

# 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.

## 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 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

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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:

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

Here  $\rho_t$ ,  $t \geq 0$  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  $\rho_0$  localized in  $X \subset \mathbb{R}^d$  and for any  $c > \kappa$ , the probability that the system in the state  $\rho_t$  is localized in  $\mathcal{H}_E \cap X_{ct}^c$  is arbitrarily small, asymptotically as  $t \rightarrow \infty$ , where  $\mathcal{H}_E$  is the spectral subspace

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

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

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

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  $\kappa$ .

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,

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

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

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

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

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  $C_A = \text{ad}_A : B \rightarrow [A, B]$  and  $p_q = -i\partial_{x_q}$ . Then, for every  $1 \leq q \leq d$ ,

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

*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

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

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*

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

*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  $\kappa$  as in (1.17), this solution satisfies*

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

*for all  $t > 0$*

*and all smooth cutoff functions  $g$  with  $\text{supp}(g) \subset (-\infty, E]$  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  $\kappa$  defined in (1.17), we have the following estimate:

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

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

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

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

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

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  $\kappa$  in Theorem 1.1. Physically,  $\kappa$  bounds the propagation speed (also called “speed of sound”) in the energy-constrained open quantum system. Naturally,  $\kappa$  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

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

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

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

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  $\delta_X$  defined in  $X^c$  such that

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

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

where  $c_1, c_2, C_\alpha$  are positive constants independent of  $X$ . Let  $f_{\epsilon_0} : \mathbb{R} \rightarrow \mathbb{R}$  be a  $C^\infty$  function such that  $f_{\epsilon_0}(x) = 0$  if  $x \leq \epsilon_0/2$ , and  $f_{\epsilon_0}(x) = x - \epsilon_0$  if  $x \geq \epsilon_0$ . We can then define

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

and verify that it satisfies the conditions above.

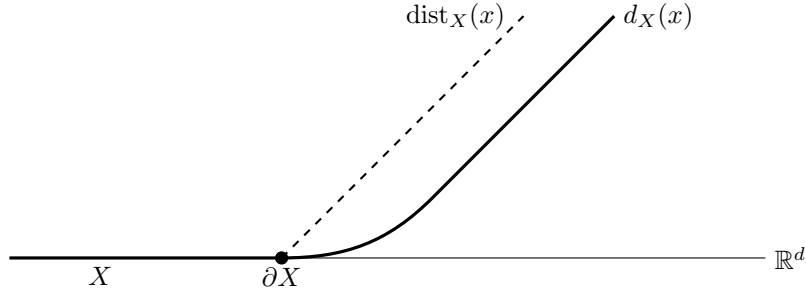


FIGURE 1. Schematic diagram illustrating  $d_X \equiv d_{X,\epsilon}$  in (1.11).

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

$$(1.13) \quad g(\mu) \equiv 1 \text{ for } \mu \leq E - \epsilon, \quad g(\mu) \equiv 0 \text{ for } \mu \geq E,$$

and define the *smooth energy cutoff* operator

$$(1.14) \quad g := g(H).$$

*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

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

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

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

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

$$(1.17) \quad \kappa := \|\gamma\| < \infty,$$

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

$$(1.18) \quad \gamma \equiv \gamma(X, E) = L'(d_X^E),$$

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  $n \geq 1$ . The assumptions made in [7] exclude in (1.1) the Schrödinger operators (1.3).

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

$$(1.19) \quad V(x) \text{ in (1.3) is } \Delta\text{-bounded with relative bound strictly less than 1,}$$

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  $\rho_t$ ,  $t \geq 0$ , to (1.1) satisfies

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

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  $(A, \rho) := \text{Tr}(A\rho)$ , i.e.,

$$(1.21) \quad \text{Tr}(AL\rho) = \text{Tr}((L'A)\rho),$$

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

$$(1.22) \quad L' = L'_0 + G', \quad L'_0 A = i[H, A],$$

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

with domain

$$(1.24) \quad \mathcal{D}(L') \equiv \mathcal{D}(L'_0) \equiv \{A \in \mathcal{B}(\mathcal{H}) \mid AD(H) \subset \mathcal{D}(H) \text{ and } [H, A] \text{ defined on } \mathcal{D}(A) \cap \mathcal{D}(H) \text{ extends to an operator on } \mathcal{D}(H)\}.$$

**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

$$(1.25) \quad A = O(B)$$

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

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

In all our estimates, it is understood that, if  $n = 1$ , the sums  $\sum_{k=2}^n(\dots)$  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  $j = 1, 2, \dots$ ,  $W_j$  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

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

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  $\Phi$  on  $\mathcal{H}$ , semi-bounded from below. We assume that

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

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

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

Hence

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

is finite.

Later on,  $H$  will be the Schrödinger operator (1.3) satisfying **(H)**,  $W_j$  will be bounded operators satisfying **(W1)**–**(W2)** and  $\Phi$  will be taken to be the operator

<sup>1</sup> $L'$  generates the dual Heisenberg-Lindblad evolution  $\partial_t A_t = L' A_t$  of quantum observables.

$\Phi \equiv \phi^E = g\phi g$  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

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

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

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

See Figure 2 below.

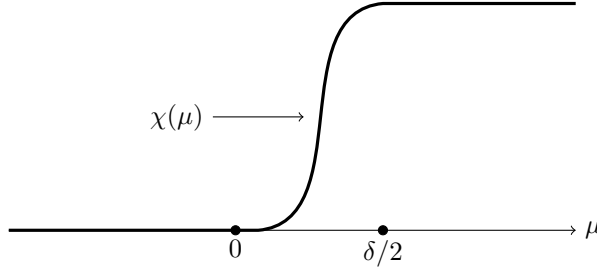


FIGURE 2. Schematic diagram illustrating  $\chi \in \mathcal{X}$ .

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  $\text{supp } w \subset (0, \delta/2)$ , then the antiderivative  $\int^x w^2 \in \mathcal{X}$ .
- (X2) If  $\xi_1, \dots, \xi_N \in \mathcal{X}$ , then  $\xi = (\xi_1^{\frac{1}{2}} + \dots + \xi_N^{\frac{1}{2}})^2$  satisfies  $\xi \in \mathcal{X}$  and  $\xi_1 + \dots + \xi_N \leq \sqrt{N}\xi$ .

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

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

Following [7], we use the method of propagation observables. Let  $\beta'_t$  be the evolution generated by the operator  $L'$ , i.e.  $\frac{d}{dt}\beta'_t(\Psi) = \beta'_t(L'\Psi)$  for all observables  $\Psi$  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

$$(2.7) \quad \frac{d}{dt}\beta'_t(\Psi_t) = \beta'_t(D\Psi_t),$$

$$(2.8) \quad D\Psi_t = L'\Psi_t + \partial_t\Psi_t.$$

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  $\chi_{ts}$  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  $\chi_{ts}$  be the operator defined in (2.6). Then there exists  $C = C(n, \chi) > 0$  and, if  $n \geq 2$ ,  $\xi^k = \xi^k(\chi) \in \mathcal{X}$ ,  $k = 2, \dots, n$ , such that as self-adjoint operators,*

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

where  $\kappa_\Phi > 0$  is as in (2.4) and  $M_k$  and  $\mu_n$  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  $r \geq 0$ ,

$$(2.10) \quad \chi_{ts}(r) := \beta'_r(\chi_{ts}) \quad \text{and} \quad \chi'_{ts}(r) := \beta'_r(\chi'_{ts}).$$

**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  $0 \leq t < s$ ,*

$$(2.11) \quad \int_0^t \chi'_{rs}(r) dr \leq C \mu_n^n \left( s \chi_{0s}(0) + \sum_{k=2}^n s^{-k+2} \xi_s^k(0) + t s^{-n} \right),$$

where  $\mu_n$  is given by (2.3).

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

$$(2.12) \quad \langle \chi_{ts} \rangle_t := \text{Tr}(\chi_{ts} \rho_t)$$

of  $\chi_{ts}$  in the state  $\rho_t$  solving (1.1) and instead of (2.7), used the relation

$$(2.13) \quad \frac{d}{dt} \langle \chi_{ts} \rangle_t = \langle D\chi_{st} \rangle_t.$$

These two formulations are related as

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

**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  $\chi_{ts}$  be the operator defined by (2.6). Then, uniformly in  $t$ , for  $s > 0$ ,*

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



where the remainder term  $\text{Rem}_H$  satisfies the estimate

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

for some  $\xi^2, \dots, \xi^n \in \mathcal{X}$  depending only on  $\chi$ , 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  $\chi_{ts}$  be the operator defined by (2.6). Then, uniformly in  $t$ , for  $s > 0$ ,*

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

where the remainder term  $\text{Rem}_W$  satisfies the estimate

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

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

*Remark 7.* The estimates above are all uniform in  $s, t, \Phi$  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  $\chi_s$  for  $\chi_{ts}$ . Also, we denote  $B_k \equiv i \text{ad}_{\Phi}^k(H)$  for  $k = 1, \dots, n+1$ . 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  $\chi$ , the hypotheses of Lemma C.2 are satisfied. Hence, by (C.4)–(C.5), we have

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

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

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  $\text{supp}(\chi^{(k)})$ . Then, we claim that

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

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

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

where

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

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

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

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

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

It follows that

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

so that

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

Now, we apply the following operator inequality

$$(2.26) \quad \pm(P^*Q + Q^*P) \leq P^*P + Q^*Q.$$

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

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

Since  $n$  is finite, we can choose  $\xi^2, \dots, \xi^n \in \mathcal{X}$  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

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

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

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

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

and for the remainder term we have

$$(2.30) \quad s^{-n} (u_s R'_n + R_n'^* u_s) \leq s^{-1} (u_s)^2 + s^{-2n+1} \|R'_n\|^2 (\tilde{\theta}_s)^2,$$

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  $\xi^2, \dots, \xi^n$  in such a way that  $\xi^l \in \mathcal{X}$  majorizes  $u^2$ ,  $\tilde{\theta}^2$  and  $(u^{(l)})^2$  for each  $l = 1, \dots, n-1$ .

Collecting all terms except for the leading order ones into the remainder term  $\text{Rem}_H$ , we obtain (2.15).  $\square$

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

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

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

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

$$(2.32) \quad \|R_{j,n+1}^{\text{right}}\|^2 \leq C \|D_{j,n+1}\|^2,$$

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

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

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

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

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

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

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  $\theta^k$  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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

This completes the proof of the claim (2.36).

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

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

Then, by writing everything as  $\text{Rem}_W$  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

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

where  $C$  is a constant depending only on  $\chi$  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

$$(2.44) \quad \begin{aligned} & W_j^* \chi_s' D_{j,1} + \text{h.c.} \\ & = u_s W_j^* D_{j,1} u_s + [W_j^*, u_s] u_s D_{j,1} + u_s W_j^* [u_s, D_{j,1}] + \text{h.c.}, \end{aligned}$$

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.  $\square$

Now we are ready to prove Theorem 2.1:

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

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

where  $C$  is some constant which depends only on  $n$  and  $\chi$ .

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

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

This completes the proof.  $\square$

### 2.3. Proof of Proposition 2.2.

*Proof of Proposition 2.2.* Within this proof, all constants  $C > 0$  depend only on  $\chi$  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  $\chi_{ts}$  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

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

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

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

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

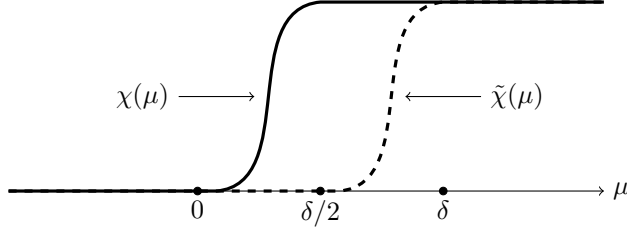
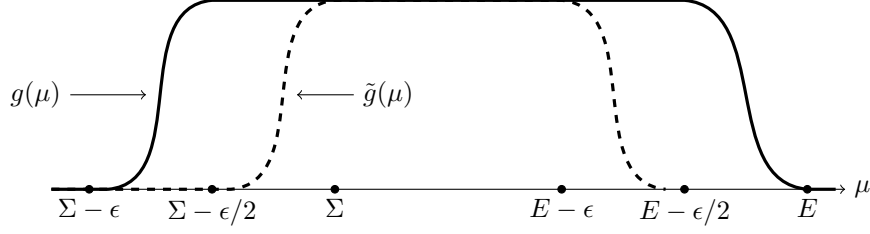
Since  $\kappa_\Phi < v$  and  $t \leq s$ , (2.48) implies, after dropping  $\chi_{ts}(t) \geq 0$ , which is due to the positive-preserving property of the flow (1.1) (see (1.20)), and multiplying by  $s(v - \kappa_\Phi)^{-1} \geq 0$ , that

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

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

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

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).  $\square$

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).

## 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  $\text{supp}(g) \subset (-\infty, E]$  (see also Remark 5) and a smooth function  $\chi$  from the space (2.5), we choose smooth cutoff functions  $\tilde{g}$  and  $\tilde{\chi}$  such that  $\text{supp}(\tilde{g}) \subset \{\chi \equiv 1\}$  and  $\text{supp}(\tilde{\chi}') \subset (\delta, +\infty) = \{\chi \equiv 1\}$ , so that

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

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

see Figs. 3–4.

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

$$(3.3) \quad \Phi := d_X^E = g(H)d_X g(H),$$

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).

To shorten notations, we introduce the following notations:

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

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

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

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

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

Recall that  $\beta'_t$  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  $\Phi$  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  $\text{supp}(g) \subset (-\infty, E]$ , 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),

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

for some  $\xi \in \mathcal{X}$  and all  $s > t$ . Taking expectation w.r.t.  $\rho_0$  on both sides of (3.7) and recalling that  $\chi_{ts}(t) := \beta'_t(\chi_{ts})$ , we find

$$(3.8) \quad \text{Tr}(\beta'_t(\chi_{ts}^E)\rho_0) \leq \text{Tr}((\chi_{0s}^E + O(s^{-1}\xi_{0s}^E))\rho_0) + O(s^{-n}).$$

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

$$(3.9) \quad \text{Tr}((\chi_{0s}^E + O(s^{-1}\xi_{0s}^E))\rho_0) = \text{Tr}(\chi_X^\# (\chi_{0s}^E + O(s^{-1}\xi_{0s}^E)) \chi_X^\# \rho_0) = O(s^{-n}).$$

The relation (3.6) implies

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

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

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

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

$$(3.12) \quad \text{Tr}(\tilde{g}\tilde{\chi}_{ts}\tilde{g}\beta'_t(\rho_0)) = O(s^{-n}).$$

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

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

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

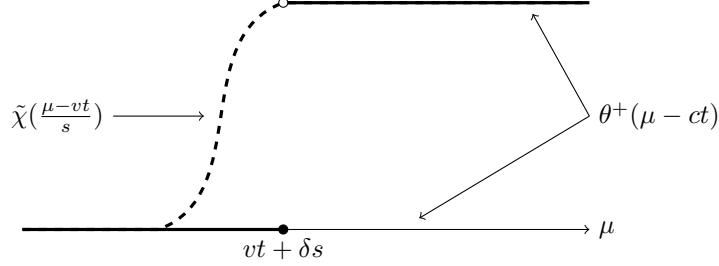


FIGURE 5. Schematic diagram illustrating estimate (3.13).

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

#### 4. ESTIMATES OF MULTIPLE COMMUTATORS

In this section, we establish some key estimates for multiple commutators of the form  $\text{ad}_{AE}^k(B)$ . More precisely, we show that the operators  $H = -\Delta + V(x)$  and  $W_j$  satisfying **(H)**–**(W2)**, with  $\Phi$  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

$$(4.1) \quad f \in \mathcal{S}^k$$

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

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

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

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

(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

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

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  $\phi \in C^\infty$ ,  $\phi \geq 0$  satisfying

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

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  $n \geq 1$ . Suppose  $H$  satisfies **(H)** and let  $\phi$  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  $E \in \mathbb{R}$ ,*

$$(4.5) \quad \left\| \text{ad}_{\phi^E}^k(H) \right\| \leq C \quad (k = 1, \dots, n+1).$$

*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

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

where

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

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

where  $\mu$  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  $\text{ad}_{\phi^E}^k(H)$  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

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

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

$$(4.9) \quad \text{ad}_{\phi^E}^1(H) = \iint d\tilde{g}(z_1) \otimes d\tilde{g}(z_2) R_H(z_1) \text{ad}_{\phi}^1(H) R_H(z_2).$$

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

Next, we compute

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

so that  $\text{ad}_{\phi}^1(H)$  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  $\text{ad}_{\phi^E}^1(H) \in \mathcal{F}^{(1)}$ , which completes the proof of the base case.

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

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

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

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

Also, we note some easy commutator relations

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

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

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

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

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

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

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

$$(4.17) \quad \begin{aligned} \phi C_{g^2}(a_k) &= \int d\tilde{g}^2 \phi R_H(\Delta a_k + 2\nabla a_k \cdot \nabla) R_H \\ &= \int d\tilde{g}^2 R_H(a_{k+1} + a_k p) R_H \\ &\quad + \int d\tilde{g}^2 R_H(a_1 + a_0 p) R_H(a_{k+2} + a_{k+1} p) R_H, \end{aligned}$$

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

$$(4.18) \quad C_{\phi}(p), \quad C_{\phi}(R_H),$$

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

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

$$(4.20) \quad \begin{aligned} C_{\phi}(R_H) &= R_H(C_{\phi} H) R_H = R_H(\Delta \phi + 2\nabla \phi \cdot \nabla) R_H \\ &= R_H(a_1 + a_0 p) R_H, \end{aligned}$$

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

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

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.  $\square$

**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:*

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

*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  $C_{\phi^E}$ . For each  $k = 1, \dots, n+1$ , we define the classes of operators on  $\mathcal{B}(\mathcal{H})$

$$(4.23) \quad \begin{aligned} \mathcal{G}_m^{(2)} &:= \{ \mathcal{L}_A \mathcal{R}_{A'} B_{rs}^{(2)} \mid A, A' \in \mathcal{F}^{(1)} \cup \{\mathbf{1}\}, \\ &\quad B_{rs}^{(2)} \equiv (\phi C_p)^r C_x^s \text{ with } r, s \geq 0 \text{ and } r + s = m \} \\ \mathcal{F}_k^{(2)} &:= \left\{ \text{polynomials of elements in } \mathcal{G}_m^{(2)}(W) \text{ for } 1 \leq m \leq k \right\}. \end{aligned}$$

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

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

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

$$(4.25) \quad \begin{aligned} C_H W &= pC_p W + (C_p W)p + C_V W \\ &= pC_p W + (C_p W)p + \int d\tilde{V}(z) R_x(z) [C_x W] R_x(z) \end{aligned}$$

and

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

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  $\tilde{V}$  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

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

which yields through Leibnitz rule that

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

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

$$\begin{aligned} \phi C_{g^2} W &= \int d\tilde{g}(z) R_H(z) \phi C_H(W) R_H(z) \\ (4.27) \quad &\quad + \int d\tilde{g}(z) R_H(z) (a_1 + a_0 p) R_H(z) [C_H W] R_H(z) \end{aligned}$$

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

$$(4.29) \quad C_{[g, \phi]g} W = [g, \phi]g W - W[g, \phi]g,$$

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  $\text{ad}_{\phi^E}^{m+1}(W_j) = C_{\phi^E}(\text{ad}_{\phi^E}^m(W_j))$ , 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

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

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

$$\begin{aligned} \mathcal{G}_m^{(3)} &:= \{ \mathcal{L}_A \mathcal{R}_{A'} B_{rs}^{(3)} \mid A, A' \in \mathcal{F}^{(1)} \cup \{1\}, B_{rs}^{(3)} \equiv (\phi^\ell C_p)^r C_x^s \\ &\quad \text{with } \ell \in \{0, 1\}, r, s \geq 0 \text{ and } r + s = m \} \\ (4.31) \quad \mathcal{F}_k^{(2)} &:= \left\{ \text{polynomials of elements in } \mathcal{G}_m^{(3)}(W) \text{ for } 1 \leq m \leq k \right\}. \end{aligned}$$

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

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  $\phi$  in place of  $\langle x \rangle$ , i.e.

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

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  $k = 0, 1 \dots$  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

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

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 Leibnitz 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  $r + s = m$ ,

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

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

$$(4.35) \quad C_p C_x = C_x C_p, \quad C_x(\phi C_p) = \phi C_p C_x$$

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

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

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

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

This completes the proof.  $\square$

**Corollary 4.3.** *Suppose that  $H = -\Delta + V(x)$  and  $W_j$  satisfy **(H)**–**(W2)**. Then, with  $\Phi$  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.  $\square$

## 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  $d_X^E = gd_Xg$  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)),*

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

*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  $X$  is also localized outside of  $X$  in position space up to small errors.

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

$$\begin{aligned} d &\equiv d_X, & d^E &\equiv d_X^E = gd_Xg, & R &= (d/s - z)^{-1}, & R^E &= (d^E/s - z)^{-1}, \\ b &= d - d^E, & \chi^E &= \chi(d^E/s), & \chi &= \chi(d/s). \end{aligned}$$

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),

$$(5.2) \quad Rd^E = Rgdg = Rdg^2 + R[g, d]g.$$

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

$$\begin{aligned} [g, d] &= \int d\tilde{g}(z) [(z - H)^{-1}, d] \\ &= - \int d\tilde{g}(z) (z - H)^{-1} \text{ad}_d^1(H) (z - H)^{-1} \\ (5.3) \quad &= \int d\tilde{g}(z) (z - H)^{-1} (\nabla \cdot (\nabla d) + \nabla d \cdot \nabla) (z - H)^{-1}. \end{aligned}$$

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

$$(5.4) \quad \|(z - H)^{-1} (\nabla \cdot (\nabla d) + \nabla d \cdot \nabla) (z - H)^{-1}\|$$

$$(5.5) \quad \leq \|B_{H,E}^{\frac{1}{2}}(\bar{z} - H)^{-1}\| \|B_{H,E}^{\frac{1}{2}}(z - H)^{-1}\|$$

$$(5.6) \quad \leq C(\langle E \rangle^{-\frac{1}{2}}|z| + \langle E \rangle^{\frac{1}{2}}|\operatorname{Im}(z)|^{-2}).$$

Using the properties of the almost analytic extension  $\tilde{g}$  (in particular the fact that it is supported in  $\{|\operatorname{Re}(z)| \leq \langle E \rangle\}$ , see (B.5) and Remark 5), this shows that the integral in (5.3) is norm convergent, which completes the proof.  $\square$

Now, using the Helffer-Sjöstrand representation (C.1) and omitting the measure  $d\tilde{\chi}$ , we write

$$(5.7) \quad \chi^E = \int R^E.$$

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

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

Plugging this expansion into (5.7) yields

$$(5.9) \quad \chi^E = \sum_{k=0}^{n-1} \chi_k + s^{-n} \operatorname{Rem}_1,$$

where

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

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

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

where the operators  $\tilde{B}_l$  and  $\tilde{M}_k$  are polynomials of operators  $\operatorname{ad}_d^k(b)$ ,  $k = 0, 1, \dots$ , (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  $\operatorname{ad}_d^k(b)$  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

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

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

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

$$(5.14) \quad Rb/s = d_s R h + R c_s, \quad \text{where}$$

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

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

$$(5.16) \quad d_s R = \mathbf{1} + zR.$$

The last two relations imply

$$(5.17) \quad Rb/s = h + Rc_s + zRh.$$

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:*

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

where

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

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

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

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  $m \geq 1$ .

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

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

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

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

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

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

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

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

This is of the form (5.18) with

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

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

where

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

satisfies (5.19).



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

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

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

$$(5.27) \quad A = A_1 + A_2 + A_3,$$

where

$$(5.28) \quad A_1 := zRh^{k+1},$$

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

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

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

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

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

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

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

The term  $A_3$  can be written as

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

where

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

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

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

which satisfies the bound (5.19) with  $k \rightarrow k + 1$ . 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

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

so that

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

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

$$(5.39) \quad \begin{aligned} RhB_{q,l}R^l &= RB'_{q,l}R^l \\ &= \sum_{r=0}^{n-l-1} (-1)^r s^{-r} \text{ad}_d^r(B'_{q,l})R^{l+r+1} + (-1)^{n-l} s^{-(n-l)} R \text{ad}_d^{n-l}(B'_{q,l})R^n. \end{aligned}$$

Using Leibniz rule for commutators and the structure of  $B_{q,l}$ , we conclude that the operators  $\text{ad}_d^r(B'_{q,l})$  are polynomials of  $\text{ad}_d^m(h)$  and  $\text{ad}_d^m(c_s)$ ,  $m = 0, 1, \dots, l+r$ , and therefore are  $(l+r)$ -operators as defined above. So, setting  $B''_{q,l+r} = (-1)^r \text{ad}_d^r(B'_{q,l})$ , expansion (5.39) becomes

$$(5.40) \quad RhB_{q,l}R^l = \sum_{r=0}^{n-l-1} s^{-r} B''_{q,l+r} R^{l+r+1} + s^{-(n-l)} RB''_{q,n} R^n.$$

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

$$(5.41) \quad \begin{aligned} A_2(q) &= \sum_{l=0}^{n-1} \sum_{r=0}^{n-l-1} s^{-(l+r)} B''_{q,l+r} R^{l+r+1} p'_{q+1,l}(z) \\ &\quad + s^{-n} \sum_{l=0}^{n-1} RB''_{q,n} R^n p'_{q+1,l}(z). \end{aligned}$$

Changing the summation index  $(l+r, l) \rightarrow (l', r')$ , the r.h.s. in line (5.41) can be written as

$$(5.42) \quad \sum_{l=0}^{n-1} \sum_{r=0}^{n-l-1} s^{-(l+r)} B''_{q,l+r} R^{l+r+1} p'_{q+1,l}(z) = \sum_{l'=0}^{n-1} \sum_{r'=0}^{l'} s^{-l'} B''_{q,l'} R^{l'+1} p'_{q+1,r'}(z).$$

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

$$(5.43) \quad \begin{aligned} A_2(q) &= \sum_{l=0}^{n-1} s^{-l} B''_{q,l} R^{l+1} p''_{q+1,l}(z) \\ &\quad + s^{-n} RB''_{q,n} R^n p''_{q+1,n}(z). \end{aligned}$$

Plugging (5.43) into (5.38) yields

$$(5.44) \quad \begin{aligned} A_2 &= \sum_{q=0}^k \sum_{l=0}^{n-1} s^{-l} B''_{q,l} R^{l+1} p''_{q+1,l}(z) \\ &\quad + s^{-n} \sum_{q=0}^k RB''_{q,n} R^n p''_{q+1,n}(z) \end{aligned}$$

Shifting the dummy index  $q \rightarrow q + 1$  and setting

$$(5.45) \quad B_{q,l}^{(3)} := B''_{q-1,l+1}, \quad p_{q,n}^{(3)}(z) := p''_{q+1,n}(z),$$

$$(5.46) \quad M_{q,n}^{(3)} := RB''_{q-1,n}R^n \text{ with } \deg_R(M_{q,n}^{(3)}) = n + 1,$$

we conclude that  $A_2$  is of the form (5.18).

This completes the proof of Lemma 5.3.  $\square$

**Corollary 5.4.** *For any  $\chi \in C^\infty(\mathbb{R})$  with compactly supported derivative and  $\chi_k = \int (Rb/s)^k R d\tilde{\chi}(z)$ ,*

$$(5.47) \quad \chi_k = h^k \chi(d_s) + \sum_{q=0}^k \sum_{l=0}^{n-1} s^{-l} B_{q,l} (\chi p_{q,l})^{(l+1)}(d_s) + s^{-n} \text{Rem}_{2,k},$$

where  $B_{q,l}$  are as in Lemma 5.3 and  $\text{Rem}_{2,k} = O(1)$ .

*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

$$(5.48) \quad \begin{aligned} \chi_k &= h^k \chi(d_s) + \sum_{q=0}^k \sum_{l=0}^{n-1} s^{-l} B_{q,l} (\chi p_{q,l})^{(l+1)}(d_s) \\ &+ s^{-n} \sum_{q=0}^k \int M_{q,n} R p_{q,n}(z) d\tilde{\chi}(z). \end{aligned}$$

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

$$(5.49) \quad \|M_{q,n}\| \leq C \sum_{j=n}^{2n} |\text{Im}(z)|^{-(j+1)} \text{ for all } q.$$

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  $(p, l) = (n + 1, n), \dots, (2n + 1, n)$  that

$$(5.50) \quad \left\| \int M_{q,n} R p_{q,n} d\tilde{\chi}(z) \right\| \leq C \int \sum_{j=n}^{2n} |\text{Im}(z)|^{-(j+2)} |p_{q,n}(z)| d\tilde{\chi}(z) \leq C.$$

Summing (5.50) over  $q$  shows that the integral on line (5.48) is  $O(1)$ . This completes the proof of Lemma 5.5.  $\square$

Since  $\chi^{(l)}(d_s) \chi_X^\# = 0$  for all  $l \geq 0$ , expansion (5.47) gives

$$(5.51) \quad \chi_k \chi_X^\# = s^{-n} \text{Rem}_{2,k} \chi_X^\# = O(s^{-n}).$$

Next, we deal with the  $\text{Rem}_1$  term in (5.9). We use the splitting

$$(5.52) \quad Rb = Rc + R_2h, \quad c := \text{ad}_d(g)g, \quad R_2 := dR,$$

which follows from (5.14). We prove:

**Lemma 5.5.** *For  $k \geq 1$ , the operator  $(Rb)^k$  has the following expansion:*

$$(5.53) \quad (Rb)^k = \sum_{l=0}^k R_2^l N_{k-l},$$

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

$$(5.54) \quad \deg_R(N_j) := \text{powers of } R \text{ in } N_j \in [j, j+2k].$$

*Proof.* We prove this by induction on  $k = 1, 2, \dots$ . 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  $k \rightarrow k+1$ . Using (5.52) and the induction hypothesis, we write

$$(5.55) \quad \begin{aligned} (Rb)^{k+1} &= (Rc + R_2h)(Rb)^k \\ &= \sum_{l=0}^k RcR_2^l N_{k-l} + \sum_{l=0}^k R_2hR_2^l N_{k-l} \\ &=: A + B. \end{aligned}$$

The goal now is to commute the bounded operator  $R_2$  successively to the left. Using the relation

$$(5.56) \quad R_2 = s(1 + zR)$$

and identity (5.20), we find

$$(5.57) \quad \text{ad}_{R_2}(D) = (s^{-1}R_2 - 1) \text{ad}_d(D)R,$$

for any operator  $D$  allowed by the domain consideration. Iterating identity (5.57) for  $p \geq 1$  times shows that there exist absolute constants  $c_1, \dots, c_l$  s.t.

$$(5.58) \quad \text{ad}_{R_2}^p(D) = \sum_{q=0}^p c_q s^{-q} R_2^q \text{ad}_d^p(D) R^p.$$

Moreover, for any bounded operators  $D, E$  and integers  $l \geq 1$ , we have

$$(5.59) \quad DE^l = E^l D + \sum_{p=1}^l (-1)^p \binom{l}{p} E^{l-p} \text{ad}_E^p(D).$$

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

$$\begin{aligned}
(5.60) \quad A &\equiv RcN_k + \sum_{l=1}^k RcR_2^l N_{k-l} \\
&= RcN_k + \sum_{l=1}^k R_2^l RcN_{k-l} \\
&\quad + \sum_{l=1}^k \sum_{p=1}^l (-1)^p \binom{l}{p} R_2^{l-p} R \operatorname{ad}_{R_2}^p(c) N_{k-l} \\
&= RcN_k + \sum_{l=1}^k R_2^l RcN_{k-l} \\
&\quad + \sum_{l=1}^k \sum_{p=1}^l \sum_{q=0}^p (-1)^p c_q s^{-q} \binom{l}{p} R_2^{l-p+q} R \operatorname{ad}_d^p(c) R^p N_{k-l}.
\end{aligned}$$

Regrouping (5.60) according to the power in  $R_2$  shows that

$$(5.61) \quad A = \sum_{l=0}^k R_2^l N_{k+1-l}^{(1)},$$

$$(5.62) \quad N_{k+1}^{(1)} := RcN_k,$$

$$(5.63) \quad N_{k+1-l}^{(1)} = RcN_{k-l}$$

$$+ \sum_{l'=l}^k \sum_{\substack{p=1, \dots, l' \\ q=0, \dots, p, \\ q-p=l-l'}} (-1)^p c_q s^{-q} \binom{l'}{p} R \operatorname{ad}_d^p(c) R^p N_{k-l'}, \quad l = 1, \dots, k.$$

Since  $\deg_R N_j \in [j, j + 2k]$ , we derive from expressions (5.62)–(5.63) that

$$(5.64) \quad \deg_R(N_j^{(1)}) \in [j + 1, j + 2k + 1], \quad j = 0, \dots, k.$$

Similarly, applying (5.58)–(5.59) to term  $B$  in (5.55) with  $D = h$  and  $E = R_2$  yields

$$\begin{aligned}
(5.65) \quad B &\equiv R_2 h N_k + \sum_{l=1}^k R_2 h R_2^l N_{k-l} \\
&= R_2 h N_k + \sum_{l=1}^k R_2^{l+1} h N_{k-l} \\
&\quad + \sum_{l=1}^k \sum_{p=1}^l (-1)^p \binom{l}{p} R_2^{l-p+1} \text{ad}_{R_2}^p(h) N_{k-l} \\
&= R_2 h N_k + \sum_{l=1}^k R_2^{l+1} h N_{k-l} \\
&\quad + \sum_{l=1}^k \sum_{p=1}^l \sum_{q=0}^p (-1)^p c_q s^{-q} \binom{l}{p} R_2^{l-p+q+1} \text{ad}_d^p(h) R^p N_{k-l}.
\end{aligned}$$

Regrouping (5.65) according to the power in  $R_2$  shows that

$$(5.66) \quad B = \sum_{l=1}^{k+1} R_2^l N_{k+1-l}^{(2)},$$

$$(5.67) \quad N_k^{(2)} := h N_k,$$

$$\begin{aligned}
(5.68) \quad N_{k+1-l}^{(2)} &= h N_{k+1-l} \\
&\quad + \sum_{l'=l}^{k+1} \sum_{\substack{p=1, \dots, l' \\ q=0, \dots, p \\ q-p=l-l'}} (-1)^p c_q s^{-q} \binom{l'-1}{p} \text{ad}_d^p(h) R^p N_{k+1-l'},
\end{aligned}$$

with  $l = 2, \dots, k+1$  and

$$(5.69) \quad \deg_R(N_j^{(2)}) \in [j, j+2k+1], \quad j = 1, \dots, k+1.$$

Combining expansions (5.61), (5.66) in line (5.55) yields

$$(5.70) \quad (Rb)^{k+1} = N_{k+1}^{(1)} + \sum_{l=1}^k R_2^l (N_{k+1-l}^{(1)} + N_{k+1-l}^{(2)}) + R_2^{k+1} N_0^{(2)},$$

which is of the form (5.53) with  $k \rightarrow k+1$ . This completes the induction and the proof of Lemma 5.5.  $\square$

Next, we have the following lemma

**Lemma 5.6.** *Let  $\text{Rem}_1$  be as in (5.10). If  $K$  is any bounded operator with  $\text{ran } d \subset \ker K$  then*

$$(5.71) \quad K \text{Rem}_1 = O(\|K\|).$$

*Proof.* We use expansion (5.53). Since  $\text{ran } d \subset \ker K$ , 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

$$(5.72) \quad K\text{Rem}_1 = \int K(Rb)^n R^E = \int KN_n R^E.$$

By the definition of  $N_n$  (see Lemma 5.5), we have

$$(5.73) \quad \|N_n\| \leq C \sum_{j=n}^{3n} |\text{Im}(z)|^{-j}.$$

Thus, by (5.72),

$$(5.74) \quad \|K\text{Rem}_1\| \leq \|K\| \sum_{j=n}^{3n} \int |\text{Im}(z)|^{-(j+1)}.$$

This, together with estimate (B.17) with  $(p, l) = (n, 0), \dots, (3n, 0)$  (recall  $n \geq 1$  to begin with), implies the desired result, (5.71).  $\square$

Applying (5.71) with  $K = \chi_X^\sharp$ , whose kernel contains  $\text{ran } d$  due to (1.11), we obtain

$$(5.75) \quad \chi_X^\sharp \text{Rem}_1 = O(1).$$

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).  $\square$

*Remark 11.* We mention the following alternative proof of Proposition 5.1. Recalling that  $\chi_{0s} = \chi(s^{-1}d_X^E)$  with  $\chi$  supported on  $[c_\delta, \infty)$  for some positive  $c_\delta$ , we write

$$\|\chi_{0s}\chi_X^\sharp\| = \|\chi_{0s}(d_X^E)^{-n}(d_X^E)^n\chi_X^\sharp\| \leq (c_\delta s)^{-n} \|(d_X^E)^n\chi_X^\sharp\|.$$

Now, with the convention  $\prod_{i=2}^n A_i = A_2 \dots A_n$ , we have

$$\begin{aligned} (d_X^E)^n &= g(H)d_X \left( \prod_{i=2}^n g^2(H)d_X \right) g(H) \\ &= g(H)d_X \langle x \rangle^{-1} \langle x \rangle \left( \prod_{i=2}^n g^2(H) \langle x \rangle^{-i+1} d_X \langle x \rangle^{-1} \langle x \rangle^i \right) g(H) \langle x \rangle^{-n} \langle x \rangle^n. \end{aligned}$$

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

$$\|(d_X^E)^n\chi_X^\sharp\| \leq C_n \|\langle x \rangle^n \chi_X^\sharp\| \leq C'_n,$$

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  $\chi$ ,  $\tilde{g}$ , and  $\tilde{\chi}$  are smooth cutoff functions such that  $\text{supp}(\tilde{g}) \subset \{g = 1\}$  and  $\text{supp}(\tilde{\chi}') \subset (\delta, +\infty) = \{\chi = 1\}$  (see Figs. 3–4). Let  $\bar{g} = 1 - g$  and  $\bar{\chi} = 1 - \chi$ . It follows that

$$(5.76) \quad \bar{g}(\mu)\tilde{g}(\mu) = 0,$$

$$(5.77) \quad \bar{\chi}(\mu)\tilde{\chi}(\mu) = 0.$$

In the remainder of this section, we use the following notations: For  $s, v, t$  as in (3.4) and  $z \in \mathbb{C}$ ,  $\text{Im}(z) \neq 0$ ,

$$d_t \equiv d_X - vt, \quad d_t^E \equiv d_X^E - vt = gd_Xg - vt,$$

$$R \equiv (d_t/s - z)^{-1}, \quad R^E \equiv (d_t^E/s - z)^{-1},$$

and

$$(5.78) \quad \xi(\mu) := \sqrt{\chi(\mu)}, \quad \bar{\xi}(\mu) = 1 - \xi(\mu),$$

$$(5.79) \quad \phi = \phi(d_t/s), \quad \phi^E = \phi(d_t^E/s) \text{ for } \phi \in \mathcal{X},$$

$$(5.80) \quad g = g(H), \quad \tilde{g} = \tilde{g}(H) \text{ for } g, \tilde{g} \text{ from (5.76)}.$$

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),*

$$(5.81) \quad \chi^E \geq \tilde{g}\tilde{\chi}\tilde{g} + O(s^{-n}).$$

*Proof.* Since  $\|\tilde{g}\tilde{\chi}\tilde{g}\| \leq 1$ , we have

$$(5.82) \quad \chi^E \geq \xi^E \tilde{g}\tilde{\chi}\tilde{g}\xi^E = \tilde{g}\tilde{\chi}\tilde{g} - \bar{\xi}^E \tilde{g}\tilde{\chi}\tilde{g} - \tilde{g}\tilde{\chi}\tilde{g}\bar{\xi}^E + \bar{\xi}^E \tilde{g}\tilde{\chi}\tilde{g}\bar{\xi}^E.$$

We now claim

$$(5.83) \quad \bar{\xi}^E \tilde{g}\tilde{\chi} = O(s^{-n}).$$

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

$$(5.84) \quad \bar{\xi}^E = \sum_{k=0}^{n-1} \bar{\xi}_k + s^{-n} \text{Rem}_1,$$

where

$$(5.85) \quad \bar{\xi}_k = \int (Rb/s)^k R d\tilde{\xi}(z) \quad \text{and} \quad \text{Rem}_1 = \int (Rb)^n R^E d\tilde{\xi}(z),$$

where  $\tilde{\xi}(z)$  is an almost analytic extension of the function  $\bar{\xi}(\mu)$ . (Below we will omit the measure  $d\tilde{\xi}(z)$  when no confusion arises.) By expansion (5.84), Claim (5.83) is equivalent to the relations

$$(5.86) \quad \bar{\xi}_k \tilde{g}\tilde{\chi} = O(s^{-n}),$$

$$(5.87) \quad \text{Rem}_1 \tilde{g}\tilde{\chi} = O(1).$$

We first prove (5.86). We write the l.h.s. of (5.86) as

$$(5.88) \quad \bar{\xi}_k \tilde{g}\tilde{\chi} = \bar{\xi}_k \tilde{\chi}\tilde{g} + \bar{\xi}_k [\tilde{g}, \tilde{\chi}].$$



Since  $\text{ad}_{d_t/s}^k(\tilde{g}) = s^{-k}\text{ad}_d^k(\tilde{g})$  is bounded for  $0 \leq k \leq n$ , we have by expansion (C.5) that

$$(5.89) \quad [\tilde{g}, \tilde{\chi}] = \sum_{k=1}^{n-1} (-1)^k \frac{s^{-k}}{k!} \tilde{\chi}^{(k)}(d_t/s) \text{ad}_d^k(\tilde{g}) + s^{-n} \text{Rem}_3,$$

where  $\text{Rem}_3 = O(1)$ . Plugging (5.89) into (5.88) yields

$$(5.90) \quad \begin{aligned} \bar{\xi}_k \tilde{g} \tilde{\chi} &= \bar{\xi}_k \tilde{\chi} \tilde{g} + \sum_{k=1}^{n-1} \frac{s^{-k}}{k!} \bar{\xi}_k \tilde{\chi}^{(k)}(d_t/s) \text{ad}_d^k(\tilde{g}) + s^{-n} \bar{\xi}_k \text{Rem}_3 \\ &=: A + B + C. \end{aligned}$$

We apply Corollary 5.4 to the function  $\bar{\xi}$  to obtain the expansion

$$(5.91) \quad \bar{\xi}_k = h^k \bar{\xi}(d_t/s) + \sum_{q=0}^k \sum_{l=0}^{n-1} s^{-l} B_{q,l} (\bar{\xi} p_{q,l})^{(l+1)}(d_t/s) + s^{-n} \text{Rem}_{2,k},$$

where  $\|h\| \leq 2$ ,  $B_{q,l} = O(1)$  are defined in Lemma 5.3, part (b), and  $\text{Rem}_{2,k} = O(1)$ . 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

$$(5.92) \quad \bar{\xi}^{(l)}(\mu) \tilde{\chi}^{(m)}(\mu) = 0 \quad \text{for any integers } l, m \geq 0,$$

see Figure 3. Thus, inserting (5.91) to (5.90) and using (5.92), we find

$$(5.93) \quad A = s^{-n} \sum_{k=0}^{n-1} \text{Rem}_{2,k} \tilde{\chi} \tilde{g} = O(s^{-n}),$$

$$(5.94) \quad B = s^{-n} \sum_{k=1}^{n-1} \sum_{l=0}^{n-1} \frac{s^{-k}}{k!} \text{Rem}_{2,l} \tilde{\chi}^{(k)} \text{ad}_d^k(\tilde{g}) = O(s^{-n}).$$

Thus we have proved (5.86).

Next, we prove (5.87) by the following lemma:

**Lemma 5.8.** For  $k = 1, \dots, n$  and  $\text{Rem}_1(k) := \int (Rb)^k R^E$ ,

$$(5.95) \quad \text{Rem}_1(k) \tilde{g} \tilde{\chi} = O(1).$$

*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

$$(5.96) \quad \begin{aligned} RbR^E &= RcR^E + R_2R^Eh + R_2[h, R^E] \\ &= RcR^E + R_2R^Eh + s^{-1}R_2R^E \text{ad}_{d^E}(h)R^E, \end{aligned}$$

where we use the relation (c.f. (5.20))

$$(5.97) \quad [B, R^E] = s^{-1}R^E \text{ad}_{d^E}(B)R^E,$$

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

$$(5.98) \quad \begin{aligned} \text{Rem}_1(1) \tilde{g} &= \int RcR^E \tilde{g} + \int s^{-1}R_2R^E \text{ad}_{d^E}(h)R^E \tilde{g} \\ &= \int RcR^E \tilde{g} + \int R^E \text{ad}_{d^E}(h)R^E \tilde{g} + \int zRR^E \text{ad}_{d^E}(h)R^E \tilde{g}. \end{aligned}$$

For  $f \in C_c^\infty(\mathbb{R})$ , the operators  $\text{ad}_{d^E}^k(f)$  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  $\|\tilde{g}\| \leq 1$ ,  $\|c\|, \|\text{ad}_{d^E}(h)\| = O(1)$ ,  $\|R\|, \|R^E\| \leq |\text{Im}(z)|^{-1}$ , 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  $k \rightarrow k+1$ . First, we note the relation  $R^E - R = RbR^E$  and so

$$\begin{aligned} \text{Rem}_1(k) &= \int (Rb)^k R + \int (Rb)^k (R^E - R) \\ (5.99) \quad &= \int (Rb)^k R + \int (Rb)^{k+1} R^E = s^k \bar{\xi}_k + \text{Rem}_1(k+1), \end{aligned}$$

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

$$(5.100) \quad \text{Rem}_1(k+1)\tilde{g}\tilde{\chi} = \text{Rem}_1(k)\tilde{g}\tilde{\chi} - s^k \bar{\xi}_k \tilde{g}\tilde{\chi}.$$

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.  $\square$

Since  $\text{Rem}_1 \equiv \text{Rem}_1(n)$  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.  $\square$

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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. 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  $\rho$ , 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

$$\begin{aligned} \|G_j(\rho)\|_1 &\leq \|W_j\rho W_j^*\|_1 + \frac{1}{2}\|\{W_j^*W_j, \rho\}\|_1 \\ &\leq \text{Tr}|W_j\rho W_j^*| + \frac{1}{2}\text{Tr}|\{W_j^*W_j, \rho\}| \\ &= \text{Tr}(W_j\rho W_j^*) + \frac{1}{2}\text{Tr}(\{W_j^*W_j, \rho\}) \\ (A.1) \qquad &= 2\text{Tr}(W_j^*W_j\rho). \end{aligned}$$

Thus,

$$(A.2) \quad \|G(\rho)\|_1 = \left\| \sum_{j \geq 1} G_j(\rho) \right\|_1 \leq 2 \sum_{j \geq 1} \text{Tr}(W_j^*W_j\rho) \leq 2 \left\| \sum_{j \geq 1} W_j^*W_j \right\| \|\rho\|_1.$$

Since  $\sum_{j \geq 1} W_j^*W_j$  is bounded by the uniform boundedness theorem, this proves  $G$  is bounded on  $\mathcal{S}_1$ , which completes the proof.  $\square$

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  $\beta_t$  as before. Note that since  $e^{L_0 t}$  is a group (defined on  $\mathbb{R}$ ), then so is  $\beta_t = e^{L t}$ .

The positivity preserving property of  $\beta_t$  follows from [9, Theorem 5.2]. We summarize the key result in the following lemma:

**Lemma A.3.** *The semigroup  $\beta_t$  is positive for all  $t \geq 0$ .*

*Proof.* First, we rewrite the vNL operator  $L$  as

$$(A.3) \quad L(\rho) = -iK_{H+iP}(\rho) + F(\rho),$$

where  $P = P^* = \frac{1}{2} \sum_{j \geq 1} W_j^*W_j$ ,  $K_A(\rho) = A\rho - \rho A^*$  and  $F(\rho) = \sum_{j \geq 1} W_j\rho W_j^*$ .

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

$$(A.4) \quad S_t(\rho) = B_t\rho B_t^*,$$

which obviously defines a positive semigroup. On the other hand, since

$$\sum_{j \geq 1} W_j\rho W_j^* \geq 0$$

for all  $\rho \geq 0$ , then  $F$  generates a positive semigroup  $e^{Ft}$ .

Finally, by Trotter-Lie formula, we have

$$(A.5) \quad \beta_t(\rho) = \lim_{n \rightarrow \infty} (S_{t/n} e^{Ft/n})^n(\rho),$$

where the limit is taken in the trace-norm. Hence the semigroup  $\beta_t$  is positive.  $\square$

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

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

Note that

$$(B.2) \quad p \leq p' \implies \mathcal{N}(f, p') \leq \mathcal{N}(f, p),$$

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  $m = 0, \dots, \nu + 2$ ,*

$$(B.3) \quad \left\| \langle x \rangle^{m-p+\rho} f^{(m)}(x) \right\|_{L^\infty} \leq C_0.$$

*Then there exists  $C > 0$  depending only on  $\rho, C_0, \nu$  such that*

$$(B.4) \quad \mathcal{N}(f, p) \leq C.$$

*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  $\rho > 0$ .  $\square$

**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  $|f^{(m)}(x)| \leq C \langle x \rangle^{l-m}$ . Since  $p \geq l + 1$ , we have (B.3) with  $\rho = 1$ .  $\square$

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

$$(B.5) \quad \tilde{f}(z) := \eta \left( \frac{y}{\langle x \rangle} \right) \sum_{k=0}^{\nu+1} f^{(k)}(x) \frac{(iy)^k}{k!},$$

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  $\mu$ . This  $\tilde{f}(z)$  induces a measure on  $\mathbb{C}$  as

$$(B.6) \quad d\tilde{f}(z) := -\frac{1}{2\pi} \partial_{\bar{z}} \tilde{f}(z) dx dy.$$

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  $0 \leq p \leq \nu$ . 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  $C = C(f, \nu, p) > 0$ :*

$$(B.7) \quad \int \left| d\tilde{f}(z) \right| |\operatorname{Im}(z)|^{-(p+1)} \leq C.$$

*Proof.* Differentiating formula (B.5), we obtain the estimate

$$(B.8) \quad \left| \partial_{\bar{z}} \tilde{f}(z) \right| \leq \eta \left( \frac{y}{\langle x \rangle} \right) \frac{|y|^{\nu+1}}{(\nu+1)!} \left| f^{(\nu+2)}(x) \right| + \sum_{k=0}^{\nu+1} \rho \left( \frac{y}{\langle x \rangle} \right) \frac{|y|^k}{k!} \left| \frac{1}{\langle x \rangle} f^{(k)}(x) \right|,$$

where

$$(B.9) \quad \rho(\mu) := |\eta'(\mu)| \langle \mu \rangle$$

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

For each fixed  $x$ , we define

$$(B.10) \quad G(x) := p.v. \int |\partial_{\bar{z}} f(z)| |y|^{-(p+1)} dy$$

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  $|y| \leq \langle x \rangle$  or  $|y| \geq 2\langle x \rangle$ , we find

$$(B.11) \quad G(x) \leq \int_{|y| \leq \langle x \rangle} \frac{|y|^{\nu-p}}{(\nu+1)!} \eta \left( \frac{y}{\langle x \rangle} \right) dy \left| f^{(\nu+2)}(x) \right|$$

$$(B.12) \quad + \sum_{k=0}^{\nu+1} \int_{\langle x \rangle < |y| < 2\langle x \rangle} \rho \left( \frac{y}{\langle x \rangle} \right) \frac{|y|^{k-p-1}}{k!} dy \left| \frac{1}{\langle x \rangle} f^{(k)}(x) \right|.$$

Since  $0 \leq \eta(\mu) \leq 1$  and  $\nu \geq p$ , the integral in line (B.11) converges and can be bounded as

$$(B.13) \quad \int_{|y| \leq \langle x \rangle} \frac{|y|^{\nu-p}}{(p+1)!} \eta \left( \frac{y}{\langle x \rangle} \right) dy \left| f^{(p+2)}(x) \right| \leq \frac{2\langle x \rangle^{\nu-p+1}}{(p+1)!} \left| f^{(p+2)}(x) \right|.$$

To bound line (B.12), we use that  $\rho(y/\langle x \rangle) < \sqrt{5}$  and  $|y|^{k-p-1} \leq \langle x \rangle^{k-p-1}$  for  $\langle x \rangle < |y| < 2\langle x \rangle$ ,  $0 \leq k \leq p+1$  (see (B.9)). Thus each integral in line (B.12) can be bounded as

$$(B.14) \quad \begin{aligned} & \sum_{k=0}^{\nu+1} \int_{\langle x \rangle < |y| < 2\langle x \rangle} \rho \left( \frac{y}{\langle x \rangle} \right) \frac{|y|^{k-p-1}}{k!} dy \left| \frac{1}{\langle x \rangle} f^{(k)}(x) \right| \\ & \leq \sum_{k=0}^{p+1} \frac{4\sqrt{5} \langle x \rangle^{k-p-1}}{k!} \left| f^{(k)}(x) \right| + \sum_{k=p+1}^{\nu+1} \frac{\sqrt{5} \cdot 2^{k-p+1} \langle x \rangle^{k-p-1}}{k!} \left| f^{(k)}(x) \right|. \end{aligned}$$

Combining (B.13)–(B.14) in (B.12), we conclude that

$$(B.15) \quad |G(x)| \leq CF(x), \quad F(x) := \sum_{m=0}^{\nu+2} \langle x \rangle^{m-p-1} \left| f^{(m)}(x) \right|.$$

Let  $G_\lambda(x) := \mathbf{1}_{[-\lambda, \lambda]} G(x)$  with  $\lambda > 0$ . Then  $G_\lambda \in L^1$  and  $|G_\lambda(x)| \leq CF(x)$  for any  $\lambda$ . 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  $\lambda \rightarrow \infty$  and using the dominated convergence theorem yields  $G \in L^1$  with

$$(B.16) \quad \|G\|_{L^1} \leq C \|F\|_{L^1}.$$

Recalling definition (B.10), we find  $(2\pi)^{-1} \|G\|_{L^1} = \text{l.h.s. of (B.7)}$ . Thus we conclude (B.7) from (B.16).  $\square$

Lemma B.3 and Corollary B.2 together imply the following results:

**Corollary B.4.** *Let  $p$  and  $l$  be two integers with  $\nu \geq p > l \geq 0$ . 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  $\nu \geq p > l \geq 0$ . Let  $P_l(x)$  be a polynomial with  $\deg \leq l$ . 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*

$$(B.17) \quad \int \left| d\tilde{f}(z) P_l(z) \right| |\text{Im}(z)|^{-(p+1)} \leq C.$$

*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

$$(B.18) \quad P_l(z) d\tilde{f}(z) = d f_l(z).$$

We compute

$$(B.19) \quad f_l^{(l+1)} = P_l^{(l+1)} f + \sum_{k=0}^l \binom{l+1}{k} P_l^{(k)} f^{(l+1-k)}.$$

The term leading term on the r.h.s. vanishes since  $\deg p \leq l$ . Each term in the sum lies in  $C_c^\infty$  since  $f^{(q)} \in C_c^\infty$  for  $q \geq 1$ . Thus  $f_l$  verifies the condition of Corollary B.4 and so (B.17) follows.  $\square$

#### APPENDIX C. COMMUTATOR EXPANSIONS

In this appendix, we take  $\tilde{f}(z), d\tilde{f}(z)$  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  $p \geq 0$ . Then for any self-adjoint operator  $A$  on  $\mathcal{H}$ ,*

$$(C.1) \quad \frac{1}{p!} f^{(p)}(A) = \int_{\mathbb{C}} d\tilde{f}(z) (z - A)^{-(p+1)},$$

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  $\Phi$  be a lower semi-bounded self-adjoint operator on  $\mathcal{H}$ . Let  $f_s := f(s^{-1}(\Phi - \alpha))$  for some fixed  $\alpha$  and all  $s > 0$ . Suppose there exists  $c \geq 0$  such that*

$$(C.2) \quad (\Phi + c)^{-1} \mathcal{D}(A) \subset \mathcal{D}(A),$$

and

$$(C.3) \quad B_k := \text{ad}_{\Phi}^k(A) \in \mathcal{B}(\mathcal{H}) \quad (1 \leq k \leq n+1).$$

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

$$(C.4) \quad [A, f_s] = - \sum_{k=1}^n \frac{s^{-k}}{k!} B_k f_s^{(k)} - s^{-(n+1)} \text{Rem}_{\text{left}}(s)$$

$$(C.5) \quad = \sum_{k=1}^n (-1)^k \frac{s^{-k}}{k!} f_s^{(k)} B_k + (-1)^{n+1} s^{-(n+1)} \text{Rem}_{\text{right}}(s),$$

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

$$(C.6) \quad \|\text{Rem}_{\text{left}}(s)\|_{\text{op}} + \|\text{Rem}_{\text{right}}(s)\|_{\text{op}} \leq c \|B_{n+1}\|.$$

*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  $|\text{Im}(z)|$  and therefore for all  $z$  with  $\text{Im}(z) \neq 0$ .

It follows that

$$(C.7) \quad [A, R] = -s^{-1} R \text{ad}_{\Phi}(A) R$$

holds in the sense of quadratic forms on  $\mathcal{D}(A)$ . Since  $R$  is bounded and  $\text{ad}_{\Phi}(A)$  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  $B_k := \text{ad}_{\Phi}^k(A)$  to left and right, respectively. This way we obtain

$$(C.8) \quad [A, R] = - \sum_{k=1}^n s^{-k} B_k R^{k+1} - s^{-(n+1)} R B_{n+1} R^{n+1}$$

$$(C.9) \quad = \sum_{k=1}^n (-1)^k s^{-k} R^{k+1} B_k + (-1)^{n+1} s^{-(n+1)} R^{n+1} B_{n+1} R,$$

which hold on all of  $\mathcal{H}$  since  $B_k$ 's are bounded operators by assumption (C.3).

Since  $f$  may not decay at  $\infty$ , 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  $\lambda$ . 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

$$(C.10) \quad [A, f_s^\lambda] = \int df^\lambda(z) [A, R],$$

which holds a priori on  $\mathcal{D}(A)$ .

Plugging expansions (C.8)–(C.9) into (C.10) yields

$$(C.11) \quad [A, f_s^\lambda] = - \sum_{k=1}^n \frac{s^{-k}}{k!} B_k \int df^\lambda(z) R^{k+1} - s^{-(n+1)} \text{Rem}_{\text{left}}^\lambda(s),$$

$$(C.12) \quad = \sum_{k=1}^n (-1)^k \frac{s^{-k}}{k!} \int df^\lambda(z) R^{k+1} B_k + (-1)^{n+1} s^{-(n+1)} \text{Rem}_{\text{right}}^\lambda(s),$$

where

$$(C.13) \quad \text{Rem}_{\text{left}}^\lambda(s) = \int df^\lambda(z) R B_{n+1} R^{(n+1)},$$

$$(C.14) \quad \text{Rem}_{\text{right}}^\lambda(s) = \int df^\lambda(z) R^{(n+1)} B_{n+1} R.$$

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

$$(C.15) \quad \begin{aligned} & \left\| \text{Rem}_{\text{left}}^\lambda(s) \right\|_{\text{op}} + \left\| \text{Rem}_{\text{right}}^\lambda(s) \right\|_{\text{op}} \\ & \leq 2 \|B_{n+1}\| \int |df^\lambda(z)| R^{n+2} \\ & \leq 2 \|B_{n+1}\| \int |df^\lambda(z)| |\text{Im}(z)|^{-(n+2)}. \end{aligned}$$

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  $\lambda$ .

By (B.2) and the assumption  $\mathcal{N}(f, 1) \leq C$ ,  $f$  satisfies condition (B.4) with  $p = 1, \dots, n+1$ . Hence, sending  $\lambda \rightarrow \infty$  in (C.11)–(C.14) and using (C.1) for  $p = 1, \dots, n$  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.  $\square$

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