject to similar conditions as (4.1.5), see e.g. [12, 13, 17, 18, 45, 73] and, for applications to natural sciences, [1, 11], as well as the references therein. For regularity theory of nonlocal evolution equations, see [30, 35, 36] For an excellent recent review on nonlocal diffusion operators with integrable kernels, see [61]. Note however that all of the cited works above are concerned with, instead of Hamiltonian evolution equation as in (4.1.1), gradient flows of the form $\partial_t u = -Hu$ with H of the form (4.1.2). This distinction should be made clear since the Hamiltonian structure of (4.1.1) is used crucially in proving the recursive monotonicity estimate (RME) for $\mathcal{A}_s(t, \chi)$ (wherefore in all other results from Section 1.2 as well), see Remark 3.

Equation (4.1.1) arises from the study of nonlinear nonlocal Schrödinger (NLS) equations of the form

$$i\partial_t u = H_0 u + Wu + f(|u|^2)u, \quad f \in C(\mathbb{R}_{\geq 0}, \mathbb{R}), \tag{4.1.6}$$

where W is a bounded external potential (possibly time-dependent). Eq. (4.1.6) has a Hamiltonian structure inherited from the nonlocal generalization of the Ginzburg-Landau free-energy functional in the presence of external potential:

$$E(u) = \frac{1}{4} \iint K(x, y) |u(x) - u(y)|^2 + \int W |u|^2 + F(|u|^2), \quad F' = f.$$

Indeed, if $v_t \in L^\infty \cap L^2$ solves (4.1.6), then v_t satisfies (4.1.1) with $V(t) := W + f(|v_t|)$ bounded for each t. This convolution-type model for phase transitions was proposed in [5] and the associated L^2-gradient flow (the nonlocal Allen-Cahn equation) has been studied in [3–5, 13, 45]. See [4, Sect. 1] for a discussion on the connection between $E(u)$ above and the classical Ginzburg-Landau energy functional.

Lastly, we mention that results concerning the asymptotic localization of states are recently announced in [50] for general nonlinear non-autonomous Schrödinger equations similar to (4.1.6), but with the standard Schrödinger operators, i.e. $-\Delta$ in place of H_0. See also [10] for similar propagation estimates for open quantum systems involving the standard Schrödinger operators.

4.2 Results

In this section, we take the ambient Hilbert space to be $\mathfrak{h} := L^2(\mathbb{R}^d)$, $d \geq 1$. Denote by $\mathcal{D} \equiv \mathcal{D}(H_0)$ the (dense) domain of $H(t)$ in (4.1.1). For a Lipschitz function ϕ, denote by $\mathrm{Lip}(\phi)$ the infimum of all L such that $|\phi(x) - \phi(y)| \leq L|x - y|$ for all $x, y \in \mathbb{R}^d$. For a measurable set $S \subset \mathbb{R}^d$, denote by $\mathbf{1}_S$ the characteristic function of S. Without specification, $\|\cdot\|$ denotes either the L^2-norm $\|\cdot\|_{\mathfrak{h}}$ or the operator norm $\|\cdot\|_{\mathfrak{h}\to\mathfrak{h}}$. We make no distinction in notations between a function and the associated multiplication operator acting on $\mathfrak{h}$. Our results below are valid for the von Neumann equation $\partial_t \rho = i[H, \rho]$ with ρ_t, $t \geq 0$ given by a path of density operators under the same assumption (4.1.3).

By the standing assumption, the evolution of a state $u \in \mathcal{D}$ according to (4.1.1) is given by

$$u_t = U(t, 0)u, \tag{4.2.1}$$

where $U(t, s)$, $s, t \in \mathbb{R}$ is the propagator for $H(t) = H_0 + V(t)$ in (4.1.1). For self-adjoint H_0 and bounded $V(t)$, the propagator $U(t, s)$ is bounded on $\mathfrak{h}$ by elementary perturbation theory. The evolution of an observable A, dual to the evolution of states $u \mapsto U(t,0)u$ w.r.t. the coupling $(A,u) \mapsto \langle u, Au\rangle$, is given by

$$\alpha_t(A) := Y(t,0)AU(t,0), \tag{4.2.2}$$

where $Y(t,s) = U(t,s)^*$ is the backward propagator.

Recall the definition

$$\mathcal{X} := \left\{ \chi \in C^\infty(\mathbb{R}, \mathbb{R}_{\ge 0}) \,\middle|\, \begin{array}{l} \operatorname{supp}\chi \subset (0,\infty),\ \chi' \ge 0, \\ \sqrt{\chi'} \in C_c^\infty,\ \operatorname{supp}\chi' \subset (0,\delta) \end{array} \right\}. \tag{4.2.3}$$

For $X \subset \mathbb{R}^d$ and $d_X(x) := \inf_{y\in X}|x-y|$, denote by $\mathbf{1}_X$ the characteristic function of X, the set $X_a^{\mathrm{c}} \equiv \left\{x \in \mathbb{R}^d : d_X(x) > a\right\}$ for $a \ge 0$, and $X^{\mathrm{c}} \equiv X_0^{\mathrm{c}}$. We define, according to (3.0.1), the multiplication operators

$$\mathcal{A}_s(t,\chi) := \chi(s^{-1}(d_X - ct)). \tag{4.2.4}$$

Observables $\mathcal{A}_s(t,\chi)$ play the role of ASTLOs, as described in Section 1.2. Indeed, if we view each $\chi \in \mathcal{X}$ as a cutoff function supported in $(0,\infty)$, then $\mathcal{A}_s(t,\chi)$ roughly amounts to a cutoff function supported on the set X_{ct}^{c}. Controlling the evolution of $\mathcal{A}_s(t)$, therefore, amounts to controlling the probability inside the evolving exterior regions X_{ct}^{c}.

Let $\varphi \in \mathcal{D}$, $\varphi_t = U(t,0)\varphi$. Our main result is the following:

Theorem 4.1 (Propagation estimates for (4.1.1))**.** *Suppose* (4.1.3) *holds for $n \ge 1$. Then, for every $c > \kappa$ with κ from* (4.1.3)*, there exists $C = C(n,c,\kappa) > 0$ such that for all subset $X \subset \mathbb{R}^d$, function $f(t) > ct$, and $t \ge 1$,*

$$\left\| \mathbf{1}_{X^{\mathrm{c}}_{f(t)}} \varphi_t \right\|^2 \le (1 + C(f(t)-ct)^{-1}) \left\| \mathbf{1}_{X^{\mathrm{c}}}\varphi \right\|^2 + Ct(f(t)-ct)^{-(n+1)} \left\|\varphi\right\|^2. \tag{4.2.5}$$

Theorem 4.1 is proved in Section 3.3.

Remark 4. Estimate (4.2.5) is a consequence of Thms. 1.1–1.2 and Proposition 3.3 with the choice $\phi = d_X$. To see that (4.2.5) implies the localization of evolving states according to (4.1.1), fix $\epsilon > 0$ and define $f(t) = (c+\epsilon)t$. Assuming the initial condition φ is localized in X in the sense that $\|\mathbf{1}_{X^{\mathrm{c}}}\varphi\| \le \epsilon$, we conclude from (4.2.5) that $\left\|\mathbf{1}_{X^{\mathrm{c}}_{ct}}\varphi_t\right\|^2_{L^2} \lesssim \epsilon + t^{-1} + \epsilon^{-(n+1)}t^{-n}$ for all t.

Proof of Theorem 4.1. Fix $X \subset \mathbb{R}^d$, $t \ge 1$, and $\chi \in \mathcal{X}$ with $\chi(\mu) \equiv 1$ for $\mu \ge 1$. Below, all estimates are independent of these parameters.

First, let $\phi := d_X \equiv \inf\{|x-y| : y \in X\}$ in (ASTLO) (see (3.0.1)). We verify the assumptions of Theorem 1.1. Since $H = H_0 + V$ in (4.1.1) with $[V,\phi] = 0$, the evolution condition (H) is satisfied with H_0 given by (4.1.2). By Corollary 4.4, the Hamiltonian H_0 from (4.1.2) and $\phi = d_X$ verify the commutator condition (A), with κ_p's independent of X. We have shown that the assumptions of Theorem 1.1 hold. Thus, by Theorem 1.1–Theorem 1.2, estimate (ME) holds.

Next, define $s = s(t) := f(t) - ct > 0$ and write $\mathcal{A}(t,\chi) \equiv \mathcal{A}_s(t,\chi)$ with this choice of s for the observables from (3.0.1). Then, by estimate (ME), there exists a constant $C > 0$ and a function $\xi \in \mathcal{X}$ such that

$$\begin{aligned} \langle \varphi_t,\, \mathcal{A}(t,\chi)\varphi_t\rangle \le \langle \varphi,\, \mathcal{A}(0,\chi)\varphi\rangle + (f(t)-ct)^{-1}\langle\varphi,\, \mathcal{A}_s(0,\xi)\varphi\rangle \\ + Ct(f(t)-ct)^{-(n+1)}\left\|\varphi\right\|^2. \end{aligned} \tag{4.2.6}$$

Lastly, we use Proposition 3.3. The function χ clearly satisfies condition (3.3.1). If the function $\xi \not\equiv 0$ in (4.2.6), then ξ also satisfy (3.3.1). (If $\xi \equiv 0$ then we drop the second term in the r.h.s. of (4.2.6)). Hence, applying (3.3.3)–(3.3.4) with $\eta = \chi, \xi$ in (4.2.6), we conclude the desired estimate, (4.2.5), from estimate (4.2.6). □

As a consequence of the localization estimate (4.2.5), we have the following a priori estimate on the propagation speed of traveling wave solutions to the nonlinear nonlocal Schrödinger equation (4.1.6):

Corollary 4.2. *Suppose* (4.1.3) *holds for* $n \geq 1$. *Suppose* $\phi_t \in L^2 \cap L^\infty$, $t \geq 0$ *solves the NLS equation* (4.1.6) *and* $\phi_t = U(\cdot - \beta t)$ *for some fixed velocity* $\beta \in \mathbb{R}^d$ *and profile* U *with the following property: There exists a bounded subset* $X \subset \mathbb{R}^d$ *such that* $\|\mathbf{1}_{X^c} U\|^2 < \|U\|^2/2$. *Then* $|\beta| \leq \kappa$.

Proof. Since ϕ_t solves (4.1.1) by freezing coefficients, ϕ_t satisfies (4.2.5) and therefore we have that

$$\left\|\mathbf{1}_{X^c_{ct}} U(x - \beta t)\right\|^2 \leq \|U\|^2/2 + Ct^{-n}, \tag{4.2.7}$$

for all $c > \kappa$. Suppose now $|\beta| > \kappa$. Then, on the one hand, we can choose $c \in (\kappa, |\beta|)$ such that (4.2.7) holds. On the other hand, since $c < |\beta|$, there is a large $T \gg 1$ depending only on $|\beta| - c$ and $\operatorname{diam}(X)$ such that

$$\left\|\mathbf{1}_{X^c_{ct}} U(\cdot - \beta t)\right\|^2 \geq \|\mathbf{1}_X U\|^2 > \|U\|^2/2 \tag{4.2.8}$$

for all $t \geq T$ (see Figure 4.1). This is a contradiction to (4.2.7).

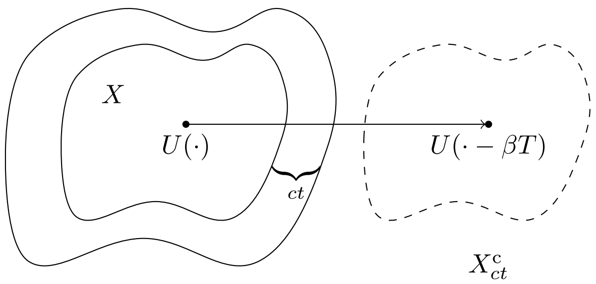

Figure 4.1: Schematic diagram illustrating relation (4.2.8).

□

4.3 Multiple commutator estimates

In this section, we prove that condition (4.1.3) implies uniform estimates on mutiple commutators $\mathrm{ad}^k_\phi(H)$ for eeach $1 \leq k \leq n+1$ with (multiplication operator by) Lipschitz ϕ. In particular, (2.2.4) holds with H_0 from (4.1.2) and $\phi = d_X$.

Lemma 4.3. *Let* $n \geq 1$. *Suppose* A *is an operator acting on* $L^2(\mathbb{R}^d)$ *as*

$$A[u](x) = \int_{\mathbb{R}^d} (V(x)u(x) - u(y))K(x,y)\,dy \tag{4.3.1}$$

for $V \in L^\infty(\mathbb{R}^d)$ *and integral kernel* $K(x,y)$ *satisfying*

$$M := \sup_{1 \leq p \leq n+1} \left(\sup_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} |K(x,y)|\,|x-y|^p \right) \times \left(\sup_{y \in \mathbb{R}^d} \int_{x \in \mathbb{R}^d} |K(x,y)|\,|x-y|^p \right) < \infty. \tag{4.3.2}$$

Then for every Lipschtiz function f *on* $\mathbb{R}^d$ *such that for some* $L > 0$,

$$|f(x) - f(x)| \leq L\,|x-y| \quad (x, y \in \mathbb{R}^d), \tag{4.3.3}$$

there holds

$$\left\|\mathrm{ad}^k_f(A)\right\| \leq L^k M \quad (1 \leq k \leq n+1). \tag{4.3.4}$$

Proof. We first prove that for each fixed $f : \mathbb{R}^d \to \mathbb{C}$ and all $1 \le k \le n+1$, we have

$$\mathrm{ad}_f^k(A)[u] = -\int (f(y) - f(x))^k K(x,y) u(y)\, dy. \tag{4.3.5}$$

We prove this by a simple induction. Clearly, the V term in (4.3.1) does not contribute to the commutators $\mathrm{ad}_f^k(A)$, since $[V, f] \equiv 0$. Hence below we take $V \equiv 0$ in (4.3.1).

For the base case $k = 1$, we compute, for fixed f and every u,

$$A[fu](x) = -\int K(x,y) f(y) u(y)\, dy,$$
$$f(x)A[u](x) = -\int f(x) K(x,y) u(y)\, dy.$$

Taking the difference yields (4.3.5) with $k = 1$. Now assume (4.3.5) holds for k. Then we have

$$\mathrm{ad}_f^k(A)[fu](x) = -\int (f(y) - f(x))^k K(x,y) f(y) u(y)\, dy,$$
$$f(x)\,\mathrm{ad}_f^k(A)[u] = -\int f(x)(f(y) - f(x))^k K(x,y) u(y)\, dy.$$

Since $\mathrm{ad}_f^{k+1}(A) = [\mathrm{ad}_f^k(A), f]$, taking the difference of the last two expressions yields (4.3.5) for $k+1$. This completes the induction.

Formula (4.3.5), together with the Schur test for integral operators, implies

$$\begin{aligned} \left\| \mathrm{ad}_f^k(A) \right\|^2 \le & \left(\sup_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} |K(x,y)| \, |f(x) - f(y)|^k \right) \\ & \times \left(\sup_{y \in \mathbb{R}^d} \int_{x \in \mathbb{R}^d} |K(x,y)| \, |f(x) - f(y)|^k \right). \end{aligned} \tag{4.3.6}$$

Now we compute, using assumptions (4.3.2) and (4.3.3), that

$$\begin{aligned} & \sup_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} |K(x,y)| \, |f(x) - f(y)|^k \\ \le & L^k \sup_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} |K(x,y)| \, |x - y|^k \le L^k M. \end{aligned}$$

This bounds the first term in the r.h.s. of (4.3.6). Similarly we can derive the same bound for the second term in the r.h.s. of (4.3.6). Plugging the results back to (4.3.6) yields estimate (4.3.4). □

Corollary 4.4. *Suppose H in (4.1.1) satisfies (4.1.3). Then for every $X \subset \mathbb{R}^d$, the distance function $d_X(x) \equiv \mathrm{dist}(\{x\}, X)$ we have*

$$\left\| \mathrm{ad}_{d_X}^k(H) \right\| \le \kappa \quad (1 \le k \le n+1).$$

Proof. All d_X satisfies (4.3.3) with $L = 1$. □

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Paper A

Light cones for open quantum systems

LIGHT CONES FOR OPEN QUANTUM SYSTEMS

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Abstract. We consider Markovian open quantum dynamics (MOQD). We show that, up to small-probability tails, the supports of quantum states evolving under such dynamics propagate with finite speed in any finite-energy subspace.

More precisely, we prove that if the initial quantum state is localized in space, then any finite-energy part of the solution of the von Neumann-Lindblad equation is approximately localized inside an energy-dependent light cone. We also obtain an explicit upper bound for the slope of this light cone.

Contents

1. Introduction

While non-relativistic quantum theory does not possess the strict light cone of relativistic theories, it has been shown in many contexts that its dynamics nonetheless exhibits a maximal speed bound up to small-probability leakage. By analogy, one speaks of a (system-dependent) *light cone* also in these cases. Existence of such light cones has been rigorously derived in standard QM [4, 21, 36, 39], for

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non-relativistic QED models [5], and for nonlinear Schrödinger equations [3]. Famously, Lieb and Robinson [27] first derived the existence of light cones in quantum spin systems. Their eponymous Lieb-Robinson bounds have developed into an extremely active research area starting in the early 2000s [18, 19, 20, 28, 29] and continues to grow in scope, e.g., with recent extensions to lattice fermions [17, 30], lattice bosons [13, 14, 26, 35, 38, 42, 43] and long-range interactions [15, 17, 41]. The existence of a maximal speed bound in a quantum theory is a fundamental statement about its non-equilibrium properties which serves as the backbone of many proofs. For instance, it played an essential role in scattering theory [10, 37] and, in quantum information theory Lieb-Robinson bounds were used to prove the celebrated area law for entanglement entropy [18] and bounds on quantum state transfer [11]. They are also central to the notion of quantum phase defined via quasi-adiabatic continuation [20, 31].

In this paper, we consider quantum particles governed by the Schrödinger operator $H = -\Delta + V$ that interact with an environment. We show that the corresponding Markovian open quantum dynamics (MOQD) exhibit an energy-dependent light cone, i.e., initially localized states propagate at most with a maximal speed. Previous results about maximal speed bounds of MOQD either concerned lattice systems (where the mechanism for maximal speed is different [32, 34]) or it excluded the most interesting case when the Hamiltonian H is a standard Schrödinger operator [7]. In this paper, we resolve this question and show that coupling quantum-mechanical particles to an environment cannot lead to acceleration of any finite-energy portion. For this purpose, we develop microlocalization techniques involving functions of noncommuting operators H and x_j. To fix ideas, we work on $L^2(\mathbb{R}^d)$ but we expect that our approach could be extended to abstract Hilbert space with abstract noncommuting self-adjoint operators H and x_j.

1.1. **Setup and main result.** We study the long-time behaviour of solutions to the von Neumann-Lindblad (vNL) equation:

$$\frac{\partial \rho_t}{\partial t} = -i[H, \rho_t] + \frac{1}{2}\sum_{j\geq 1}\big([W_j, \rho_t W_j^*] + [W_j\rho_t, W_j^*]\big). \tag{1.1}$$

Here ρ_t, $t \geq 0$ is a family of density operators (i.e. non-negative-definite operators with unit trace) on a Hilbert space $\mathcal{H}$, H is the quantum Hamiltonian, a self-adjoint operator on $\mathcal{H}$, and the $\{W_j\}$ are bounded operators, arising from interaction with the environment.

We show that, for any E, there exists $\kappa = \kappa(E) > 0$ such that, for any initial condition ρ_0 localized in $X \subset \mathbb{R}^d$ and for any $c > \kappa$, the probability that the system in the state ρ_t is localized in $\mathcal{H}_E \cap X_{ct}^{\mathrm{c}}$ is arbitrarily small, asymptotically as $t \to \infty$, where $\mathcal{H}_E$ is the spectral subspace

$$\mathcal{H}_E := \{H \leq E\} \equiv \mathrm{Ran}(\mathbf{1}_{(-\infty,E]}(H))$$

and $X_{ct}^{\mathrm{c}} = \mathbb{R}^d \setminus X_{ct}$ with

$$X_{ct} \equiv \big\{x \in \mathbb{R}^d : d_X(x) \leq ct\big\} \tag{1.2}$$

the light cone corresponding to a smoothed out distance function $d_X(\cdot)$ defined in (1.11) below. Put differently, there exists an energy-dependent light cone for (1.1) with slope κ.

Throughout this article, we let $\mathcal{H} = L^2(\mathbb{R}^d)$, $d \geq 1$. We make no distinction in our notation between functions and the operators of multiplication defined by those functions. For an operator A on $\mathcal{H}$, denote by $\mathcal{D}(A) \subset \mathcal{H}$ the domain of A.

We now set out the main assumptions in this paper. We take the Hamiltonian H in (1.1) to be the standard Schrödinger operator,

$$H = -\Delta + V(x), \quad V : \mathbb{R}^d \to \mathbb{R}. \tag{1.3}$$

Then, for some fixed integer $n \geq 1$, we assume

(H) There exist $\rho > 0$ and $C > 0$ such that

$$|\partial^\alpha V(x)| \leq C \langle x \rangle^{-|\alpha|-\rho} \quad (x \in \mathbb{R}^d,\ 0 \leq |\alpha| \leq n). \tag{1.4}$$

Here and below, we write $\langle \cdot \rangle = \sqrt{1 + |\cdot|^2}$.

Remark 1. If V satisfies **(H)**, then it is bounded and therefore H is self-adjoint on $\mathcal{D}(-\Delta)$ (see e.g. [8]) and bounded from below.

For the operators W_j, $j \geq 1$ in (1.1), we assume, for the same integer $n \geq 1$ as in **(H)**:

- **(W1)** For all integers $j \geq 1$, $W_j \in \mathcal{B}(\mathcal{H})$ and the series $\sum_{j=1}^\infty W_j^* W_j$ converges strongly in $\mathcal{B}(\mathcal{H})$ (and consequently, $\sum_{j=1}^\infty W_j^* W_j \in \mathcal{B}(\mathcal{H})$);
- **(W2)** Let $C_A = \mathrm{ad}_A : B \to [A, B]$ and $p_q = -i\partial_{x_q}$. Then, for every $1 \leq q \leq d$,

$$\sum_{j=1}^\infty \sum_{\substack{\sum(k_i+\ell_i)=n+1 \\ k_i,\, \ell_i \geq 0}} \| \prod_i \left[(\langle x \rangle C_{p_q})^{k_i} C_{x_q}^{\ell_i} W_j \right] \|^2 < \infty. \tag{1.5}$$

Remark 2. Assumptions **(W1)** and **(W2)** can be ensured for example by taking the W_j's to be suitable pseudodifferential operators. See also [7, Section 1.4] and [12, Section 4]

Remark 3. Let $\mathcal{S}_1$ stand for the Schatten space of trace-class operators. Conditions **(H)** and **(W1)** guarantee global well-posedness for (1.1) in the space

$$\mathcal{D} := \{\rho \in \mathcal{S}_1 \mid \rho\mathcal{D}(H) \subset \mathcal{D}(H) \text{ and } [H, \rho] \in \mathcal{S}_1\}, \tag{1.6}$$

see below.

For each subset $X \subset \mathbb{R}^d$, let $X^c := \mathbb{R}^d \setminus X$ and $\chi_X^\sharp$ stand for the characteristic function of X. The main result of this paper is the following:

Theorem 1.1 (Main result)**.** *Suppose Assumptions **(H)** and **(W1)**–**(W2)** hold. Let $X \subset \mathbb{R}^d$ be a bounded and closed subset. Suppose $\rho_0 \in \mathcal{D}$ (see (1.6)) is supported in X in the sense that*

$$\mathrm{Tr}(\chi_{X^c}^\sharp \rho_0) = 0. \tag{1.7}$$

Then (1.1) has a unique solution $\rho_t \in \mathcal{D}$, $t \geq 0$, and for any $E \in \sigma(H)$ and $c > \kappa$ with κ as in (1.17), this solution satisfies

$$\mathrm{Tr}(g(H)\chi_{X_{ct}^c}^\sharp g(H)\rho_t) \leq C_{n,E} t^{-n}, \tag{1.8}$$

for all $t > 0$ and all smooth cutoff functions g with $\mathrm{supp}(g) \subset (-\infty, E]$ and $0 \leq g \leq 1$, where $X_{ct}^c \equiv (X_{ct})^c$ and $C_{n,E}$ is a positive constant depending on n and E.

Remark 4. For the energy-dependent speed κ defined in (1.17), we have the following estimate:

$$\kappa \le C(1+|E|)^{1/2} \text{ for some fixed } C>0 \text{ and all } X \subset \mathbb{R}^d, E \in \mathbb{R}. \tag{1.9}$$

Moreover, the constant $C_{n,E}$ in (1.8) grows polynomially with E.

Theorem 1.1 solves an open problem from [7], namely, to derive a light cone for MOQD when the Hamiltonians is a standard Schrödinger operator $-\Delta + V$ (a situation not covered by the methods in [7]).

Theorem 1.1 is proved in Section 3. Theorem 1.1 implies that "microlocally" the propagation speed for (1.1) is finite, and yields an upper bound for the maximal speed of propagation of initially localized states. Indeed, define the probability

$$\mathrm{Prob}_{\rho_t,E}(Y) := \mathrm{Tr}(g_E(H)\chi_Y^\sharp g_E(H)\rho_t) \tag{1.10}$$

for the system in the state ρ_t to be in the part of the state (phase) space where $x \in Y$ and $H \le E$. With notation (1.10) and, recall, $X_{ct}^{\mathrm{c}} \equiv (X_{ct})^{\mathrm{c}}$, the exterior of the light cone X_{ct} in (1.2), Theorem 1.1 says that

$$\mathrm{Prob}_{\rho_t,E}(X_{ct}^{\mathrm{c}}) \le C_{n,E}t^{-n}.$$

The constant $C_{n,E}$ in (1.8) depends on the difference $c-\kappa>0$ (through (2.49) below). For brevity of notation, we do not display the dependence on $c-\kappa$.

In equations (1.16)-(1.17) below, we provide an explicit formula for the number κ in Theorem 1.1. Physically, κ bounds the propagation speed (also called "speed of sound") in the energy-constrained open quantum system. Naturally, κ depends on the system parameters and the energy cutoff.

We first introduce some notations. For each closed set $X \subset \mathbb{R}^d$, we define the *smoothed distance function* to X, $d_X \in C^\infty(\mathbb{R}^d)$ in the following way. Let $\epsilon_0 > 0$ be a fixed parameter (the estimate (1.8), in particular, depends on this arbitrary parameter). Let

$$d_X(x) \equiv d_{X,\epsilon_0}(x) \begin{cases} = 0, & \mathrm{dist}_X(x) = 0, \\ \ge 0, & 0 < \mathrm{dist}_X(x) < c_1\epsilon_0, \\ = \delta_X(x) - \epsilon_0, & \mathrm{dist}_X(x) \ge c_1\epsilon_0, \end{cases} \tag{1.11}$$

where $\delta_X \in C^\infty(\mathbb{R}^d)$ satisfies $c_1 \,\mathrm{dist}_X(x) \le \delta_X(x) \le c_2 \,\mathrm{dist}_X(x)$ for some $c_1, c_2 > 0$, and

$$\mathrm{dist}_X^{|\alpha|-1}(x)\,|\partial^\alpha d_X(x)| \le C_\alpha \quad (x \in \mathbb{R}^d,\ 0 \le |\alpha|), \tag{1.12}$$

for some absolute constants $C_\alpha > 0$. In one-dimension, such functions are easy to construct, see the schematic diagram Figure 1. In any dimension, one can proceed as follows. By the extension theorem of Whitney (see e.g. [40, Theorem 6.2.2]), there exists a function δ_X defined in X^c such that

$$c_1 \,\mathrm{dist}_X(x) \le \delta_X(x) \le c_2 \,\mathrm{dist}_X(x), \quad \text{for all } x \in X^c$$

$$\delta_X \text{ is } C^\infty \text{ in } X^c \text{ and } \mathrm{dist}_X^{|\alpha|-1}(x)\partial^\alpha\delta_X(x) \le C_\alpha, \quad \text{for all } x \in X^c \text{ and } |\alpha| \ge 0,$$

where c_1, c_2, C_α are positive constants independent of X. Let $f_{\epsilon_0} : \mathbb{R} \to \mathbb{R}$ be a C^∞ function such that $f_{\epsilon_0}(x) = 0$ if $x \le \epsilon_0/2$, and $f_{\epsilon_0}(x) = x - \epsilon_0$ if $x \ge \epsilon_0$. We can then define

$$d_X(x) := f_{\epsilon_0}(\delta_X(x))$$

and verify that it satisfies the conditions above.

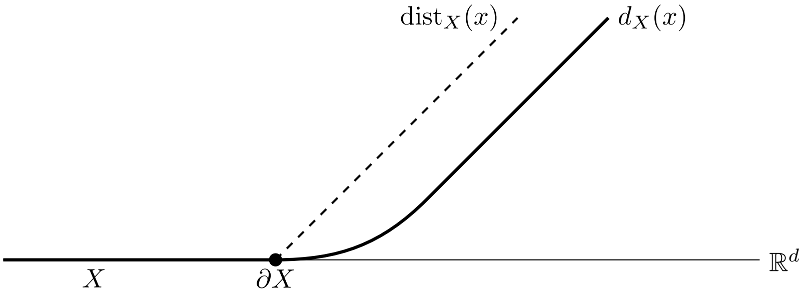

FIGURE 1. Schematic diagram illustrating $d_X \equiv d_{X,\epsilon}$ in (1.11).

We fix $E \in \sigma(H)$ and a function $g \in C^\infty(\mathbb{R})$ satisfying $0 \le g \le 1$ and, for some small $\epsilon > 0$,

$$g(\mu) \equiv 1 \text{ for } \mu \le E - \epsilon, \quad g(\mu) \equiv 0 \text{ for } \mu \ge E, \tag{1.13}$$

and define the *smooth energy cutoff* operator

$$g := g(H). \tag{1.14}$$

Remark 5. Since $g(H) = (g\chi^{\#}_{\sigma(H)})(H)$, the values of g outside of $\sigma(H)$ are irrelevant. Since, moreover, H is bounded from below by **(H)**, one can always take g to have compact support if needed.

Considering the multiplication operator d_X by the smoothed distance function $d_X(x)$, introduced in (1.11) above, we define the spectrally localized distance function

$$d_X^E := g d_X g \qquad \text{defined on} \qquad \{u \in \mathcal{H} : gu \in \mathcal{D}(d_X)\}. \tag{1.15}$$

Now, we define the *energy-dependent velocity operator*

$$\gamma \equiv \gamma(X, E) := i[H, d_X^E] + \frac{1}{2}\sum_{j\ge 1}\big(W_j^*[d_X^E, W_j] + [W_j^*, d_X^E]W_j\big). \tag{1.16}$$

It is shown in Section 4 that γ is bounded on $\mathcal{H}$:

$$\kappa := \|\gamma\| < \infty, \tag{1.17}$$

provided assumptions **(H)** and **(W2)** hold. Notice that the bound on κ is independent of X, see (1.9). Formally, the velocity operator (1.16) has a simple origin:

$$\gamma \equiv \gamma(X, E) = L'(d_X^E), \tag{1.18}$$

where L' is the operator acting on the space of observables $\mathcal{B}(\mathcal{H})$, which is dual to the operator L defined by the r.h.s. of (1.1), see (1.21) below.

Under a different set of assumptions, an estimate similar to (1.8) is shown in [7] with $O(t^{-n})$ remainder for any $n \ge 1$. The assumptions made in [7] exclude in (1.1) the Schrödinger operators (1.3).

It is straightforward to show that under the conditions **(W1)**,

(1.19) $V(x)$ in (1.3) is Δ-bounded with relative bound strictly less than 1, and for any $\rho_0 \in \mathcal{D}$ (see (1.6)), Eq. (1.1) has a solution in $\mathcal{D}$. For more detailed discussions, see Appendix A below and Refs. [9, Section 5.5], [12, Appendix A], [33]. Note that Condition (1.19) holds e.g. for every $V \in L^2(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ and is much weaker than **(H)**.

One can show further (see [1, 9, 12, 24, 25] and Appendix A) that the operator L defines a completely positive, trace-preserving, strongly continuous semigroup of contractions. In particular, for any initial state $\rho_0 \in \mathcal{D}$, the solution ρ_t, $t \geq 0$, to (1.1) satisfies

$$\rho_t \geq 0, \quad \text{if} \quad \rho_0 \geq 0, \quad \text{and} \quad \mathrm{Tr}\rho_t = \mathrm{Tr}\rho_0. \tag{1.20}$$

Finally, we give the explicit expression of the operator L' in (1.18) and its domain. Let L be the operator defined by the r.h.s. of (1.1) on its natural domain $\mathcal{D}$ (see (1.6)), and L' be the operator acting on the space of observables $\mathcal{B}(\mathcal{H})$, which is dual to L with respect to the coupling $(A, \rho) := \mathrm{Tr}(A\rho)$, i.e.,

$$\mathrm{Tr}(AL\rho) = \mathrm{Tr}((L'A)\rho), \tag{1.21}$$

for $\rho \in \mathcal{D}(L)$ and $A \in \mathcal{D}(L') \subset \mathcal{B}(\mathcal{H})$. [1] Explicitly, the dual vNL operator L' defined in (1.21) is given by:

$$L' = L_0' + G', \qquad L_0'A = i[H, A], \tag{1.22}$$

$$G'A := \frac{1}{2}\sum_{j\geq 1}(W_j^*[A, W_j] + [W_j^*, A]W_j), \tag{1.23}$$

with domain

$$\begin{aligned} \mathcal{D}(L') \equiv \mathcal{D}(L_0') \equiv \big\{&A \in \mathcal{B}(\mathcal{H}) \,|\, A\mathcal{D}(H) \subset \mathcal{D}(H) \text{ and} \\ &[H, A] \text{ defined on } \mathcal{D}(A) \cap \mathcal{D}(H) \text{ extends to an operator on } \mathcal{D}(\mathcal{H})\big\}. \end{aligned} \tag{1.24}$$

Notation. In the remainder of this paper, $\|\cdot\|$ stands either for the norm of vectors in $\mathcal{H}$, or for the norm of operators on $\mathcal{H}$, which one is meant is always clear from the context. For two bounded operators A, B, the notation

$$A = O(B) \tag{1.25}$$

means that $\|A\| \leq C_{n,E}\,\|B\|$ for some $C_{n,E} > 0$ independent of $A\,, B\,, t\,, s$. As above, we will write

$$X_a := \big\{x \in \mathbb{R}^d : d_X(x) \leq a\big\} \text{ for } a \geq 0, \quad X_{ct}^{\mathrm{c}} \equiv (X_{ct})^{\mathrm{c}}.$$

In all our estimates, it is understood that, if $n = 1$, the sums $\sum_{k=2}^n(\cdots)$ should be dropped.

2. Recursive monotonicity estimate

We work in this section in an abstract setting, with H a self-adjoint operator on a Hilbert space $\mathcal{H}$ and, for $j = 1, 2, \ldots$, W_j bounded operators in $\mathcal{H}$ such that $\sum_{j\geq 1} W_j^* W_j$ strongly converges in $\mathcal{H}$. We consider the vNL operator

$$L\rho = -i[H, \rho] + \frac{1}{2}\sum_{j\geq 1}\big([W_j, \rho W_j^*] + [W_j\rho, W_j^*]\big),$$

[1] L' generates the dual Heisenberg-Lindblad evolution $\partial_t A_t = L'A_t$ of quantum observables.

defined on the domain (1.6), as well as the dual operator L' defined as in (1.21)–(1.24).

We consider in addition a self-adjoint operator Φ on $\mathcal{H}$, semi-bounded from below. We assume that

$$(\Phi + c)^{-1}\mathcal{D}(H) \subset \mathcal{D}(H), \tag{2.1}$$

for some $c \geq 0$ and there is an integer $n \geq 1$ such that, for all $k = 1, \ldots, n+1$,

$$M_k := 1 + \left\|\mathrm{ad}_{\Phi}^{k}(H)\right\|^2 + \|\sum_{j\geq 1} W_j^* W_j\| + \sum_{j\geq 1}\left\|\mathrm{ad}_{\Phi}^{k}(W_j)\right\|^2 < \infty. \tag{2.2}$$

Hence

$$\mu_n := \max_{2\leq k\leq n+1} M_k \tag{2.3}$$

is finite.

Later on, H will be the Schrödinger operator (1.3) satisfying **(H)**, W_j will be bounded operators satisfying **(W1)**–**(W2)** and Φ will be taken to be the operator $\Phi \equiv \phi^E = g\phi g$ with $g \equiv g(H)$ described in (1.13) and some $\phi \in C^\infty(\mathbb{R}^d)$, see Section 4.

As in (1.16)–(1.17) we set

$$\kappa_\Phi := \left\| i[H,\Phi] + \frac{1}{2}\sum_{j\geq 1}\left(W_j^*[\Phi, W_j] + [W_j^*, \Phi]W_j\right)\right\|. \tag{2.4}$$

The main result of this section is a key differential inequality, (2.9). The proof of this inequality is *the only place* where the information about equation (1.1) is used.

2.1. **ASTLO and RME.** We construct a class of observables, which we call *adiabatic spacetime localization observables (ASTLOs)*, which play the central role in our analysis.

For a constant $\delta > 0$ specified later on, we define a set of smooth cutoff functions

$$\mathcal{X} \equiv \mathcal{X}_\delta := \left\{ \chi \in C^\infty(\mathbb{R}) \,\middle|\, \begin{array}{l} \operatorname{supp}\chi \subset \mathbb{R}_{\geq 0}, \operatorname{supp}\chi' \subset (0, \delta/2) \\ \chi' \geq 0,\ \sqrt{\chi'} \in C^\infty(\mathbb{R}) \end{array} \right\}. \tag{2.5}$$

See Figure 2 below.

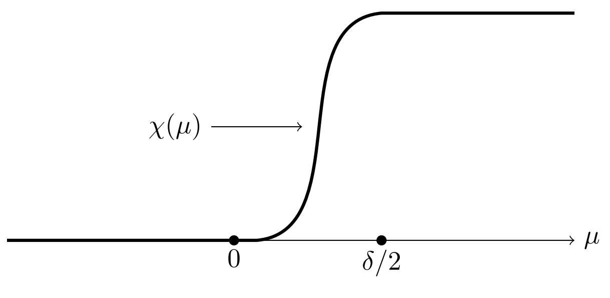

FIGURE 2. Schematic diagram illustrating $\chi \in \mathcal{X}$.

We note that $\chi \geq 0$ for $\chi \in \mathcal{X}$, and the following two properties hold:

(X1) If $w \in C_c^\infty$ and $\operatorname{supp} w \subset (0, \delta/2)$, then the antiderivative $\int^x w^2 \in \mathcal{X}$.

(X2) If $\xi_1, \ldots, \xi_N \in \mathcal{X}$, then $\xi = (\xi_1^{\frac{1}{2}} + \cdots + \xi_N^{\frac{1}{2}})^2$ satisfies $\xi \in \mathcal{X}$ and $\xi_1 + \cdots + \xi_N \leq \sqrt{N}\xi$.

For a function $\chi \in \mathcal{X}$, a densely defined self-adjoint operator Φ, a constant $v \in (\kappa, c)$ and $s > t \geq 0$, we define a family of self-adjoint operators

$$\chi_{ts} = \chi\left(\frac{\Phi - vt}{s}\right). \tag{2.6}$$

Following [7], we use the method of propagation observables. Let β_t' be the evolution generated by the operator L', i.e. $\frac{d}{dt}\beta_t'(\Psi) = \beta_t'(L'\Psi)$ for all observables Ψ in $\mathcal{D}(L') \subset \mathcal{B}(\mathcal{H})$. For a differentiable family of bounded operators $\Psi_t \in \mathcal{D}(L')$, $t \geq 0$, we then have the relation

$$\frac{d}{dt}\beta_t'(\Psi_t) = \beta_t'(D\Psi_t), \tag{2.7}$$

$$D\Psi_t = L'\Psi_t + \partial_t \Psi_t. \tag{2.8}$$

As in [7], we call the operation D the *Heisenberg derivative.*

Note that the condition (2.1) ensures that for all t, s, the bounded observable χ_{ts} belongs to the domain of L' and also that the commutator expansion Lemma C.2 can be applied. The main result of this section is the following:

Theorem 2.1 (recursive monotonicity estimate)**.** *Suppose that* (2.1)–(2.2) *hold. Let $\chi \in \mathcal{X}$ and let χ_{ts} be the operator defined in* (2.6)*. Then there exists $C = C(n, \chi) > 0$ and, if $n \geq 2$, $\xi^k = \xi^k(\chi) \in \mathcal{X}$, $k = 2, \ldots, n$, such that as self-adjoint operators,*

$$D\chi_{ts} \leq -\frac{v - \kappa_\Phi}{s}\chi_{ts}' + \sum_{k=2}^{n} \frac{M_k}{s^k}(\xi^k)_{ts}' + C\frac{\mu_n}{s^{n+1}}, \tag{2.9}$$

where $\kappa_\Phi > 0$ is as in (2.4) *and M_k and μ_n are defined in* (2.2) *and* (2.3)*.*

This theorem is proved in Section 2.2.

Since the second, remainder term on the r.h.s. is of the same form as the leading, negative term, we call (2.9) the *recursive monotonicity estimate (RME).* It can be bootstrapped as in Proposition 2.2 to obtain an integral inequality with $O(s^{-n})$ remainder. We write, for $r \geq 0$,

$$\chi_{ts}(r) := \beta_r'(\chi_{ts}) \qquad \text{and} \qquad \chi_{ts}'(r) := \beta_r'(\chi_{ts}'). \tag{2.10}$$

Proposition 2.2. *Suppose the assumptions of Theorem 2.1 hold. Then, for all $c > \kappa_\Phi$ and $\chi \in \mathcal{X}$, there exist $C = C(n, \chi) > 0$ and $\xi^k \in \mathcal{X}$, $2 \leq k \leq n$ (dropped for $n = 1$), such that for all $0 \leq t < s$,*

$$\int_0^t \chi_{rs}'(r)dr \leq C\mu_n^n\Big(s\chi_{0s}(0) + \sum_{k=2}^{n} s^{-k+2}\ \xi_s^k(0) + ts^{-n}\Big), \tag{2.11}$$

where μ_n is given by (2.3)*.*

Remark 6. Instead of the evolution $\chi_{rs}(t)$, we could have used the expectation:

$$\langle \chi_{ts} \rangle_t := \operatorname{Tr}(\chi_{ts}\rho_t) \tag{2.12}$$

of χ_{ts} in the state ρ_t solving (1.1) and instead of (2.7), used the relation

$$\frac{d}{dt}\langle\chi_{ts}\rangle_t = \langle D\chi_{st}\rangle_t \,. \tag{2.13}$$

These two formulations are related as

$$\langle\chi_{ts}\rangle_t = \langle\chi_{ts}(t)\rangle_0 \,. \tag{2.14}$$

2.2. **Proof of Theorem 2.1.** To prove the recursive monotonicity estimate, Theorem 2.1, we first need a totally symmetrized commutator expansion. Our next results, Proposition 2.3 and Proposition 2.4, generalize the commutator expansion for bounded operators, first obtained in [36], and subsequently improved in e.g. [16, 22, 23, 39]. We refer to [22] for details and references.

Recall that the dual vNL operator L' satisfies $L' = i[H, A] + G'A$ for all A in $\mathcal{D}(L')$, where G' is given by (1.23).

Proposition 2.3. *Suppose that* (2.1) *and* (2.2) *hold. Let* $\chi \in \mathcal{X}$ *and let* χ_{ts} *be the operator defined by* (2.6). *Then, uniformly in* t, *for* $s > 0$,

$$i[H, \chi_{ts}] = s^{-1}\sqrt{\chi'_{ts}}\, i[H, \Phi]\sqrt{\chi'_{ts}} + \mathrm{Rem}_H \tag{2.15}$$

where the remainder term Rem_H *satisfies the estimate*

$$\pm\mathrm{Rem}_H \le \sum_{k=2}^{n} \frac{M_k}{s^k}(\xi^k)'_{ts} + C\frac{M_{n+1}}{s^{n+1}} \tag{2.16}$$

for some $\xi^2, ..., \xi^n \in \mathcal{X}$ *depending only on* χ, *with* M_k *as in* (2.2) *and for some constant* $C = C(n, \chi) > 0$.

Proposition 2.4. *Suppose that* (2.1) *and* (2.2) *hold. Let* $\chi \in \mathcal{X}$ *and let* χ_{ts} *be the operator defined by* (2.6). *Then, uniformly in* t, *for* $s > 0$,

$$G'(\chi_{ts}) = s^{-1}\sqrt{\chi'_{ts}}\, G'(\Phi)\sqrt{\chi'_{ts}} + \mathrm{Rem}_W, \tag{2.17}$$

where the remainder term Rem_W *satisfies the estimate*

$$\pm\mathrm{Rem}_W \le \sum_{k=2}^{n} \frac{M_k}{s^k}(\xi^k)'_{ts} + C\frac{\mu_n}{s^{n+1}} \tag{2.18}$$

for some $\xi^2, ..., \xi^n \in \mathcal{X}$ *depending only on* χ, *for some constant* $C = C(n, \chi) > 0$, *with* M_k *and* μ_n *as in* (2.2) *and* (2.3).

Remark 7. The estimates above are all uniform in s, t, Φ and, in particular, are valid for the operator $\phi^E = g\phi g$ such as (3.3).

Remark 8. We note that the error term in Theorem 1.1 arises in the symmetrization procedure above, and can be improved as the expansion continues to higher order.

Proof of Proposition 2.3. In this proof, the time t is fixed and is omitted from the notation, so we write χ_s for χ_{ts}. Also, we denote $B_k \equiv i\mathrm{ad}^k_\Phi(H)$ for $k = 1, ..., n+1$. In this case, since H is self-adjoint, we have $B_k^* = (-1)^{k-1}B_k$.

1. By (2.1)–(2.2) and the assumption on χ, the hypotheses of Lemma C.2 are satisfied. Hence, by (C.4)–(C.5), we have

$$i[H, \chi_s] = \frac{1}{2}\sum_{k=1}^{n} \frac{s^{-k}}{k!}\left(\chi_s^{(k)}B_k + B_k^*\chi_s^{(k)}\right) + \frac{1}{2}s^{-(n+1)}\left(R_{n+1} + R_{n+1}^*\right), \tag{2.19}$$

where $\|R_{n+1}\| \leq c\|B_{n+1}\|$ for some constant $c > 0$ depending only on χ.

2. Next, we claim that every term on the r.h.s. of (2.19), except for the leading term ($k = 1$), are uniformly bounded by $(\chi_1)'_s$ for some $\chi_1 \in \mathcal{X}$.

To show this, for each k, we choose some smooth function $\theta^k \in C_c^\infty((0, \delta/2))$ that takes value 1 on $\operatorname{supp}(\chi^{(k)})$. Then, we claim that

$$\chi_s^{(k)} B_k = \chi_s^{(k)} B_k \theta_s^k + O(s^{-(n+1-k)}), \tag{2.20}$$

where $\theta_s^k \equiv \theta^k(s^{-1}(\Phi - vt))$. Indeed, using commutator expansion and the fact that $\mathrm{ad}_\Phi^l(B_k) = B_{k+l}$, we have

$$\begin{aligned} \chi_s^{(k)} B_k = \chi_s^{(k)} \theta_s^k B_k &= \chi_s^{(k)} B_k \theta_s^k + \chi_s^{(k)} [\theta_s^k, B_k] \\ &= \chi_s^{(k)} B_k \theta_s^k - \chi_s^{(k)} \sum_{l=1}^{n-k} \frac{(-1)^l s^{-l}}{l!} (\theta^k)_s^{(l)} B_{k+l} \\ &\quad + (-1)^{n+1-k} s^{-(n+1-k)} \chi_s^{(k)} \mathrm{Rem}_{\mathrm{right}}(s), \end{aligned} \tag{2.21}$$

where

$$\mathrm{Rem}_{\mathrm{right}}(s) = \int d\widetilde{\theta^k}(z) R^{n+1-k} B_{n+1} R. \tag{2.22}$$

Since θ^k has compact support, $\mathrm{Rem}_{\mathrm{right}}(s)$ is bounded so that

$$\chi_s^{(k)} B_k = \chi_s^{(k)} B_k \theta_s^k - \chi_s^{(k)} \sum_{l=1}^{n-k} \frac{(-1)^l s^{-l}}{l!} (\theta^k)_s^{(l)} B_{k+l} + O(s^{-(n+1-k)}). \tag{2.23}$$

Next, since $\theta^k \equiv 1$ on $\operatorname{supp}(\chi^{(k)})$, we have $\operatorname{supp}((\theta^k)^{(l)}) \cap \operatorname{supp}(\chi^{(k)}) = \varnothing$ for all $l \geq 1$ so that

$$\chi_s^{(k)} \sum_{l=1}^{n-k} \frac{(-1)^l s^{-l}}{l!} (\theta^k)_s^{(l)} B_{k+l} = 0. \tag{2.24}$$

It follows that

$$\chi_s^{(k)} B_k = \chi_s^{(k)} B_k \theta_s^k + O(s^{-(n+1-k)})$$

so that

$$s^{-k}(\chi_s^k B_k + B_k^* \chi_s^k) = s^{-k}(\chi_s^k B_k \theta_s^k + \theta_s^k B_k^* \chi_s^k) + O(s^{-(n+1)}). \tag{2.25}$$

Now, we apply the following operator inequality

$$\pm(P^* Q + Q^* P) \leq P^* P + Q^* Q. \tag{2.26}$$

with $P = \chi_s^{(k)}$ and $Q = B_k \theta_s^k$ on (2.25) to obtain

$$s^{-k}(\chi_s^k B_k + B_k^* \chi_s^k) \leq s^{-k} \left((\chi_s^{(k)})^2 + \|B_k\|^2 (\theta_s^k)^2 \right) + O(s^{-(n+1)}). \tag{2.27}$$

Since n is finite, we can choose $\xi^2, ..., \xi^n \in \mathcal{X}$ such that $(\xi^k)'$ majorizes $(\chi^{(k)})_s^2 + \|B_k\|^2 (\theta_s^k)^2$ for each k.

3. Now, we symmetrize the leading order term. Let $u = (\chi')^{1/2}$. Since u is smooth by assumption, we use (C.1) to expand the leading order terms and obtain

$$\begin{aligned}(u_s)^2 B_1 + B_1 (u_s)^2 &= 2u_s B_1 u_s + u_s[u_s, B_1] + [B_1, u_s]u_s \\ &= 2u_s B_1 u_s + \sum_{l=1}^{n-1} \frac{s^{-l}}{l!} \left(u_s u_s^{(l)} B_{1+l} + B_{1+l}^* u_s^{(l)} u_s \right) \\ &\quad + s^{-n}(u_s R_n' + R_n'^* u_s),\end{aligned} \tag{2.28}$$

where $\|R_n'\| \le c' \|B_{n+1}\|$ for some constant $c' > 0$ depending only on u.

Again, using operator estimate (2.26), for each $l = 1, ..., n-1$, we have

$$s^{-l}(u_s u_s^{(l)} B_{1+l} + B_{1+l}^* u_s^{(l)} u_s) \le s^{-1} \|B_{1+l}\|^2 (u_s^{(l)})^2 + s^{-2l+1}(u_s)^2, \tag{2.29}$$

and for the remainder term we have

$$s^{-n}(u_s R_n' + R_n'^* u_s) \le s^{-1}(u_s)^2 + s^{-2n+1} \|R_n'\|^2 (\tilde{\theta}_s)^2, \tag{2.30}$$

where $\tilde{\theta}$ is again some smooth cutoff function supported in $(0, \delta/2)$ that takes value 1 on the support of u and $\tilde{\theta}_s \equiv \tilde{\theta}(s^{-1}(\Phi - vt))$. Since u, $u^{(l)}$ and $\tilde{\theta}$ are supported in $(0, \delta/2)$, we can modify $\xi^2, ..., \xi^n$ in such a way that $\xi^l \in \mathcal{X}$ majorizes u^2, $\tilde{\theta}^2$ and $(u^{(l)})^2$ for each $l = 1, ..., n-1$.

Collecting all terms except for the leading order ones into the remainder term Rem_H, we obtain (2.15). □

Proof of Proposition 2.4. In this proof, we also fix t and omit it from the notation. Furthermore, we fix $j \ge 1$ and denote $D_{j,k} \equiv \mathrm{ad}_\Phi^k(W_j)$. In particular, we obtain $\mathrm{ad}_\Phi^k(W_j^*) = (-1)^k (\mathrm{ad}_\Phi^k(W_j))^* = (-1)^k D_{j,k}^*$.

1. First, using Lemma C.2 and the boundedness of W_j, we have

$$[\chi_s, W_j] = -\sum_{k=1}^{n} \frac{s^{-k}}{k!} \chi_s^{(k)} D_{j,k} - s^{-(n+1)} R_{j,n+1}^{\mathrm{right}} \tag{2.31}$$

where $R_{j,n+1}^{\mathrm{right}}$ is given in (C.14) and satisfies the estimate

$$\|R_{j,n+1}^{\mathrm{right}}\|^2 \le C \|D_{j,n+1}\|^2, \tag{2.32}$$

for some constant C independent of j. Similarly, we have

$$[W_j^*, \chi_s] = -\sum_{k=1}^{n} \frac{s^{-k}}{k!} D_{j,k}^* \chi_s^{(k)} - (-1)^{n+1} s^{-(n+1)} \widetilde{R}_{j,n+1}^{\mathrm{left}}, \tag{2.33}$$

where $\widetilde{R}_{j,n+1}^{\mathrm{left}} = (-1)^{n+1} (R_{j,n+1}^{\mathrm{right}})^*$. Combining (2.31) and (2.33), we have

$$\begin{aligned}G_j'(\chi_s) &= W_j^*[\chi_s, W_j] + [W_j^*, \chi_s]W_j \\ &= -\sum_{k=1}^{n} \frac{s^{-k}}{k!} \left(W_j^* \chi_s^{(k)} D_{j,k} + D_{j,k}^* \chi_s^{(k)} W_j \right) \\ &\quad - s^{-(n+1)} \left(W_j^* R_{j,n+1}^{\mathrm{right}} + (R_{j,n+1}^{\mathrm{right}})^* W_j \right),\end{aligned} \tag{2.34}$$

where $G_j'(\cdot) = W_j^*[\cdot, W_j] + [W_j^*, \cdot]W_j$.

2. We now verify that the r.h.s. of (2.34) is summable in $j \geq 1$. We begin with the remainder terms. Using the operator estimate (2.26), we obtain

$$\pm\left(W_j^* R_{j,n+1}^{\text{left}} + (R_{j,n+1}^{\text{left}})^* W_j\right) \leq W_j^* W_j + \|R_{j,n+1}^{\text{left}}\|^2, \tag{2.35}$$

which are summable in $j \geq 1$ since $\sum_j W_j^* W_j$ strongly converges in $\mathcal{H}$, and since (2.2) and (2.32) hold.

Next, we estimate the k-th terms in the first two lines of (2.34). Let θ^k be some smooth cutoff function supported in $(0, \delta/2)$ such that $\theta^k \equiv 1$ on $\text{supp}(\chi^{(k)})$. It follows that $\chi_s^{(k)} = \theta_s^k \chi_s^{(k)} \theta_s^k$, where $\theta_s^k \equiv \theta^k(s^{-1}(\Phi - vt))$. Then, we claim that

$$\begin{aligned} &W_j^* \chi_s^{(k)} D_{j,k} + D_{j,k}^* \chi_s^{(k)} W_j \\ &\quad = \theta_s^k \left(W_j^* \chi_s^{(k)} D_{j,k} + D_{j,k}^* \chi_s^{(k)} W_j\right) \theta_s^k + s^{-(n+1-k)} C_k \|D_{j,n+1}\|^2, \end{aligned} \tag{2.36}$$

where C_k is some constant depending only on $\chi^{(k)}$.

If (2.36) holds, then using (2.26), we have

$$\begin{aligned} &\pm\left(W_j^* \chi_s^{(k)} D_{j,k} + D_{j,k}^* \chi_s^{(k)} W_j\right) \\ &\quad \leq \theta_s^k W_j^* W_j \theta_s^k + \|D_{j,k}\|^2 \|\chi^{(k)}\|^2 (\theta_s^k)^2 + C_k s^{-(n+1-k)} \|D_{j,n+1}\|^2, \end{aligned} \tag{2.37}$$

which are also summable in $j \geq 1$ by (2.2).

3. Now, we prove the claim (2.36). By a direct calculation, we have

$$\begin{aligned} &W_j^* \chi_s^{(k)} D_{j,k} - \theta_s^k W_j^* \chi_s^{(k)} D_{j,k} \theta_s^k \\ &\quad = [W_j^*, \theta_s^k] \chi_s^{(k)} D_{j,k} + \theta_s^k W_j^* \chi_s^{(k)} [\theta_s^k, D_{j,k}] \end{aligned} \tag{2.38}$$

and a similar expression for $D_{j,k}^* \chi_s^{(k)} W_j$. Thus, it suffices to show that $[W_j^*, \theta_s^k]$ and $[\theta_s^k, D_{j,k}]$ are $O(s^{-(n-k)})$.

3.1. For the first term, we use (2.33) to obtain

$$[W_j^*, \theta_s^k] = -\sum_{l=1}^{n} \frac{s^{-l}}{l!} D_{j,l}^* (\theta^k)_s^{(l)} - s^{-(n+1)} R_{j,n+1}^*, \tag{2.39}$$

where $R_{j,n+1}$ is given by (C.14) and satisfies the estimate $\|R_{j,n+1}\| \leq C\|D_{j,n+1}\|$. Since $\theta^k \equiv 1$ on $\text{supp}(\chi^{(k)})$, then we have $(\theta^k)_s^{(l)} \chi_s^{(k)} = 0$ for $l \geq 1$ so that

$$[W_j^*, \theta_s^k] \chi_s^{(k)} D_{j,k} = -s^{(n+1)} R_{j,n+1}^* \chi_s^{(k)} D_{j,k}, \tag{2.40}$$

which is $O(s^{-(n+1)})$ and summable in $j \geq 1$, by the Cauchy-Schwarz inequality and (2.2).

3.2. For the second term, we proceed similarly, using (2.31), to obtain

$$[\theta_s^k, D_{j,k}] = -\sum_{l=1}^{n-k} \frac{s^{-l}}{l!} (\theta^k)_s^{(l)} D_{j,k+l} + s^{-(n+1-k)} \widetilde{R}_{j,n+1-k}, \tag{2.41}$$

where $\widetilde{R}_{j,n+1-k}$ is given by (C.13) with n replaced by $n-k$ and satisfies the estimate $\|\widetilde{R}_{j,n+1-k}\| \leq C\|D_{j,n+1-k}\|$ with C only depending on θ^k. Using the same reason as above, since $\chi_s^{(k)} (\theta^k)_s^{(l)} = 0$ for all $l \geq 1$, we conclude that

$$\theta_s^k W_j^* \chi_s^{(k)} [\theta_s^k, D_{j,k}] = s^{-(n+1-k)} \theta_s^k W_j^* \chi_s^{(k)} \widetilde{R}_{j,n+1-k}. \tag{2.42}$$

This completes the proof of the claim (2.36).

4. Now we choose $\xi^2, ..., \xi^n \in \mathcal{X}$ such that

$$\left(\| \sum_{j\geq 1} W_j^* W_j \| + \sum_{j\geq 1} \|D_{j,k}\|^2 \right) (\theta^k)^2 \leq M_k (\xi^k)'.$$

Then, by writing everything as Rem_W in (2.34) except for the leading order terms (obtained for $k = 1$), we obtain, up to some terms coming from the leading order terms which will be dealt with below, the estimate

$$\pm \mathrm{Rem}_W \leq \sum_{k=2}^{n+1} \frac{M_k}{s^k} (\xi^k)'_s + \frac{C\mu_n}{s^{n+1}}, \tag{2.43}$$

where C is a constant depending only on χ and n.

5. Finally, we deal with the leading order terms (obtained for $k = 1$) in (2.34). Following the same lines as in the proof for Proposition 2.3, we define $u = \sqrt{\chi'}$ and use (C.1) to obtain

$$\begin{aligned} & W_j^* \chi'_s D_{j,1} + \text{h.c.} \\ =& u_s W_j^* D_{j,1} u_s + [W_j^*, u_s] u_s D_{j,1} + u_s W_j^* [u_s, D_{j,1}] + \text{h.c.}, \end{aligned} \tag{2.44}$$

where h.c. means the adjoint of the terms before it. Without repeating the same calculation as above, using (C.1) and (2.26), we can show that the commutators are summable in $j \geq 1$. Then, we modify $\xi^k \in \mathcal{X}$ to majorize $(u^{(k)})^2$ and u^2 as well. This completes the proof. □

Now we are ready to prove Theorem 2.1:

Proof of Theorem 2.1. Given Proposition 2.3–2.4, we choose $\xi^2, ..., \xi^n$ depending on χ, in such a way that

$$\mathrm{Rem}_H + \mathrm{Rem}_W \leq \sum_{k=2}^{n} \frac{M_k}{s^k} (\xi^k)'_{ts} + C \frac{\mu_n}{s^{n+1}}, \tag{2.45}$$

where C is some constant which depends only on n and χ.

It remains to calculate $\partial_t \chi_{ts}$. Using the chain rule, we immediately obtain

$$\partial_t \chi_{ts} = -s^{-1} v \chi'_{ts}. \tag{2.46}$$

This completes the proof. □

2.3. **Proof of Proposition 2.2.**

Proof of Proposition 2.2. Within this proof, all constants $C > 0$ depend only on χ and n.

We will use the relation (2.7). First, we observe that, by Condition (2.1) and Definition (2.5), for $\chi \in \mathcal{X}$ and all $0 < t \leq s$, the operator χ_{ts} maps $\mathcal{D}(H)$ into itself. Moreover, (2.19) in the proof of Proposition 2.3 shows that $[H, \chi_{ts}] \in \mathcal{B}(\mathcal{H})$. Hence $\chi_{ts} \in \mathcal{D}(L')$.

Next, for each fixed s, integrating the formula (2.7) with $\Psi_t \equiv \chi_{ts}$ in t gives

$$\chi_{ts}(t) - \int_0^t \beta'_r(D\chi_{rs})\,dr = \chi_{0s}(0). \tag{2.47}$$

The positive-preserving property of the flow (1.1) (see (1.20)) extends by duality to β'_r, so that we can apply the inequality (2.9) to the second term on the l.h.s. of (2.47) to obtain

$$\begin{aligned}&\chi_{ts}(t) + (v-\kappa_\Phi)s^{-1}\int_0^t \chi'_{rs}(r)\,dr\\ &\le \chi_{0s}(0) + C\mu_n\left(\sum_{k=2}^n s^{-k}\int_0^t (\xi^k)'_{rs}(r)\,dr + ts^{-(n+1)}\right),\end{aligned} \tag{2.48}$$

where we recall that the second term in the r.h.s. is dropped for $n=1$.

Since $\kappa_\Phi < v$ and $t \le s$, (2.48) implies, after dropping $\chi_{ts}(t) \ge 0$, which is due to the positive-preserving property of the flow (1.1) (see (1.20)), and multiplying by $s(v-\kappa_\Phi)^{-1} \ge 0$, that

$$\int_0^t \chi'_{rs}(r)\,dr \le C\mu_n\left(s\chi_{0s}(0) + \sum_{k=2}^n s^{-k+1}\int_0^t (\xi^k)'_{rs}(r)\,dr + ts^{-n}\right). \tag{2.49}$$

3. If $n=1$, then (2.49) gives (2.11). If $n \ge 2$, applying (2.49) to the term $\int_0^t (\xi^k)'_{rs}(r)\,dr$ and using the property (X2), we obtain

(2.50)
$$\int_0^t \chi'_{rs}(r)\,dr \le C\mu_n^2\Big(s\chi_{0s}(0) + \xi^2_{0s}(0) + \sum_{k=3}^n s^{-k+2}\int_0^t (\eta^k)'_{rs}(r)\,dr + ts^{-n}\Big),$$

where the third term in the r.h.s. is dropped for $n=2$, and $\eta^k = \eta^k(\xi^2,\xi^k) \in \mathcal{X}, k=3,\dots,n$. Bootstrapping this procedure, we arrive at (2.11). □

3. Proof of Theorem 1.1

We formulate the technical relations mentioned in Theorem 1.1. Given a smooth, non-negative cutoff functions g with $\mathrm{supp}(g) \subset (-\infty, E]$ (see also Remark 5)and a smooth function χ from the space (2.5), we choose smooth cutoff functions $\tilde{g}$ and $\tilde{\chi}$ such that $\mathrm{supp}(\tilde{g}) \subset \{g \equiv 1\}$ and $\mathrm{supp}(\tilde{\chi}') \subset (\delta, +\infty) = \{\chi \equiv 1\}$, so that

$$\bar{\chi}(\mu)\tilde{\chi}(\mu) = 0, \tag{3.1}$$

$$\bar{g}(\mu)\tilde{g}(\mu) = 0. \tag{3.2}$$

see Figs. 3–4.

We also specify the self-adjoint operator Φ in Theorem 2.1 and definition (2.6) as

$$\Phi := d_X^E = g(H)d_X g(H), \tag{3.3}$$

where, recall, $X \subset \mathbb{R}^d$ is a bounded subset with smooth boundary and $d_X \in C^\infty(\mathbb{R}^d)$ is the smoothed distance function to X given in (1.11) for some $\epsilon_0 > 0$ and satisfies (1.12).

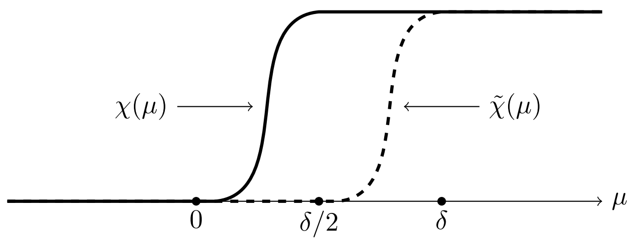

FIGURE 3. Schematic diagram illustrating $\tilde{\chi}$ satisfying (3.1).

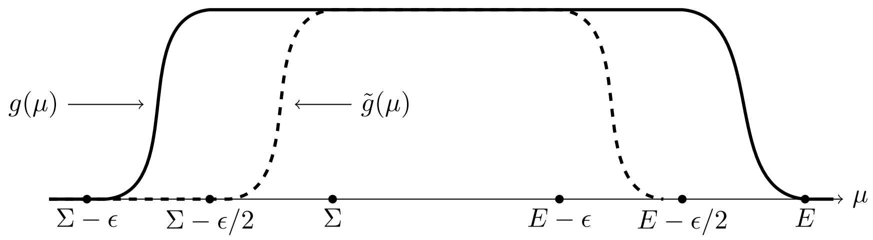

FIGURE 4. Schematic diagram illustrating $\tilde{g}$ satisfying (3.2). Here $\Sigma := \inf \sigma(H)$ (see Remark 5).

To shorten notations, we introduce the following notations:

$$\chi_{ts}^E := \chi((d_X^E - vt)/s), \quad \chi_{ts} := \chi((d_X - vt)/s). \tag{3.4}$$

Now, for any $\chi \in \mathcal{X}$ and $\tilde{g}$, $\tilde{\chi}$ as above, we claim that

$$\chi_X^\sharp \chi_{0s}^E \chi_X^\sharp = O(s^{-n}), \tag{3.5}$$

$$\chi_{ts}^E \geq \tilde{g}\tilde{\chi}_{ts}\tilde{g} + O(s^{-n}), \tag{3.6}$$

where we recall that $\chi_X^\sharp$ stands for the characteristic function of X. We discuss these claims in Section 5.

Recall that β_t' denotes the evolution generated by the operator L' and that $\chi_{ts}^E(t) := \beta_t'(\chi_{ts}^E)$, $(\chi')_{ts}^E(t) := \beta_t'((\chi')_{ts}^E)$. We are now ready to prove Theorem 1.1.

Proof of Theorem 1.1. We want to apply Proposition 2.2 to $H = -\Delta + V(x)$ and W_j satisfying **(H)–(W2)**, with Φ given by (3.3). Hence we need to verify that the abstract conditions (2.1)–(2.2) are satisfied.

First, we fix any $c > 0$ and justify that $(d_X^E + c)^{-1}$ maps $\mathcal{D}(H)$ into itself. Recalling that $d_X^E = g(H) d_X g(H)$ with $\operatorname{supp}(g) \subset (-\infty, E]$, we have

$$\begin{aligned}(d_X^E + c)^{-1} &= \chi^\#_{(-\infty,E]}(H)(d_X^E + c)^{-1} + \chi^\#_{(E,\infty)}(H)(d_X^E + c)^{-1} \\ &= \chi^\#_{(-\infty,E]}(H)(d_X^E + c)^{-1} + c^{-1}\chi^\#_{(E,\infty)}(H).\end{aligned}$$

The first term is a bounded operator from $\mathcal{H}$ to $\mathcal{D}(H)$ while the second term obviously preserves $\mathcal{D}(H)$. This shows that $(d_X^E + c)^{-1}$ maps $\mathcal{D}(H)$ into itself

Next, condition (2.2) is verified in Section 4, see Corollary 4.3. Therefore Proposition 2.2 with $\Phi = d_X^E$ applies.

Now we take $\chi \in \mathcal{X}$ with $\chi(\mu) \equiv 1$ for $\mu \geq \delta/2$. Retaining the first term in the l.h.s. of (2.48) in the proof of Proposition 2.2 and dropping the second one, which is non-negative since $\chi' \geq 0$ and $v > \kappa$, we obtain

$$\chi_{ts}^E(t) \leq \chi_{0s}^E(0) + C_{n,E}\left(\sum_{k=2}^n s^{-k+1}\int_0^t ((\xi^k)')_{rs}^E(r)dr + ts^{-(n+1)}\right).$$

Here we used that the constant $\mu_n = \max_{2\leq k\leq n+1} M_k$ appearing in the r.h.s. of (2.48) is bounded by $C_{n,E}$ for some positive constant depending on n and E. Applying (2.11) to the second term on the r.h.s.,

we deduce that, with the notation as in (1.25),

$$\chi_{ts}^E(t) \leq \chi_{0s}^E(0) + O(s^{-1}\xi_{0s}^E(0)) + O(s^{-n}), \tag{3.7}$$

for some $\xi \in \mathcal{X}$ and all $s > t$. Taking expectation w.r.t. ρ_0 on both sides of (3.7) and recalling that $\chi_{ts}(t) := \beta_t'(\chi_{ts})$, we find

$$\mathrm{Tr}\left(\beta_t'(\chi_{ts}^E)\rho_0\right) \leq \mathrm{Tr}\left(\left(\chi_{0s}^E + O(s^{-1}\xi_{0s}^E)\right)\rho_0\right) + O(s^{-n}). \tag{3.8}$$

By the localization assumption (1.7) on the initial state, we have $\rho_0 = \chi_X^\sharp \rho_0 \chi_X^\sharp$. By this fact, we find

$$\mathrm{Tr}\left(\left(\chi_{0s}^E + O(s^{-1}\xi_{0s}^E)\right)\rho_0\right) = \mathrm{Tr}\left(\chi_X^\sharp\left(\chi_{0s}^E + O(s^{-1}\xi_{0s}^E)\right)\chi_X^\sharp\rho_0\right) = O(s^{-n}). \tag{3.9}$$

The relation (3.6) implies

$$\chi_{ts}^E \geq \tilde{g}\tilde{\chi}_{ts}\tilde{g} + O(s^{-n}), \tag{3.10}$$

where we recall that $\tilde{g}$ is a smooth non-negative cutoff function with $\mathrm{supp}(\tilde{g}) \subset \{g \equiv 1\}$ and $\tilde{\chi}$ is a smooth function such that $\tilde{\chi} \equiv 1$ on $(\delta, +\infty)$. It follows that, by applying the dual evolution β_t',

$$\beta_t'(\tilde{g}\tilde{\chi}_{ts}\tilde{g}) \leq \beta_t'(\chi_{ts}^E) + O(s^{-n}). \tag{3.11}$$

Plugging the estimates (3.9), (3.10) and (3.11) to (3.8) yields

$$\mathrm{Tr}(\tilde{g}\tilde{\chi}_{ts}\tilde{g}\beta_t(\rho_0)) = O(s^{-n}). \tag{3.12}$$

Finally, recalling the definition (1.11), we find, for all $v \in (\kappa, c)$,

$$\chi_{X_{ct}^c}^\sharp = \theta^+(d_{X_{ct}}) = \theta^+(d_X - ct) \leq \tilde{\chi}_{ts}, \tag{3.13}$$

where θ^+ is the Heaviside function, provided $\delta = c - v$ and $s = t$. See Figure 5.

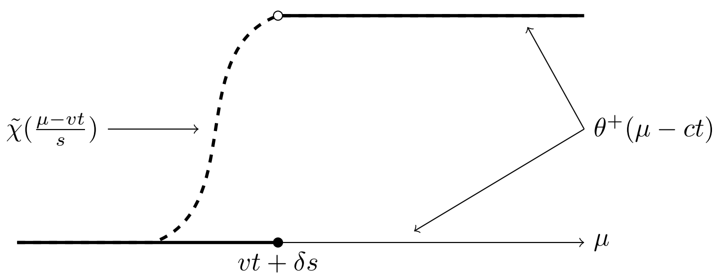

FIGURE 5. Schematic diagram illustrating estimate (3.13).

Hence we conclude estimate (1.8) from (3.12)–(3.13). This completes the proof of Theorem 1.1. □

4. Estimates of multiple commutators

In this section, we establish some key estimates for multiple commutators of the form $\mathrm{ad}^k_{A^E}(B)$. More precisely, we show that the operators $H = -\Delta + V(x)$ and W_j satisfying **(H)**–**(W2)**, with Φ given by (3.3), verify that the abstract conditions (2.2) used to prove the recursive monotonicity estimate in Section 2.

First, we introduce some notation. For an integer k and a function $f \in C^{n+1}(\mathbb{R}^d)$, we write

$$f \in \mathcal{S}^k \tag{4.1}$$

if there exists $C = C(n, f) > 0$ such that for all multi-indices α with $0 \le |\alpha| \le n+1$ and $x \in \mathbb{R}^d$,

$$|\partial^\alpha f(x)| \le C \langle x \rangle^{-k-|\alpha|} . \tag{4.2}$$

For any multi-index β with order $0 \le |\beta| \le n+1$, $f \in \mathcal{S}^k$ and $g \in \mathcal{S}^l$, it follows immediately from the definition and Leibnitz's rule that

$$\partial^\beta f \in \mathcal{S}^{k+|\beta|}, \quad fg \in \mathcal{S}^{k+l}, \tag{4.3}$$

(with the obvious observation that $\partial^\beta f \in C^{n+1-|\beta|}$ if $f \in C^{n+1}$). To simplify notation, for a fixed operator A on $\mathcal{H}$, define

$$C_A : B \mapsto \mathrm{ad}_A(B) \equiv [A, B]$$

on the set of linear operators on $\mathcal{H}$. We also omit the subindices in x_j and p_j. Restoring these subindices is straightforward.

Results in this section are valid for functions $\phi \in C^\infty, \phi \ge 0$ satisfying

$$\langle x \rangle^{|\alpha|-1} |\partial^\alpha \phi(x)| \le M \quad (x \in \mathbb{R}^d,\ 0 \le |\alpha| \le n+1), \tag{4.4}$$

for some absolute constant $M > 0$.

In particular, the smoothed-out distance function d_X verifies (4.4). Later on, we choose $\phi(x)$ to be a smoothed-out distance function from x to X, see (1.11).

The main result of this section are the following two propositions:

Proposition 4.1. *Let $n \ge 1$. Suppose H satisfies **(H)** and let ϕ be as above. Let $\phi^E := g\phi g$, where g is defined in* (1.13)-(1.14). *Then there exists $C = C(n, M, E) > 0$ such that, for all $E \in \mathbb{R}$,*

$$\left\| \mathrm{ad}^k_{\phi^E}(H) \right\| \le C \quad (k = 1, \dots, n+1). \tag{4.5}$$

Proof. 1. In the following, we denote the resolvent $(z - A)^{-1}$ of the operator A by $R_A(z)$ and R_A if the argument is not important. For measures, if it is clear from the context, we will also drop the arguments for simplicity.

2. The proof is based on the mapping property of certain derivations. Before we proceed, we define a class of operators

$$\mathcal{F}^{(1)} := \left\{ \text{ polynomials of operators of the form } B^{(1)} \right\}, \tag{4.6}$$

where

$$B^{(1)} = \int d\mu(z_1, \dots, z_\nu) \left(\prod_{j=1}^{\nu} R_H(z_j)^{m_j^1} \right) \left(\prod_{q=1}^{N} \prod_{r=1}^{\nu} a_{k_q} p^{\ell_q} R_H(z_r)^{m_r^q} \right), \tag{4.7}$$

$$\sum_{j=1}^{\nu} m_j^1 \geq 1,\ 0 \leq \ell_q \leq \min(1, \sum_{r=1}^{\nu} m_r^q),\ \ k_q \geq 0,\ \ \forall q = 2, \dots N,$$

where μ is some finite measure on $\mathbb{C}^\nu$, $\nu \geq 2$, N is some finite integer, and a_k stands for a generic function belonging to $\mathcal{S}^k$ (see (4.1)). Since $\ell_q \leq \sum_{r=1}^{\nu} m_r^q$ and $k_q \geq 0$ for each q, the second factor in the integrand of (4.7) is bounded, and therefore

$$\mathcal{F}^{(1)} \subset \mathcal{B}(\mathcal{H}).$$

Our goal is to show $\mathrm{ad}^k_{\phi^E}(H)$ lies in $\mathcal{F}^{(1)}$ for all $1 \leq k \leq n+1$ by induction, whence (4.5) follows.

3. For the base case $k = 1$, since $[g, H] = 0$, we find by Leibnitz's rule that

$$\mathrm{ad}^1_{\phi^E}(H) = g \mathrm{ad}^1_\phi(H) g. \tag{4.8}$$

Using formula (C.1) for each g, we can rewrite (4.8) using Fubini's theorem as

$$\mathrm{ad}^1_{\phi^E}(H) = \iint d\widetilde{g}(z_1) \otimes d\widetilde{g}(z_2) R_H(z_1) \mathrm{ad}^1_\phi(H) R_H(z_2). \tag{4.9}$$

By Remark 5, we can modify g to have compact support. Thus, we can choose the measure $d\widetilde{g} \otimes d\widetilde{g}$ to have compact support in $\mathbb{C}^2$ (see (B.5) and Appds. B–C for details).

Next, we compute

$$\mathrm{ad}^1_\phi(H) = \Delta\phi + 2\nabla\phi \cdot \nabla, \tag{4.10}$$

so that $\mathrm{ad}^1_\phi(H)$ is a linear combination of terms of the forms a_1 or $a_0 p$ with $a_j \in \mathcal{S}^j$, by assumption (4.4). Plugging this into (4.9) shows that $\mathrm{ad}^1_{\phi^E}(H) \in \mathcal{F}^{(1)}$, which completes the proof of the base case.

4. Now, assuming $\mathrm{ad}^k_{\phi^E}(H) \in \mathcal{F}^{(1)}$, we will prove $\mathrm{ad}^{k+1}_{\phi^E}(H) \in \mathcal{F}^{(1)}$. It is immediately clear that the induction step is equivalent to showing

$$C_{\phi^E}(\mathcal{F}^{(1)}) \subset \mathcal{F}^{(1)}. \tag{4.11}$$

To establish (4.11), we use the crucial fact that the map C_A is a derivation, i.e. a linear operator satisfying the Leibnitz rule. In particular, with $A = \phi^E = g\phi g = \phi g^2 + [g, \phi] g$, we have

$$C_{\phi^E} = \phi C_{g^2} + C_\phi(\cdot) g^2 + C_{[g,\phi]g}. \tag{4.12}$$

Also, we note some easy commutator relations

$$C_A R_H = R_H (C_A H) R_H \quad \text{ for all operators } A \text{ s.t. } R_H : \mathcal{D}(A) \to \mathcal{D}(A), \tag{4.13}$$

$$C_H p = i\nabla V,\ C_\phi p = i\nabla\phi,\ C_\phi H = -C_H \phi = \Delta\phi + 2\nabla\phi \cdot \nabla. \tag{4.14}$$

We will show that each of the three maps in (4.12) maps $\mathcal{F}^{(1)}$ into itself using the relations (4.13)–(4.14).

4.1 First, we show $\phi C_{g^2}(\mathcal{F}^{(1)}) \subset \mathcal{F}^{(1)}$. Since $\phi C_{g^2}(R_H) = 0$, it suffices, by the induction hypothesis, formula (4.7) and Leibnitz's rule, to evaluate the operators

$$\phi C_{g^2}(p), \quad \phi C_{g^2}(a_k). \tag{4.15}$$

Using (4.13)–(4.14), together with the relation $C_{g^2}A = -\int d\widetilde{g^2}R_H(C_HA)R_H$ and the fact that $\nabla V \in \mathcal{S}^1$ by Hypothesis **(H)**, we compute, using (4.14)

$$\begin{aligned}\phi C_{g^2}(p) &= \int d\widetilde{g^2}\phi R_H(i\nabla V)R_H \\ &= \int d\widetilde{g^2}R_H a_0 R_H + \int d\widetilde{g^2}R_H(a_1+a_0p)R_H a_1 R_H, \qquad (4.16)\end{aligned}$$

where in the second equality we commuted ϕ through R_H and used again (4.14) together with (4.4). Similarly,

$$\begin{aligned}\phi C_{g^2}(a_k) &= \int d\widetilde{g^2}\phi R_H(\Delta a_k + 2\nabla a_k\cdot\nabla)R_H \\ &= \int d\widetilde{g^2}R_H(a_{k+1}+a_kp)R_H \\ &\quad + \int d\widetilde{g^2}R_H(a_1+a_0p)R_H(a_{k+2}+a_{k+1}p)R_H, \qquad (4.17)\end{aligned}$$

which are indeed of the desired form in order to deduce that $\phi C_{g^2}(\mathcal{F}^{(1)}) \subset \mathcal{F}^{(1)}$.

4.2 Next, we show $C_\phi(\mathcal{F}^{(1)})g^2 \subset \mathcal{F}^{(1)}$. Since $C_\phi(a_k) = 0$ for all k, it suffices, by induction hypothesis, formula (4.7) and Leibnitz's rule, to evaluate the following operators

$$C_\phi(p), \quad C_\phi(R_H), \qquad (4.18)$$

where, recall, R_H stands for the resolvent of H. Using the relations (4.13)–(4.14), we compute

$$C_\phi(p) = \nabla\phi \in \mathcal{S}^0, \qquad (4.19)$$

$$\begin{aligned}C_\phi(R_H) &= R_H(C_\phi H)R_H = R_H(\Delta\phi + 2\nabla\phi\cdot\nabla)R_H \\ &= R_H(a_1+a_0p)R_H, \qquad (4.20)\end{aligned}$$

which, inserted into (4.7), allows us to conclude that $C_\phi(\mathcal{F}^{(1)})g^2 \subset \mathcal{F}^{(1)}$.

4.3 Finally, we show $C_{[g,\phi]g}(\mathcal{F}^{(1)}) \subset \mathcal{F}^{(1)}$. By the induction hypothesis and the Leibnitz rule, it suffices to show that $[g,\phi]\,g$ is of the form (4.7). To this end we use (C.1) so that

$$\begin{aligned}[g,\phi]\,g &= \left(\int d\widetilde{g}(z_1)\,[R_H(z),\phi]\right)\left(\int d\widetilde{g}(z_2)R_H(z_2)\right) \\ &= -\left(\int d\widetilde{g}(z_1)R_H(z_1)\left(\mathrm{ad}^1_\phi(H)\right)R_H(z_1)\right)\left(\int d\widetilde{g}(z_2)R_H(z_2)\right). \qquad (4.21)\end{aligned}$$

Since $C_\phi(H) = a_1 + a_0p$ from (4.14), Eq. (4.21) shows that $C_{[g,\phi]g}(\mathcal{F}^{(1)}) \subset \mathcal{F}^{(1)}$.

This completes the induction. □

Proposition 4.2. *Suppose Assumption **(W2)** holds and let $\phi \in C^\infty(\mathbb{R}^d)$ satisfy condition* (4.4). *Let $\phi^E = g\phi g$ where g is defined in* (1.13)-(1.14). *Then, the following estimates hold:*

$$\sum_j \left\|\mathrm{ad}^k_{\phi^E}(W_j)\right\|^2 < \infty \quad (k = 0,\dots,n+1). \qquad (4.22)$$

Proof. Within this proof we fix some j and write $W \equiv W_j$. We will use the same strategy and adapt the same notations in the proof of Proposition 4.1 to establish mapping property for the derivation C_{ϕ^E}. For each $k = 1, \dots, n+1$, we define the classes of operators on $\mathcal{B}(\mathcal{H})$

$$\mathcal{G}_m^{(2)} := \{\mathcal{L}_A \mathcal{R}_{A'} B_{rs}^{(2)} \mid A, A' \in \mathcal{F}^{(1)} \cup \{\mathbf{1}\}, \quad B_{rs}^{(2)} \equiv (\phi C_p)^r C_x^s \text{ with } r, s \geq 0 \text{ and } r+s=m\}$$

$$\mathcal{F}_k^{(2)} := \Big\{ \text{ polynomials of elements in } \mathcal{G}_m^{(2)}(W) \text{ for } 1 \leq m \leq k \Big\}. \tag{4.23}$$

Here $\mathcal{L}, \mathcal{R}$ are left- and right-multiplication operator in $\mathcal{B}(\mathcal{H})$, respectively, $\mathcal{F}^{(1)}$ is defined in (4.6), and $\mathcal{G}_m^{(2)}(W)$ means operators in $\mathcal{G}_m^{(2)}$ acting on W.

1. Our first claim is that

$$\mathrm{ad}_{\phi^E}^k(W) \in \mathcal{F}_k^{(2)} \tag{4.24}$$

for every $k = 1, \dots, n+1$. We prove the this claim by induction in k. For $k = 1$, we first compute

$$\begin{aligned} C_H W &= pC_pW + (C_pW)p + C_V W \\ &= pC_pW + (C_pW)p + \int d\widetilde{V}(z) R_x(z)[C_xW]R_x(z) \end{aligned} \tag{4.25}$$

and

$$\begin{aligned} \phi C_V W &= \int d\widetilde{V}(z)\phi(x) R_x(z)[C_xW]R_x(z) \\ &= a_0 \int d\widetilde{V}(z)(\mathbf{1} - (z-i)R_x(z))[C_xW]R_x(z), \end{aligned} \tag{4.26}$$

using the identity $R_x(z) = (x-i)^{-1}[\mathbf{1} - (z-i)R_x(z)]$ and noting that $\phi(x-i)^{-1} \in \mathcal{S}^0$. Note that the integral in (4.26) is convergent, as follows from the fact that $V \in \mathcal{S}^\rho$ for some $\rho > 0$ (see Hypothesis **(H)**) together with the properties of the almost analytic extension $\widetilde{V}$ described in Appendix B.

Here and below, to simplify the proof we take $d = 1$. For $d \geq 1$, we use the Helffer-Sjöstrand representation (C.1) for several variables to write

$$V(x_1, \dots, x_d) = \int d\widetilde{V}(z_1, \dots, z_d)(z - x_1)^{-1} \dots (z - x_d)^{-1},$$

which yields through Leibnitz rule that

$$\begin{aligned} \phi C_V W = &\int d\widetilde{V}(z)\phi(x) R_{x_1}(z)[C_{x_1}W]R_{x_1}(z)R_{x_2}(z)\cdots R_{x_d}(z) + \dots \\ &+ \int d\widetilde{V}(z)\phi(x)R_{x_1}(z)\cdots R_{x_d}(z)[C_{x_d}W]R_{x_d}(z). \end{aligned}$$

One can handle each of the d terms on the r.h.s. exactly as in (4.26) and then sum over the results.

Eqs. (4.25)–(4.26) show that $\phi C_H W \in \mathcal{F}_1^{(2)}$. Now, using (4.12)–(4.14) and that fact that $g^2, [g,\phi]g \in \mathcal{F}^{(1)}$, as shown in Proposition 4.1, we have

$$\phi C_{g^2}(W) = \int d\widetilde{g}(z) R_H(z) \phi C_H(W) R_H(z) + \int d\widetilde{g}(z) R_H(z)(a_1 + a_0 p) R_H(z)[C_H W] R_H(z) \tag{4.27}$$

$$C_\phi(W) g^2 = \int d\widetilde{\phi}(z) R_x(z)[C_x W] R_x(z) g^2(H), \tag{4.28}$$

$$C_{[g,\phi]g} W = [g,\phi] g W - W [g,\phi] g, \tag{4.29}$$

so that $C_{\phi^E} W \in \mathcal{F}_1^{(1)}$. This completes the proof for the base case.

2. Now, assuming (4.24) holds for $k = m$, we prove it for $k = m+1$. Since $\mathrm{ad}_{\phi^E}^{m+1}(W_j) = C_{\phi^E}(\mathrm{ad}_{\phi^E}^m(W_j))$, by inductive assumption, it suffices to show that $C_{\phi^E}(AB_m A') \in \mathcal{F}_m^{(2)}$ for all $AB_m A' \in \mathcal{G}_m^{(2)}$. By Leibnitz rule, we have

$$C_{\phi^E}(AB_m A') = (C_{\phi^E} A) B_m A' + A (C_{\phi^E} B_m) A' + A B_m (C_{\phi^E} A'). \tag{4.30}$$

The first and the last term on the r.h.s. of (4.30) is taken cared by Proposition 4.1. We now have to compute the second term. To this end, we define another set of operators

$$\mathcal{G}_m^{(3)} := \{\mathcal{L}_A \mathcal{R}_{A'} B_{rs}^{(3)} \mid A, A' \in \mathcal{F}^{(1)} \cup \{\mathbf{1}\}, B_{rs}^{(3)} \equiv (\phi^\ell C_p)^r C_x^s \text{ with } \ell \in \{0,1\}, r, s \geq 0 \text{ and } r+s = m\}$$

$$\mathcal{F}_k^{(2)} := \Big\{\text{polynomials of elements in } \mathcal{G}_m^{(3)}(W) \text{ for } 1 \leq m \leq k\Big\}. \tag{4.31}$$

We remark that the operator product $(\phi^\ell C_p)^r$ means that products of the form $(\phi C_p)^{r_1}(C_p)^{r_2}...(\phi C_p)^{r_{2n-1}}(C_p)^{r_{2n}}$ for any $r_1, ..., r_{2n} \geq 0$ and $r_1 + ... + r_{2n} = r$.

Write $\phi = b\langle x\rangle$ with $b(x) := \phi(x)/\langle x\rangle \in \mathcal{S}^0$ by (4.4) with $\alpha = 0$. We successively commute the bounded operators b's to the left. Then condition (1.5) implies the same estimate but with ϕ in place of $\langle x\rangle$, i.e.

$$\sum_{j=1}^{\infty} \sum_{\substack{\sum(k_i+\ell_i)=n+1 \\ k_i, \ell_i \geq 0}} \| \prod_i \left[(\phi C_{p_q})^{k_i} C_{x_q}^{\ell_i} W_j\right] \|^2 < \infty. \tag{4.32}$$

By (4.32) and the fact that $\mathcal{F}^{(1)} \subset \mathcal{B}(\mathcal{H})$, it follows that

$$\mathcal{F}_{n+1}^{(3)} \subset \mathcal{B}(\mathcal{H}).$$

We now claim that for $k = 0, 1 \ldots$ and every $B_k^{(2)} \in \mathcal{G}_k^{(2)}$, there exist

$$A,\, A' \in \mathcal{F}^{(1)} \cup \{\mathbf{1}\}, \quad B_k^{(3)}(W) \in \mathcal{F}^{(3)}$$

such that

$$B_k^{(2)}(W) = A B_k^{(3)}(W) A'. \tag{4.33}$$

This relation implies $\mathcal{F}^{(2)} \subset \mathcal{F}^{(3)}$. This, together with (4.24) and the inclusion $\mathcal{F}_{n+1}^{(3)} \subset \mathcal{B}(\mathcal{H})$, leads to (4.22).

2.1 Again, we prove (4.33) by induction. For $k = 1$, it is trivial from the definition.

2.2 Next, assuming (4.33) holds for $k = m$, we prove it for $k = m+1$. Again, by Proposition 4.1 and by the induction hypothesis and the Leibniz rule, it suffices therefore to show that, for any $B_m^{(3)} = (\phi^\ell C_p)^r C_x^s$ for some $\ell \in \{0,1\}$ and $r, s \geq 0$ such that $r + s = m$,

$$\phi C_p(B_m^{(2)}(W)), C_x(B_m^{(2)}(W)) \in \mathcal{F}_{m+1}^{(3)}. \tag{4.34}$$

For the former term, it is trivial. For the latter case, we use the fact that

$$C_p C_x = C_x C_p, \qquad C_x(\phi C_p) = \phi C_p C_x \tag{4.35}$$

so that $C_x(B_m^{(3)} W) = B_m^{(3)} C_x W = (\phi^\ell C_p)^r C_x^{s+1} W$. This completes the induction.

3. Now we return back to our previous induction proof. Since every operator in $\mathcal{G}_m^{(2)}(W)$ can be expanded as a finite sum of terms in $\mathcal{F}_m^{(3)}$, it suffices to calculate $C_{\phi^E}(B_m^{(3)}(W))$ for some $B_m^{(3)} = (\phi^\ell C_p)^r C_x^s \in \mathcal{G}_m^{(3)}$. As in the calculation for the base case, it suffices to compute the terms $\phi C_H(B_m^{(3)}(W))$ and $C_x(B_m^{(3)}(W))$. The latter term is contained in $\mathcal{F}_{m+1}^{(3)}$ trivially. For the former term, we have

$$\begin{aligned} \phi C_H(B_m^{(3)}(W)) &= \phi p C_p(B_m^{(3)}(W)) + \phi C_p(B_m^{(3)}(W))p + \phi C_V(B_m^{(3)}(W)) \\ &= p(\phi C_p B_m^{(3)}(W)) + (\phi C_p B_m^{(3)}(W))p \\ &\quad + (C_p\phi)B_m^{(3)}(W) + \phi C_V(B_m^{(3)}(W)). \end{aligned} \tag{4.36}$$

Obviously the first three terms in the last line of (4.36) belong in $\mathcal{F}_{m+1}^{(3)}$. For the last term, we have

$$\begin{aligned} \phi C_V B_m^{(3)} &= a_0 \int d\widetilde{\phi}(z)[\mathbf{1} - (z-i)R_x(z)](C_x B_m^{(3)}(W))R_x(z) \\ &= a_0(C_x B_m^{(3)}(W))a_0 - \int d\widetilde{\phi}(z)(z-i)R_x(z)(C_x B_m^{(3)}(W))R_x(z). \end{aligned} \tag{4.37}$$

This completes the proof. □

Corollary 4.3. *Suppose that $H = -\Delta + V(x)$ and W_j satisfy **(H)–(W2)**. Then, with Φ given by* (3.3)*, condition* (2.2) *holds.*

Proof. Since $d_X(x)$ satisfies condition (4.4), it suffices to apply Propositions 4.1–4.2. □

5. Proof of Claims (3.5)–(3.6)

5.1. **Proof of Claim** (3.5)**.** Recall that $\chi_X^\sharp$, $X \subset \mathbb{R}^d$, denotes the characteristic functions of X. Recall also that the set of smooth cutoff functions $\mathcal{X}$ is defined in (2.5) and that $d_X^E = g d_X g$ with $g = g^E(H)$ (see (1.13)–(1.15)) and d_X the smooth distance function defined in (1.11). We reproduce Claim (3.5) below:

Proposition 5.1. *For every $\chi \in \mathcal{X}$ and $\chi_{0s} = \chi(s^{-1}d_X^E)$ (see* (3.4)*),*

$$\chi_X^\sharp \chi_{0s} \chi_X^\sharp = O(s^{-n}). \tag{5.1}$$

Remark 9. This is a semiclassical estimate which physically says that a quantum particle that is essentially localized in phase space inside an energy ball and outside of X (by way of d_X^E) is also localized outside of X in position space up to small errors. A technical challenge here is that the operator d_X is unbounded.

Proof of Proposition 5.1. In the remainder of this proof, we use the following notations: For $z \in \mathbb{C}$ with $\mathrm{Im}(z) \neq 0$, d as in (1.11), and g as in (1.14),

$$d \equiv d_X, \qquad d^E \equiv d^E_X = g d_X g, \qquad R = (d/s - z)^{-1}, \qquad R^E = (d^E/s - z)^{-1},$$
$$b = d - d^E, \qquad \chi^E = \chi(d^E/s), \qquad \chi = \chi(d/s).$$

We begin with

Lemma 5.2. *The operator Rb is bounded.*

Proof. Since $b = d - d^E$ and Rd is bounded as the multiplication operator by a bounded function, it suffices to show that Rd^E is bounded. For the latter, we have, by (1.15),

$$Rd^E = Rgdg = Rdg^2 + R[g, d]g. \tag{5.2}$$

Since g is bounded and $Rd = s(1 + zR)$ so that $\|Rd\| \leq s(1 + |z|\,|\mathrm{Im}(z)|^{-1})$, it remains to show that $[g, d]$ is bounded. Using the HS representation (C.1) with $k = 0$ and formula (4.10), we have

$$\begin{aligned}
[g, d] &= \int d\widetilde{g}(z) \left[(z - H)^{-1}, d\right] \\
&= -\int d\widetilde{g}(z)(z - H)^{-1} \mathrm{ad}^1_d(H)(z - H)^{-1} \\
&= \int d\widetilde{g}(z)(z - H)^{-1} \left(\nabla \cdot (\nabla d) + \nabla d \cdot \nabla\right)(z - H)^{-1}.
\end{aligned} \tag{5.3}$$

Next we multiply by i and use the operator Cauchy-Schwarz inequality

$$\begin{aligned}
&i\nabla \cdot (\nabla d) + \nabla d \cdot i\nabla \\
\leq& -\langle E\rangle^{-1/2} \Delta + \langle E\rangle^{1/2} |\nabla d|^2 \\
\leq& \frac{H}{\langle E\rangle^{1/2}} + \|V\|_\infty + 1 + \langle E\rangle^{1/2} |\nabla d|^2 =: B_{H,E}.
\end{aligned}$$

By (1.12), we have $|\nabla d| \leq C$. This, together with condition (1.4) on V and the HS representation (C.1) with $k = 1$, shows that

$$\left\|(z - H)^{-1} \left(\nabla \cdot (\nabla d) + \nabla d \cdot \nabla\right)(z - H)^{-1}\right\| \tag{5.4}$$
$$\leq \left\|B^{\frac{1}{2}}_{H,E}(\bar{z} - H)^{-1}\right\|\left\|B^{\frac{1}{2}}_{H,E}(z - H)^{-1}\right\| \tag{5.5}$$
$$\leq C\left(\langle E\rangle^{-\frac{1}{2}}|z| + \langle E\rangle^{\frac{1}{2}}|\mathrm{Im}(z)|^{-2}\right). \tag{5.6}$$

Using the properties of the almost analytic extension $\tilde{g}$ (in particular the fact that it is compactly supported, see (B.5) and Remark 5), this shows that the integral in (5.3) is norm convergent, which completes the proof. □

Now, using the Helffer-Sjöstrand representation (C.1) and omitting the measure, we write

$$\chi^E = \int R^E. \tag{5.7}$$

Using that the operator Rb is bounded and expanding $R^E = (d^E/s - z)^{-1} = (d/s - z - b/s)^{-1}$ in powers of Rb/s up to the order $n-1$, we obtain

$$R^E = (d/s - z - b/s)^{-1} = \sum_{k=0}^{n-1} s^{-k}(Rb)^k R + s^{-n}(Rb)^n R^E. \tag{5.8}$$

Plugging this expansion into (5.7) yields

$$\chi^E = \sum_{k=0}^{n-1} \chi_k + s^{-n}\mathrm{Rem}_1, \tag{5.9}$$

where

$$\chi_k = \int (Rb/s)^k R \quad \text{and} \quad \mathrm{Rem}_1 = \int (Rb)^n R^E. \tag{5.10}$$

Our goal is to move the R's in the first integrand to the right. Using the relations $Rb = bR + [R, b]$ and $[R, b] = -s^{-1}R\mathrm{ad}_d(b)R$, we would like to obtain an expansion of the form

$$(Rb)^k R = \sum_l s^{-i_l}\tilde{B}_l R^{l+1} + s^{-n}\tilde{M}_k, \tag{5.11}$$

where the operators $\tilde{B}_l$ and $\tilde{M}_k$ are polynomials of operators $\mathrm{ad}_d^k(b), k = 0, 1, \dots,$ (and R for $\tilde{M}_k$), and then use $\int R^{l+1} = (-1)^{l+1}\chi^{(l)}$ (see (C.1)) and $\chi^{(l)}\chi_X^{\#} = 0$ for all $l \geq 0$. The problem here is that the operators $\mathrm{ad}_d^k(b)$ are not bounded, so $\tilde{B}_l$ and $\tilde{M}_k$ are not guaranteed to be bounded operators. Hence, we proceed differently.

We transform the product $(Rb/s)^k$ as follows. We use the relation

$$b = gd\bar{g} + \bar{g}d = dh - \mathrm{ad}_d(\bar{g})g, \tag{5.12}$$

$$\text{where } \bar{g} = 1 - g \text{ and } h := \bar{g}(1 + g), \tag{5.13}$$

and the definition $R = (d/s - z)^{-1}$ to write

$$Rb/s = d_s Rh + Rc_s, \text{ where} \tag{5.14}$$

$$d_s := d/s, \quad c := \mathrm{ad}_d(g)g, \quad c_s = c/s. \tag{5.15}$$

Notice that the operators c_s, h and $d_s R$ are bounded and

$$d_s R = \mathbf{1} + zR. \tag{5.16}$$

The last two relations imply

$$Rb/s = h + Rc_s + zRh. \tag{5.17}$$

Our goal is to move the R's to the extreme right to obtain the following:

Lemma 5.3. *The operator $(Rb/s)^k$ has the following expansion:*

$$(Rb/s)^k = h^k + \sum_{q=0}^{k}\sum_{l=0}^{n-1} s^{-l}B_{q,l}R^{l+1}p_{q,l}(z) + s^{-n}\sum_{q=0}^{k} M_{q,n}p_{q,n}(z), \tag{5.18}$$

where

(a) $k = 1, ..., n-1,$
(b) the operators $B_{q,l}$ are polynomials of bounded operators $\mathrm{ad}_d^m(h)$ and $\mathrm{ad}_d^m(c_s)$, with $0 \leq m \leq l$,

(c) the operators $M_{q,n}$ are polynomials of bounded operators R, $\mathrm{ad}_d^m(h)$ and $\mathrm{ad}_d^m(c_s)$, with $0 \le m \le n$ and

$$\deg_R(M_{q,n}) := \text{powers of } R \text{ in } M_{q,n} \in [n+1, n+k]. \tag{5.19}$$

(d) $p_{q,l}(z)$ are polynomials in z of the degree $\le q$.

We call the operators described in (b) as *l-operators*. Note that if B_l is an l-operator, then it is also an $(l+m)$-operator for $m \ge 1$.

Remark 10. The negative powers of s come from the commutator relation

$$[R, B] = -s^{-1} R \,\mathrm{ad}_d(B) R, \tag{5.20}$$

valid for any bounded operator B and $\mathrm{Im}(z) \neq 0$.

Proof of Lemma 5.3. We prove (5.18) by induction on k.

For the base case $k = 1$, we use the commutator expansion

$$RB = \sum_{r=0}^{p-1} (-1)^r s^{-r} \,\mathrm{ad}_d^r(B) R^{r+1} + (-1)^p s^{-p} R \,\mathrm{ad}_d^p(B) R^p, \tag{5.21}$$

valid for any bounded operators B and integer $p \ge 1$. Applying (5.21) to $B = h$ and c_s (see (5.14)), we find

$$\begin{aligned} Rb/s =& h + Rc_s + zRh \\ =& h + \sum_{r=0}^{n-1} (-1)^r s^{-r} \,\mathrm{ad}_d^r(c_s) R^{r+1} + (-1)^n s^{-n} R \,\mathrm{ad}_d^n(c_s) R^n \\ &+ z \left(\sum_{r=0}^{n-1} (-1)^r s^{-r} \,\mathrm{ad}_d^r(h) R^{r+1} + (-1)^n s^{-n} R \,\mathrm{ad}_d^n(h) R^n \right). \end{aligned} \tag{5.22}$$

This is of the form (5.18) with

$$B_{0,r} := (-1)^r \,\mathrm{ad}_d^r(c_s), \quad M_{0,n} := (-1)^n R \,\mathrm{ad}_d^n(c_s) R^n, \tag{5.23}$$

$$B_{1,r} := (-1)^r \,\mathrm{ad}_d^r(h), \quad M_{1,n} := (-1)^n R \,\mathrm{ad}_d^n(h) R^n, \tag{5.24}$$

where

$$\deg_R(M_{0,n}) = \deg_R(M_{1,n}) = n + 1 \tag{5.25}$$

satisfies (5.19).

Now we assume (5.18) for a given $k \ge 1$ and prove it for $k \to k+1$. We use (5.17) to write

$$\begin{aligned} (Rb/s)^{k+1} &= (zRh + Rc_s + h)^{k+1} \\ &= zRh(Rb/s)^k + Rc_s(Rb/s)^k + h(Rb/s)^k \\ &=: A + B + C. \end{aligned} \tag{5.26}$$

Using the induction hypothesis, we see that the third term on the r.h.s. of (5.26) is already in the desired form (notice that the term h^{k+1} in (5.18) comes from this contribution). The first two terms on the r.h.s. of (5.26) are treated similarly, so we only consider the first term.

We transform the term A in line (5.26) as

$$A = A_1 + A_2 + A_3, \tag{5.27}$$

where

$$A_1 := zRh^{k+1}, \tag{5.28}$$

$$A_2 := zRh\sum_{q=0}^{k}\sum_{l=0}^{n-1} s^{-l}B_{q,l}R^{l+1}p_{q,l}(z), \tag{5.29}$$

$$A_3 := s^{-n}zRh\sum_{q=0}^{k} M_{q,n}p_{q,n}(z). \tag{5.30}$$

The term A_1 can be handled using expansion (5.21) as

$$A_1 = z\left(\sum_{l=0}^{n-1}(-1)^l s^{-l}\operatorname{ad}_d^l(h^{k+1})R^{l+1} + (-1)^n s^{-n}R\operatorname{ad}_d^n(h^{k+1})R^n\right). \tag{5.31}$$

By Leibniz's rule, for each l, $\operatorname{ad}_d^l(h^{k+1})$ is an l-operator as defined in part (b) of Lemma 5.3, and so A_1 is of the form (5.18) with

$$B_{1,l}^{(1)} := (-1)^l s^{-l}\operatorname{ad}_d^l(h^{k+1}), \quad p_{q,l}^{(1)} := \delta_{1q}z, \tag{5.32}$$

$$M_{1,n}^{(1)} := (-1)^n s^{-n}R\operatorname{ad}_d^n(h^{k+1})R^n \text{ satisfying } \deg_R(M_{1,n}^{(1)}) = n+1. \tag{5.33}$$

The term A_3 can be written as

$$A_3 = \sum_{q=0}^{k}(RhM_{q,n})(zp_{q,n}(z)) = \sum_{q=1}^{k+1} M_{q,n}^{(2)}p_{q,n}^{(2)}, \tag{5.34}$$

where

$$M_{q,n}^{(2)} := RhM_{q-1,n}, \quad p_{q,n}^{(2)} := zp_{q-1,n}(z), \tag{5.35}$$

with notations as in parts (c)-(d) of Lemma 5.3. Since $\deg_R M_{q,n} \le n+k$, we have

$$\deg_R M_{q,n}^{(2)} \in [n+2, n+k+1], \tag{5.36}$$

which satisfies the bound (5.19) with $k \to k+1$. Thus A_3 is of the form (5.18).

To bring the term A_2 into the desired form, we commute R's in (5.28) to the right using expansion (5.21). For each $q = 0, \dots, k$, we consider the sum

$$A_2(q) := \sum_{l=0}^{n-1} s^{-l}zRhB_{q,l}R^{l+1}p_{q,l}(z), \tag{5.37}$$

so that

$$A_2 = \sum_{q=0}^{k} A_2(q). \tag{5.38}$$

Let $B'_{q,l} = hB_{q,l}$. Using (5.21), we have, for each $l = 0, \dots, n-1$,

(5.39)

$$\begin{aligned} RhB_{q,l}R^l &= RB'_{q,l}R^l \\ &= \sum_{r=0}^{n-l-1}(-1)^r s^{-r}\operatorname{ad}_d^r(B'_{q,l})R^{l+r+1} + (-1)^{n-l}s^{-(n-l)}R\operatorname{ad}_d^{n-l}(B'_{q,l})R^n. \end{aligned}$$

Using Leibniz rule for commutators and the structure of $B_{q,l}$, we conclude that the operators $\operatorname{ad}_d^r(B'_{q,l})$ are polynomials of $\operatorname{ad}_d^m(h)$ and $\operatorname{ad}_d^m(c_s)$, $m = 0, 1, ..., l +$

r, and therefore are $(l+r)$-operators as defined above. So, setting $B''_{q,l+r} = (-1)^r \operatorname{ad}_d^r(B'_{q,l})$, expansion (5.39) becomes

$$RhB_{q,l}R^l = \sum_{r=0}^{n-l-1} s^{-r} B''_{q,l+r} R^{l+r+1} + s^{-(n-l)} RB''_{q,n} R^n. \tag{5.40}$$

Substituting (5.40) into (5.37) and setting $p'_{q+1,l}(z) := zp_{q,l}(z)$ for $l = 0, \dots, n-1$, we obtain

$$\begin{aligned} A_2(q) =& \sum_{l=0}^{n-1} \sum_{r=0}^{n-l-1} s^{-(l+r)} B''_{q,l+r} R^{l+r+1} p'_{q+1,l}(z) \\ &+ s^{-n} \sum_{l=0}^{n-1} RB''_{q,n} R^n p'_{q+1,l}(z). \end{aligned} \tag{5.41}$$

Changing the summation index $(l+r, l) \to (l', r')$, the r.h.s. in line (5.41) can be written as

$$\sum_{l=0}^{n-1} \sum_{r=0}^{n-l-1} s^{-(l+r)} B''_{q,l+r} R^{l+r+1} p'_{q+1,l}(z) = \sum_{l'=0}^{n-1} \sum_{r'=0}^{l'} s^{-l'} B''_{q,l'} R^{l'+1} p'_{q+1,r'}(z). \tag{5.42}$$

Setting $p''_{q+1,n} := \sum_{l=0}^{n-1} p'_{q+1,l}(z)$ in (5.41) and $p''_{q+1,l'} := \sum_{r'=0}^{l'} p'_{q+1,r'}$ for each $l' = 0, \dots, n-1$ in (5.42), we conclude that

$$\begin{aligned} A_2(q) =& \sum_{l=0}^{n-1} s^{-l} B''_{q,l} R^{l+1} p''_{q+1,l}(z) \\ &+ s^{-n} RB''_{q,n} R^n p''_{q+1,n}(z). \end{aligned} \tag{5.43}$$

Plugging (5.43) into (5.38) yields

$$\begin{aligned} A_2 =& \sum_{q=0}^{k} \sum_{l=0}^{n-1} s^{-l} B''_{q,l} R^{l+1} p''_{q+1,l}(z) \\ &+ s^{-n} \sum_{q=0}^{k} RB''_{q,n} R^n p''_{q+1,n}(z) \end{aligned} \tag{5.44}$$

Shifting the dummy index $q \to q+1$ and setting

$$B^{(3)}_{q,l} := B''_{q-1,l+1}, \quad p^{(3)}_{q,n}(z) := p''_{q+1,n}(z), \tag{5.45}$$

$$M^{(3)}_{q,n} := RB''_{q-1,n} R^n \text{ with } \deg_R(M^{(3)}_{q,n}) = n+1, \tag{5.46}$$

we conclude that A_2 is of the form (5.18).

This completes the proof of Lemma 5.3. □

Corollary 5.4. *For any $\chi \in C^\infty(\mathbb{R})$ with compactly supported derivative and $\chi_k = \int (Rb/s)^k R \, d\tilde{\chi}(z)$,*

$$\chi_k = h^k \chi(d_s) + \sum_{q=0}^{k} \sum_{l=0}^{n-1} s^{-l} B_{q,l} (\chi p_{q,l})^{(l+1)}(d_s) + s^{-n} \mathrm{Rem}_{2,k}, \tag{5.47}$$

where $B_{q,l}$ are as in Lemma 5.3 and $\mathrm{Rem}_{2,k} = O(1)$.

Proof. We have by the Heffler-Sjörstrand representation (C.1) that $\int R^{l+1} p_l(z) = (-1)^{l+1} (\chi p_l)^{(l)}(d_s)$ (see (C.1)).

This, together with the definition $\chi_k = \int (Rb/s)^k R$ and expansion (5.18), implies

$$\chi_k = h^k \chi(d_s) + \sum_{q=0}^{k} \sum_{l=0}^{n-1} s^{-l} B_{q,l} (\chi p_{q,l})^{(l+1)}(d_s)$$

$$+ s^{-n} \sum_{q=0}^{k} \int M_{q,n} R p_{q,n}(z)\, d\tilde{\chi}(z). \tag{5.48}$$

Thus it remains to show the integral on line (5.48) is $O(1)$.

Using the estimate $\|R\| \leq |\text{Im}(z)|^{-1}$ and the degree bound (5.19) and that $k \leq n-1$, we have

$$\|M_{q,n}\| \leq C \sum_{j=n}^{2n} |\text{Im}(z)|^{-(j+1)} \text{ for all } q. \tag{5.49}$$

Since $p_{q,n}$ has degree at most n and $\tilde{\chi}$ has compactly supported derivatives, we find by expression (5.49) and Corollary B.5 with $(p,l) = (n+1, n), \ldots, (2n+1, n)$ that

$$\left\| \int M_{q,n} R p_{q,n}\, d\widetilde{\chi}(z) \right\| \leq C \int \sum_{j=n}^{2n} |\text{Im}(z)|^{-(j+2)}\ |p_{q,n}(z)|\ d\widetilde{\chi}(z) \leq C. \tag{5.50}$$

Summing (5.50) over q shows that the integral on line (5.48) is $O(1)$. This completes the proof of Corollary 5.4. □

Since $\chi^{(l)}(d_s)\chi_X^{\#} = 0$ for all $l \geq 0$, expansion (5.47) gives

$$\chi_k \chi_X^{\#} = s^{-n} \text{Rem}_{2,k} \chi_X^{\sharp} = O(s^{-n}). \tag{5.51}$$

Next, we deal with the Rem_1 term in (5.9). We use the splitting

$$Rb = Rc + R_2 h, \quad c := \text{ad}_d(g) g, \quad R_2 := dR, \tag{5.52}$$

which follows from (5.14). We prove:

Lemma 5.5. *For $k \geq 1$, the operator $(Rb)^k$ has the following expansion:*

$$(Rb)^k = \sum_{l=0}^{k} R_2^l N_{k-l}, \tag{5.53}$$

where the operators N_j are polynomials of bounded operators R, $\text{ad}_d^m(h)$ and $\text{ad}_d^m(c)$ with $0 \leq m \leq k-1$ and

$$\deg_R(N_j) := \textit{powers of } R \textit{ in } N_j \in [j, j+2k]. \tag{5.54}$$

Proof. We prove this by induction on $k = 1, 2, \ldots$. For the base case $k = 1$, we use expansion (5.52), which is of the form (5.53) with $N_1 = Rc$ and $N_0 = h$, satisfying degree bound (5.54).

Suppose now (5.53) holds with some $k \geq 1$, and we prove it for $k \to k+1$. Using (5.52) and the induction hypothesis, we write

$$(Rb)^{k+1} = (Rc + R_2 h)(Rb)^k$$

$$= \sum_{l=0}^{k} RcR_2^l N_{k-l} + \sum_{l=0}^{k} R_2 h R_2^l N_{k-l}$$

$$=: A + B. \tag{5.55}$$

The goal now is to commute the bounded operator R_2 successively to the left. Using the relation

$$R_2 = s(1 + zR) \tag{5.56}$$

and identity (5.20), we find

$$\mathrm{ad}_{R_2}(D) = (s^{-1}R_2 - 1)\,\mathrm{ad}_d(D)R, \tag{5.57}$$

for any operator D allowed by the domain consideration. Iterating identity (5.57) for $p \geq 1$ times shows that there exist absolute constants $c_1, \ldots, c_l$ s.t.

$$\mathrm{ad}^p_{R_2}(D) = \sum_{q=0}^{p} c_q s^{-q} R_2^q \mathrm{ad}^p_d(D) R^p. \tag{5.58}$$

Moreover, for any bounded operators D, E and integers $l \geq 1$, we have

$$DE^l = E^l D + \sum_{p=1}^{l} (-1)^p \binom{l}{p} E^{l-p} \mathrm{ad}^p_E(D). \tag{5.59}$$

Applying (5.58)–(5.59) to term A in (5.55) with $D = c$ and $E = R_2$, and using that $[R_2, R] = 0$, we find

$$\begin{aligned} A \equiv & RcN_k + \sum_{l=1}^{k} RcR_2^l N_{k-l} \\ = & RcN_k + \sum_{l=1}^{k} R_2^l RcN_{k-l} \\ & + \sum_{l=1}^{k}\sum_{p=1}^{l} (-1)^p \binom{l}{p} R_2^{l-p} R\ \mathrm{ad}^p_{R_2}(c) N_{k-l} \\ = & RcN_k + \sum_{l=1}^{k} R_2^l RcN_{k-l} \\ & + \sum_{l=1}^{k}\sum_{p=1}^{l}\sum_{q=0}^{p} (-1)^p c_q s^{-q} \binom{l}{p} R_2^{l-p+q} R\ \mathrm{ad}^p_d(c) R^p N_{k-l}. \end{aligned} \tag{5.60}$$

Regrouping (5.60) according to the power in R_2 shows that

$$A = \sum_{l=0}^{k} R_2^l N^{(1)}_{k+1-l}, \tag{5.61}$$

$$N^{(1)}_{k+1} := RcN_k, \tag{5.62}$$

$$\begin{aligned} N^{(1)}_{k+1-l} = & RcN_{k-l} \\ & + \sum_{l'=l}^{k} \sum_{\substack{p=1,\ldots,l' \\ q=0,\ldots,p, \\ q-p=l-l'}} (-1)^p c_q s^{-q} \binom{l'}{p} R\ \mathrm{ad}^p_d(c) R^p N_{k-l'}, \quad l = 1, \ldots, k. \end{aligned} \tag{5.63}$$

Since $\deg_R N_j \in [j, j+2k]$, we derive from expressions (5.62)–(5.63) that

$$\deg_R(N^{(1)}_j) \in [j+1, j+2k+1], \quad j = 0, \ldots k. \tag{5.64}$$

Similarly, applying (5.58)–(5.59) to term B in (5.55) with $D = h$ and $E = R_2$ yields

$$\begin{aligned} B \equiv & R_2 h N_k + \sum_{l=1}^{k} R_2 h R_2^l N_{k-l} \\ = & R_2 h N_k + \sum_{l=1}^{k} R_2^{l+1} h N_{k-l} \\ & + \sum_{l=1}^{k} \sum_{p=1}^{l} (-1)^p \binom{l}{p} R_2^{l-p+1} \operatorname{ad}_{R_2}^p(h) N_{k-l} \\ = & R_2 h N_k + \sum_{l=1}^{k} R_2^{l+1} h N_{k-l} \\ & + \sum_{l=1}^{k} \sum_{p=1}^{l} \sum_{q=0}^{p} (-1)^p c_q s^{-q} \binom{l}{p} R_2^{l-p+q+1} \operatorname{ad}_d^p(h) R^p N_{k-l}. \end{aligned} \tag{5.65}$$

Regrouping (5.65) according to the power in R_2 shows that

$$B = \sum_{l=1}^{k+1} R_2^l N_{k+1-l}^{(2)}, \tag{5.66}$$

$$N_k^{(2)} := h N_k, \tag{5.67}$$

$$\begin{aligned} N_{k+1-l}^{(2)} = & h N_{k+1-l} \\ & + \sum_{l'=l}^{k+1} \sum_{\substack{p=1,\dots,l' \\ q=0,\dots,p, \\ q-p=l-l'}} (-1)^p c_q s^{-q} \binom{l'-1}{p} \operatorname{ad}_d^p(h) R^p N_{k+1-l'}, \end{aligned} \tag{5.68}$$

with $l = 2, \dots, k+1$ and

$$\deg_R(N_j^{(2)}) \in [j, j+2k+1], \quad j = 1, \dots k+1. \tag{5.69}$$

Combining expansions (5.61), (5.66) in line (5.55) yields

$$(Rb)^{k+1} = N_{k+1}^{(1)} + \sum_{l=1}^{k} R_2^l (N_{k+1-l}^{(1)} + N_{k+1-l}^{(2)}) + R_2^{k+1} N_0^{(2)}, \tag{5.70}$$

which is of the form (5.53) with $k \to k+1$. This completes the induction and the proof of Lemma 5.5. □

Next, we have the following lemma

Lemma 5.6. *Let* Rem_1 *be as in* (5.10). *If* K *is any bounded operator with* $\operatorname{ran} d \subset \ker K$ *then*

$$K \mathrm{Rem}_1 = O(\|K\|). \tag{5.71}$$

Proof. We use expansion (5.53). Since $\operatorname{ran} d \subset \ker K$, we have $KR_2 = (Kd)R = 0$ by definition (5.52). Thus only the leading term in (5.53) survives left multiplication by K, yielding

$$K \mathrm{Rem}_1 = \int K (Rb)^n R^E = \int K N_n R^E. \tag{5.72}$$

By the definition of N_n (see Lemma 5.5), we have

$$\|N_n\| \le C \sum_{j=n}^{3n} |\mathrm{Im}(z)|^{-j}\,. \tag{5.73}$$

Thus, by (5.72),

$$\|K\mathrm{Rem}_1\| \le \|K\| \sum_{j=n}^{3n} \int |\mathrm{Im}(z)|^{-(j+1)}\,. \tag{5.74}$$

This, together with estimate (B.17) with $(p,l) = (n,0), \dots, (3n,0)$ (recall $n \ge 1$ to begin with), implies the desired result, (5.71). □

Applying (5.71) with $K = \chi_X^\sharp$, whose kernel contains $\operatorname{ran} d$ due to (1.11), we obtain

$$\chi_X^\sharp \mathrm{Rem}_1 = O(1). \tag{5.75}$$

Finally, plugging (5.51) and (5.75) back to expansion (5.9) yields the desired estimate (5.1). This completes the proof of (5.1). □

Remark 11. We mention the following alternative proof of Proposition 5.1. Recalling that $\chi_{0s} = \chi(s^{-1}d_X^E)$ with χ supported on $[c_\delta, \infty)$ for some positive c_δ, we write

$$\left\|\chi_{0s}\chi_X^\sharp\right\| = \left\|\chi_{0s}\left(d_X^E\right)^{-n}\left(d_X^E\right)^n\chi_X^\sharp\right\| \le (c_\delta s)^{-n}\left\|\left(d_X^E\right)^n\chi_X^\sharp\right\|.$$

Now, with the convention $\prod_{i=2}^n A_i = A_2 \dots A_n$, we have

$$\begin{aligned}\left(d_X^E\right)^n &= g(H)d_X\Big(\prod_{i=2}^n g^2(H)d_X\Big)g(H)\\ &= g(H)d_X\langle x\rangle^{-1}\langle x\rangle\Big(\prod_{i=2}^n g^2(H)\langle x\rangle^{-i+1}d_X\langle x\rangle^{-1}\langle x\rangle^i\Big)g(H)\langle x\rangle^{-n}\langle x\rangle^n.\end{aligned}$$

A standard induction argument shows that $\langle x\rangle^i g^2(H)\langle x\rangle^{-i}$ is a bounded operator for any positive integer i (since H is the Schrödinger operator $H = -\Delta + V$), and likewise with g instead of g^2. Since in addition $d_X\langle x\rangle^{-1}$ is bounded, we deduce that

$$\left\|\left(d_X^E\right)^n\chi_X^\sharp\right\| \le C_n\left\|\langle x\rangle^n\chi_X^\sharp\right\| \le C_n',$$

since X is bounded. This establishes Proposition 5.1. (Note that if X is unbounded, the same holds, replacing $\langle x\rangle$ by $\langle d_X\rangle$ in the argument above.)

The proof we gave in Section 5.1 has the advantage of being more robust. Moreover the arguments we used are also crucial in our proof of (3.6) given in the next section.

5.2. **Proof of Claim** (3.6)**.** Recall χ, $\tilde g$, and $\tilde\chi$ are smooth cutoff functions such that $\mathrm{supp}(\tilde g) \subset \{g = 1\}$ and $\mathrm{supp}(\tilde\chi') \subset (\delta, +\infty) = \{\chi = 1\}$ (see Figs. 3–4). Let $\bar g = 1 - g$ and $\bar\chi = 1 - \chi$. It follows that

$$\bar g(\mu)\tilde g(\mu) = 0, \tag{5.76}$$

$$\bar\chi(\mu)\tilde\chi(\mu) = 0. \tag{5.77}$$

In the remainder of this section, we use the following notations: For s, v, t as in (3.4) and $z \in \mathbb{C}$, $\mathrm{Im}(z) \neq 0$,

$$d_t \equiv d_X - vt, \qquad d_t^E \equiv d_X^E - vt = g d_X g - vt,$$
$$R \equiv (d_t/s - z)^{-1}, \qquad R^E \equiv (d_t^E/s - z)^{-1},$$

and

$$\xi(\mu) := \sqrt{\chi(\mu)}, \quad \bar{\xi}(\mu) = 1 - \xi(\mu), \tag{5.78}$$

$$\phi = \phi(d_t/s), \quad \phi^E = \phi(d_t^E/s) \text{ for } \phi \in \mathcal{X}, \tag{5.79}$$

$$g = g(H), \quad \tilde{g} = \tilde{g}(H) \text{ for } g,\ \tilde{g} \text{ from (5.76)}. \tag{5.80}$$

Using these notations, we reproduce Claim 3.6 as follows:

Proposition 5.7. *For every $\chi \in \mathcal{X}$ and $\tilde{g}$, $\tilde{\chi}$ as in* (5.76)–(5.77)*,*

$$\chi^E \geq \tilde{g}\tilde{\chi}\tilde{g} + O(s^{-n}). \tag{5.81}$$

Proof. Since $\|\tilde{g}\tilde{\chi}\tilde{g}\| \leq 1$, we have

$$\chi^E \geq \xi^E \tilde{g}\tilde{\chi}\tilde{g}\xi^E = \tilde{g}\tilde{\chi}\tilde{g} - \bar{\xi}^E\tilde{g}\tilde{\chi}\tilde{g} - \tilde{g}\tilde{\chi}\tilde{g}\bar{\xi}^E + \bar{\xi}^E\tilde{g}\tilde{\chi}\tilde{g}\bar{\xi}^E. \tag{5.82}$$

We now claim

$$\bar{\xi}^E\tilde{g}\tilde{\chi} = O(s^{-n}). \tag{5.83}$$

If (5.83) holds, then the last three terms on the r.h.s. of (5.82) are $O(s^{-n})$ and we are done.

Since the operator $b \equiv d - d^E = d_t - d_t^E$ as in the proof of Proposition 5.1, proceeding as in (5.9)–(5.10), we find the expansion

$$\bar{\xi}^E = \sum_{k=0}^{n-1} \bar{\xi}_k + s^{-n}\mathrm{Rem}_1, \tag{5.84}$$

where

$$\bar{\xi}_k = \int (Rb/s)^k R\, d\tilde{\bar{\xi}}(z) \quad \text{and} \quad \mathrm{Rem}_1 = \int (Rb)^n R^E\, d\tilde{\bar{\xi}}(z), \tag{5.85}$$

where $\tilde{\bar{\xi}}(z)$ is an almost analytic extension of the function $\bar{\xi}(\mu)$. (Below we will omit the measure $d\tilde{\bar{\xi}}(z)$ when no confusion arises.) By expansion (5.84), Claim (5.83) is equivalent to the relations

$$\bar{\xi}_k\tilde{g}\tilde{\chi} = O(s^{-n}), \tag{5.86}$$

$$\mathrm{Rem}_1\tilde{g}\tilde{\chi} = O(1). \tag{5.87}$$

We first prove (5.86). We write the l.h.s. of (5.86) as

$$\bar{\xi}_k\tilde{g}\tilde{\chi} = \bar{\xi}_k\tilde{\chi}\tilde{g} + \bar{\xi}_k[\tilde{g}, \tilde{\chi}]. \tag{5.88}$$

Since $\mathrm{ad}_{d_t/s}^k(\tilde{g}) = s^{-k}\mathrm{ad}_d^k(\tilde{g})$ is bounded for $0 \leq k \leq n$, we have by expansion (C.5) that

$$[\tilde{g}, \tilde{\chi}] = \sum_{k=1}^{n-1} (-1)^k \frac{s^{-k}}{k!}\tilde{\chi}^{(k)}(d_t/s)\mathrm{ad}_d^k(\tilde{g}) + s^{-n}\mathrm{Rem}_3, \tag{5.89}$$

where $\mathrm{Rem}_3 = O(1)$. Plugging (5.89) into (5.88) yields

$$\begin{aligned}\bar{\xi}_k\tilde{g}\tilde{\chi} =&\bar{\xi}_k\tilde{\chi}\tilde{g} + \sum_{k=1}^{n-1}\frac{s^{-k}}{k!}\bar{\xi}_k\tilde{\chi}^{(k)}(d_t/s)\mathrm{ad}_d^k(\tilde{g}) + s^{-n}\bar{\xi}_k\mathrm{Rem}_3\\ =&:A+B+C.\end{aligned} \tag{5.90}$$

We apply Corollary 5.4 to the function $\bar{\xi}$ to obtain the expansion

$$\bar{\xi}_k =h^k\bar{\xi}(d_t/s) + \sum_{q=0}^{k}\sum_{l=0}^{n-1} s^{-l}B_{q,l}(\bar{\xi}p_{q,l})^{(l+1)}(d_t/s) + s^{-n}\mathrm{Rem}_{2,k}, \tag{5.91}$$

where $\|h\| \le 2$, $B_{q,l} = O(1)$ are defined in Lemma 5.3, part (b), and $\mathrm{Rem}_{2,k} = O(1)$. Thus $\bar{\xi}_k = O(1)$ and so the term C in line (5.90) is $O(s^{-n})$. By definition (5.78), we have

$$\bar{\xi}^{(l)}(\mu)\tilde{\chi}^{(m)}(\mu) = 0 \quad \text{for any integers } l, m \ge 0, \tag{5.92}$$

see Figure 3 . Thus, inserting (5.91) to (5.90) and using (5.92), we find

$$A =s^{-n}\sum_{k=0}^{n-1}\mathrm{Rem}_{2,k}\tilde{\chi}\tilde{g} = O(s^{-n}), \tag{5.93}$$

$$B =s^{-n}\sum_{k=1}^{n-1}\sum_{l=0}^{n-1}\frac{s^{-k}}{k!}\mathrm{Rem}_{2,l}\tilde{\chi}^{(k)}\mathrm{ad}_d^k(\tilde{g}) = O(s^{-n}). \tag{5.94}$$

Thus we have proved (5.86).

Next, we prove (5.87) by the following lemma:

Lemma 5.8. *For $k = 1, \dots, n$ and $\mathrm{Rem}_1(k) := \int (Rb)^k R^E$,*

$$\mathrm{Rem}_1(k)\tilde{g}\tilde{\chi} = O(1). \tag{5.95}$$

Proof. We prove this by induction on k. We have by expansion (5.52) that $Rb = Rc + R_2h$. For the base case $k = 1$, we write

$$\begin{aligned}RbR^E =&RcR^E + R_2R^Eh + R_2[h, R^E]\\ =&RcR^E + R_2R^Eh + s^{-1}R_2R^E\mathrm{ad}_{d^E}(h)R^E,\end{aligned} \tag{5.96}$$

where we use the relation (c.f. (5.20))

$$[B, R^E] = s^{-1}R^E\,\mathrm{ad}_{d^E}(B)R^E, \tag{5.97}$$

valid for any operator B allowed by the domain consideration.

The second term (5.96) is a priori large $O(s)$ but it is removed by $\tilde{g}$. Indeed, since $h\tilde{g} = 0$ by (5.13) and the relation (5.77) (c.f. Figure 4), and $s^{-1}R_2 = 1 + zR$ by (5.56), we have

$$\begin{aligned}\mathrm{Rem}_1(1)\,\tilde{g} =& \int RcR^E\tilde{g} + \int s^{-1}R_2R^E\mathrm{ad}_{d^E}(h)R^E\tilde{g}\\ =& \int RcR^E\tilde{g} + \int R^E\mathrm{ad}_{d^E}(h)R^E\tilde{g} + \int zRR^E\mathrm{ad}_{d^E}(h)R^E\tilde{g}.\end{aligned} \tag{5.98}$$

For $f \in C_c^\infty(\mathbb{R})$, the operators $\mathrm{ad}_{d^E}^k(f)$ are $O(1)$ by results from Section 4, see (4.5) and [22, eqn. (B.20)]. Thus the three integrals in line (5.98) are $O(1)$ by the estimates $\|\tilde{g}\| \le 1$, $\|c\|, \|\mathrm{ad}_{d^E}(h)\| = O(1)$, $\|R\|$, $\left\|R^E\right\| \le |\mathrm{Im}(z)|^{-1}$, and Corollary B.5 with $(p, l) = (1, 0)$, $(2, 1)$. This shows (5.95) with $k = 1$.

Suppose now (5.95) holds with some $k \geq 1$, and we prove it for $k \to k+1$. First, we note the relation $R^E - R = RbR^E$ and so

$$\begin{aligned} \mathrm{Rem}_1(k) &= \int (Rb)^k R + \int (Rb)^k (R^E - R) \\ &= \int (Rb)^k R + \int (Rb)^{k+1} R^E = s^k \bar{\xi}_k + \mathrm{Rem}_1(k+1), \end{aligned} \tag{5.99}$$

where $\bar{\xi}_k$ is defined by (5.85). Right-multiplying $\tilde{g}\tilde{\chi}$ on both sides of (5.99) and rearranging, we find

$$\mathrm{Rem}_1(k+1)\tilde{g}\tilde{\chi} = \mathrm{Rem}_1(k)\tilde{g}\tilde{\chi} - s^k \bar{\xi}_k \tilde{g}\tilde{\chi}. \tag{5.100}$$

The first term on the r.h.s. is $O(1)$ by induction hypothesis. The second term is $O(s^{k-n})$ by (5.86) proved earlier. Since $k \leq n$, this completes the induction and the proof of Lemma 5.8. □

Since $\mathrm{Rem}_1 \equiv \mathrm{Rem}_1(n)$ in Lemma 5.8, estimate (5.95) implies (5.87). This, together with (5.86), implies the claim (5.83). This completes the proof of Proposition 5.7. □

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- Data availability: Data sharing is not applicable to this article as no datasets were generated or analysed during the current study.

Appendix A. Existence of unique solution to vNL equation

In this section, we prove existence of unique mild solution to (1.1) in the Schatten space S^1 of trace-class operators. Throughout the section, we assume **(W1)**, i.e. $\sum_{j\geq 1} W_j^* W_j$ with W_j in (1.1) converges strongly.

The main mechanism is the following theorem (see e.g. [6, Theorem 3.1.33]):

Theorem A.1. *Let U be a strongly continuous semigroup on the Banach space X with generator S and let P be a bounded operator on X. Then, $S + P$ generates a strongly continuous semigroup U^P.*

In our case, X is the Schatten space $\mathcal{S}^1$ with trace-norm $\|\cdot\|_1$, the strongly continuous semigroup U is the unitary semigroup generated by $-i[H, \cdot]$ and the perturbation P is the Lindblad operator G (see (1.1)).

In the next lemma, we show that G is norm closed and bounded, so that Theorem A.1 indeed applies.

Lemma A.2. *The Lindblad operator G defined in* (1.1) *is bounded on $\mathcal{S}_1$.*

Proof. Without loss of generality, we assume $\rho \in \mathcal{S}^1$ is positive. Let $G_j(\cdot) = W_j\,(\cdot)\,W_j^* - \frac{1}{2}\{W_j^* W_j, (\cdot)\}$. For a positive ρ, it is clear the operators $W_j \rho W_j^*$ and $\{W_j^* W_j, \rho\}$ are positive for all j. Then, by cyclicity of the trace, we have

$$\begin{aligned} \|G_j(\rho)\|_1 &\le \|W_j\rho W_j^*\|_1 + \frac{1}{2}\|\{W_j^*W_j,\rho\}\|_1 \\ &\le \operatorname{Tr}|W_j\rho W_j^*| + \frac{1}{2}\operatorname{Tr}|\{W_j^*W_j,\rho\}| \\ &= \operatorname{Tr}(W_j\rho W_j^*) + \frac{1}{2}\operatorname{Tr}(\{W_j^*W_j,\rho\}) \\ &= 2\operatorname{Tr}(W_j^*W_j\rho). \end{aligned} \tag{A.1}$$

Thus,

$$\|G(\rho)\|_1 = \left\|\sum_{j\ge 1} G_j(\rho)\right\|_1 \le 2\sum_{j\ge 1}\operatorname{Tr}(W_j^*W_j\rho) \le 2\left\|\sum_{j\ge 1} W_j^*W_j\right\|\|\rho\|_1. \tag{A.2}$$

Since $\sum_{j\ge 1} W_j^* W_j$ is bounded by the uniform boundedness theorem, this proves G is bounded on $\mathcal{S}_1$, which completes the proof. □

Theorem A.1 shows that (1.1) has a unique strong solution in $\mathcal{D}(L)$ and a unique mild solution in $\mathcal{S}_1$. We denote the semigroup generated by vNL operator L by β_t as before. Note that since $e^{L_0 t}$ is a group (defined on $\mathbb{R}$), then so is $\beta_t = e^{Lt}$.

The positivity preserving property of β_t follows from [9, Theorem 5.2]. We summarize the key result in the following lemma:

Lemma A.3. *The semigroup β_t is positive for all $t \ge 0$.*

Proof. First, we rewrite the vNL operator L as

$$L(\rho) = -iK_{H+iP}(\rho) + F(\rho), \tag{A.3}$$

where $P = P^* = \frac{1}{2}\sum_{j\ge 1} W_j^* W_j$, $K_A(\rho) = A\rho - \rho A^*$ and $F(\rho) = \sum_{j\ge 1} W_j \rho W_j^*$.

Let $B_t = e^{-iHt-Pt}$, which is well-defined since P is bounded by assumption. It is easy to check that the semigroup S_t generated by $-iK_{H+iP}$ is given by

$$S_t(\rho) = B_t \rho B_t^*, \tag{A.4}$$

which obviously defines a positive semigroup. On the other hand, since

$$\sum_{j\ge 1} W_j \rho W_j^* \ge 0$$

for all $\rho \ge 0$, then F generates a positive semigroup e^{Ft}.

Finally, by Trotter-Lie formula, we have

$$\beta_t(\rho) = \lim_{n\to\infty} (S_{t/n} e^{Ft/n})^n(\rho), \tag{A.5}$$

where the limit is taken in the trace-norm. Hence the semigroup β_t is positive. □

Note that (A.5) yields another way to construct the semigroup $\beta_t = e^{Lt}$.

Appendix B. Remainder estimates

In this appendix and the next one, we present some estimates and commutator expansions, first derived in [36] and then improved in [16, 22, 23, 39]. We adapt some of the arguments from [22] and refer to this paper for details and references.

Throughout this section we fix an integer $\nu \geq 0$. For integers $p \geq 0$ and smooth functions $f \in C^{\nu+2}(\mathbb{R})$, we define a weighted norm

$$\mathcal{N}(f,p) := \sum_{m=0}^{\nu+2} \int_{\mathbb{R}} \langle x\rangle^{m-p-1} \left| f^{(m)}(x) \right| dx. \tag{B.1}$$

Note that

$$p \leq p' \implies \mathcal{N}(f,p') \leq \mathcal{N}(f,p), \tag{B.2}$$

and we have the following property:

Lemma B.1. *Let $p \geq 0$ be an integer. Suppose $f \in C^{\nu+2}$ and there exist C_0, $\rho > 0$ such that, for $m = 0, \ldots, \nu+2$,*

$$\left\| \langle x\rangle^{m-p+\rho} f^{(m)}(x) \right\|_{L^\infty} \leq C_0. \tag{B.3}$$

Then there exists $C > 0$ depending only on ρ, C_0, ν such that

$$\mathcal{N}(f,p) \leq C. \tag{B.4}$$

Proof. We have

$$\begin{aligned}\mathcal{N}(f,p) \leq & \sum_{m=0}^{\nu+2} \left\| \langle x\rangle^{m-p+\rho} f^{(m)}(x) \right\| \int_{\mathbb{R}} \langle x\rangle^{-1-\rho} dx \\ \leq & (\nu+3) C_0 \int_{\mathbb{R}} \langle x\rangle^{-1-\rho} dx,\end{aligned}$$

and the integral converges for $\rho > 0$. □

Corollary B.2. *Let p and l be two integers with $p > l \geq 0$. If $f \in C^\infty(\mathbb{R})$ and $f^{(l+1)}$ has compact support, then* (B.4) *holds.*

Proof. It suffices to verify condition (B.3) for the function f, whence (B.4) follows from Lemma B.1. For $m \geq l+1$, (B.3) holds since $f^{(m)} \in C_c^\infty$. For $m \leq l$, integrating $f^{(l+1)}$ shows that $\left|f^{(m)}(x)\right| \leq C \langle x\rangle^{l-m}$. Since $p \geq l+1$, we have (B.3) with $\rho = 1$. □

Write $z = x + iy \in \mathbb{C}$. In what follows, as in [22, Eq. (B.5)], for $f \in C^{\nu+2}(\mathbb{R})$, we take $\tilde{f}(z)$ to be an almost analytic extension of f defined by

$$\tilde{f}(z) := \eta\left(\frac{y}{\langle x\rangle}\right) \sum_{k=0}^{\nu+1} f^{(k)}(x) \frac{(iy)^k}{k!}, \tag{B.5}$$

where $\eta \in C_c^\infty(\mathbb{R})$ is a cutoff function with $\eta(\mu) \equiv 1$ for $|\mu| \leq 1$, $\eta(\mu) \equiv 0$ for $|\mu| \geq 2$, and $|\eta'(\mu)| \leq 1$ for all μ. This $\tilde{f}(z)$ induces a measure on $\mathbb{C}$ as

$$d\tilde{f}(z) := -\frac{1}{2\pi} \partial_{\bar{z}} \tilde{f}(z) dx\, dy. \tag{B.6}$$

In the remainder of this appendix, we derive integral estimate for various functions against the measure (B.6).

The next result is obtained by adapting the argument in [22, Lem. B.1]:

Lemma B.3 (Remainder estimate)**.** *Let* $0 \le p \le \nu$*. Let* $f \in C^{\nu+2}(\mathbb{R})$ *satisfy* (B.4)*. Then the extension* $\tilde{f}$ *from* (B.5) *satisfies the following estimate for some* $C = C(f, \nu, p) > 0$:

$$\int \left| d\widetilde{f}(z) \right| |\mathrm{Im}(z)|^{-(p+1)} \le C. \tag{B.7}$$

Proof. Differentiating formula (B.5), we obtain the estimate

$$\left|\partial_{\bar{z}} \tilde{f}(z)\right| \le \eta\left(\frac{y}{\langle x\rangle}\right) \frac{|y|^{\nu+1}}{(\nu+1)!} \left|f^{(\nu+2)}(x)\right| + \sum_{k=0}^{\nu+1} \rho\left(\frac{y}{\langle x\rangle}\right) \frac{|y|^k}{k!} \left|\frac{1}{\langle x\rangle} f^{(k)}(x)\right|, \tag{B.8}$$

where

$$\rho(\mu) := |\eta'(\mu)| \langle \mu \rangle \tag{B.9}$$

is supported on $1 < |\mu| < 2$.

For each fixed x, we define

$$G(x) := p.v. \int |\partial_{\bar{z}} f(z)| \, |y|^{-(p+1)} \, dy \tag{B.10}$$

by integrating (B.8) against $|y|^{-(p+1)}$. Using that $\eta(y/\langle x\rangle) \equiv 0$ for $|y| > \langle x\rangle$ and $\rho(y/\langle x\rangle) \equiv 0$ for $|y| \le \langle x\rangle$ or $|y| \ge 2\langle x\rangle$, we find

$$G(x) \le \int_{|y| \le \langle x\rangle} \frac{|y|^{\nu-p}}{(\nu+1)!} \eta\left(\frac{y}{\langle x\rangle}\right) dy \left|f^{(\nu+2)}(x)\right| \tag{B.11}$$

$$+ \sum_{k=0}^{\nu+1} \int_{\langle x\rangle < |y| < 2\langle x\rangle} \rho\left(\frac{y}{\langle x\rangle}\right) \frac{|y|^{k-p-1}}{k!} \, dy \left|\frac{1}{\langle x\rangle} f^{(k)}(x)\right|. \tag{B.12}$$

Since $0 \le \eta(\mu) \le 1$ and $\nu \ge p$, the integral in line (B.11) converges and can be bounded as

$$\int_{|y| \le \langle x\rangle} \frac{|y|^{\nu-p}}{(p+1)!} \eta\left(\frac{y}{\langle x\rangle}\right) dy \left|f^{(p+2)}(x)\right| \le \frac{2\langle x\rangle^{\nu-p+1}}{(p+1)!} \left|f^{(p+2)}(x)\right|. \tag{B.13}$$

To bound line (B.12), we use that $\rho(y/\langle x\rangle) < \sqrt{5}$ and $|y|^{k-p-1} \le \langle x\rangle^{k-p-1}$ for $\langle x\rangle < |y| < 2\langle x\rangle$, $0 \le k \le p+1$ (see (B.9)). Thus each integral in line (B.12) can be bounded as

$$\sum_{k=0}^{\nu+1} \int_{\langle x\rangle < |y| < 2\langle x\rangle} \rho\left(\frac{y}{\langle x\rangle}\right) \frac{|y|^{k-p-1}}{k!} \, dy \left|\frac{1}{\langle x\rangle} f^{(k)}(x)\right|$$

$$\le \sum_{k=0}^{p+1} \frac{4\sqrt{5}\langle x\rangle^{k-p-1}}{k!} \left|f^{(k)}(x)\right| + \sum_{k=p+1}^{\nu+1} \frac{\sqrt{5} \cdot 2^{k-p+1} \langle x\rangle^{k-p-1}}{k!} \left|f^{(k)}(x)\right|. \tag{B.14}$$

Combining (B.13)–(B.14) in (B.12), we conclude that

$$|G(x)| \le CF(x), \quad F(x) := \sum_{m=0}^{\nu+2} \langle x\rangle^{m-p-1} \left|f^{(m)}(x)\right|. \tag{B.15}$$

Let $G_\lambda(x) := \mathbf{1}_{[-\lambda,\lambda]} G(x)$ with $\lambda > 0$. Then $G_\lambda \in L^1$ and $|G_\lambda(x)| \le CF(x)$ for any λ. By assumption (B.4) and definition(B.1), we have $\|F\|_{L^1} = \mathcal{N}(f, p) < \infty$

and so $F \in L^1$. Therefore, sending $\lambda \to \infty$ and using the dominated convergence theorem yields $G \in L^1$ with

$$\|G\|_{L^1} \le C \|F\|_{L^1}. \tag{B.16}$$

Recalling definition (B.10), we find $(2\pi)^{-1} \|G\|_{L^1}$ =l.h.s. of (B.7). Thus we conclude (B.7) from (B.16). □

Lemma B.3 and Corollary B.2 together imply the following results:

Corollary B.4. *Let p and l be two integers with $\nu \ge p > l \ge 0$. If $f \in C^\infty(\mathbb{R})$ and $f^{(l+1)}$ has compact support, then there exists $C > 0$ such that the extension $\tilde{f}$ from* (B.5) *satisfies the remainder estimate* (B.7).

Corollary B.5. *Let p and l be two integers with $\nu \ge p > l \ge 0$. Let $P_l(x)$ be a polynomial with* deg $\le l$. *Let $f \in C^\infty(\mathbb{R})$ have compactly supported derivatives. Then there exists $C > 0$ such that the extension $\tilde{f}$ from* (B.5) *satisfies*

$$\int \left| d\widetilde{f}(z) P_l(z) \right| |\mathrm{Im}(z)|^{-(p+1)} \le C. \tag{B.17}$$

Proof. Let $f_l(x) := P_l(x)\chi(x)$. Observe that since $\partial_{\bar{z}} P_l(z) = 0$, we have by (B.6) that

$$P_l(z) d\widetilde{f}(z) = d\widetilde{f_l}(z). \tag{B.18}$$

We compute

$$f_l^{(l+1)} = P_l^{(l+1)} f + \sum_{k=0}^{l} \binom{l+1}{k} P_l^{(k)} f^{(l+1-k)}. \tag{B.19}$$

The term leading term on the r.h.s. vanishes since $\deg p \le l$. Each term in the sum lies in C_c^∞ since $f^{(q)} \in C_c^\infty$ for $q \ge 1$. Thus f_l verifies the condition of Corollary B.4 and so (B.17) follows. □

Appendix C. Commutator expansions

In this appendix, we take $\tilde{f}(z)$, $d\widetilde{f}(z)$ to be as in (B.5)–(B.6).

We frequently use the following result, taken from [22, Lemma B.2]:

Lemma C.1. *Let $f \in C^{\nu+2}(\mathbb{R})$ satisfy* (B.4) *for some $p \ge 0$. Then for any self-adjoint operator A on $\mathcal{H}$,*

$$\frac{1}{p!} f^{(p)}(A) = \int_{\mathbb{C}} d\tilde{f}(z)(z - A)^{-(p+1)}, \tag{C.1}$$

where the integral converges absolutely in operator norm and is uniformly bounded in A.

Remark 12. Note that (B.4) ensures $f^{(p)}$ is bounded independent of A and the remainder estimate in Lemma B.3 ensures the norm convergence of the r.h.s. of (C.1).

We call Equation (C.1) the *Helffer-Sjöstrand (HS) representation.* It is possible to obtain stronger results with less regularity assumption on f using some technical estimates from [2, Sec. 5]. We do not pursue this generality here, as the assumption (B.4) already suffices for our purposes.

The HS representation (C.1), together with the remainder estimate (B.7), implies the following commutator expansion:

Lemma C.2. *Let $n \geq 1$. Let $f \in C^{n+3}(\mathbb{R})$ satisfy* (B.4) *with $p = 1$. Let A be an operator on $\mathcal{H}$. Let Φ be a lower semi-bounded self-adjoint operator on $\mathcal{H}$. Let $f_s := f(s^{-1}(\Phi - \alpha))$ for some fixed α and all $s > 0$. Suppose there exists $c \geq 0$ such that*

$$(\Phi + c)^{-1}\mathcal{D}(A) \subset \mathcal{D}(A), \tag{C.2}$$

and

$$B_k := \mathrm{ad}_\Phi^k(A) \in \mathcal{B}(\mathcal{H}) \quad (1 \leq k \leq n+1). \tag{C.3}$$

Then $[A, f_s] \in \mathcal{B}(\mathcal{H})$, and we have the expansion

$$[A, f_s] = -\sum_{k=1}^{n} \frac{s^{-k}}{k!} B_k f_s^{(k)} - s^{-(n+1)} \mathrm{Rem}_{\mathrm{left}}(s) \tag{C.4}$$

$$= \sum_{k=1}^{n} (-1)^k \frac{s^{-k}}{k!} f_s^{(k)} B_k + (-1)^{n+1} s^{-(n+1)} \mathrm{Rem}_{\mathrm{right}}(s), \tag{C.5}$$

where the remainders are defined by these relations and given explicitly by (C.13)–(C.14)*. Moreover, there exists $c > 0$ depending only on n and $\mathcal{N}(f, n+1)$, such that*

$$\|\mathrm{Rem}_{\mathrm{left}}(s)\|_{\mathrm{op}} + \|\mathrm{Rem}_{\mathrm{right}}(s)\|_{\mathrm{op}} \leq c \|B_{n+1}\|. \tag{C.6}$$

Proof. Within this proof we write $R = (z - x_s)^{-1}$ with $x_s = s^{-1}(\Phi - \alpha)$. Hypothesis (C.2) shows that

$$R = (\Phi + c)^{-1}(z(\Phi + c)^{-1} - x_s(\Phi + c)^{-1})^{-1}$$

maps $\mathcal{D}(A)$ into itself for z with large $|\mathrm{Im}(z)|$ and therefore for all z with $\mathrm{Im}(z) \neq 0$.

It follows that

$$\big[A, R\big] = -s^{-1} R \, \mathrm{ad}_\Phi(A) R \tag{C.7}$$

holds in the sense of quadratic forms on $\mathcal{D}(A)$. Since R is bounded and $\mathrm{ad}_\Phi(A)$ is bounded by assumption, the r.h.s. of (C.7) is bounded and so $[A, R]$ extends to a bounded operator on $\mathcal{H}$.

Using (C.7), we proceed by commuting successively the commutators $B_k := \mathrm{ad}_\Phi^k(A)$ to left and right, respectively. This way we obtain

$$[A, R]$$

$$= -\sum_{k=1}^{n} s^{-k} B_k R^{k+1} - s^{-(n+1)} R B_{n+1} R^{n+1} \tag{C.8}$$

$$= \sum_{k=1}^{n} (-1)^k s^{-k} R^{k+1} B_k + (-1)^{n+1} s^{-(n+1)} R^{n+1} B_{n+1} R, \tag{C.9}$$

which hold on all of $\mathcal{H}$ since B_k's are bounded operators by assumption (C.3).

Since f may not decay at ∞, we cannot directly express $f_s = f(s^{-1}(\Phi - \alpha))$ using the HS representation C.1. We therefore introduce a cutoff as follows. Let $\eta^\lambda \in C_c^\infty(\mathbb{R})$, $\lambda > 0$ be cutoff functions with $\eta^\lambda(x) \equiv 1$ for $|x| \leq \lambda$, $\eta(x) \equiv 0$ for $|\mu| \geq \lambda + 1$, and $\|\eta^\lambda\|_{C^{n+3}} \leq C$ for all λ. Set $f^\lambda := \eta^\lambda f$. Since $f^\lambda \in C_c^{n+3}$, it satisfies (B.4) for all $p \geq 0$. Thus the HS representation C.1 holds with $p = 0$ and so

$$[A, f_s^\lambda] = \int d\widetilde{f^\lambda}(z)\big[A, R\big], \tag{C.10}$$

which holds a priori on $\mathcal{D}(A)$.

Plugging expansions (C.8)–(C.9) into (C.10) yields

$$\begin{aligned}
&[A, f_s^\lambda] \\
&= -\sum_{k=1}^{n} \frac{s^{-k}}{k!} B_k \int d\widetilde{f^\lambda}(z) R^{k+1} - s^{-(n+1)} \mathrm{Rem}^\lambda_{\mathrm{left}}(s), && \text{(C.11)}\\
&= \sum_{k=1}^{n} (-1)^k \frac{s^{-k}}{k!} \int d\widetilde{f^\lambda}(z) R^{k+1} B_k + (-1)^{n+1} s^{-(n+1)} \mathrm{Rem}^\lambda_{\mathrm{right}}(s), && \text{(C.12)}
\end{aligned}$$

where

$$\mathrm{Rem}^\lambda_{\mathrm{left}}(s) = \int d\widetilde{f^\lambda}(z) R B_{n+1} R^{(n+1)}, \tag{C.13}$$

$$\mathrm{Rem}^\lambda_{\mathrm{right}}(s) = \int d\widetilde{f^\lambda}(z) R^{(n+1)} B_{n+1} R. \tag{C.14}$$

Since the operator B_{n+1} is bounded independent of λ, z, and $\|R\| \leq |\mathrm{Im}(z)|^{-1}$, we have

$$\begin{aligned}
&\left\|\mathrm{Rem}^\lambda_{\mathrm{left}}(s)\right\|_{\mathrm{op}} + \left\|\mathrm{Rem}^\lambda_{\mathrm{right}}(s)\right\|_{\mathrm{op}} \\
&\leq 2\|B_{n+1}\| \int |d\widetilde{f^\lambda}(z)| R^{n+2} \\
&\leq 2\|B_{n+1}\| \int |d\widetilde{f^\lambda}(z)| |\mathrm{Im}(z)|^{-(n+2)}. && \text{(C.15)}
\end{aligned}$$

Similarly we could bound the sums in (C.11)–(C.12). Thus we see $[A, f_s^\lambda]$ extends to a bounded operator on $\mathcal{H}$ for each λ.

By (B.2) and the assumption $\mathcal{N}(f, 1) \leq C$, f satisfies condition (B.4) with $p = 1, \ldots, n+1$. Hence, sending $\lambda \to \infty$ in (C.11)–(C.14) and using (C.1) for $p = 1, \ldots, n$ and the remainder estimate (B.7) for $p = n+1$, we conclude that $[A, f_s] \in \mathcal{B}(\mathcal{H})$ and expansions (C.4)–(C.5) and estimate (C.6) hold. □

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Paper B

On propagation of information in quantum many-body systems

ON PROPAGATION OF INFORMATION IN QUANTUM MANY-BODY SYSTEMS

ISRAEL MICHAEL SIGAL AND JINGXUAN ZHANG

ABSTRACT. We prove bounds on the minimal time for quantum messaging, propagation/creation of correlations, and control of states for *general* lattice quantum many-body systems. The proofs are based on a maximal velocity bound, which states that the many-body evolution stays, up to small leaking probability tails, within a light cone of the support of the initial conditions. This estimate is used to prove the light-cone approximation of dynamics and Lieb-Robinson-type bound, which in turn yield the results above. Our conditions cover long-range interactions.

CONTENTS

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Key words and phrases. Maximal propagation speed; Lieb-Robinson bounds; quantum many-body systems; quantum information; quantum light cones.

1. Introduction

The finite speed of propagation of particles and fields is a fundamental law of nature. It provides powerful constraints in relativistic physics. It is remarkable that such constraints also effectively exist in non-relativistic quantum theory, the only quantum theory with a solid mathematical foundation and physical consistency. This was discovered by Lieb and Robinson ([35]) 50 years ago, for quantum spin lattice systems, in a form of space-time bounds on the commutators of observables with disjoint space-time supports.

About 40 years later, starting with the work of Hastings ([23]) on the Lieb-Schultz-Mattis theorem and followed by Nachtergaele and Sims ([38]) on exponential decay of correlations in condensed matter physics, Bravyi, Hastings and Verstraete ([7]), Bravyi and Hastings ([6]), Eisert and Osborn ([12]) and Hastings ([25, 26]) on quantum messaging, correlation creation, scaling and area laws for the entanglement entropy and belief propagation in Quantum Information Science (QIS), it transpired that Lieb-Robinson bounds (LRBs) are among the very few effective and general tools that are available for analyzing quantum many-body systems.[1]

In the last 15 years, following these works, a new active area of theoretical and mathematical physics dealing with dynamics of quantum information sprung to life. A variety of improvements of the original LRB, e.g., extensions to long-range spin interactions, fermionic lattice gases and finally to bosonic systems, have been achieved, and their applications expanded and deepened to include, e.g. the state transport ([14, 16]) and the error bounds on quantum simulation algorithms (see e.g. [47, 49]) in QIS, the equilibration ([20]) in condensed matter physics, thermodynamic limit of dynamics ([36, 37, 40]) in Statistical Mechanics and scrambling time in Quantum Field Theory [43]. See the survey papers [30, 39] and brief reviews in [15, 16].

Independently and using a different approach, it was shown in [45] that in Quantum Mechanics the "essential support" of the wave functions, i.e. the support up to negligible probability tails, spreads with finite speed. The result was improved in [1, 28, 46] and extended to the nonrelativistic QED in [3] and to condensed matter physics, i.e. to systems with positive particle densities, in [15, 16].

[1] It is clear in hindsight that Lieb-Robinson-type bounds on the propagation of information would play a central role in QIS.

In this paper, we prove bounds on the minimal time for quantum messaging, propagation/creation of correlations (scrambling time[2]) and control of states, for general quantum many-body lattice systems.[3] Fixing a lattice $\mathcal{L} \subset \mathbb{R}^d$, $d \geq 1$, such systems are described by the Hamiltonians [4]

$$H_\Lambda := \sum_{x,y\in\Lambda} h_{xy} a_x^* a_y + \frac{1}{2} \sum_{x,y\in\Lambda} a_x^* a_y^* v_{xy} a_y a_x, \tag{1.1}$$

for subsets Λ of $\mathcal{L}$, acting on the bosonic Fock spaces[5] $\mathcal{F}_\Lambda$ over the 1-particle Hilbert spaces $\mathfrak{h}_\Lambda := \ell^2(\Lambda)$. Here a_x and a_x^* are the annihilation and creation operators, respectively, h_{xy} is the operator kernel (matrix) of an 1-particle Hamiltonian h acting on $\mathfrak{h}$ and v_{xy} is a 2-particle pair potential. We assume that h is hermitian, i.e. $h_{xy} = \overline{h_{yx}}$ and v is real-symmetric, i.e. $v_{xy} = \overline{v_{xy}} = v_{yx}$.

Our main results are given in Theorems 2.1–2.8 below. Our starting point is the maximal velocity bound (MVB), Theorem 2.1, which states that the many-body evolution stays, up to small leaking tails, within a light cone of the support of the initial conditions. We use the MVB to derive Theorem 2.2 on the light-cone approximation of quantum dynamics, which, in turn, yields the weak LRB, Theorem 2.3. The latter establishes power-law decay of commutators of evolving observables and holds (uniformly) on *a subset of localized states*.

Theorems 2.4–2.7 provide general constraints on propagation/creation of correlation, quantum messaging, state control times, and the relation between a spectral gap and the decay of correlations. They are derived readily from Theorems 2.2 and 2.3. Theorem 2.8 describes macroscopic particle transport. Its proof extends in an essential way the proof of Theorem 2.1.

For pure states, the correlation signifies entanglement and Theorem 2.4 gives bounds on the time for propagation/creation of entanglement between different regions within a given spatial domain.

To emphasize, our results yield the existence of a linear light cone for general lattice quantum many-body systems, providing powerful constraints on the evolution of information for such systems.

The bounds on the maximal speed of propagation are given in terms of the norm of the 1-particle group velocity operator $i[h, x]$, where x is the 1-particle Hamiltonian entering (1.1) and the position observable, respectively.

The Hamiltonians under consideration in this paper are characterized by two decay rates, one for h_{xy} and the other, for v_{xy}. We assume that there exists $n \geq 1$

[2]The scrambling time could be defined as the time an initially uncorrelated subsystem stays uncorrelated (i.e. the time needed to create correlations). In particular, our results imply non-existence of fast scramling, c.f. [9, 31].

[3]From the condensed matter physics viewpoint, such systems arise in the standard tight-binding approximation, see e.g. [18] and, for rigorous results, [2, 22]. We consider them to avoid inessential technicalities in the proof of the approximation result, Theorem 2.2.

[4]For background on the second quantization and quantum many-body systems, see [5, 21].

[5]See Appendix A for the definitions and discussions of Fock spaces.

s.th.

$$\kappa_n := \sup_{x\in\Lambda} \sum_{y\in\Lambda} |h_{xy}|\,|x-y|^{n+1} < \infty, \tag{1.2}$$

$$\nu_n := \sup_{x\in\Lambda} \sum_{y\in\Lambda} |v_{xy}|\,|x-y|^{n} < \infty. \tag{1.3}$$

Moreover, in Theorem 2.1, we do not use condition (1.3) and allow v_{xy} to be arbitrary (apart from the standing assumption $v_{xy} = \overline{v_{xy}} = v_{yx}$). The parameter $n \geq 1$ in (1.2)–(1.3) determines the time-/ space-decay rate in various statements.

All our results hold for bosonic systems with long-range interactions[6], say, $|h_{xy}| \leq C(1+|x-y|)^{-\alpha}$ with $\alpha > d+n+1$ and similarly for v, which suffices for (1.2)–(1.3). Taking $n = 1$, we see that, for $d > 1$ and $\alpha \in (d+2, 2d+1)$, our result gives a linear light cone as defined in terms of the weak LRB (2.17). On the other hand, fast state-transfer and entanglement-generation protocols [13, 33, 34, 48, 50] show that linear light cones, defined in terms of the LRB, do not exist for $\alpha < 2d+1$. See [49] for the phase diagram summarizing the situation for the Lieb-Robinson light cones and [4, 10] for reviews of the effect of the long-range interactions on quantum many-body dynamics and, in particular, on the transmission of quantum information. Thus our bounds narrow the class of systems for which long-range interactions lead to speed-up of the spreading of information[7].

Our results can be extended to Hamiltonians with time-dependent and few-body interactions and adapted to long-range fermionic systems.

1.1. **Related results.** Results similar to Theorems 2.1–2.3, 2.5–2.6, and 2.8, but for the Bose-Hubbard model, were obtained in [15,16]. Our proofs of those theorems follow the corresponding proofs in [15, 16]. The rendition in the present paper is more geometric, which streamlines the derivations and makes the arguments more transparent. Furthermore, we view the results in Theorem 2.6 as bounds on quantum control time, rather than those on the time for state transfer as in [14,16].

Earlier on, results similar to Thms 2.1 and 2.2 and 2.3 have previously been obtained in [44], [51] and [34], respectively (the last two papers deal with the Bose-Hubbard model), for detailed comparisons, see Remark 8 in Section 2.9. Moreover, LRB for a special class of bosonic lattice systems was proved in [41].

The constraints imposed by the LRB on the propagation/creation of correlations were first discussed in [7], with rigorous results for fermionic systems given in [36].

The relation between spectral gap and the decay of correlations (clustering) for fermionic systems was established in [23, 24, 27, 38], with the sharpest results given in [38].

As we were preparing the present paper for publication, a new preprint [32] was posted with deep results related to those in Thms. 2.1–2.2 for rather general finite-range quantum many-body Hamiltonians. Assuming the initial state satisfies a uniform low density condition, the authors of [32] proved the existence of the superlinear light cone $|x| \sim t \log t$ (resp. $|x| \sim t^d \operatorname{polylog} t$, where d is the dimension

[6]In the present context, H is said to be short-/long-range if h_{xy}, v_{xy} decay exponentially/polynomially in $|x-y|$.

[7]We are grateful to Marius Lemm for pointing this out to us.

and polylog is the polylogarithmic function) for particle transport (resp. the light-cone approximation of observables), up to fast decaying leaking probability tails.

1.2. **Organization of the paper.** In Section 2, we describe the dynamics generated by the Hamiltonian (1.1) and formulate the main results of this paper, Theorems 2.1-2.8. Their proofs are given in Sects. 3–11. The technicalities are deferred to the appendices, with Appendix A containing some general facts about the Fock spaces. In Section 2.9, we comment on possible extensions of the main theorems.

1.3. **Notation.** Throughout the paper, we fix the underlying lattice $\mathcal{L}$, with grid size ≥ 1, and the domain $\Lambda \subset \mathcal{L}$, and we do not display these in our notations, e.g., we write H, $\mathcal{F}$, and $\mathfrak{h}$ for H_Λ, $\mathcal{F}_\Lambda$, and $\mathfrak{h}_\Lambda$.

We denote by $\mathcal{D}(A)$ the domain of an operator A and $\|\cdot\|$, the norm of operators on $\mathcal{F}$ and sometimes on $\mathfrak{h}$. For a bounded operator A on $\mathfrak{h}$, we denote by A_{xy}, $x, y \in \Lambda$, the operator kernel (matrix) of A. We make no distinction in our notation between a function $f \in \mathfrak{h}$ and the associated multiplication operator $\psi(x) \mapsto f(x)\psi(x)$ on $\mathfrak{h}$.

All quantities and equations we work with are dimensionless. In particular, in our units, the Planck constant is set to 2π and speed of light, to one ($\hbar = 1$ and $c = 1$).

2. Setup and main results

For symmetric h and v, the Hamiltonian H in (1.1) is symmetric and therefore self-adjoint. To show the latter, one can use the canonical commutator relations to show that the number operator

$$N \equiv N_\Lambda, \quad \text{where} \quad N_X := \sum_{x \in X} a_x^* a_x, \tag{2.1}$$

commutes with H. Since the operators $H_n := H \restriction_{\{N=n\}}$, $n = 0, 1, \ldots$, are symmetric and bounded, they are self-adjoint. Hence so is $H = \oplus_{n=0}^\infty H_n$ as an infinite direct sum of self-adjoint operators. Therefore the propagator e^{-itH} is well-defined for every $t \in \mathbb{R}$.

It is convenient to extend the state space $\mathcal{F}$ by going to the space $S(\mathcal{F})$ of density operators on $\mathcal{F}$, i.e. positive trace-class operators ρ on $\mathcal{F}$, which we identify with positive linear functionals (i.e. expectations) of observables, $\omega(A) \equiv \omega_\rho(A) := \mathrm{Tr}(A\rho)$. Consequently, we pass from the Schrödinger equation $i\partial_t \psi = H\psi$ on $\mathcal{F}$, to the von Neumann equation

$$\partial_t \rho_t = -i[H, \rho_t] \quad \text{or} \quad \partial_t \omega_t(A) = \omega_t(i[H, A]). \tag{2.2}$$

The domain of $\mathrm{ad}_H : A \mapsto [A, H]$ in the space $S(\mathcal{F})$ of density operators over the Fock space $\mathcal{F}$ is given by

$$\mathcal{D} := \{\rho \in S(\mathcal{F}) \mid \rho\mathcal{D}(H) \subset \mathcal{D}(H) \text{ and } [H, \rho] \in S(\mathcal{F})\}, \tag{2.3}$$

We write $\omega \in \mathcal{D}$ if $\omega = \omega_\rho$ for some $\rho \in \mathcal{D}$. For each $\rho \in \mathcal{D}$, the Cauchy problem (2.2) with initial configuration ρ has a unique solution given by

$$\rho_t \equiv \alpha_t'(\rho) := e^{-itH} \rho e^{itH}. \tag{2.4}$$

It is straightforward to check that the evolution (2.4) preserves total probability and positivity, i.e.,

$$\mathrm{Tr}(\rho_t) \equiv \mathrm{Tr}(\rho) \quad \text{and} \quad \rho \geq 0 \implies \rho_t \geq 0 \quad (t \in \mathbb{R}), \tag{2.5}$$

as well as the eigenvalues of ρ.

The evolution of observables, dual to α_t' in (2.4) w.r.t. the coupling $(A, \rho) \mapsto \mathrm{Tr}(A\rho)$, is given by

$$A_t \equiv \alpha_t(A) := e^{itH} A e^{-itH}. \tag{2.6}$$

In terms of linear functionals with initial condition ω, evolution (2.4) becomes $\omega_t(A) = \omega(A_t)$, where $\omega_t = \omega \circ \alpha_t$, and relations (2.5) become $\omega_t(\mathbf{1}) \equiv \omega(\mathbf{1})$ and $\omega \geq 0 \implies \omega_t \geq 0$.

Below, we evaluate our inequalities on states ω (which we also consider as initial conditions for (2.2)) satisfying the following conditions:

$$\omega \in \mathcal{D}, \quad \omega(N^2) < \infty, \tag{2.7}$$

where, recall, $N \equiv N_\Lambda$ is the total number operator. In what follows, for a subset $X \subset \Lambda$, we denote by $X^c := \Lambda \setminus X$ its complement in Λ, $d_X(x) \equiv \mathrm{dist}(\{x\}, X) := \inf_{y \in X} |x - y|$ the distance function to X, $X_\xi := \{x \in \Lambda : d_X(x) \leq \xi\}$ (see Figure 1 below), and X_ξ^c is always understood as $(X_\xi)^c$.

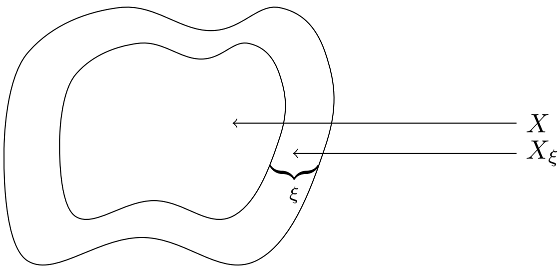

FIGURE 1. Schematic diagram illustrating X_ξ.

Finally, let

$$\kappa \equiv \kappa_0 = \sup_{x \in \Lambda} \sum_{y \in \Lambda} |h_{xy}| \, |x - y| \,. \tag{2.8}$$

The number κ bounds the norm of the 1-particle group velocity operator $i[h, x]$, see Remark 6 below.

2.1. **Maximal velocity bound.** The main result in this section gives an estimate on the maximal velocity of propagation of particles into empty regions. Continuing with terminology of [15, 16, 45], we call such an estimate the *maximal velocity bound* (MVB).

Theorem 2.1 (MVB for lattice quantum many-body system)**.** *Suppose* (1.2) *holds with some $n \geq 1$. Then, for every $c > \kappa$, there exists $C = C(n, \kappa_n, c) > 0$ s.th. for all $\eta \geq 1$, $X \subset \Lambda$, we have the following estimate for all $|t| < \eta / c$:*

$$\alpha_t(N_{X_\eta^c}) \leq C(N_{X^c} + \eta^{-n} N). \tag{2.9}$$

Theorem 2.1 is proved in Section 3, with an outline given in Section 3.1. Here and below, an operator inequality $A \leq B$ means that $\omega(A) \leq \omega(B)$ for all states ω satisfying (2.7).

Estimate (2.9) shows that, if the initial condition ω satisfies (2.7) and is localized in X, then, up to polynomially vanishing probability tails, the particles propagate within the light cone

$$X_{ct} \equiv \{d_X(x) \leq ct\}$$

for every fixed $c > \kappa$ and all t. More precisely, if we assume the initial state satisfies

$$\omega(N_{X^c}) = 0, \tag{2.10}$$

and use the observation, due to M. Lemm, that under (2.10),

$$\omega(N^p) = \omega(N_X^p) \qquad (p = 1, 2), \tag{2.11}$$

we find, for all $|t| < \eta/c$,

$$\omega_t(N_{X_\eta^c}) = \omega(\alpha_t(N_{X_\eta^c})) \leq C\eta^{-n}\omega(N_X). \tag{2.12}$$

Put differently, the probability that particles are transported from X to any test (or probe) domain Y outside the light cone X_{ct} is of the order $O(\eta^{-n})$, where $\eta = \mathrm{dist}(X, Y)$.

2.2. **Light-cone approximation of evolution** (2.6)**.** The main result of this section and the next one concerns the evolution of general *local observables.* We say that an operator A acting on $\mathcal{F}$ is *localized* in $X \subset \Lambda$ if

$$\left[A, a_x^\sharp\right] = 0 \quad \forall x \in X^c, \tag{2.13}$$

where $a_x^\#$ stands for either a_x or a_x^*. Denote by $\mathrm{supp}\, A$ the intersection of all X s.th. (2.13) holds. Then A is localized in X if and only if

$$\mathrm{supp}\, A \subset X.$$

The support of an initially localized observable generally spreads over the entire space immediately for any $t > 0$. Nonetheless, in Theorem 2.2 below, we show that the evolution of local observables under (2.6) can be approximated by a family of observables localized within the light cone of the initial support.

To state our result, we introduce some notations. For a subset $X \subset \Lambda$, define the *localized evolution* of observables as

$$\alpha_t^X(A) := e^{itH_X} A e^{-itH_X}, \tag{2.14}$$

where H_X is defined by (1.1) but with X in place of Λ, and the set of operators

$$\mathcal{B}_X := \{A \in \mathcal{B}(\mathcal{F}) : [A, N] = 0, \mathrm{supp}\, A \subset X\}, \tag{2.15}$$

where $\mathcal{B}(\mathcal{F})$ is the space of bounded operators on $\mathcal{F}$. One can check using definitions (2.13), (2.14), and the relation $[H_X, N] = 0$ that, for all $A \in \mathcal{B}_X$, the evolution $\alpha_t^X(A)$ lies in $\mathcal{B}_X$ for all t.

The main result of this section is that the full evolution $\alpha_t(A)$ can be well approximated by the localized evolution $\alpha_t^{X_\xi}(A)$, supported inside the light cone of $\mathrm{supp}\, A$:

Theorem 2.2 (Light-cone approximation of quantum evolution)**.** *Suppose* (1.2)–(1.3) *hold with some* $n \geq 1$*. Suppose a state* ω *satisfies* (2.7) *and* (2.10)*, with some* $X \subset \Lambda$*. Then, for every* $c > 2\kappa$*, there exists* $C = C(n, \kappa_n, \nu_n, c) > 0$ *s.th. for all*

$\xi \geq 1$ and operator $A \in \mathcal{B}_X$ (see (2.15)), the full evolution $\alpha_t(A)$ is approximated by the local evolution $\alpha_t^{X_\xi}(A)$ for all $|t| < \xi/c$, as

$$\left|\omega\Big(\alpha_t(A) - \alpha_t^{X_\xi}(A)\Big)\right| \leq C\,|t|\,\xi^{-n}\,\|A\|\,\omega(N_X^2). \tag{2.16}$$

Theorem 2.2 follows from Theorem 2.9. We sketch the proof of Theorem 2.2 in Section 5.

2.3. **Lieb-Robinson-type bounds.** Using Theorem 2.2, we prove a Lieb-Robinson-type bound for general interacting quantum many-body systems:

Theorem 2.3 (Weak Lieb-Robinson bound)**.** *Suppose the assumptions of Theorem 2.2 hold with $n \geq 1$, $X \subset \Lambda$. Then, for every $c > 2\kappa$, there exists $C = C(n, \kappa_n, \nu_n, c) > 0$ s.th. for all $\xi \geq 1$, $Y \subset \Lambda$ with $\mathrm{dist}(X, Y) \geq 2\xi$, and operators $A \in \mathcal{B}_X$, $B \in \mathcal{B}_Y$, we have the following estimate for all $|t| < \xi/c$:*

$$|\omega([\alpha_t(A), B])| \leq C\,|t|\,\|A\|\,\|B\|\,\xi^{-n}\omega(N_X^2). \tag{2.17}$$

Theorem 2.3 is proved in Section 6. We call a bound of the form (2.17) the *weak Lieb-Robinson bound (LRB)*. Unlike the classical LRB, estimate (2.17) depends on a subclass of states and provides power-law, rather than exponential, decay.

Estimate (2.17) shows that, with the probability approaching 1 as $t \to \infty$, an evolving family of observable $A_t = \alpha_t(A)$ remains commuting with any other observable supported outside the light cone

$$\{x \in \Lambda \mid \mathrm{dist}(x, \mathrm{supp}\, A) \leq ct\},$$

for any fixed $c > 2\kappa$, provided the supports of these observables are separated by initially empty regions.

2.4. **Propagation/creation of correlations.** In this section we address the following questions (c.f. [7, 36]):

- Assuming the initial state ω is weakly correlated in a domain $Z^c \subset \Lambda$, how long does it take for the correlations in Z to spread, under the evolution (2.6), into Z^c? Put differently, how long does it take to create correlations in Z^c?

To begin with, we define what we mean by weakly correlated states.

Definition 2.1. Let $Z \subset \Lambda$. For subsets X, $Y \subset \Lambda$, let $d_{XY} := \mathrm{dist}(X, Y)$ and

$$d_{XY}^Z := \min(d_{XY}, d_{XZ}, d_{YZ}). \tag{2.18}$$

We say a state ω is *weakly correlated in a subset Z^c at a scale* $\lambda > 0$, or $\mathrm{WC}(Z^c, \lambda)$, if there exists $C > 0$ s.th. for all subsets X, $Y \subset Z^c$ with $d_{XY}^Z > 0$ and operators $A \in \mathcal{B}_X$, $B \in \mathcal{B}_Y$ (see (2.15)), the following estimate holds:

$$|\omega^c(AB)| \leq C\,\|A\|\,\|B\|\,(d_{XY}^Z/\lambda)^{1-n}, \tag{2.19}$$

where $\omega^c(A, B) := \omega(AB) - \omega(A)\omega(B)$ is a (2-point) *connected correlation function.*

Clearly, λ plays the same role as the correlation length for exponentially decaying correlations. The main result of this section, proved in Section 7, shows that the maximal speed for the propagation/creation of correlations is bounded by 3κ:

Theorem 2.4 (Propagation/creation of correlation)**.** *Suppose* (1.2)–(1.3) *hold with some* $n \geq 1$*. Let* $Z \subset \Lambda$ *and suppose the initial state* ω *is* $\mathrm{WC}(Z^{\mathrm{c}}, \lambda)$ *and satisfies* (2.7) *and*

$$\omega(N_{Z^{\mathrm{c}}}) = 0. \tag{2.20}$$

Then, ω_t *is* $\mathrm{WC}(Z^{\mathrm{c}}, 3\lambda)$ *for all* $|t| < \lambda/3\kappa$*; specifically, for any operators* $A \in \mathcal{B}_X$*,* $B \in \mathcal{B}_Y$ *supported in* $X, Y \subset Z^{\mathrm{c}}$ *with* $d^Z_{XY} > 0$ *and for* $|t| < \lambda/3\kappa$*,*

$$|\omega^{\mathrm{c}}_t(AB)| \leq C \, \|A\| \, \|B\| \, (d^Z_{XY}/3\lambda)^{1-n} \omega(N^2_Z), \tag{2.21}$$

For short-range (i.e. exponentially decaying) interactions, (2.21) *holds for all* $n \geq 1$*.*

For the second statement, we note that for short-range interactions, conditions (1.2)–(1.3) are valid for all n.

2.5. **Constraint on the propagation of quantum signals.** The weak LRB (2.17) imposes a direct constraint on the propagation of information through the quantum channel defined by the time evolution α'_t of quantum states (see e.g. [7,16, 42]). For example, assume that Bob at a location Y is in possession of a state ρ and an observable B and would like to send a signal through the quantum channel α'_t to Alice who is at X and who possesses the same state ρ and an observable A. To send a message, Bob uses B as a Hamiltonian to evolve ρ for a time $r > 0$, and then sends Alice the resulting state $\rho_r = \tau_r(\rho)$, where $\tau_r(\rho) := e^{-iBr}\rho e^{iBr}$, as $\alpha'_t(\rho_r)$. To see whether Bob sent his message, Alice computes the difference between the expectations of A in the states $\alpha'_t(\rho_r)$ and $\alpha'_t(\rho)$, which we call the signal detector, SD:

$$\mathrm{SD}(t, r) := \mathrm{Tr}\big[A\alpha'_t(\rho_r) - A\alpha'_t(\rho)\big]. \tag{2.22}$$

The main result of this section gives an upper bound on this difference:

Theorem 2.5. *Let the assumptions of Theorem 2.2 hold with* $n \geq 1$*,* $X \subset \Lambda$ *and* $\omega(\cdot) = \mathrm{Tr}((\cdot)\rho)$*. Then, for every* $c > 4\kappa$*, there exists* $C = C(n, \kappa_n, \nu_n, c) > 0$ *s.th. for all* $\xi \geq 2$*,* $X, Y \subset \Lambda$ *with* $\mathrm{dist}(X, Y) \geq 2\xi$*, and operators* $A \in \mathcal{B}_X$*,* $B \in \mathcal{B}_Y$*, with the operator kernel of* B *satisfying* (1.2) *with* $n \geq 1$*, we have the following estimate for all* $r, |t| < \xi/c$*:*

$$|\mathrm{SD}(t, r)| \leq Cr \, |t| \, \xi^{-n} \, \|A\| \, \|B\| \, \mathrm{Tr}(N^2_X \rho). \tag{2.23}$$

The proof of this theorem is found in Section 8.

2.6. **Bound on quantum state control.** In this section, we derive a bound on the information-theoretic task of state control. For any subset $S \subset \Lambda$, we denote by $\mathcal{F}_S$ the Fock space over the one-particle Hilbert space $\ell^2(S)$, see Appendix A for the definitions and discussions. Due to the tensorial structure $\mathcal{F} \simeq \mathcal{F}_Y \otimes \mathcal{F}_{Y^{\mathrm{c}}}$ (see (A.5)), we can define the partial trace $\mathrm{Tr}_{\mathcal{F}_{Y^{\mathrm{c}}}}$ over $\mathcal{F}_{Y^{\mathrm{c}}}$, e.g. by the equation $\mathrm{Tr}_{\mathcal{F}_Y}(A\mathrm{Tr}_{\mathcal{F}_{Y^{\mathrm{c}}}}\rho) = \mathrm{Tr}((A \otimes \mathbf{1}_{\mathcal{F}_{Y^{\mathrm{c}}}})\rho)$ for every bounded operator A acting on $\mathcal{F}_Y$. This allows one to define a *restriction* of a state ρ to the density operators on the local Fock space $\mathcal{F}_Y$, $Y \subset \Lambda$, by $\rho_Y := \mathrm{Tr}_{\mathcal{F}_{Y^{\mathrm{c}}}}\rho$.

Let τ be a quantum map (or *state control map*) supported in X. Given a density operator ρ, our task is to design τ so that at some time t, the evolution $\rho^\tau_t := \alpha_t(\rho^\tau)$ of the density operator $\rho^\tau := \tau(\rho)$ has the restriction $[\rho^\tau_t]_Y$ to $S(\mathcal{F}_Y)$, which is close to a desired state, say σ.

To measure the success of the transfer operation, one can use the figure of merit

$$F([\rho_t^\tau]_Y, \sigma), \tag{2.24}$$

where $F(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_{S_1}$ is the *fidelity.* Here $\|\rho\|_{S_1}$ denotes the Schatten 1-norm. Note that $0 \leq F(\rho, \sigma) \leq 1$, with $F(\rho, \sigma) = 1$ if and only if $\rho = \sigma$. If $\sigma = |\phi\rangle\langle\phi|$, then $F(\rho, \sigma) = \sqrt{\langle \phi, \rho\phi\rangle}$ and therefore $F(\rho, \sigma) = 0$ if $\rho\phi = 0$. So, one would like to find τ maximizing (2.24). Using this figure of merit, one might be able to estimate the upper bound on the state transfer time.

On the other hand, to show that the state transfer is impossible in a given time interval, we would compare ρ_t^τ and $\rho_t := \alpha_t(\rho)$ by using (c.f. [14, 16])

$$F([\rho_t^\tau]_Y, [\rho_t]_Y), \tag{2.25}$$

as a figure of merit, and try to show that it is close to 1 for $t \leq t_*$ and for all state preparation (unitary) maps τ localized in X. If this is true, then clearly using τ's localized in X does not affect states in Y.

Specifically, we take τ to be of the form $\tau(\rho) = U\rho U^* \equiv \rho^U$, where U is a unitary operator. Our result in this setting is the following lower bound on the fidelity of quantum state control:

Theorem 2.6 (Quantum control bound)**.** *Suppose the assumptions of Theorem 2.2 hold with $n \geq 1$, $X \subset \Lambda$, and $\omega(\cdot) = \mathrm{Tr}((\cdot)\rho)$, where ρ is a pure state. Then, for every $c > 8\kappa$, there exists $C = C(n, \kappa_n, \nu_n, c) > 0$ s.th. for all $\xi \geq 4$, $Y \subset \Lambda$ with $\mathrm{dist}(X, Y) \geq 2\xi$, and unitary operator $U \in \mathcal{B}_X$ (see (2.15)), we have the following lower bound for all $|t| < \xi/c$:*

$$F(\mathrm{Tr}_{Y^c}(\alpha_t'(\rho)), \mathrm{Tr}_{Y^c}(\alpha_t'(\rho^U))) \geq 1 - C\,|t|\,\xi^{-n}\,\mathrm{Tr}(N_X^2\rho). \tag{2.26}$$

The proof of this theorem is found in Section 9 As noted at the begining of this section, Theorem 2.6 imposes a constraint on the best-possible quantum state transfer protocols for the quantum many-body dynamics.

2.7. **Spectral gap and decay of correlation.** Denote by Ω the normalized ground state of the Hamiltonian H in (1.1). The main result of this section is the following:

Theorem 2.7 (Gap at the ground state implies decay of ground state correlations)**.** *Suppose H in (1.1) has a spectral gap of size $\gamma > 0$ at the ground state energy E. Suppose the assumptions of Theorem 2.2 hold with $n \geq 1$, $X \subset \Lambda$, and $\omega = \langle \Omega, (\cdot)\Omega\rangle$. Then, there exists $C = C(n, \kappa_n, \nu_n) > 0$ s.th. for all $\xi \geq 1$, $Y \subset \Lambda$ with $\mathrm{dist}(X, Y) \geq 2\xi$, and operators $A \in \mathcal{B}_X$, $B \in \mathcal{B}_Y$, we have the following bound:*

$$|\langle \Omega,\, BA\Omega\rangle| \leq C\,\|A\|\,\|B\|\,(\gamma^{-1}\xi^{-2} + \xi^{1-n}\,\langle \Omega,\, N_X^2\Omega\rangle). \tag{2.27}$$

This theorem is proved in Section 10.

2.8. **Light cone in macroscopic particle transport.** In this section, we derive an estimate on the macroscopic particle transport for states evolving according to (2.2). To begin with, for a given subset $S \subset \Lambda$, we define the (macroscopic) local relative particle numbers as

$$\bar{N}_S := \frac{N_S}{N_\Lambda}. \tag{2.28}$$

For $0 \le \nu \le 1$, we write $P_{\bar{N}_S \ge \nu}$ for the spectral projection associated to the self-adjoint operator $\bar{N}_S$ onto the spectral interval $[\nu, 1]$.

The main result of this section is the following:

Theorem 2.8. *Suppose* (1.2) *holds with some* $n \ge 1$*. Suppose the initial state* $\omega \in \mathcal{D}$ *satisfies*

$$\omega(P_{\bar{N}_{X^c} \ge \nu}) = 0, \tag{2.29}$$

with some $\nu \ge 0$, $X \subset \Lambda$*. Then, for all* $\nu' > \nu$, $c > \kappa$*, there exists* $C = C(n, \kappa_n, c, \nu' - \nu) > 0$ *s.th. for every* $\eta \ge 1$*, we have the following estimate for all* $|t| < \eta/c$*:*

$$\omega_t \left(P_{\bar{N}_{X^c_\eta} \ge \nu'} \right) \le C\eta^{-n}. \tag{2.30}$$

Theorem 2.8 is proved in Section 11. Note that estimate (2.30) holds for rather general initial states (including ones with particle densities uniformly bounded from below) and it controls macroscopic fractions of particles.

2.9. **Discussions of the results and extensions.** We begin with a number of remarks on Theorems 2.1–2.3.

Remark 1. Recall that the grid size for the underlying lattice is fixed throughout the paper. Consequently, estimates obtained in this paper are all implicitly dependent on the grid size and in general blow up as the latter shrinks to 0. This has to do with the implicit momentum cutoff baked into the discretization process.

Remark 2. At the quantum energies in nature and laboratories (besides particle accelerators), the maximal speed of propagation implied by Theorem 2.1 is much below the speed of light, so the non-relativistic nature of Quantum Mechanics is unimportant here.

Remark 3. The factor $\omega(N_X^2)$ in Thms. 2.3-2.7 originates in Theorem 2.2.

Remark 4. The conclusion of Theorem 2.8 is thermodynamically stable, in the sense that it does not change as $|\Lambda|$, $\omega(N) \to \infty$ with $\omega(N^p) \le C\,|\Lambda|^p$, $p = 1, 2$.

Remark 5. From the proof of Theorem 2.1, one can see that the constant in (2.9) is inversely proportional to the difference $c - \kappa > 0$. See the proof of Proposition 3.4, particularly estimate (3.29).

Remark 6. The conclusion of Theorem 2.1 holds under a slightly weaker assumption. Indeed, let h be the 1-particle Hamiltonian in (1.1). Then condition (1.2) implies that there exists $C = C(n) > 0$ s.th. for every subset $X \subset \Lambda$, the multiple commutators $\mathrm{ad}^p_{d_X}(h)$ satisfies

$$\kappa_p' := \left\| \mathrm{ad}^{p+1}_{d_X}(h) \right\| \le C \quad (p = 0, 1, \dots, n). \tag{2.31}$$

This important consequence is proved in Lemma B.1. The statement of Theorem 2.1 is valid under assumption (2.31), with $\kappa \equiv \kappa_0$ replace by

$$\kappa' \equiv \kappa_0' = \| i[h, d_X] \| \,. \tag{2.32}$$

Here $i[h, d_X]$ is related to the the group velocity operator $i[h, x]$, where x is the 1-particle position observable.

Remark 7. A sufficient condition for (1.2) (and therefore the weaker condition (2.31)) is

$$|h_{xy}| \leq C(1+|x-y|)^{-(n+d+2)}$$

and similarly for (1.3).

Remark 8. [44] obtains a result similar to Theorem 2.1, but with the exponential error bound, while having an additional prefactor (coming from the summation over the sites of X_η^{c}), essentially, $|\Lambda|$. Apart from Theorems 2.8, whose proof uses results of the proof of Theorem 2.1, we could have used this result in Theorems 2.2, 2.3, 2.4-2.7, instead of Theorem 2.1 to obtain the exponential decay with the prefactor $|\Lambda|$, instead of the power-law decay. We also note that the result of [44] requires $h = -\Delta$ (the negative of lattice Laplacian) and uses a bound on the matrix of the imaginary time propagator $e^{\tau\Delta t}$, while our analysis requires only commutators of h with (functions of) x.

In [34], the authors derive an approximation result similar to that of Theorem 2.2 but with a logarithmically modified light cone and with (2.10) replaced by the low-density condition $\sup_{x\in\Lambda} \omega(e^{c_0 n_x}) \leq M$.

In [51], a weak LRB similar to Theorem 2.3 is proven for the steady state $e^{-\mu N}$.

Remark 9. Estimate (2.12) and other results can be extended in a straightforward way to initial states of the form $\omega = \alpha\omega_* + \beta\omega'$, where ω_* is a stationary state, ω' satisfies (2.10), and α, $\beta \geq 0$ with $\alpha + \beta = 1$. Then (2.12) implies that $0 \leq \omega_t(N_{X_\eta^{\mathrm{c}}}) - \alpha\omega_*(N_{X_\eta^{\mathrm{c}}}) \leq C\eta^{-n}\omega'(N_X)$.

Remark 10. Theorem 2.2 follows from the following result, proved in Appendix D:

Theorem 2.9. *Suppose* (1.2)–(1.3) *hold with some* $n \geq 1$. *Let a state* ω *satisfy* (2.7). *Then, for every* $c > 2\kappa$, *there exists* $C = C(n, \kappa_n, \nu_n, c) > 0$ *s.th. for all* $\xi \geq 1$, $X, Y \subset \Lambda$ *with* $\mathrm{dist}(X,Y) \geq 2\xi$, *and operators* $A \in \mathcal{B}_X$, $B \in \mathcal{B}_Y$, *we have, for all* $|t| < \xi/c$:

$$\begin{aligned} &|\omega\big(B(\alpha_t(A) - \alpha_t^{X_\xi}(A))\big)| \\ &\quad \leq C\,|t|\,\|A\|\,\|B\|\left(\omega\left(N_{X_{2\xi}\setminus X}N\right) + \xi^{-n}\omega(N^2)\right). \end{aligned} \tag{2.33}$$

Note that $\omega(N_S N) \geq 0$ since N and N_S commute.

Theorem 2.9 implies Theorem 2.2: Applying estimate (2.33) with $B = \mathbf{1}$, and the relations $N_{X_{2\xi}\setminus X} \leq N_{X^{\mathrm{c}}}$ and

$$\omega(N_{X^{\mathrm{c}}}N) \leq \omega(N^2)^{1/2}\omega(N_{X^{\mathrm{c}}}^2)^{1/2}, \tag{2.34}$$

and using condition (2.10), we find the desired estimate (2.16). □

We compare (2.33) with $B = \mathbf{1}$ with the corresponding result for the Hubbard model, i.e. $v_{xy} = \lambda\delta_{xy}$ for some $\lambda \in \mathbb{R}$, see (5.6) below.

Next, we comment on various extensions of the results from preceding sections. Theorems 2.1-2.7 can be extended to (a) time-dependent one-particle and two-particle operators h and v satisfying (1.2)–(1.3) uniformly in time; (b) k-body potentials (added to or replacing the second term on the r.h.s. of (1.1))

$$V = \sum_k \sum_{x_1\ldots x_k} \prod_i a_{x_i}^* v_{x_1\ldots x_k} \prod_i a_{x_i}$$

under appropriate conditions on $v_{x_1 \ldots x_k}$.

Through Corollary 2.10 below, Theorems 2.3–2.7 can be generalized to relative $N^{\nu/2}$-bounded observables with $0 < \nu < \infty$. By definition, this class of operators contains all polynomials in $\{a_x, a_x^*\}_{x\in\Lambda}$ with degree at most ν. Precise definitions and further comments are delegated to Appendix E.

Corollary 2.10. *Suppose* (1.2) *holds with some* $n \geq 1$. *Let* $\nu, q \geq 0$. *Then, for all* $c > \kappa$, *there exists* $C = C(n, \kappa_n, c) > 0$ *s.th. for every* $\eta \geq 1$ *and two subsets* $X \subset S \subset \Lambda$, *we have the following estimate for all* $|t| < \eta/c$:

$$\alpha_t^S(N_{S\setminus X_\eta}^{q+1} N^\nu) \leq C\left(N_{S\setminus X} N^{\nu+q} + \eta^{-n} N^{\nu+q+1}\right), \tag{2.35}$$

where α_t^S *is as in* (2.14).

Proof. We use Theorem 2.1 with $\alpha_t^S(\cdot)$ in place of $\alpha_t(\cdot)$, which is possible because H_S also satisfies (1.2) with the same $n \geq 1$ as in the assumption. This gives estimate (2.9) with $S\setminus(\cdot)$ in place of $(\cdot)^{\mathrm{c}}$. This, together with the relations $N_{S\setminus X_\eta}^{q+1} \leq N_{S\setminus X_\eta} N^q$, $[N, H_S] = 0$, and $N_S \leq N$, implies that

$$\begin{aligned}\alpha_t^S\left(N_{S\setminus X_\eta}^{q+1} N^\nu\right) &\leq \alpha_t^S\left(N_{S\setminus X_\eta}\right) N^{\nu+q}\\ &\leq C\left(N_{S\setminus X} + \eta^{-n} N_S\right) N^{\nu+q}\\ &\leq C\left(N_{S\setminus X} N^{\nu+q} + \eta^{-n} N^{\nu+q+1}\right).\end{aligned}$$

This gives (2.35). □

3. Proof of Theorem 2.1

3.1. **Outline of the proof of Theorem 2.1.** The proofs of Theorems 2.2–2.3 and the subsequent applications are based on Theorem 2.1, whose proof we outline now.

3.1.1. *Propagation identifier observables.* Recall that the second quantization $\mathrm{d}\Gamma$ of 1-particle operators on $\mathfrak{h} \equiv \ell^2(\Lambda)$ is given by

$$\mathrm{d}\Gamma(b) := \sum_{\Lambda\times\Lambda} b_{xy} a_x^* a_y, \tag{3.1}$$

where b_{xy} is the matrix ("integral" kernel) of an operator b on $\ell^2(\Lambda)$. As we identify a function $f : \Lambda \to \mathbb{C}$ with the multiplication operator induced by it on $\mathfrak{h} \equiv \ell^2(\Lambda)$, we write

$$\hat{f} \equiv \mathrm{d}\Gamma(f) := \sum_{x\in\Lambda} f(x) a_x^* a_x. \tag{3.2}$$

We denote by $\chi_S^\sharp$ the characteristic function of a subset $S \subset \Lambda$. For $f = \chi_S^\sharp$, the above gives the local particle number operators $N_S \equiv \mathrm{d}\Gamma(\chi_S^\sharp)$ in (2.1). For a differentiable real function f, we write $\hat{f}' \equiv \mathrm{d}\Gamma(f')$ and $\hat{f}'_{ts} \equiv \mathrm{d}\Gamma(f'_{ts})$, where $f'_{ts} \equiv f'\left(\frac{d_X - vt}{s}\right)$.

As in [15, 16], we control the time evolution associated to (1.1) by monotonicity formulae for a class of observables called *adiabatic spacetime localization observables (ASTLOs)*, defined as

$$\hat{\chi}_{ts} := \mathrm{d}\Gamma(\chi_{ts}). \tag{3.3}$$

Here $s > 0$, $t \in \mathbb{R}$, and χ_{ts} is the family of multiplication operators by real functions

$$\chi_{ts} = \chi\left(\frac{d_X - vt}{s}\right), \tag{3.4}$$

where d_X is the distance function to X, $v \in (\kappa, c)$, with κ from (2.8) and c from the statement of Theorem 2.1. We assume that χ belongs to the following set of functions:

$$\mathcal{X} \equiv \mathcal{X}_\delta := \left\{ \chi \in C^\infty(\mathbb{R}) \,\middle|\, \begin{array}{l} \operatorname{supp}\chi \subset \mathbb{R}_{\geq 0},\ \operatorname{supp}\chi' \subset (0,\delta) \\ \chi' \geq 0,\ \sqrt{\chi'} \in C^\infty(\mathbb{R}) \end{array} \right\}, \tag{3.5}$$

for some $\delta > 0$. Later on, we will choose the number δ in (3.5) as $\delta = c - v$ with c and v given in the statement of Theorem 2.1 and (3.4), respectively. We note that $\chi \geq 0$ for each $\chi \in \mathcal{X}$. Additional properties of $\mathcal{X}$ will be stated in Section 3.2. Physically, $\hat{\chi}_{ts}$ is a smoothed local particle number operator, measuring fraction of the particles outside the light cone of X. We also write $\chi'_{ts} = (\chi')_{ts}$.

3.1.2. *Recursive monotonicity formula.* For a differentiable family of observables, define the Heisenberg derivative

$$DA(t) = \frac{\partial}{\partial t} A(t) + i[H, A(t)], \tag{3.6}$$

so that

$$\partial_t \alpha_t(A(t)) = \alpha_t(DA(t)) \iff \partial_t \omega_t(A(t)) = \omega_t(DA(t)), \tag{3.7}$$

where $\omega_t = \omega \circ \alpha_t$ is the evolution of state associated to (2.2) with initial state ω. We will use the identity (3.7) to prove a key differential inequality:

Theorem 3.1 (Recursive monotonicity of $\hat{\chi}_{ts}$)**.** *Suppose the assumptions of Theorem 2.1 hold. Then, for every $\chi \in \mathcal{X}$, there exist $C = C(n, \kappa_n, \chi) > 0$ and, if $n \geq 2$, $\xi^k = \xi^k(\chi) \in \mathcal{X}$, $k = 2, \ldots, n$, each supported in $\operatorname{supp}\chi$, s.th. for all $s > 0$, $t \in \mathbb{R}$,*

$$D\hat{\chi}_{ts} \leq -\frac{v - \kappa}{s}\hat{\chi}'_{ts} + C\sum_{k=2}^{n} s^{-k}\widehat{(\xi^k)'}_{ts} + Cs^{-(n+1)}N. \tag{3.8}$$

(The sum in the r.h.s. is dropped if $n = 1$.)

Theorem 3.1 is deduced at the end of this section. Since the second term on the r.h.s. is of the same form as the leading, negative term (recall $v > \kappa$ in (3.4)), estimate (3.8) can be bootstrapped to obtain an integral inequality with $O(s^{-n})$ remainder, see Proposition 3.4 below. Hence, we call (3.17) the *recursive monotonicity estimate.*

For the next step, we observe that the second quantization (3.2) has the properties

$$\mathrm{d}\Gamma(v + cw) = \mathrm{d}\Gamma(v) + c\,\mathrm{d}\Gamma(w), \tag{3.9}$$

$$\mathrm{d}\Gamma(v^*) = \mathrm{d}\Gamma(v)^*, \tag{3.10}$$

$$\mathrm{d}\Gamma(v) \leq \mathrm{d}\Gamma(w) \iff v \leq w, \tag{3.11}$$

$$\mathrm{ad}^k_{\mathrm{d}\Gamma(v)}(\mathrm{d}\Gamma(w)) = \mathrm{d}\Gamma(\mathrm{ad}^k_v(w)), \quad k = 1, 2, \ldots, \tag{3.12}$$

for all 1-particle operators v and w acting on $\mathfrak{h}$ and scalars c. These properties are either obvious or are obtained by direct computation using the canonical commutator relations, see e.g. [15, p.9]. Moreover, the second term on the r.h.s. of (1.1), which we denote by V, satisfies

$$[V, \mathrm{d}\Gamma(f)] = 0 \quad \forall f \in \ell^\infty(\Lambda). \tag{3.13}$$

Relations (3.9)–(3.13) allow us to reduce estimates on $D\hat{\chi}_{ts}$ to those on $d\chi_{ts}$, where db is the 1-particle Heisenberg derivative, defined as

$$db(t) := \partial_t b(t) + i[h, b(t)], \tag{3.14}$$

for a differentiable path of 1-particle operator $b(t)$ on $\mathfrak{h}$. Indeed, let $H_0 := \mathrm{d}\Gamma(h)$ and define the free Heisenberg derivative as

$$D_0 A(t) = \frac{\partial}{\partial t} A(t) + i[H_0, A(t)]. \tag{3.15}$$

Then, by (3.12), we have $D_0\, \mathrm{d}\Gamma\big(b\big) = \mathrm{d}\Gamma\big(db\big)$. This, together with property (3.13), gives

$$D\, \mathrm{d}\Gamma\big(f\big) = \mathrm{d}\Gamma\big(df\big) \iff D\hat{f} = \widehat{df}, \tag{3.16}$$

for every multiplication operator (by a function) f.

In Section 4, we prove the following:

Proposition 3.2. *Suppose the assumptions of Theorem 2.1 hold. Then, for every $\chi \in \mathcal{X}$, there exist $C = C(n, \kappa_n, \chi) > 0$ and, if $n \geq 2$, $\xi^k = \xi^k(\chi) \in \mathcal{X}$, $k = 2, \dots, n$, each supported in* $\operatorname{supp}\chi$*, s.th. for all $s > 0$, $t \in \mathbb{R}$,*

$$d\chi_{ts} \leq -\frac{v-\kappa}{s}\chi'_{ts} + C\left(\sum_{k=2}^{n} s^{-k}(\xi^k)'_{ts} + s^{-(n+1)}\right). \tag{3.17}$$

(The sum in the r.h.s. is dropped if $n = 1$.)

This proposition, together with relation (3.16), implies Theorem 3.1.

3.2. **Proof of Theorem 2.1 assuming Proposition 3.2.** Recall that $\chi_S^\sharp$, $S \subset \Lambda$ denotes the characteristic function of S. The main result of this section is the following:

Theorem 3.3. *Let the assumptions of Theorem 2.1 hold. Suppose Proposition 3.2 holds and, for all $\chi \in \mathcal{X}$ with $\|\chi\|_{L^\infty} = 1$, $s = \eta/c$, and $|t| < s$, the following holds:*

$$\chi_{0s} \leq \chi^{\#}_{X^c}, \tag{3.18}$$

$$\chi^{\#}_{X^c_\eta} \leq \chi_{ts}. \tag{3.19}$$

Then the conclusion of Theorem 2.1 holds.

The proof of Theorem 3.3 is found at the end of this section. It uses the following properties of the set $\mathcal{X}$ from (3.5):

- (X1) If $w \in C^\infty$ and $\operatorname{supp} w \subset (0, \delta)$, then the antiderivative $\int^x w^2 \in \mathcal{X}$.
- (X2) If $\xi_1, \dots, \xi_N \in \mathcal{X}$, then there exists $\xi \in \mathcal{X}$ s.th. $\xi_1 + \ldots + \xi_N \leq \xi$.

For the 1-particle Hamiltonian h in (1.1) and operators b acting on $\mathfrak{h}$, let β_t be the 1-particle evolution

$$\beta_t(b) := e^{ith} b e^{-ith}, \tag{3.20}$$

c.f. (2.6), and note that

$$\partial_t \beta_t(b(t)) = \beta_t(db(t)), \tag{3.21}$$

c.f. (3.7). We denote

$$\chi_s(t) := \beta_t(\chi_{ts}) \qquad \text{and} \qquad \chi'_s(t) := \beta_t(\chi'_{ts}). \tag{3.22}$$

We now bootstrap (3.17) to obtain the following integral estimate:

Proposition 3.4. *Let the assumptions of Theorem 2.1 hold. Suppose Proposition 3.2 holds. Then, for every $\chi \in \mathcal{X}$, there exist $C = C(n, \kappa_n, \chi, v - \kappa) > 0$ (with v and κ from* (3.4) *and* (2.8)*, resp.) and, if $n \geq 2$, $\xi^k = \xi^k(\chi) \in \mathcal{X}$, $2 \leq k \leq n$, each supported in* $\operatorname{supp}\chi$*, s.th. for all $s > 0$, $t \geq 0$,*

$$\int_0^t \chi'_s(r)dr \leq C\Big(s\chi_s(0) + \sum_{k=2}^n s^{-k+2}\ \xi^k_s(0) + ts^{-n}\Big), \tag{3.23}$$

where the sum should be dropped if $n = 1$.

Remark 11. Proposition 3.4 can be reformulated in terms of expectation. Indeed, instead of the evolution $\chi_s(t)$, we could have used the expectation:

$$\omega_t\left(\chi_{ts}\right) \equiv \operatorname{Tr}(\chi_{ts}\rho_t) \tag{3.24}$$

of χ_{ts} in the state ρ_t solving (2.6) and instead of (3.7), used the relation

$$\frac{d}{dt}\omega_t\left(\chi_{ts}\right) = \omega_t\left(D\chi_{st}\right). \tag{3.25}$$

These two formulations are related through the identity

$$\omega_t\left(\chi_{ts}\right) = \omega\left(\chi_s(t)\right). \tag{3.26}$$

Proof of Proposition 3.4. For each fixed s, integrating formula (3.21) with $b(t) \equiv \chi_{ts}$ in t gives

$$\chi_s(t) - \int_0^t \beta_r(d\chi_{sr})\,dr = \chi_s(0). \tag{3.27}$$

We apply inequality (3.17) to the second term on the l.h.s. of (3.27) to obtain

$$\begin{aligned} &\chi_s(t) + (v-\kappa)s^{-1}\int_0^t \chi'_s(r)\,dr \\ &\leq \chi_s(0) + C\left(\sum_{k=2}^n s^{-k}\int_0^t (\xi^k)'_s(r)\,dr + ts^{-(n+1)}\right), \end{aligned} \tag{3.28}$$

where $C = C(n, \kappa_n, \chi) > 0$ and the second term in the r.h.s. is dropped for $n = 1$. Since $\chi_s(t) \geq 0$ due to the positive-preserving property of β_t (c.f. (3.20)), $\kappa < v$ and $s > 0$, inequality (3.28) implies, after dropping $\chi_s(t)$ and multiplying both sides by $s(v-\kappa)^{-1} \geq 0$, that

$$\int_0^t \chi'_s(r)\,dr \leq C\left(s\chi_s(0) + \sum_{k=2}^n s^{-k+1}\int_0^t (\xi^k)'_s(r)\,dr + ts^{-n}\right), \tag{3.29}$$

where the second term in the r.h.s. is dropped for $n = 1$. Note that from this point onward, the constant $C > 0$ depends also on $v - \kappa$.

If $n = 1$, then (3.29) gives (3.23). If $n \geq 2$, applying (3.29) to the term $\int_0^t (\xi^k)'_s(r)\,dr$ for $k = 2$, we obtain

$$\int_0^t \chi'_s(r)\,dr \leq C\Big(s\chi_s(0) + \xi^2_s(0) + \sum_{k=3}^n s^{-k+1}\int_0^t (\eta^k)'_s(r)\,dr + ts^{-n}\Big), \tag{3.30}$$

where the third term in the r.h.s. is dropped for $n = 2$, and $\eta^k = \eta^k(\xi^2, \xi^k) \in \mathcal{X}, k = 3, \ldots, n$. Bootstrapping this procedure, we arrive at (3.23). □

Proof of Theorem 3.3. To fix ideas, we take $t \geq 0$ within this proof. The case $t \leq 0$ follows from time reflection.

Fix $\chi \in \mathcal{X}$ with $\|\chi\|_{L^\infty} = 1$ and consider (3.28). Retaining the first term in the l.h.s. of (3.28) and dropping the second one, which is non-negative since $\chi' \geq 0$ and $v > \kappa$ (see (3.4)), we obtain

$$\chi_s(t) \leq \chi_s(0) + C\left(\sum_{k=2}^{n} s^{-k}\int_0^t (\xi^k)'_s(r)dr + ts^{-(n+1)}\right), \tag{3.31}$$

Applying (3.23) to the second term on the r.h.s. and using property (X2), we deduce that

$$\chi_s(t) \leq \chi_s(0) + Cs^{-1}\xi_s(0) + Cs^{-n}, \tag{3.32}$$

for some fixed $\xi \in \mathcal{X}$, $C > 0$ and all $s > t$.

Let $s = \eta/c$ and $\eta > ct$. We first consider the r.h.s. of (3.32). Using $\chi_s(0) \equiv \chi_{0s}$ in (3.18) and noting $\operatorname{supp}\xi^k \subset \operatorname{supp}\chi$ for each k, we find that

$$\chi_s(0) + Cs^{-1}\xi_s(0) \leq (1 + Cs^{-1})\chi^\sharp_{X^c}. \tag{3.33}$$

By (3.33) and property (3.11), we have

$$\widehat{\chi_s(0)} + Cs^{-1}\widehat{\xi_s(0)} \leq (1 + Cs^{-1})N_{X^c}. \tag{3.34}$$

Next, consider the l.h.s. of (3.32). Applying β_t to (3.19), we find that

$$\beta_t(\chi^\sharp_{X^c_\eta}) \leq \chi_s(t), \tag{3.35}$$

We show in Appendix B, Lemma B.3, that for every function f on Λ and $\hat{f} \equiv \mathrm{d}\Gamma(f)$,

$$\alpha_t(\hat{f}) = \mathrm{d}\Gamma(\beta_t(f)). \tag{3.36}$$

This, together with (3.35), yields

$$\alpha_t(N_{X^c_\eta}) \leq \widehat{\chi_s(t)}. \tag{3.37}$$

Finally, combining estimates (3.32), (3.34), (3.37) and recalling the assumption $\eta \geq 1$, we conclude that for all $t < s = \eta/c$,

$$\alpha_t(N_{X^c_\eta}) \leq C(N_{X^c} + \eta^{-n}N),$$

which is (2.9). This completes the proof of Theorem 3.3. □

Theorem 2.1 follows from Proposition 3.2, Theorem 3.3, and the following lemma, proved in Section 4.2:

Lemma 3.5. *Let $v \in (c, \kappa)$, $s = \eta/c$, and $\delta = c - v$ in definitions* (3.4)–(3.5)*. Then* (3.18)–(3.19) *hold for the family* (3.4) *with* $\|\chi\|_{L^\infty} = 1$.

This completes the proof of Theorem 2.1, modulo the proofs of Proposition 3.2 and Lemma 3.5, given in the next section. □

4. Proofs of Proposition 3.2 and Lemma 3.5

In this section, we prove the 1-particle recursive monotonicity estimate, Proposition 3.2, and the geometric estimates (3.18)–(3.19).

4.1. **Proof of Proposition 3.2.** Recall the definition of the operators χ_{ts} in (3.4). To begin with, we prove the following lemma:

Lemma 4.1. *Suppose* (1.2) *holds with some* $n \geq 1$. *Then, for every* $\chi \in \mathcal{X}$, *there exist* $\xi^k = \xi^k(\chi) \in \mathcal{X}$, $k = 2, \dots, n$ *(dropped if* $n = 1$*), each supported in* $\operatorname{supp}\chi$, *and some* $C = C(n, \kappa_n, \chi) > 0$ *s.th. for all* $t \in \mathbb{R}$, $s > 0$,

$$L\chi_{ts} \leq s^{-1}\kappa\chi'_{ts} + C\left(\sum_{k=2}^{n} s^{-k}(\xi^k)'_{ts} + s^{-(n+1)}\right), \tag{4.1}$$

where $L = i\,[h, \cdot]$ *and* κ *is as in* (2.8). *(The sum in the r.h.s. is dropped if* $n = 1$.*)*

Proof. Throughout the proof we fix t and write $\chi_s \equiv \chi_{ts}$. Since $\chi' \geq 0$ for $\chi \in \mathcal{X}$, expansion (C.3) with $A = ih$, $\Phi = d_X$ yields (see Corollary C.2):

$$\begin{aligned} L\chi_s =& s^{-1}\sqrt{\chi'_s}(Ld_X)\sqrt{\chi'_s} \\ &+ \sum_{k=2}^{n} s^{-k} \sum_{m=1}^{N_k} g^{(m)}(s) v_s^{(m)} B_k v_s^{(m)} + s^{-(n+1)}R(s), \end{aligned} \tag{4.2}$$

where the sum in the second line is dropped for $n = 1$. For $n \geq 2$, $1 \leq k \leq n$, $1 \leq m \leq N_k$, the functions $v^{(m)}$ are piece-wise smooth and satisfy

$$\operatorname{supp} v^{(m)} \subset \operatorname{supp}\chi', \quad \left\| v^{(m)} \right\|_{L^\infty} \leq C(\chi), \tag{4.3}$$

$g^{(m)}(s)$ are piece-wise constant and take values in ± 1, and $B_k = \operatorname{ad}^k_{d_X}(ih)$. Furthermore, by condition (1.2), Lemma B.1, and the remainder estimate (C.4), the operators B_k and $R(s)$ are bounded on $\mathfrak{h}$, satisfying

$$\|Ld_X\| \leq \kappa \equiv \kappa_0, \quad \|B_k\| \leq \kappa_{k-1}, \quad \|R(s)\| \leq C(n, \chi)\kappa_n, \tag{4.4}$$

with κ_p's given in (1.2).

Next, adding the adjoint to both sides of (4.2), using the self-adjointness of the first term on both sides, and then dividing the result by two, we find

$$\begin{aligned} L\chi_s = s^{-1}\sqrt{\chi'_s}(Ld_X)\sqrt{\chi'_s} + \frac{1}{2}\sum_{k=1}^{n} s^{-k} \sum_{m=1}^{N_k} g^{(m)}(s) v_s^{(m)} \left(B_k + B_k^*\right) v_s^{(m)} \\ + \frac{1}{2} s^{-(n+1)} \left(R(s) + R(s)^*\right). \end{aligned} \tag{4.5}$$

We can now derive an operator inequality from expansions (4.5) and uniform estimates (4.4) as

$$L\chi_s \leq \kappa\chi'_s + C\left(\sum_{k=2}^{n} s^{-k}(U_s^k)^2 + s^{-(n+1)}\right), \tag{4.6}$$

where the sum in the r.h.s. of (4.6) is dropped for $n = 1$ and $C = C(n, \kappa_n, \chi) > 0$. For $n \geq 2$, each $U^k \in C_c^\infty$ and is supported in $\operatorname{supp}\chi'$.

Lastly, in view of property (X1), we find that for each $2 \leq k \leq n$, there exists $\xi^k \in \mathcal{X}$ s.th. $(U_s^k)^2 \leq (\xi^k)'_s$. Plugging this back to (4.6) and substituting back $\chi_s \equiv \chi_{ts}$ etc. yields (4.1). This completes the proof. □

Proof of Proposition 3.2. We compute

$$\frac{\partial}{\partial t}\chi_{ts} = -s^{-1}v\,\chi'_{ts}. \tag{4.7}$$

By (4.1), we find

$$L\chi_{ts} \le \kappa s^{-1}\chi'_{ts} + C\left(\sum_{k=2}^{n} s^{-k}(\xi^k)'_{ts} + s^{-(n+1)}\right),$$

where $C = C(n, \kappa_n, \chi)$ and the second term in the r.h.s. is dropped for $n = 1$. This, together with (4.7) and definition (3.6), implies (3.17). □

4.2. **Proof of Lemma 3.5.** First, by (3.5), we have $\operatorname{supp}\chi \subset (0,\infty)$, and therefore $\operatorname{supp}\chi\left(\frac{\cdot}{s}\right) \subset (0,\infty)$ for any $s > 0$. This implies

$$\chi_{0s} \equiv \chi\left(\frac{d_X}{s}\right) \le \theta(d_X) \equiv \chi^\sharp_{X^c}, \tag{4.8}$$

where $\theta : \mathbb{R} \to \mathbb{R}$ is the characteristic function of $\mathbb{R}_{>0}$ (see Figure 2). By these facts, we conclude (3.18).

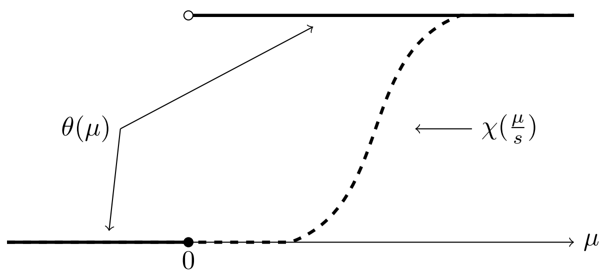

FIGURE 2. Schematic diagram illustrating (4.8)

Next, again by the definition of $\mathcal{X}$, we have $\chi(\frac{\mu-vt}{s}) \equiv 1$ for all $\mu \ge v\,|t| + (c-v)s$ by setting $\delta = c - v > 0$. Now, we choose $s = \eta/c$. Then, for all $|t| < \eta/c$ and $v < c$, we have $\chi(\frac{\mu-vt}{s}) \equiv 1$ for $\mu \ge \eta$. This implies the estimate

$$\chi((\mu - vt)/s) \ge \theta(\mu - \eta), \tag{4.9}$$

see Figure 3.

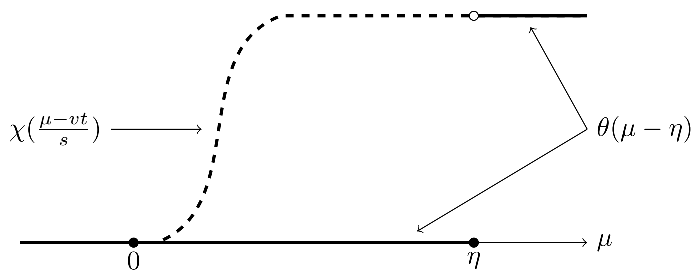

FIGURE 3. Schematic diagram illustrating (4.9).

Since $X^c_\eta = \{d_X(x) > \eta\}$, we have $\chi^\sharp_{X^c_\eta} = \theta(d_X - \eta)$. This, together with (4.9), implies (3.19). This completes the proof of Lemma 3.5. □

5. Main ideas of the proof of Theorem 2.2

Recall the notations $X^c := \Lambda \setminus X$, $X_\xi \equiv \{x \in \Lambda : d_X(x) \le \xi\}$ for $\xi \ge 0$ (see Figure 1), and that an observable (i.e. bounded operator) A is said to be localized in $X \subset \Lambda$ if (2.13) holds, written as $\operatorname{supp} A \subset X$. Next, we use the notation

$$A_s^\xi \equiv \alpha_s^{X_\xi}(A) = e^{isH_{X_\xi}} A e^{-isH_{X_\xi}}, \tag{5.1}$$

where H_Y, $Y \subset \Lambda$ is the Hamiltonian defined by (1.1) with Y in place of Λ. By definition (2.13), we see that if $\operatorname{supp} A \subset X$, then $\operatorname{supp} A_s^\xi \subset X_\xi$ for all $s \in \mathbb{R}$, $\xi \ge 0$.

Let $A_t = \alpha_t(A)$ be the full evolution (2.6). By the fundamental theorem of calculus, we have

$$A_t - A_t^\xi = \int_0^t \partial_r \alpha_r(\alpha_{t-r}^{X_\xi}(A))\, dr.$$

Using identity (3.7) for α_r and $\alpha_{t-r}^{X_\xi}$ in the integrand above, as well as the fact that $\alpha_{t-r}^{X_\xi}([H_{X_\xi}, A]) = [H_{X_\xi}, \alpha_{t-r}^{X_\xi}(A)]$, we find

$$A_t - A_t^\xi = \int_0^t \alpha_r(i[R', A_{t-r}^\xi])\, dr, \tag{5.2}$$

where $R' := H - H_{X_\xi}$. Since A_s^ξ is localized in X_ξ, only terms in R' which connect X_ξ and X_ξ^c contribute to $[R', A_{t-r}^\xi]$ (see Figure 4).

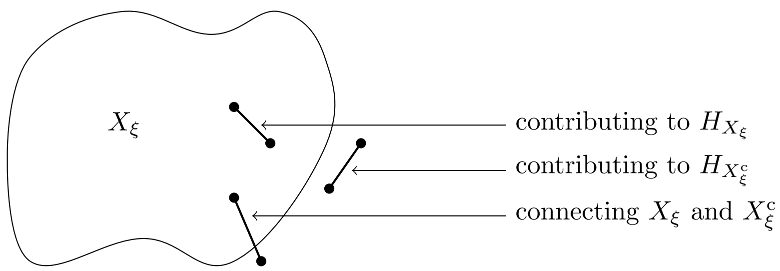

Figure 4. Schematic diagram illustrating the splitting of H.

Let $s := t - r$. Assuming first that h and v are finite-range, we see that the commutator $i[R', A_s^\xi]$ is localized near the boundary ∂X_ξ. Considering for simplicity the *Hubbard model*, i.e. $v_{xy} = \lambda \delta_{xy}$ for some $\lambda \in \mathbb{R}$, and assuming A and therefore A_s^ξ are self-adjoint, $i[R', A_s^\xi]$ can be bounded, in essence, as

$$i[R', A_s^\xi] \le C \|A\| N_{\partial X_\xi}. \tag{5.3}$$

Next, we take X so that X^c is 'bounded', i.e. independent of Λ (see Figure 5 below) and set $Y := X_\xi^c$, so that $X^c = Y_\xi$. Then MVB (2.9) gives the 'incoming' light cone estimate, for $r \le \xi/c$, $c > 2\kappa$,

$$\alpha_r(N_Y) \le C(N_{Y_\xi} + \xi^{-n} N). \tag{5.4}$$

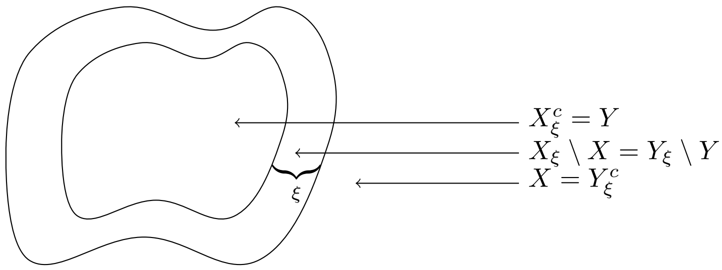

FIGURE 5. Schematic diagram illustrating Y, Y_ξ, Y_ξ^c.

Now, by the MVB (5.4), for any $r \le \xi/c,\ c > 2\kappa$, we have

$$\alpha_r(N_{\partial X_\xi}) \le C(N_{(\partial X_\xi)_\xi} + \xi^{-n}N). \tag{5.5}$$

This, together with (5.2), (5.3) and the observation $(\partial X_\xi)_\xi = X_{2\xi\setminus X}$, yields

$$\left|\omega\big(\alpha_t(A) - \alpha_t^{X_\xi}(A)\big)\right| \le C\,|t|\,\|A\|\,\big(\omega(N_{X_{2\xi}\setminus X}) + \xi^{-n}\omega(N)\big)\,, \tag{5.6}$$

This, together with (2.11), gives (2.16) in the finite-range case.

For h and v of infinite-range, we refine the argument presented above. Let $X_{a,b} = X_b \setminus X_a$ for $b > a \ge 0$. To estimate $i[R', A_s^\xi]$ in (5.2), we split the annulus $X_{0,2\xi}$ into four annuli, say

$$X_{0,\frac{3}{4}\xi}, \quad X_{\frac{3}{4}\xi,\xi}, \quad X_{\xi,\frac{5}{4}\xi,}, \quad X_{\frac{5}{4}\xi,2\xi}. \tag{5.7}$$

In the second and the third annuli, we use the MVB from Theorem 2.1 and in the first and the fourth ones, the decay properties of h_{xy} and v_{xy} as $|x-y| \to \infty$. See Appendix D for details.

6. Proof of Theorem 2.3

We introduce the remainder term for (2.16):

$$\mathrm{Rem}_t(A) := \alpha_t(A) - \alpha_t^{X_\xi}(A). \tag{6.1}$$

Since A (and therefore the evolution $\alpha_t^{X_\xi}(A)$) and B are respectively localized in X_ξ and $Y \subset X_{2\xi}^c$, $\alpha_t^{X_\xi}(A)$ and B commute, yielding

$$[\alpha_t(A), B] = [\mathrm{Rem}_t(A), B]. \tag{6.2}$$

Next, we use Theorem 2.9, which implies that for $c > 2\kappa$, there exists $C = C(n, \kappa_n, \nu_n, c) > 0$ s.th. for $|t| < \xi/c$,

$$|\omega\,(B\,\mathrm{Rem}_t(A))| \le C\,|t|\,\|A\|\,\|B\|\,\big(\omega\,\big(N_{X_{2\xi}\setminus X}N\big) + \xi^{-n}\omega(N^2)\big)\,. \tag{6.3}$$

Since $|\omega(\mathrm{Rem}_t(A)B)| = |\omega(B^*(\mathrm{Rem}_t(A))^*)|$ and $(\mathrm{Rem}_t(A))^* = \mathrm{Rem}_t(A^*)$ (see (6.1)), replacing A, B in (6.3) by A^*, B^* yields the same estimate on $|\omega(\mathrm{Rem}_t(A)B)|$, namely $|\omega(\mathrm{Rem}_t(A)\,B)| \le$r.h.s. of (6.3) for all $|t| < \xi/c$. Then the desired estimate (2.17) follows from the triangle inequality $|\omega\,([\mathrm{Rem}_t(A), B])| \le |\omega\,(\mathrm{Rem}_t(A)B)| + |\omega\,(B\,\mathrm{Rem}_t(A))|$, assumption (2.10) and equality (2.11). □

7. Proof of Theorem 2.4

To fix ideas, we let $t \geq 0$. We write $C_{AB} \equiv C\,\|A\|\,\|B\|\,\omega(N_Z^2)$ with $C > 0$ independent of A, B, N, Λ. Then (2.21) becomes

$$|\omega_t^c(A,B)| \leq C_{AB}(d_{XY}^Z/(3\lambda))^{1-n} \tag{7.1}$$

for any two bounded operators A, B localized in X, Y with $d_{XY}^Z \geq 3\lambda$. (For $0 < d_{XY}^Z < 3\lambda$, (7.1) holds trivially.)

To prove (7.1), we use the equality $\omega_t^c(A,B) = \omega^c(A_t, B_t)$ and write $A_t = A_t^\xi + \mathrm{Rem}_t(A)$ with $\xi := d_{XY}^Z/3$ (see (6.1)) and the same for B_t. This way we arrive at

$$\begin{aligned}\omega_t^c(A,B) =& \omega^c(A_t,B_t) = \omega^c(A_t^\xi, B_t^\xi)\\ &+ \omega(\mathrm{Rem}_t(A)B_t) + \omega(A_t\mathrm{Rem}_t(B))\\ &+ \omega(\mathrm{Rem}_t(A)\mathrm{Rem}_t(B))\\ &+ \omega(\mathrm{Rem}_t(A))\omega(B_t) + \omega(\mathrm{Rem}_t(B))\omega(A_t)\\ &+ \omega(\mathrm{Rem}_t(A))\omega(\mathrm{Rem}_t(B)).\end{aligned} \tag{7.2}$$

Since A_t^ξ and B_t^ξ are localized in two disjoint sets X_ξ and Y_ξ at the distance $d_{X_\xi,Y_\xi}^Z = d_{XY}^Z - 2\xi = d_{XY}^Z/3 \geq \lambda$, then, by the $\mathrm{WC}(Z^c,\lambda)$ assumption on ω, the leading term is bounded as

$$\left|\omega^c(A_t^\xi B_t^\xi)\right| \leq C_{AB}^1(d_{X_\xi Y_\xi}^Z/\lambda)^{1-n} \leq C_{AB}^1(d_{XY}^Z/3\lambda)^{1-n},$$

with $C_1 > 0$ as in (2.21).

For the 6 trailing terms in the r.h.s. of (7.2), we use (2.33) and similar estimates with the roles of A and B interchanged, together with (2.34), (2.20), and (2.11). Since $X_{2\xi} \equiv X_{2d_{XY}^Z/3}$, $Y_{2\xi} \equiv Y_{2d_{XY}^Z/3} \subset Z^c$, we have $N_{X_{2\xi}}, N_{Y_{2\xi}} \leq N_{Z^c}$. Hence, due to (2.34), the leading term in the r.h.s. of (2.33) drops out. Thus, these 6 terms can be bounded by $C_{AB}^2\xi^{1-n} = C_{AB}^2(d_{XY}^Z/3)^{1-n}$ uniformly for all $t < \xi/3\kappa$.

In conclusion, since $d_{XY}^Z \geq 3\lambda$ and therefore $\xi \geq \lambda$, we find

$$|\omega_t^c(A,B)| \leq C_{AB}(d_{XY}^Z/(3\lambda))^{1-n}, \tag{7.3}$$

for some $C = C(n, C_1, C_2) > 0$ and all $t < \lambda/c$. We conclude the claim from here. □

8. Proof of Theorem 2.5

Let $\mathrm{SD} \equiv \mathrm{SD}(t,r)$ as defined in (2.22). The fundamental theorem of calculus yields

$$\mathrm{SD} = \int_0^r \mathrm{Tr}\big[A\alpha_t'(\tau_s(i[\rho,B]))\big]\,ds. \tag{8.1}$$

Since $\tau_s(i[\rho,B]) = i[\tau_s(\rho),\tau_s(B)]$ and $\tau_s(B) = B$, moving α_t' from the state to the observable A in eq. (8.1) gives

$$\begin{aligned}\mathrm{SD} &= \int_0^r ds\mathrm{Tr}\big[\alpha_t(A)i[\tau_s(\rho),B]\big]\\ &= \int_0^r ds\omega_s\big(i[B,\alpha_t(A)]\big),\end{aligned} \tag{8.2}$$

where $\omega_s := \mathrm{Tr}((\cdot)\tau_s(\rho))$ is the evolution generated by B. (8.2) implies the upper bound

$$|\mathrm{SD}| \le r \sup_{0\le s\le r} \left|\omega_s\big([B,\alpha_t(A)]\big)\right| . \tag{8.3}$$

Let $\xi' := \xi/2 \ge 1$, $c' := c/2 > 2\kappa$, and $N_{\gamma,\xi} := N_{X_{(1-\gamma)\xi,(1+\gamma)\xi}}$ (c.f. (D.12)). Note that A and B are localized in $\mathcal{B}_{X_{\xi'}}$ and $\mathcal{B}_Y$, respectively, with $\mathrm{dist}(X_{\xi'}, Y) \ge \xi'$. Hence, by estimate (2.33) (which, importantly, is independent of state ω) and the relation $X_{\xi/2,3\xi/2} = (X_{\xi'})_{0,2\xi'}$, we have

$$|\omega_s\left([B,\alpha_t(A)]\right)| \le C\,|t|\,\|A\|\,\|B\|\left(\omega_s\left(N_{1/2,\xi}N\right)+\xi^{-n}\omega_s\left(N^2\right)\right), \tag{8.4}$$

for some $C = C(n,\kappa_n,\nu_n,c) > 0$ and all $|t| < \xi'/c'$. To bound the r.h.s. of (8.4), we apply Corollary 2.10 to the evolution ω_s generated by B to find

$$\omega_s\left(N_{X^{\mathrm{c}}_{\xi/2}}N\right) \le C\left(\omega\left(N_{X^{\mathrm{c}}}N\right)+\xi^{-n}\omega(N^2)\right), \tag{8.5}$$

for some $C > 0$ and all $0 \le s < \xi'/c'$, and use that $\omega_s(N^p) \equiv \omega(N^p)$. Now, plugging (8.4)–(8.5) back to (8.3), using the assumption $s \le r < \xi/c = \xi'/c'$, taking ω satisfying (2.10) and therefore $\omega(N_{X^{\mathrm{c}}}N) = 0$ by (2.34), and using relations (2.11), we arrive at the desired estimate (2.23). This completes the proof. □

9. Proof of Theorem 2.6

We apply Theorem 2.2 so that $U_t^\xi \equiv \alpha_t^{X_\xi}(U)$ is localized in $X_\xi \subset Y^{\mathrm{c}}$ (see (2.14)). Consequently, conjugation by U_t^ξ does not affect the partial trace $\mathrm{Tr}_{Y^{\mathrm{c}}}$. This leads to

$$\begin{aligned} F\left(\mathrm{Tr}_{Y^{\mathrm{c}}}(\rho_t), \mathrm{Tr}_{Y^{\mathrm{c}}}(\rho_t^{U_t})\right) &= F\left(\mathrm{Tr}_{Y^{\mathrm{c}}}\left(\rho_t^{U_t^\xi}\right), \mathrm{Tr}_{Y^{\mathrm{c}}}\left(\rho_t^{U_t}\right)\right) \\ &\ge F\left(\rho_t^{U_t^\xi}, \rho_t^{U_t}\right), \end{aligned}$$

where the last line follows from the data processing inequality for the fidelity, see [17, Lem. B.4].

Since ω is a pure state, $\omega = \langle\varphi, (\cdot)\varphi\rangle$ for some $\varphi \in \mathcal{D}(H)\cap\mathcal{D}(N)$. For rank-one projections $\rho_t = |\varphi_t\rangle\langle\varphi_t|$ generated by the initial state $|\varphi\rangle\langle\varphi|$, we compute

$$F\left(\rho_t^{U_t^\xi}, \rho_t^{U_t}\right) = \left|\left\langle U_t^\xi\varphi_t,\, U_t\varphi_t\right\rangle\right| .$$

Since U_t is unitary, so is U_t^ξ (again, see (2.14)). Writing $U_t = U_t^\xi + \mathrm{Rem}_t(U)$ and using $(U_t^\xi)^*U_t^\xi = 1$, we arrive at

$$\left|\left\langle U_t^\xi\varphi_t,\, U_t\varphi_t\right\rangle\right| \ge 1 - \left|\left\langle \varphi_t,\, (U_t^\xi)^*\mathrm{Rem}_t(U)\varphi_t\right\rangle\right| . \tag{9.1}$$

Let $\xi' := \xi/4 \ge 1$, $c' := c/2 > 2\kappa$, and $N_{\gamma,\xi} := N_{X_{(1-\gamma)\xi,(1+\gamma)\xi}}$ (c.f. (D.12)). We view U as an observable in $\mathcal{B}_{X_{3\xi/4}}$, so that $B \in \mathcal{B}_Y$ with $\mathrm{dist}(X_{3\xi/4}, Y) \ge \xi'$. Take the pair (φ,ψ) in estimate (D.51) to be $(U_t^\xi\varphi, \varphi)$. Then, by estimate (2.33) (which, importantly, is independent of state ω) and the relation $X_{3\xi/4,5\xi/4} = (X_{3\xi/4})_{0,2\xi'}$, we have for all $|t| < \xi'/c' = \xi/c$ that

$$\left|\left\langle \varphi,\, (U_t^\xi)^*\mathrm{Rem}_t(U)\varphi\right\rangle\right| \le C\,|t|\,\tau_{1/4}(\varphi)^{1/2}\tau_{1/4}(U_t^\xi\varphi)^{1/2}, \tag{9.2}$$

$$\text{where } \tau_\alpha(\phi) := \langle\phi,\, N_{\alpha,\xi}N\phi\rangle + (\gamma\xi)^{-n}\left\langle\phi,\, N^2\phi\right\rangle, \tag{9.3}$$

for some $C = C(n, \kappa_n, \nu_n, c) > 0$ and small γ with $(1-\gamma)c' > 2\kappa$. Note that $\|U\|$ is dropped for unitary U.

Let $\tilde\varphi_t = e^{-itH_{X_\xi}}\varphi$. By Corollary 2.10, the first term in the second factor on the r.h.s. of (9.2) can be bounded as follows:

$$\left\langle U_t^\xi\varphi,\, N_{1/4,\xi}NU_t^\xi\varphi\right\rangle = \left\langle \tilde\varphi_t,\, U^*\alpha_{-t}^{X_\xi}(N_{1/4,\xi}N)U\tilde\varphi_t\right\rangle \le C\tau_{1/2}(U\tilde\varphi_t). \tag{9.4}$$

which holds for fixed $C = C(n, \kappa_n, c)$ and all $|t| < \xi/(4c')$ by (2.10).

Since $U \in \mathcal{B}_X$ and $\operatorname{supp} N_{1/2,\xi} \subset X^{\mathrm{c}}$, we have $[U, N] = [U, N_{1/2,\xi}] = 0$. By this and the relation $U^*U = 1$, the leading term in the last line of (9.4) can be bounded as

$$\left\langle \tilde\varphi_t,\, U^*N_{1/2,\xi}NU\tilde\varphi_t\right\rangle = \left\langle \tilde\varphi_t,\, N_{1/2,\xi}N\tilde\varphi_t\right\rangle \le C\tau_1(\varphi), \tag{9.5}$$

which holds for fixed $C = C(n, \kappa_n, c)$ and all $|t| < \xi/(2c')$. We also have for all t that

$$\left\langle U_t^\xi\varphi,\, N^2U_t^\xi\varphi\right\rangle = \left\langle \varphi,\, N^2\varphi\right\rangle. \tag{9.6}$$

Plugging (9.4)–(9.6) back to (9.2), we conclude that, for some fixed $C = C(n, \kappa_n, c)$ and all $|t| < \xi/(4c')$,

$$\left|\left\langle \varphi,\, (U_t^\xi)^*\mathrm{Rem}_t(U)\varphi\right\rangle\right| \le C\,|t|\,\tau_1(\varphi). \tag{9.7}$$

Plugging (9.7) back to (9.1) and using the choice $c' = c/4$ and the localization conditions (2.10)–(2.11) on the initial state ω, we get the desired lower bound (2.26) for all $|t| < \xi/c$. This completes the proof. ☐

10. Proof of Theorem 2.7

We adapt the argument of [38]. We shift H in (1.1) so that the new Hamiltonian, which we still denote by H, has the ground state energy 0 and so $H \ge 0$.

Since $H = \oplus_n H_n$ and each $H_n := H\restriction_{\{N=n\}}$, $n = 0, 1, \dots$, is bounded, $e^{izH} = \prod_n e^{izH_n}$ is an entire operator-valued function of z. Consequently,

$$f(z) := \langle \Omega,\, B\alpha_z(A)\Omega\rangle \quad (z \in \mathbb{C}),$$

with $\alpha_z(A) = e^{izH}Ae^{-izH}$ (c.f. (2.6)), is well-defined and entire. Now, we claim that, for all $A \in \mathcal{B}_X$, $B \in \mathcal{B}_Y$, and all small $b > 0$,

$$|f(ib)| \le C_{AB}(\gamma^{-1}\xi^{-2} + \xi^{1-n}\omega(N_X^2)). \tag{10.1}$$

Here and in the remainder of the proof, $C_{AB} = C\,\|A\|\,\|B\|$ with $C > 0$ depending only on n, κ_n, ν_n, and b. Then the desired estimate (2.27) follows from the relation $f(0) = \langle \Omega,\, BA\Omega\rangle$ by taking $b \to 0+$.

Now we prove (10.1). Let $\mathbb{C}^\pm := \{z \in \mathbb{C} : \pm\mathrm{Im} z > 0\}$. Since Ω is an eigenvector with eigenvalue 0, we have $f(z) = \left\langle \Omega,\, Be^{izH}A\Omega\right\rangle$. This, together with the spectral theorem and the gap assumption on H, implies

$$f(z) = \int_\gamma^\infty e^{iz\lambda}\, d\,\langle \Omega,\, BP_\lambda A\Omega\rangle\,, \tag{10.2}$$

where P_λ is the projection-valued spectral measure corresponding to H. To estimate the integral on the r.h.s. of (10.2), we pass to Riemann sums to obtain, for all

$z \in \mathbb{C}^+$,

$$|f(z)| \le e^{-\mathrm{Im} z\gamma} \lim \sum_i |\langle \Omega,\, BP_{\Delta_i} A\Omega\rangle| \,, \tag{10.3}$$

where the sum is taken over a partition of $[\gamma, \infty)$ into subintervals Δ_i's. Next, using Cauchy-Schwartz inequality, we estimate

$$\begin{aligned} \sum |\langle \Omega,\, BP_{\Delta_i} A\Omega\rangle| &\le \sum \|P_{\Delta_i} B^*\Omega\| \, \|P_{\Delta_i} A\Omega\| \\ &\le \Big(\sum \|P_{\Delta_i} B^*\Omega\|^2\Big)^{1/2} \Big(\sum \|P_{\Delta_i} A\Omega\|^2\Big)^{1/2} \\ &\le \|B^*\Omega\| \, \|A\Omega\| \,, \end{aligned} \tag{10.4}$$

with the norms on the r.h.s. taken in the Fock space $\mathcal{F}$. Since (10.4) is uniform in all partitions, combining (10.3)–(10.4) yields

$$|f(z)| \le \|A\| \, \|B\| \, e^{-\mathrm{Im} z\gamma}. \tag{10.5}$$

Next, fix $T > 0$ to be chosen later. Since $f(z)$ is entire, by the Cauchy integral formula, for every $0 < b < T$, we have

$$f(ib) = \frac{1}{2\pi i}\left(\int_{\Gamma_T^+} \frac{f(z)dz}{z - ib} + \int_{-T}^{T} \frac{f(t)\, dt}{t - ib}\right), \tag{10.6}$$

where $\Gamma_T^+ \subset \mathbb{C}^+$ denotes the semicircle with radius T in the upper half-plane $\mathbb{C}^+$. Moreover, for all sufficiently small b, we have $|z - ib| > T/2$ for all $z \in \Gamma_T^+$, whence

$$\left|\int_{\Gamma_T^+} \frac{f(z)dz}{z - ib}\right| \le \frac{\|A\| \, \|B\|}{T} \int_0^\pi e^{-\gamma T \sin\theta}\, d\theta \le \frac{C^1_{AB}}{\gamma T^2}, \tag{10.7}$$

by estimate (10.5). This bounds the first term in the r.h.s. of (10.6).

To bound the second term in the r.h.s. of (10.6), we take some $0 < \delta < T$ to be determined later, split the interval $I_T = I_\delta \cup (I_T \setminus I_\delta)$ (where $I_a := [-a, a]$), and write, for every $t \in I_T$,

$$f(t) = \langle \Omega,\, \alpha_t(A)B\Omega\rangle + \langle \Omega,\, [B, \alpha_t(A)]\Omega\rangle =: \mathrm{I}(t) + \mathrm{II}(t). \tag{10.8}$$

Then we have

$$\begin{aligned} \left|\int_{-T}^{T} \frac{f(t)\, dt}{t - ib}\right| \le& \left|\int_{-T}^{T} \frac{\mathrm{I}(t)\, dt}{t - ib}\right| + \left|\int_{-\delta}^{\delta} \frac{\mathrm{II}(t)\, dt}{t - ib}\right| + \left|\int_{I_T \setminus I_\delta} \frac{\mathrm{II}(t)\, dt}{t - ib}\right| \\ =:& F + G_1 + G_2. \end{aligned} \tag{10.9}$$

To bound F, we note that by the Cauchy–Goursat theorem, $F = \left|\int_{\Gamma_T^-} \frac{\mathrm{I}(z)\, dz}{z - ib}\right|$, where and $\Gamma_T^- \subset \mathbb{C}^-$ denotes the semicircle with radius T in the lower half-plane $\mathbb{C}^-$. Therefore, by the same argument as (10.7), we find that F satisfies the estimate

$$F \le \frac{C^1_{AB}}{\gamma T^2}. \tag{10.10}$$

To bound G_1, we note that since $\mathrm{II}(t)$ is analytic and vanishes at $t = 0$, we have $|\mathrm{II}(t)| \le C^2_{AB}\, |t|$ for all small t. This implies

$$G_1 \le \int_{-\delta}^{\delta} \frac{|\mathrm{II}(t)|\, dt}{|t|} \le C^2_{AB}\delta. \tag{10.11}$$

To bound G_2, we note that by the weak LRB (2.17), $\mathrm{II}(t)$ satisfies the uniform estimate $|\mathrm{II}(t)| \le C^3_{AB}\,|t|\,\xi^{-n}\omega(N^2_X)$ for all real t with $|t| < \xi/(3\kappa)$. Hence,

$$G_2 \le \int_{I_T \setminus I_\delta} \frac{|\mathrm{II}(t)|\ dt}{|t|} \le C^3_{AB}(T-\delta)\xi^{-n}\omega(N^2_X), \tag{10.12}$$

provided $T < \xi/(3\kappa)$. Combining (10.9)–(10.12) yields an estimate on the second term in the r.h.s. of (10.6):

$$\left|\int_{-T}^{T} \frac{f(t)\,dt}{t-ib}\right| \le C_{AB}(\gamma^{-1}T^{-2} + \delta + (T-\delta)\xi^{-n}\omega(N^2_X)). \tag{10.13}$$

Finally, choosing $\delta = \xi^{-n}/(10\kappa) < T = \xi/(6\kappa)$ (recall $\xi \ge 1$), and plugging (10.7), (10.13) back to (10.6), we find

$$|f(ib)| \le C_{AB}(\gamma^{-1}\xi^{-2} + \xi^{-n} + \xi^{1-n}\omega(N^2_X)).$$

We conclude claim (10.1) from here. This completes the proof □

11. Proof of Theorem 2.8

We follow the argument in Sects. 3–4. For $\chi \in \mathcal{X}$ (see (3.5)) and two numbers $|t| < s$, define the ASTLOs

$$\bar{\chi}_{ts} := \hat{\chi}_{ts}/N, \tag{11.1}$$

where, recall, $\hat{\chi}_{ts}$ is given by (3.3). By relation (3.12), we see that $\bar{\chi}_{ts}$ commutes with $\bar{\xi}_{t's'}$ for any two functions χ, ξ. Define a set of smooth cutoff functions

$$\mathcal{G} \equiv \mathcal{G}_{\nu,\nu'} := \left\{ f \in C^\infty(\mathbb{R}) \;\middle|\; \begin{array}{l} \operatorname{supp} f \subset \mathbb{R}_{\ge 0},\ \operatorname{supp} f' \subset (\nu,\nu') \\ f' \ge 0,\ \sqrt{f'} \in C^\infty(\mathbb{R}) \end{array} \right\}. \tag{11.2}$$

For any $f \in \mathcal{G}$, $\chi \in \mathcal{X}$, we consider the two parameter family of operators

$$f_{ts} := f(\bar{\chi}_{ts}). \tag{11.3}$$

We now claim that this family satisfies a recursive monotonicity estimate similar to (3.8): Namely, there exist constant $C > 0$ and function $\xi_k \in \mathcal{X}$ s.th. for all $t \in \mathbb{R}$, $s > 0$,

$$Df_{ts} \le f'_{ts}\left(\frac{\kappa - v}{s}\overline{\chi'}_{ts} + \sum_{k=2}^{n} s^{-k}\overline{(\xi^k)'}_{ts} + Cs^{-(n+1)}\right), \tag{11.4}$$

where, recall, $D = \partial_t + i[H,\cdot]$ is the Heisenberg derivative from (3.6), $f'_{ts} \equiv f'(\bar{\chi}_{ts})$, and $\overline{\chi'}_{ts} \equiv \hat{\chi}'_{ts}/N$. (The sum in the r.h.s. is dropped for $n = 1$.)

Let $R_{ts}(z) = (z - \bar{\chi}_{ts})^{-1}$ for $\mathrm{Im} z \ne 0$. Since f is smooth and has compactly supported derivatives, by the Helffer-Sjörstrand formula (see [29, Lem. B.2]),

$$f^{(p)}_{ts} = \int R^{p+1}_{ts}(z)\,d\tilde{f}(z), \quad p = 0, 1, \tag{11.5}$$

for some finite measure $d\tilde{f}(z)$ on $\mathbb{C}$ vanishing for $\mathrm{Im} z = 0$. By (11.5), together with the relations $Df_{ts} = \int DR_{ts}(z)\,d\tilde{f}(z)$ and $DR_{ts} = R_{ts}(D\bar{\chi}_{ts})R_{ts}$, we compute

$$Df_{ts} = \int R_{ts}(z) D\bar{\chi}_{ts} R_{ts}(z)\,d\tilde{f}(z). \tag{11.6}$$

(One can consider (11.6) as an *integral chain rule* for the Heisenberg derivative.) Since $[H, N] = 0$, by definition (11.1), we have $D\bar{\chi}_{ts} = D\hat{\chi}_{ts}N^{-1}$. Plugging this back to (11.6) and applying the recursive monotonicity estimate (3.8), we find

$$Df_{ts} \leq \int R_{ts}(z)\left(-\frac{v-\kappa}{s}\overline{\chi'}_{ts} + \sum_{k=2}^{n} s^{-k}\overline{(\xi^k)'}_{ts} + Cs^{-(n+1)}\right)R_{ts}(z)\,d\tilde{f}(z), \tag{11.7}$$

for some $\xi_k \in \mathcal{X}$ and $C = C(n, \kappa_n, \chi) > 0$. (The sum in the r.h.s. is dropped for $n = 1$.) Finally, using that $[R_{ts}(z), \bar{\eta}_{ts}] = 0$ for $\eta = \chi', \xi_k'$, estimate (11.7), and representation formula (11.5), we conclude claim (11.4).

With the recursive monotonicity estimate (11.4), we can proceed exactly as in the proof of Proposition 3.4 and the derivation of (3.32) to obtain

$$\alpha_t(f_{ts}) \leq C\left(f_{0s} + s^{-n}\right), \tag{11.8}$$

for some $C = C(n, \kappa_n, c, \nu' - \nu) > 0$ and all $s > |t|$. Following the same argument as in Section 4.2, for appropriately chosen $f \in \mathcal{G}$, we obtain the estimates

$$f_{0s} \leq P_{\bar{N}_{X^c} \geq \nu}, \quad P_{\bar{N}_{X^c_\eta} \geq \nu'} \leq f_{ts}, \tag{11.9}$$

c.f. (3.18)–(3.19) as well as [15, Eq. (15)]. By assumption (2.29) and estimates (11.8)–(11.9), we conclude (11.2). □

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Declarations

- Conflict of interest: The Authors have no conflicts of interest to declare that are relevant to the content of this article.
- Data availability: Data sharing is not applicable to this article as no datasets were generated or analysed during the current study.

Appendix A. Fock spaces

In this appendix we discuss some general properties of Fock spaces used in this paper, see [11, 19].

Given a (1-particle) Hilbert space $\mathfrak{h}$, one defines the Fock space (over $\mathfrak{h}$) as

$$\mathcal{F} \equiv \mathcal{F}(\mathfrak{h}) := \oplus_{n=0}^{\infty} \otimes^n \mathfrak{h}, \tag{A.1}$$

where $\otimes^n \mathfrak{h} = \mathbb{C}$ for $n = 0$, $= \mathfrak{h}$ for $n = 1$, and is the symmetric (or anti-symmetric) tensor product of $\mathfrak{h}$'s for $n > 1$.

For any two (1-particle) Hilbert spaces $\mathfrak{h}_1$ and $\mathfrak{h}_2$, there is a unitary map $U \equiv U_{(\mathfrak{h}_1,\mathfrak{h}_2)}$ s.t.

$$U : \Gamma(\mathfrak{h}_1 \oplus \mathfrak{h}_2) \to \Gamma(\mathfrak{h}_1) \otimes \Gamma(\mathfrak{h}_2). \tag{A.2}$$

Let p_i be the projection from $\mathfrak{h}_1 \oplus \mathfrak{h}_2$ to $\mathfrak{h}_i$. Then the map U is defined as follows

$$U\big|_{\otimes^n(\mathfrak{h}_1\oplus\mathfrak{h}_2)} := \sum_{k=0}^{n} \begin{pmatrix} n \\ k \end{pmatrix}^{1/2} p_1^{\otimes(n-k)} \otimes p_2^{\otimes k}, \tag{A.3}$$

where $p_i^{\otimes m}$ denotes the m-fold tensor product $p_i \otimes \cdots \otimes p_i$.

Furthermore, the decoupling operator $U \equiv U_{(\mathfrak{h}_1,\mathfrak{h}_2)}$ can also be constructed using creation and annihilation operators by setting

$$\begin{aligned} &U_{(\mathfrak{h}_1,\mathfrak{h}_2)}\Omega := \Omega_1 \otimes \Omega_2, \\ &U_{(\mathfrak{h}_1,\mathfrak{h}_2)}a^\sharp(f) = \big(a^\sharp(f_1) \otimes \mathbf{1} + \mathbf{1} \otimes a^\sharp(f_2)\big)U_{(\mathfrak{h}_1,\mathfrak{h}_2)}, \end{aligned} \tag{A.4}$$

for $f = f_1 \oplus f_2 \in \mathfrak{h}_1 \oplus \mathfrak{h}_2$, and using these formulae to define $U_{(\mathfrak{h}_1,\mathfrak{h}_2)}$ on an arbitrary vector in $\Gamma(\mathfrak{h}_1 \oplus \mathfrak{h}_2)$. Here, $\Omega_\sharp$ is the vacuum in $\mathcal{F}_\sharp$ and $a^\sharp(f) = \sum_{x\in\Lambda} a_x^\sharp f(x)$ with $a^\sharp$ standing for either a or a^*.

A natural example of the splitting $\mathfrak{h} = \mathfrak{h}_1 \oplus \mathfrak{h}_2$ is the splitting of the Hilbert space $\ell^2(\Lambda)$ as

$$\ell^2(\Lambda) = \ell^2(S) \oplus \ell^2(S^{\mathrm{c}})$$

for any $S \subset \Lambda$ and with $S^{\mathrm{c}} = \Lambda \setminus S$. Denoting the corresponding unitary map by U_S, we have

$$U_S : \mathcal{F} \to \mathcal{F}_S \otimes \mathcal{F}_{S^{\mathrm{c}}}, \tag{A.5}$$

where $\mathcal{F}_S$ is the Fock space over the 1-particle Hilbert space $\ell^2(S)$,

$$\mathcal{F}_S := \Gamma(\ell^2(S)) \equiv \mathcal{F}(\ell^2(S)).$$

Then, an observable A on the Fock space $\mathcal{F}$ is supported (or localized) in S in the sense of (2.13) if and only if it is of the form

$$U_S A U_S^* = A_S \otimes \mathbf{1}_{S^{\mathrm{c}}}, \tag{A.6}$$

where A_S is the restriction of A on $\mathcal{F}_S$ and similar for $\mathbf{1}_{S^{\mathrm{c}}}$.

Appendix B. Technical estimates

Throughout this section, let Λ be a connected subset of a lattice $\mathcal{L} \subset \mathbb{R}^d$, $d \geq 1$ with grid size ≥ 1. Denote by $\mathfrak{h} := \ell^2(\Lambda)$ and by $\mathcal{F}$ the (fermionic or bosonic) Fock space over $\mathfrak{h}$.

Lemma B.1. *Let $n \geq 1$. Suppose A is an operator acting on $\mathfrak{h}$ with operator kernel (matrix) A_{xy} satisfying*

$$M := \left(\sup_{x\in\Lambda} \sum_{y\in\Lambda} |A_{xy}|\,|x-y|^{n+1}\right)\left(\sup_{y\in\Lambda} \sum_{x\in\Lambda} |A_{xy}|\,|x-y|^{n+1}\right) < \infty. \tag{B.1}$$

Then for every function f on Λ s.th. for some $L > 0$,

$$|f(x) - f(x)| \leq L\,|x-y| \quad (x, y \in \Lambda), \tag{B.2}$$

we have

$$\left\|\mathrm{ad}_f^k(A)\right\| \leq L^k M \quad (1 \leq k \leq n+1). \tag{B.3}$$

Proof. For every $f : \Lambda \to \mathbb{C}$, a simply induction shows that for all k,

$$\left(\mathrm{ad}_f^k(A)\right)_{xy} = A_{xy}(f(y) - f(x))^k. \tag{B.4}$$

This formula, together with the Schur test for matrices, implies

$$\left\|\mathrm{ad}_f^k(A)\right\|^2 \le \left(\sup_{x\in\Lambda}\sum_{y\in\Lambda}|A_{xy}|\,|f(x)-f(y)|^k\right)\left(\sup_{y\in\Lambda}\sum_{x\in\Lambda}|A_{xy}|\,|f(x)-f(y)|^k\right). \tag{B.5}$$

If f satisfies (B.2), then

$$\sup_{x\in\Lambda}\sum_{y\in\Lambda}|A_{xy}|\,|f(x)-f(y)|^k \le L^k \sup_{x\in\Lambda}\sum_{y\in\Lambda}|A_{xy}|\,|x-y|^k \le L^k M, \tag{B.6}$$

where the last estimate follows from assumptions (B.1) and that the grid size of Λ is at least 1. Similarly we can show that the second term in the r.h.s. of (B.5) satisfies the same bound as (B.6). Plugging the results back to (B.5) completes the proof. □

Corollary B.2. *Suppose H in* (1.1) *satisfies* (1.2). *Then, for every $X \subset \Lambda$ and the distance function $d_X(x) = \mathrm{dist}(\{x\}, X)$, we have*

$$\left\|\mathrm{ad}_{d_X}^k(H)\right\| \le M \quad (1 \le k \le n+1).$$

Proof. Every d_X is uniformly Lipschitz and satisfies (B.2) with $L = 1$. □

Lemma B.3. *Let α_t (resp. β_t) be the many-body (resp.* 1*-body) evolutions generated by $H = \mathrm{d}\Gamma(h) + V$ (resp. h). Suppose V satisfies* (3.13). *Then for every function f on Λ and its second quantization $\hat{f}$ as in* (3.2),

$$\alpha_t(\hat{f}) = \mathrm{d}\Gamma(\beta_t(f)). \tag{B.7}$$

Proof. Without loss of generality, we take $t \ge 0$ within this proof. Write $H_0 := \mathrm{d}\Gamma(h)$. We decompose the evolution α_t into a composition of two maps:

$$\alpha_t = \alpha_t^{\mathrm{int}} \circ \alpha_t^{\mathrm{loc}}, \tag{B.8}$$

$$\alpha_t^{\mathrm{loc}}(A) = e^{itH_0} A e^{-itH_0}, \tag{B.9}$$

$$\alpha_t^{\mathrm{int}}(A) = e^{itH} e^{-itH_0} A e^{itH_0} e^{-itH}. \tag{B.10}$$

For every function $f : \Lambda \to \mathbb{C}$ and $f_r := \beta_r(f)$, we compute using (B.9) that

$$\frac{1}{i}\partial_r \alpha_{t-r}^{\mathrm{loc}}(\mathrm{d}\Gamma(f_r)) = \alpha_{t-r}^{\mathrm{loc}}\left(-[H_0, \mathrm{d}\Gamma(f_r)] + \mathrm{d}\Gamma([h, f_r])\right).$$

Applying (3.12) to the second term on the r.h.s., we see that $\partial_r \alpha_{t-r}^{\mathrm{loc}}(\mathrm{d}\Gamma(f_r)) = 0$. Hence

$$\mathrm{d}\Gamma(f_t) - \alpha_t^{\mathrm{loc}}(\hat{f}) = \int_0^t \partial_r \alpha_{t-r}^{\mathrm{loc}}(\mathrm{d}\Gamma(f_r))\, dr = 0, \tag{B.11}$$

where, recall, $\hat{f} = \mathrm{d}\Gamma(f)$.

Next, using (B.10), we compute, for every observable A,

$$\frac{1}{i}\partial_r \alpha_r^{\mathrm{int}}(A) = \alpha_r^{\mathrm{int}}\left(\left[\alpha_r^{\mathrm{loc}}(V), A\right]\right), \tag{B.12}$$

and therefore

$$\begin{aligned}\alpha_t(\hat{f}) - \alpha_t^{\rm loc}(\hat{f}) =& \int_0^t \partial_r \left(\alpha_r^{\rm int} \circ \alpha_t^{\rm loc}(\hat{f})\right) dr \\ =& i \int_0^t \alpha_r^{\rm int} \left(\left[\alpha_r^{\rm loc}(V), \alpha_t^{\rm loc}(\hat{f})\right]\right) dr \\ =& i \int_0^t \alpha_r \left(\left[V, \alpha_{t-r}^{\rm loc}(\hat{f})\right]\right) dr \\ =& i \int_0^t \alpha_r \left([V, {\rm d}\Gamma(f_{t-r})]\right) = 0,\end{aligned} \tag{B.13}$$

where in the last line we use (B.11) and property (3.13). Combining (B.11)–(B.13) gives (B.7). □

Appendix C. Symmetrized commutator expansion

In this appendix, we establish the following symmetrized commutator expansion (c.f. [8, 15]):

Proposition C.1. *Let $A \in \mathcal{B}(\mathfrak{h})$ and Φ be a self-adjoint operator on $\mathfrak{h}$ s.th. for some $n \geq 1$,*

$$\mathrm{ad}_\Phi^k(A) \in \mathcal{B}(\mathfrak{h}) \quad (1 \leq k \leq n+1). \tag{C.1}$$

Then, for every $\chi \in C^\infty(\mathbb{R})$ s.th. χ' has compact support and operators

$$\chi_{ts} := \chi(s^{-1}(\Phi - vt)) \tag{C.2}$$

with s, $t \in \mathbb{R}$ (c.f. (3.4)), we have the expansion

$$\begin{aligned}[A, \chi_{ts}] =& s^{-1}\sqrt{|\chi_{ts}'|}\,\mathrm{sgn}(\chi_{ts}')[A, \Phi]\sqrt{|\chi_{ts}'|} \\ &+ \sum_{k=2}^n s^{-k} \sum_{m=1}^{N_k} v_{ts}^{(m)} g_{ts}^{(m)}\,\mathrm{ad}_\Phi^k(A) v_{ts}^{(m)} + s^{(n+1)} R(t,s).\end{aligned} \tag{C.3}$$

The r.h.s. of (C.3) is dropped for $n = 1$. Moreover, if $n \geq 2$,

1. *$v^{(m)}$ are piece-wise smooth functions supported in $\mathrm{supp}(\chi')$;*
2. *$g^{(m)}$ are piece-wise constant functions taking values in ± 1 on $\mathrm{supp}(v^{(m)})$;*
3. *$v_{ts}^{(m)}$, $g_{ts}^{(m)}$ are defined as (C.2);*
4. *$R(t,s)$ is bounded for all s, t, and satisfies*

$$\|R(t,s)\| \leq C \left\|\mathrm{ad}_\Phi^{n+1}(A)\right\|, \tag{C.4}$$

   for some $C = C(n, \chi) > 0$;
5. *$1 \leq N_k \leq C(n)$ for some $C(n) > 1$ and all $k = 2, \ldots, n$.*

Since $\chi \in \mathcal{X}$ and h satisfies (1.2), by definition (3.5) and Corollary B.2, the hypotheses of Proposition C.1 are satisfied with $\chi \in \mathcal{X}$, $A = ih$ (see (1.1)), and $\Phi = d_X$ for any $X \subset \Lambda$. This gives :

Corollary C.2. *Let $\Phi = d_X$ in (C.2). Then the operators χ_{ts} satisfies (C.3) with $A = ih$, $\Phi = d_X$.*

Proof of Proposition C.1. Throughout the proof, we fix t in (3.4) and the *self-adjoint operator* Φ satisfying (C.1). Then we consider the one-parameter family of (bounded) operators $\chi_s \equiv \chi_{ts}$, see (C.2). In the proof below, all estimates are independent of Φ, v, t.

1. Since $\chi \in C^\infty$ and χ' has compact support, the hypotheses of [29, Lems. B.1–2] are satisfied. Hence, by the commutator expansion formula [29, Eq. (B.14)], we have

$$[A, \chi_s] = \sum_{k=1}^{n} s^{-k} E^{(0)}(k,s) + s^{-(n+1)} R^{(0)}(s),$$
$$E^{(0)}(k,s) := \frac{1}{k!}\chi_s^{(k)} \operatorname{ad}_\Phi^k(A).$$

with $R^{(0)}(s)$ satisfying the remainder estimate,

$$\left\| R^{(0)}(s) \right\| \le C \left\| \operatorname{ad}_\Phi^{n+1}(A) \right\|,$$

where $C = C(n, \chi) > 0$ and the r.h.s. is finite by condition (C.1). We proceed to symmetrize $E^{(0)}(k,s)$, $k = 1, \ldots, n$ w.r.t. the functions $G_k^{(0)}(s) := \chi_s^{(k)}$. For each k, let

$$v_k^{(0)}(s) \equiv \left(v_k^{(0)}\right)_s := \sqrt{\left|G_k^{(0)}(s)\right|}, \quad g_k^{(0)}(s) \equiv \operatorname{sgn}(G_k^{(0)}(s)).$$

Then we have

$$G_k^{(0)}(s) \operatorname{ad}_\Phi^k(A) = g_k^{(0)}(s) v_k^{(0)}(s) \operatorname{ad}_\Phi^k(A) v_k^{(0)}(s) + g_k^{(0)}(s) v_k^{(0)}(s) \left[v_k^{(0)}(s), \operatorname{ad}_\Phi^k(A) \right]. \tag{C.5}$$

By the assumption on χ, each $v_k^{(0)}$ is a piece-wise smooth function supported $\operatorname{supp}\chi'$. Hence, we can again expand the commutator in the r.h.s. of (C.5) via [29, Eq. (B.14)]. This way we obtain

$$[v_k^{(0)}(s), \operatorname{ad}_\Phi^k(A)] = -\sum_{m=1}^{n-k} \frac{s^{-m}}{m!} G_{m,k}^{(1)}(s) \operatorname{ad}_\Phi^{k+m}(A) + s^{-(n-k+1)} R_k^{(1)}(s), \tag{C.6}$$

where

(a) the sum is dropped if $k = n$;
(b) $\operatorname{supp} G_k^{(1)}(s) \subset \operatorname{supp} v_k^{(0)}(s) \subset \operatorname{supp} \chi_s'$, with $\left\| G_k^{(1)}(s) \right\|_{L^\infty} \le C$ for some $C = C(\chi)$ and all k, s;
(c) and $\left\| R_k^{(1)}(s) \right\| \le C \left\| \operatorname{ad}_\Phi^{n+1}(A) \right\|$ for some $C = C(n, \chi) > 0$ and all k, s.

If $n = 1$, then the first term in (C.6) is dropped. Hence, plugging (C.6) into (C.5), we find

$$[A, \chi_s] = g_1^{(0)}(s) v_1^{(0)}(s) \operatorname{ad}_\Phi^1(A) v_1^{(0)}(s) + s^{-2}(R^{(0)}(s) + R_1^{(1)}(s)).$$

This establishes expansion (C.3) for $n = 1$.

2. If $n \geq 2$, then we iterate Step 1 as follows. First, plugging (C.6) into (C.5), we find

$$\begin{aligned}
[A, \chi_s] = &\sum_{k=1}^{n} s^{-k}\Big(S^{(1)}(k,s) + \sum_{m=1}^{n-k+1} s^{-m} E^{(1)}(k,m,s)\Big) \\
&+ s^{-(n+1)}\Big(R^{(0)}(s) + R^{(1)}(s)\Big),\\
S^{(1)}(k,s) :=& \frac{1}{k!} g_k^{(0)}(s) v_k^{(0)}(s)\, \mathrm{ad}_\Phi^k(A) v_k^{(0)}(s),\\
E^{(1)}(k,m,s) :=& -\frac{1}{m!} g_k^{(0)}(s) v_k^{(0)}(s) G_{k,m}^{(1)}(s)\, \mathrm{ad}_\Phi^{k+m}(A),\\
R^{(1)}(s) :=& \sum_{k=1}^{n} \frac{1}{k!} g_k^{(0)}(s) v_k^{(0)}(s) R_k^{(1)}(s).
\end{aligned}$$

Fix $1 \leq k \leq n-1$. We symmetrize each of $E^{(1)}(k,m,s)$, $m = 1, \ldots, n-k+1$ w.r.t. the function

$$-\frac{1}{m!} g_k^{(0)}(s) v_k^{(0)}(s) G_{k,m}^{(1)}(s) \tag{C.7}$$

in place of $G_k^{(0)}(s)$ in Step 1. This will introduce symmetrized operators $S^{(2)}(k,m,s)$, uniformly bounded operators $E^{(2)}(k,m,l,s)$, and remainders $R_{k,m}^{(2)}(s)$ as before.

3. From here one can see that this process can be iterated for exactly $(n-1)$–times. At the end, we obtain an expansion of $[A, \chi_s]$ into a sum of the form

$$[A, \chi_s] = \sum_{k=1}^{n} s^{-k} \sum_{p=1}^{n-1} \sum S^{(p)}(k_1, \ldots, k_p) + \sum_{k=0}^{k} R^{(k)}(s), \tag{C.8}$$

where the third sum is over some combinations of $k_i \geq 1$ with $\sum_{i=1}^{p} k_i = k$. Each $S^{(p)}$, $p = 1, \ldots, n-1$ is of the form

$$S^{(p)}(k_1, \ldots, k_p, t, s) = (-1)^{p-1} \frac{1}{k_p!} g_{k_1 \ldots k_p}^{(p-1)}(s) v_{k_1 \ldots k_p}^{(p-1)}(s)\, \mathrm{ad}_\Phi^{k_1 + \ldots + k_p}(A) v_{k_1 \ldots k_p}^{(p-1)}(s),$$

where the functions $v_{k_1 \ldots k_p}^{(p-1)}$ are piece-wise smooth, uniformly bounded by a constant $C = C(\chi)$, and supported in $\operatorname{supp} \chi'$. $\left|g_{k_1 \ldots k_p}^{(p-1)}(s)\right|$ are piece-wise constant functions, taking values in ± 1. This establishes expansion (C.3). The uniform bound on the remainder follows from corresponding uniform estimates obtained above. □

Appendix D. Proof of Theorem 2.9

Within this proof we assume $t \geq 0$. The case $t \leq 0$ follows by the time reflection. Recall the notations $A_t = \alpha_t(A)$ and $A_t^\xi = \alpha_t^{X_\xi}(A)$ for $\xi \geq 0$, see (2.14).

For a mixed state ω, we decompose $\omega = \sum p_i P_{\psi^i}$, where P_ψ is the rank-one projection onto $\mathbb{C}\psi$, with $p_i \geq 0$, $\sum p_i < \infty$, and use linearity to reduce the problem to estimating $\left|\left\langle \varphi, (A_t - A_t^\xi)\psi \right\rangle\right|$ for appropriate φ and ψ. The latter is done in Step 4 at the end of the proof.

1. We fix an operator $A \in \mathcal{B}_X$ and define the remainder operator

$$\mathrm{Rem}_t \equiv \mathrm{Rem}_t(A) = A_t - A_t^\xi,$$

c.f. (6.1), as well as the (X_ξ-X_ξ^c)-coupling operator (c.f. R' in (5.2))

$$R = H - H_{X_\xi} - H_{X_\xi^c} = R' - H_{X_\xi^c}.$$

Using these definitions and that $[H_{X_\xi^c}, A_s^\xi] = 0$ for all $s \in \mathbb{R}, \xi \geq 0$, since $\operatorname{supp} A_s^\xi \subset X_\xi$ (see (5.1)), we find from (5.2) that

$$\text{Rem}_t = \int_0^t \alpha_r \left(i \left[R, A_{t-r}^\xi \right] \right) dr. \tag{D.1}$$

Next, we use the standing assumptions $h_{xy} = \overline{h_{yx}}$ and $v_{xy} = v_{yx} = \overline{v_{xy}}$ to split the (X_ξ-X_ξ^c)-coupling term R into two terms arising respectively from the kinetic and potential terms in (1.1) (see Figure 4):

$$R := S + W, \tag{D.2}$$

$$S := S' + (S')^*, \quad S' := \sum_{x \in X_\xi, y \in X_\xi^c} h_{xy} a_x^* a_y, \tag{D.3}$$

$$W := \sum_{x \in X_\xi, y \in X_\xi^c} V_{xy} \quad \text{with } V_{xy} := a_x^* a_y^* v_{xy} a_y a_x. \tag{D.4}$$

Eqs. (D.1)–(D.2) imply, for any $\varphi,\ \psi \in \mathcal{D}(N) \cap \mathcal{D}(H)$,

$$|\langle \varphi, \text{Rem}_t \psi \rangle| \ \leq \ t \sup_{0 \leq r \leq t} \left(\left| \left\langle \varphi_r,\ \left[S, A_{t-r}^\xi \right] \psi_r \right\rangle \right| + \left| \left\langle \varphi_r,\ \left[W, A_{t-r}^\xi \right] \psi_r \right\rangle \right| \right), \tag{D.5}$$

where $\phi_r = e^{-irH}\phi$. In the rest of the proof we estimate the r.h.s. of this expression.

2. We first estimate the first term in the r.h.s. of (D.5). Within this step, all constants $C > 0$ depend only on n, κ_n, and c.

Let $s := t - r$. By formula (D.3), we have the estimate

$$\begin{aligned} &\left| \left\langle \varphi_r,\ \left[S', A_s^\xi \right] \psi_r \right\rangle \right| \\ \leq &\sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left(\left| \left\langle \varphi_r,\ a_x^* a_y A_s^\xi \psi_r \right\rangle \right| + \left| \left\langle \varphi_r,\ A_s^\xi a_x^* a_y \psi_r \right\rangle \right| \right) \\ = &\sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left(\left| \left\langle a_x \varphi_r,\ a_y A_s^\xi \psi_r \right\rangle \right| + \left| \left\langle a_x (A_s^\xi)^* \varphi_r,\ a_y \psi_r \right\rangle \right| \right). \end{aligned}$$

Using the Cauchy-Schwarz inequality and the fact that $\|a_z \varphi_r\| = \langle \varphi_r,\ n_z \varphi_r \rangle^{1/2}$ (recall $n_z = a_z^* a_z$), we find

$$\left| \left\langle \varphi_r,\ \left[S', A_s^\xi \right] \psi_r \right\rangle \right| \leq \text{I}^{1/2} \text{II}^{1/2} + \text{III}^{1/2} \text{IV}^{1/2}, \tag{D.6}$$

$$\text{I} := \sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left\langle \varphi_r,\ n_x \varphi_r \right\rangle, \tag{D.7}$$

$$\text{II} := \sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left\langle \psi_r,\ (A_s^\xi)^* n_y A_s^\xi \psi_r \right\rangle, \tag{D.8}$$

$$\text{III} := \sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left\langle \psi_r,\ n_y \psi_r \right\rangle, \tag{D.9}$$

$$\text{IV} := \sum_{x \in X_\xi, y \in X_\xi^c} |h_{xy}| \left\langle \varphi_r,\ A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle. \tag{D.10}$$

We now estimate the terms in the r.h.s. of (D.6). Given $c > 2\kappa$, we fix a number $0 < \gamma < 1/3$ in the remainder of the proof s.th.

$$c_1 := \frac{(1-\gamma)c}{2} > \kappa. \tag{D.11}$$

We introduce the local number operators counting the number of particles in the curved annular regions (c.f. (5.7) and Figure 6 below):

$$N_{\gamma,\xi} := N'_{\gamma,\xi} + N''_{\gamma,\xi}, \quad N'_{\gamma,\xi} := N_{X_{(1-\gamma)\xi,\xi}}, \quad N''_{\gamma,\xi} := N_{X_{\xi,(1+\gamma)\xi}}. \tag{D.12}$$

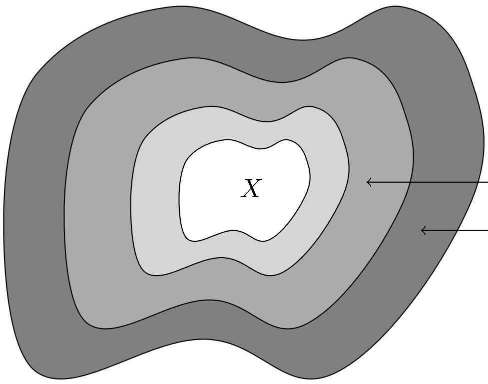

FIGURE 6. Schematic diagram illustrating the region associated to the local number operators in (D.12).

In what follows, we will use the following estimate for the particle number in curved annular regions (c.f. [16, Thm. 2.3]):

$$\langle \varphi_r, N_{\gamma_1,\xi}\varphi_r\rangle \le C\left(\langle\varphi, N_{\gamma_2,\xi}\varphi\rangle + ((\gamma_2-\gamma_1)\xi)^{-n}\langle\varphi, N\varphi\rangle\right), \tag{D.13}$$

valid for any two numbers $1 \ge \gamma_2 > \gamma_1 \ge 0$, $c > \kappa$, and $r < (\gamma_2-\gamma_1)\xi/c$. Estimate (D.13) follows from the 'incoming' light cone estimate, (5.4).

2.1. To estimate the term I from (D.7), we use the decomposition

$$X_\xi = X_{(1-\gamma)\xi} \cup X_{(1-\gamma)\xi,\xi}, \tag{D.14}$$

c.f. Figure 6, and that $|x-y| \ge \gamma\xi$ for all $x \in X_{(1-\gamma)\xi}$ and $y \in X_\xi^c$, to compute

$$\begin{aligned}
\mathrm{I} &= \sum_{y\in X_\xi^c} |h_{xy}| \left(\sum_{x\in X_{(1-\gamma)\xi,\xi}} \langle\varphi_r, n_x\varphi_r\rangle + \sum_{x\in X_{(1-\gamma)\xi}} \langle\varphi_r, n_x\varphi_r\rangle \right) \\
&\le \left(\sup_{x\in\Lambda}\sum_{y\in X_\xi^c}|h_{xy}|\right) \sum_{x\in X_{(1-\gamma)\xi,\xi}} \langle\varphi_r, n_x\varphi_r\rangle \\
&\quad + (\gamma\xi)^{-n}\left(\sup_{x\in\Lambda}\sum_{y\in X_\xi^c}|h_{xy}||x-y|^n\right) \sum_{x\in X_{(1-\gamma)\xi}} \langle\varphi_r, n_x\varphi_r\rangle.
\end{aligned}$$

Recalling definition (1.2) and noting the fact that $\sup_{x\in\Lambda}\sum_{y\in X_\xi^c}|h_{xy}| \le \kappa_{n-1}$ as the grid size of the underlying lattice is at least 1 (see (1.2)), we conclude

$$\mathrm{I} \le \kappa_{n-1}\left(\langle\varphi_r, N'_{\gamma,\xi}\varphi_r\rangle + (\gamma\xi)^{-n}\langle\varphi_r, N\varphi_r\rangle\right), \tag{D.15}$$

where, recall, $N'_{\gamma,\xi} \equiv N_{X_{(1-\gamma)\xi,\xi}}$ (see (D.12)).

To estimate the first term in line (D.15), we use the relation $N'_{\gamma,\xi} \le N_{\gamma,\xi}$ and apply (D.13) with $c \to c_1 > \kappa$ (see the choice (D.11)) to obtain, for all $0 \le r < (1-\gamma)\xi/c_1$,

$$\left\langle \varphi_r,\, N'_{\gamma,\xi}\varphi_r \right\rangle \le C\tau_0(\varphi), \tag{D.16}$$

$$\tau_0(\phi) := \langle \phi,\, N_{1,\xi}\phi\rangle + (\gamma\xi)^{-n}\langle \phi,\, N\phi\rangle. \tag{D.17}$$

Plugging estimate (D.16) back to (D.15) and using the conservation N, we find that

$$\mathrm{I} \le C\tau_0(\varphi), \tag{D.18}$$

uniformly for all r with $0 \le r < (1-\gamma)\xi/c_1$.

2.2. To estimate the term II from (D.8), we use the decomposition

$$X_\xi^{\mathrm{c}} = X_{(1+\gamma)\xi}^{\mathrm{c}} \cup X_{\xi,(1+\gamma)\xi}, \tag{D.19}$$

c.f. Figure 6, and the notation $\widetilde{n_y} := (A_s^\xi)^* n_y A_s^\xi$, to compute

$$\begin{aligned}
\mathrm{II} &= \sum_{x\in X_\xi} |h_{xy}| \left(\sum_{y\in X_{\xi,(1+\gamma)\xi}} \langle \psi_r,\, \widetilde{n_y}\psi_r\rangle + \sum_{y\in X^{\mathrm{c}}_{(1+\gamma)\xi}} \langle \psi_r,\, \widetilde{n_y}\psi_r\rangle \right) \\
&\le \left(\sup_{y\in\Lambda} \sum_{x\in X_\xi} |h_{xy}| \right) \sum_{y\in X_{\xi,(1+\gamma)\xi}} \langle \psi_r,\, \widetilde{n_y}\psi_r\rangle \\
&\quad + (\gamma\xi)^{-n} \left(\sup_{y\in\Lambda} \sum_{x\in X_\xi} |h_{xy}||x-y|^n \right) \sum_{y\in X^{\mathrm{c}}_{(1+\gamma)\xi}} \langle \psi_r,\, \widetilde{n_y}\psi_r\rangle \\
&\le \kappa_{n-1}\left(\left\langle \psi_r,\, (A_s^\xi)^* N''_{\gamma,\xi} A_s^\xi \psi_r \right\rangle + (\gamma\xi)^{-n} \left\langle \psi_r,\, (A_s^\xi)^* N A_s^\xi \psi_r\right\rangle \right).
\end{aligned} \tag{D.20}$$

To estimate the first term in line (D.20), we note that since $\operatorname{supp} A_s^\xi \subset X_\xi$ for all s and $\operatorname{supp} N''_{\gamma,\xi} \subset X_\xi^{\mathrm{c}}$ by construction (see (D.12)), we have $\left[A_s^\xi, N''_{\gamma,\xi}\right] \equiv 0$ for all s. By this fact, the first term in line (D.20) can be bounded as

$$\begin{aligned}
&\left\langle \psi_r,\, (A_s^\xi)^* N''_{\gamma,\xi} A_s^\xi \psi_r \right\rangle \\
&= \left\langle \psi_r,\, (N''_{\gamma,\xi})^{1/2} (A_s^\xi)^* A_s^\xi (N''_{\gamma,\xi})^{1/2} \psi_r \right\rangle \\
&\le \left\| A_s^\xi \right\|^2 \left\langle \psi_r,\, N''_{\gamma,\xi}\psi_r \right\rangle = \|A\|^2 \left\langle \psi_r,\, N''_{\gamma,\xi}\psi_r \right\rangle.
\end{aligned} \tag{D.21}$$

Using the relation $N''_{\gamma,\xi} \le N_{\gamma,\xi}$ and applying Corollary 2.10 to the r.h.s. above with $c \to c_1 > \kappa$, we obtain that for all $0 \le r < (1-\gamma)\xi/c_1$,

$$\left\langle \psi_r,\, (A_s^\xi)^* N''_{\gamma,\xi} A_s^\xi \psi_r \right\rangle \le C\|A\|^2 \tau_0(\psi). \tag{D.22}$$

To estimate the second term in line (D.20), we use the relation $[A_s^\xi, N] = 0$ (see (5.1)) and the conservation of the expectation of N to get

$$\left\langle \psi_r,\, (A_s^\xi)^* N A_s^\xi \psi_r \right\rangle \le \left\| A_s^\xi \right\|^2 \langle \psi_r,\, N\psi_r\rangle = \|A\|^2 \langle \psi,\, N\psi\rangle.$$

Plugging the two preceding inequalities back to (D.20), we obtain

$$\mathrm{II} \le C\|A\|^2 \tau_0(\psi). \tag{D.23}$$

uniformly for all r with $0 \le r < (1-\gamma)\xi/c_1$.

2.3. The term III in (D.9) can be bounded as (D.20). (It is actually simpler because there is no A's in (D.9).) Here we record the result:

$$\mathrm{III} \le C\tau_0(\psi), \tag{D.24}$$

which holds uniformly for all $0 \le r < (1-\gamma)\xi/c_1$.

2.4. To bound the term IV in (D.10), we use the decomposition (D.14) to compute

$$\mathrm{IV} = \sum_{y \in X_\xi^c} |h_{xy}| \sum_{x \in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle \tag{D.25}$$

$$+ \sum_{y \in X_\xi^c} |h_{xy}| \sum_{x \in X_{(1-\gamma)\xi,\xi}} \left\langle \varphi_r,\, A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle . \tag{D.26}$$

Using the relation $[A_s^\xi, N] = 0$ (see (5.1)) and the conservation of N, we bound the term in line (D.25) as

$$\begin{aligned} &\sum_{y \in X_\xi^c} |h_{xy}| \sum_{x \in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle \\ &\le (\gamma\xi)^{-n} \sum_{y \in X_\xi^c} |h_{xy}||x-y|^n \sum_{x \in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle \\ &\le \kappa_{n-1} (\gamma\xi)^{-n} \left\langle \varphi_r,\, A_s^\xi N (A_s^\xi)^* \varphi_r \right\rangle \\ &\le \kappa_{n-1} \|A\|^2 (\gamma\xi)^{-n} \langle \varphi,\, N\varphi \rangle . \end{aligned} \tag{D.27}$$

To bound the term in line (D.26), we define $\varphi_{r,s} := e^{-isH_{X_\xi}} \varphi_r$ and recall $N'_{\gamma,\xi} \equiv N_{X_{(1-\gamma)\xi,\xi}}$. Then, we have, by definition (5.1) for the local evolution,

$$\begin{aligned} &\sum_{y \in X_\xi^c} |h_{xy}| \sum_{x \in X_{(1-\gamma)\xi,\xi}} \left\langle \varphi_r,\, A_s^\xi n_x (A_s^\xi)^* \varphi_r \right\rangle \\ \le& \kappa_{n-1} \left\langle \varphi_r,\, A_s^\xi N'_{\gamma,\xi} (A_s^\xi)^* \varphi_r \right\rangle \\ =& \kappa_{n-1} \left\langle A^* \varphi_{r,s},\, \alpha_{-s}^{X_\xi}(N'_{\gamma,\xi}) A^* \varphi_{r,s} \right\rangle . \end{aligned} \tag{D.28}$$

To estimate the quantity in the last line of (D.28), we use Corollary 2.10 with evolution $\alpha_{-s}^{X_\xi}(\cdot)$ to obtain that for all $s < \frac{1-\gamma}{2}\xi/c_1$,

$$\begin{aligned} &\left\langle A^* \varphi_{r,s},\, \alpha_{-s}^{X_\xi}(N'_{\gamma,\xi}) A^* \varphi_{r,s} \right\rangle \\ \le& C \left(\left\langle \varphi_{r,s},\, A N'_{(1+\gamma)/2,\xi} A^* \varphi_{r,s} \right\rangle + (\gamma\xi)^{-n} \langle \varphi_{r,s},\, A N A^* \varphi_{r,s} \rangle \right) . \end{aligned} \tag{D.29}$$

For the remainder estimate, we use that $0 < \gamma < 1/3$ so that $\frac{1-\gamma}{2} > \gamma$. Note that this is the only place $\gamma < 1/3$ is used.

Since $\operatorname{supp} A \subset X$ and $\operatorname{supp} N'_{(1+\gamma)/2,\xi} \subset X^{\mathrm{c}}$ by construction, we can pull out A's from (D.29) to obtain

$$\begin{aligned} &\left\langle A^* \varphi_{r,s},\, \alpha_{-s}^{X_\xi}(N'_{\gamma,\xi}) A^* \varphi_{r,s} \right\rangle \\ \le& \|A\|^2 C \left(\left\langle \varphi_{r,s},\, N'_{(1+\gamma)/2,\xi} \varphi_{r,s} \right\rangle + (\gamma\xi)^{-n} \langle \varphi_{r,s},\, N \varphi_{r,s} \rangle \right) . \end{aligned} \tag{D.30}$$

Now we use Corollary 2.10 twice on the first term of (D.30), first with the evolution $\alpha_s^{X_\xi}(\cdot)$ and then with $\alpha_r(\cdot)$. This way we obtain that for $r+s = t < \frac{1-\gamma}{2}\xi/c_1$,

$$\left\langle \varphi_{r,s},\, N'_{(1+\gamma)/2,\xi} \varphi_{r,s} \right\rangle \le \left\langle \varphi,\, \alpha_r \circ \alpha_s^{X_\xi}(N'_{(1+\gamma)/2,\xi}) \varphi \right\rangle \le C \tau_0(\varphi), \tag{D.31}$$

where $\tau_0(\varphi)$ is defined by (D.17). This bounds the first term in the r.h.s. of (D.30). (The derivation is similar to (9.5).) By the conservation of N, we find

$$\langle \varphi_{r,s},\, N \varphi_{r,s} \rangle = \langle \varphi,\, N\varphi \rangle \tag{D.32}$$

in the second term in the r.h.s. of (D.30).

Combining (D.27)–(D.32) yields

$$\mathrm{IV} \le C \left\|A\right\|^2 \tau_0(\varphi), \tag{D.33}$$

which holds uniformly for all

$$t < \frac{1-\gamma}{2}\xi/c_1. \tag{D.34}$$

2.5. At this point, we have uniform estimates (D.18), (D.23), (D.24), and (D.33), which are valid for all t satisfying (D.34). Plugging these estimates back to (D.6), we conclude that all t satisfying (D.34),

$$\sup_{0\le r\le t}\left|\left\langle \varphi_r,\, \left[S', A^{\xi}_{t-r}\right]\psi_r\right\rangle\right| \le C\left\|A\right\|\tau_0(\varphi)^{1/2}\tau_0(\psi)^{1/2}.$$

Since $\left|\left\langle \varphi_r,\, \left[(S')^*, A^{\xi}_{t-r}\right]\psi_r\right\rangle\right| = \left|\left\langle \psi_r,\, \left[S', (A^{\xi}_{t-r})^*\right]\varphi_r\right\rangle\right|$ and $(A^{\xi}_{t-r})^* = (A^*)^{\xi}_{t-r}$ (see (5.1)), going through Steps 2.1–4 and interchanging the roles of A^* (resp. φ_r) and A (resp. ψ_r) yields the exact same estimate for $\sup_{0\le r\le t}\left|\left\langle \varphi_r,\, \left[(S')^*, A^{\xi}_{t-r}\right]\psi_r\right\rangle\right|$ as above.

Recalling the definition of c_1 in (D.11) and the validity interval (D.34), we conclude that for every $0 \le t < \xi/c$,

$$\sup_{0\le r\le t}\left|\left\langle \varphi_r,\, \left[S, A^{\xi}_{t-r}\right]\psi_r\right\rangle\right| \le C\left\|A\right\|\tau_0(\varphi)^{1/2}\tau_0(\psi)^{1/2}. \tag{D.35}$$

This bounds the first term in the r.h.s. of (D.5).

3. Next,we estimate the second term in the last line of (D.5). Within this step, all constants $C > 0$ depend only on n, κ_n, ν_n, and c, where ν_n is as in (1.3).

By formula (D.4), the fact that $[a^\sharp_x, n_y] \equiv 0$ for all $x \in X_\xi$, $y \in X^c_\xi$ and $a^\sharp_x = a_x,\, a^*_x$, and the localization property $[A^\xi_s, a_y] = 0$, we have the estimate

$$\begin{aligned}
&\left|\left\langle \varphi_r,\, \left[W, A^\xi_s\right]\psi_r\right\rangle\right| \\
\le &\sum_{x\in X_\xi, y\in X^c_\xi} \left|v_{xy}\right| \left(\left|\left\langle \varphi_r,\, n_x n_y A^\xi_s \psi_r\right\rangle\right| + \left|\left\langle \varphi_r,\, A^\xi_s n_x n_y \psi_r\right\rangle\right|\right) \\
= &\sum_{x\in X_\xi, y\in X^c_\xi} \left|v_{xy}\right| \left(\left|\left\langle (A^\xi_s)^* n_x \varphi_r,\, n_y \psi_r\right\rangle\right| + \left|\left\langle n_x (A^\xi_s)^* \varphi_r,\, n_y \psi_r\right\rangle\right|\right).
\end{aligned}$$

Applying the Cauchy-Schwarz and triangle inequalities to the last line above, we find

$$\left|\left\langle \varphi_r,\, \left[W, A^\xi_s\right]\psi_r\right\rangle\right| \le \mathrm{V}^{1/2}\mathrm{VI}^{1/2} + \mathrm{V}^{1/2}\mathrm{VII}^{1/2}, \tag{D.36}$$

$$\mathrm{V} := \sum_{x\in X_\xi, y\in X^c_\xi} \left|v_{xy}\right| \left\langle \psi_r,\, n_y^2 \psi_r\right\rangle, \tag{D.37}$$

$$\mathrm{VI} := \sum_{x\in X_\xi, y\in X^c_\xi} \left|v_{xy}\right| \left\langle \varphi_r,\, n_x A^\xi_s (A^\xi_s)^* n_x \varphi_r\right\rangle, \tag{D.38}$$

$$\mathrm{VII} := \sum_{x\in X_\xi, y\in X^c_\xi} \left|v_{xy}\right| \left\langle \varphi_r,\, A^\xi_s n_x^2 (A^\xi_s)^* \varphi_r\right\rangle. \tag{D.39}$$

3.1. To bound the term V in (D.37), we use the fact $\sum_{x\in S} n_x^2 \le N_S^2$ and proceed exactly as in Step 2.3 above for the estimate of (D.9) (see more details in Step 3.2 below). This way we obtain that, for all $0 \le r < (1-\gamma)\xi$,

$$\text{V} \le C\tau(\psi), \tag{D.40}$$

$$\tau(\phi) := \langle \phi,\, N_{1,\xi} N\phi\rangle + (\gamma\xi)^{-n} \left\langle \phi,\, N^2\phi\right\rangle . \tag{D.41}$$

3.2. To bound the term VI in (D.38), we first use

$$\text{VI} \le \left\| A_t^\xi \right\|^2 \sum_{x\in X_\xi, y\in X_\xi^c} |v_{xy}| \left\langle \varphi_r,\, n_x^2 \varphi_r\right\rangle = \|A\|^2 \sum_{x\in X_\xi, y\in X_\xi^c} |v_{xy}| \left\langle \varphi_r,\, n_x^2\varphi_r\right\rangle .$$

Using decomposition (D.14) and the relation $\sum_{x\in S} n_x^2 \le N_S^2$, we then proceed as in the estimate of (D.7) (see Step 2.1) to obtain, in place of (D.15),

$$\begin{aligned} \text{VI} \le \|A\|^2 \Big(& \sum_{y\in X_\xi^c} |v_{xy}| \sum_{x\in X_{(1-\gamma)\xi,\xi}} \left\langle \varphi_r,\, n_x^2\varphi_r\right\rangle \\ & + (\gamma\xi)^{-n} \sum_{y\in X_\xi^c} |v_{xy}| |x-y|^n \sum_{x\in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, n_x^2\varphi_r\right\rangle \Big) \\ \le \nu_n & \left(\left\langle \varphi_r,\, \left(N'_{\gamma,\xi}\right)^2 \varphi_r \right\rangle + (\gamma\xi)^{-n} \left\langle \varphi_r,\, N\varphi_r\right\rangle \right) . \end{aligned}$$

For the first term in the last line above, we use Corollary 2.10 to obtain, for all $0 \le r < (1-\gamma)\xi/c_1$,

$$\left\langle \varphi_r,\, \left(N'_{\gamma,\xi}\right)^2 \varphi_r \right\rangle \le C\tau(\varphi). \tag{D.42}$$

Using the preceding two estimates and the conservation of N, we conclude that

$$\text{VI} \le C \|A\|^2 \tau(\varphi), \tag{D.43}$$

uniformly for all $0 \le r < (1-\gamma)\xi$.

3.3. To bound the term VII in (D.39), we proceed as in the estimate of (D.10) (see Step 2.4). Using the decomposition (D.14), we compute

$$\text{VII} = \sum_{y\in X_\xi^c} |v_{xy}| \sum_{x\in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, A_s^\xi n_x^2 (A_s^\xi)^* \varphi_r\right\rangle \tag{D.44}$$

$$+ \sum_{y\in X_\xi^c} |v_{xy}| \sum_{x\in X_{(1-\gamma)\xi,\xi}} \left\langle \varphi_r,\, A_s^\xi n_x^2 (A_s^\xi)^* \varphi_r\right\rangle . \tag{D.45}$$

The term in line (D.44) can be bounded in the same way as (D.27):

$$\sum_{y\in X_\xi^c} |v_{xy}| \sum_{x\in X_{(1-\gamma)\xi}} \left\langle \varphi_r,\, A_s^\xi n_x^2 (A_s^\xi)^* \varphi_r\right\rangle \le \nu_n (\gamma\xi)^{-n} \|A\|^2 \left\langle \varphi,\, N^2\varphi\right\rangle . \tag{D.46}$$

To bound the term in line (D.45), we first use that

$$\sum_{y\in X_\xi^c} |v_{xy}| \sum_{x\in X_{(1-\gamma)\xi,\xi}} \left\langle \varphi_r,\, A_s^\xi n_x^2 (A_s^\xi)^* \varphi_r\right\rangle \le \nu_n \left\langle A^*\varphi_{r,s},\, \alpha_{-s}^{X_\xi}((N'_{\gamma,\xi})^2) A^* \varphi_{r,s} \right\rangle ,$$

which can be derived similarly as (D.28). Applying Corollary 2.10 to the r.h.s. above, we find that for all $s < \frac{1-\gamma}{2}\xi/c_1$,

$$\begin{aligned} & \left\langle A^*\varphi_{r,s},\, \alpha_{-s}^{X_\xi}((N'_{\gamma,\xi})^2) A^*\varphi_{r,s} \right\rangle \\ \le & C \left(\left\langle \varphi_{r,s},\, AN'_{(1+\gamma)/2,\xi} N A^*\varphi_{r,s} \right\rangle + (\gamma\xi)^{-n} \left\langle \varphi_{r,s},\, AN^2A^*\varphi_{r,s}\right\rangle \right) . \end{aligned} \tag{D.47}$$

Since the local number operator $N'_{(1+\gamma)/2,\xi}$ is supported away from $X \supset \operatorname{supp} A$ (see (D.12) and Figure 6), and since $[A,N]=0$, we can pull out the A's from the first term in the r.h.s. of (D.47) as

$$\left\langle \varphi_{r,s},\, AN'_{(1+\gamma)/2,\xi} NA^*\varphi_{r,s}\right\rangle \le \|A\|^2 \left\langle \varphi_{r,s},\, N'_{(1+\gamma)/2,\xi} N\varphi_{r,s}\right\rangle, \tag{D.48}$$

c.f. (D.21). The rest of the estimate of (D.47) follows similarly as in the estimate of (D.29). Here we record the result:

$$\mathrm{VII} \le C\,\|A\|^2\,\tau(\varphi), \tag{D.49}$$

which holds uniformly for all $0\le r<t$, $s=t-r$, so long as (D.34) holds.

3.4. Combining uniform estimates (D.36), (D.40)–(D.49) yields, for every $0 \le t < \xi/c$,

$$\sup_{0\le r\le t}\left|\left\langle \varphi_r,\, \left[W, A^{\xi}_{t-r}\right]\psi_r\right\rangle\right| \le C\,\|A\|\,\tau(\varphi)^{1/2}\tau(\psi)^{1/2}. \tag{D.50}$$

4. Combining (D.35) and (D.50) in (D.5) and recalling the choice $\gamma=\gamma(c,\kappa)$ in (D.11) and definitions (D.17), (D.41), we conclude that, for $t<\eta/c$ and $c>2\kappa$,

$$|\langle \varphi,\, \mathrm{Rem}_t\psi\rangle| \le Ct\,\|A\|\,\tau(\varphi)^{1/2}\tau(\psi)^{1/2}. \tag{D.51}$$

Finally, for any mixed state ω satisfying (2.10) and any operator $B\in\mathcal{B}_Y$, we use the spectral decomposition $\omega=\sum p_i P_{\psi^i}$ with $p_i\ge 0$, $\sum p_i \le C<\infty$, and the choice $\varphi^i = B^*\psi^i$ in (D.51) to obtain

$$\begin{aligned} |\omega\big(B\,\mathrm{Rem}_t\big)| \le& \sum p_i \left|\left\langle B^*\psi^i,\, \mathrm{Rem}_t\psi^i\right\rangle\right| \\ \le& Ct\,\|A\|\sum p_i\,\tau(B^*\psi^i)^{1/2}\tau(\psi^i)^{1/2}. \end{aligned} \tag{D.52}$$

Since $B\in\mathcal{B}_Y$ and $Y\subset X^{\mathrm{c}}_{2\xi}$, we have $[B,N]=[B,N_{1,\xi}]=0$ (see (D.12)). Therefore, by definition (D.41), we have $\tau(B^*\psi^i)\le \|B\|^2\,\tau(\psi^i)$ for each i. This, together with estimate (D.52) and the facts that $\sum p_i\tau(\psi_i)=\omega\left(N_{X_{2\xi}\setminus X}N\right)+(\gamma\xi)^{-n}\omega(N^2)$ (see (D.41)) and $0<\gamma<1/3$, yields

$$|\omega\big(B\,\mathrm{Rem}_t\big)| \le C\gamma^{-n}t\,\|A\|\,\|B\|\left(\omega\left(N_{X_{2\xi}\setminus X}N\right)+\xi^{-n}\omega(N^2)\right). \tag{D.53}$$

This completes the proof of Theorem 2.9. □

Appendix E. Generalizations to unbounded observables

In this section, we sketch the extension of the main theorems in Section 2 to a large class of unbounded operators. We say that an operator A acting on $\mathcal{F}$ *has finite degree* if $[A,N]=0$ and

$$\deg A := \inf\left\{\nu\ge 0 : A,\ A^* \text{ are } N^{\nu/2}\text{-bounded}\right\} < \infty. \tag{E.1}$$

By definition, $\deg A=0$ if and only if A is bounded, and $\deg A\le 2M$ if A is a polynomial in n_x with degree at most M. For each $0\le\nu<\infty$, we define the norm

$$|||A|||_\nu := \max\left(\left\|AN^{-\nu/2}\right\|,\left\|A^*N^{-\nu/2}\right\|\right). \tag{E.2}$$

Let

$$\mathcal{B}^\nu := \left\{\text{operators } A \text{ on } \mathcal{F} \text{ with } |||A|||_\nu<\infty\right\}, \tag{E.3}$$

$$\mathcal{B}^\nu_X := \left\{A\in\mathcal{B}^\nu : \operatorname{supp} A\subset X,\ [A,N]=0\right\}. \tag{E.4}$$

Then $\mathcal{B}^\nu_X$ with $\nu=0$ coincides with (2.15), and we have the following lemma:

Lemma E.1. *Let* $0 \le \nu < \infty$, $X \subset \Lambda$, *and* $A \in \mathcal{B}^\nu_X$. *Then, for all numbers* $p, q \ge 0$ *and operator* $B \ge 0$ *with* $[B, N] = 0$, $\operatorname{supp} B \subset X^c$, *we have the following operator inequalities:*

$$A^* N^q A \le \|\!|A|\!\|_\nu^2 N^{\nu+q} \qquad \text{on } \mathcal{D}(N^{(\nu+q)/2}), \tag{E.5}$$

$$A^* N^{p/2} B^q N^{p/2} A \le \|\!|A|\!\|_\nu^2 N^{(\nu+p)/2} B^q N^{(\nu+p)/2} \qquad \text{on } \mathcal{D}(B^{q/2} N^{(\nu+p)/2}). \tag{E.6}$$

Proof. Since ν is fixed, we write $\|\!|\cdot|\!\| \equiv \|\!|\cdot|\!\|_\nu$ within this proof. Symmetrizing as

$$A^* N^q A = N^{(\nu+q)/2} N^{-(\nu+q)/2} A^* N^{q/2} N^{q/2} A N^{-(\nu+q)/2} N^{(\nu+q)/2},$$

and using definitions (E.2)–(E.4), we see that

$$A^* N^q A \le \left\| N^{q/2} A N^{-(\nu+q)/2} \right\|^2 N^{\nu+q} = \|\!|A|\!\|^2 N^{\nu+q}.$$

This gives (E.5). Next, since $\operatorname{supp} A \in X$ and $\operatorname{supp} B \subset X^c$, we have $[A, B] = [A, N] = 0$ and therefore

$$A^* N^{p/2} B^q N^{p/2} A = N^{p/2} B^{q/2} A^* A B^{q/2} N^{p/2}.$$

Applying (E.5) to the r.h.s. with $q = 0$ and then using the fact that $[N, B] = 0$, we find

$$\begin{aligned} A^* N^{p/2} B^q N^{p/2} A \le & \|\!|A|\!\|^2 N^{p/2} B^{q/2} N^\nu B^{q/2} N^{p/2} \\ = & \|\!|A|\!\|^2 N^{(\nu+p)/2} B^q N^{(\nu+p)/2}. \end{aligned}$$

This gives (E.6). □

Now we sketch the proof of Theorem 2.9 for operators $A \in \mathcal{B}^\nu_X$ with $\nu > 0$. Through this, the corresponding results for Thms. 2.2–2.3 follow readily, wherefore extensions of the results in Sects. 2.4–2.7, which are applications of Thms. 2.2–2.3, follow.

The main idea is to use Corollary 2.10 together with Lemma E.1, in places where Theorem 2.1 is used. For example, in place of (D.21), we use (E.5) with $B = N''_{\gamma,\xi}$, which is supported away from X_ξ (see (D.12)), to get

$$\left\langle \psi_r,\, (A^\xi_s)^* N''_{\gamma,\xi} A^\xi_s \psi_r \right\rangle \le \|\!|A|\!\|^2 \left\langle \psi_r,\, N''_{\gamma,\xi} N^\nu \psi_r \right\rangle. \tag{E.7}$$

Then we use Corollary 2.10 to the r.h.s. above to get

$$\left\langle \psi_r,\, N''_{\gamma,\xi} N^\nu \psi_r \right\rangle \le C \left(\langle \psi,\, N_{1,\xi} N^\nu \psi \rangle + (\gamma\xi)^{-n} \left\langle \psi,\, N^{\nu+1} \psi \right\rangle \right).$$

This, together with (E.7), yields

$$\begin{aligned} & \left\langle \psi_r,\, (A^\xi_s)^* N''_{\gamma,\xi} A^\xi_s \psi_r \right\rangle \\ \le & C \|\!|A|\!\|^2 \left(\langle \psi,\, N_{1,\xi} N^\nu \psi \rangle + (\gamma\xi)^{-n} \left\langle \psi,\, N^{\nu+1} \psi \right\rangle \right) \end{aligned} \tag{E.8}$$

in place of (D.22). Similar modifications are then made to (D.30), (D.31), (D.42), etc. This way one can obtain, for states $\varphi, \psi \in \mathcal{D}(N^{\frac{\nu+2}{2}}) \cap \mathcal{D}(H)$ and all other notations the same as in Theorem 2.9,

$$\begin{aligned} & \left| \left\langle \varphi,\, (A_t - A^\xi_t) \psi \right\rangle \right| \\ \le & C\, |t|\, \|\!|A|\!\| \left(\left\langle \varphi,\, N_{X_{2\xi} \setminus X} N^{\nu+1} \varphi \right\rangle + (\gamma\xi)^{-n} \left\langle \varphi,\, N^{\nu+2} \varphi \right\rangle \right)^{1/2} \\ & \times \left(\left\langle \psi,\, N_{X_{2\xi} \setminus X} N^{\nu+1} \psi \right\rangle + (\gamma\xi)^{-n} \left\langle \psi,\, N^{\nu+2} \psi \right\rangle \right)^{1/2}. \end{aligned}$$

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