Maximal speed for macroscopic particle transport in the Bose-Hubbard model

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The Lieb-Robinson bound asserts the existence of a maximal propagation speed for the quantum dynamics of lattice spin systems. Such general bounds are not available for most bosonic lattice gases due to their unbounded local interactions. Here we establish for the first time a general ballistic upper bound on macroscopic particle transport in the paradigmatic Bose-Hubbard model. The bound is the first to cover a broad class of initial states with positive density including Mott states, which resolves a longstanding open problem. It applies to Bose-Hubbard type models on any lattice with not too long-ranged hopping. The proof is rigorous and rests on controlling the time evolution of a new kind of adiabatic spacetime localization observable via iterative differential inequalities.

A central tenet of relativistic theory is the existence of the light cone, i.e., an absolute upper bound on the speed of propagation. It is a remarkable fact that many non-relativistic condensed-matter systems similarly display an effective "light" cone which provides a systemdependent upper bound on the maximal speed of quantum propagation. In contrast to its relativistic counterpart, this effective light cone leaks exponentially small errors as is typically unavoidable in quantum dynamics. This deep fact was discovered by Lieb and Robinson [1] for quantum spin systems on lattices. The resulting Lieb-Robinson bound showed that the ultraviolet cutoff imposed by the lattice provides a maximal speed of propagation on the many-body dynamics. The interest in Lieb-Robinson bounds rapidly surged in the early 2000s when it became clear that they are among the very few effective and general tools that are available for analyzing quantum many-body systems. Accordingly, they have played a decisive role in contexts as diverse as quantum information science [2, 3], condensed-matter theory [4–9] and high-energy physics [10-12] to name a few.

A variety of improvements of the original Lieb-Robinson bound have been achieved over the past 10 years [8, 13–24] including, e.g., extensions to long-range spin interactions and fermionic lattice gases. For a more complete discussion, see the survey papers [25–27].

Despite these celebrated successes, a nagging limitation of the Lieb-Robinson bounds has persisted over the years—the standard proofs are fundamentally limited to bounded interactions as enjoyed by quantum spin systems. Certain oscillator systems with unbounded interactions have been addressed by different methods [21]. However, for general unbounded interactions, the standard arguments only yield an unsatisfactory bound on the maximal speed which is proportional to the total particle number N, a trivial bound in the thermodynamic limit.

This limitation largely leaves out the wide field of bosonic quantum lattice gases since these naturally come with unbounded interactions, for example the paradigmatic Bose-Hubbard (BH) model [28]. Experiments with ultracold gases in optical lattices and numerical simulations have found an effective light cone for the BH model after a quench [29–34]. On the theoretical side, a fully satisfactory understanding of this fact is lacking. It is known that the problem is subtle because superballistic transport can occur in certain related examples [35].

A small number of theoretical results have established a maximal propagation speed for bosonic lattice gases for special initial states. A first maximal speed bound in the BH model was given in [36] for initial states that have no particles outside of a fixed region. This condition excludes states of positive local density, e.g., Mott states (9). Very recently, a number of groups have made progress on this problem through novel techniques: The *N*-scaling of the velocity was improved to \sqrt{N} [37]; an almost-linear light cone was derived for special initial states that are local perturbations of a stationary state satisfying certain exponential constraints on the local particle density [38]; a linear light cone was derived for commutators tested against the state $e^{-\mu N}$ [39]; and [36] was extended to propagation through vacuum [40].

In this Letter, we show for the first time the finiteness of the speed of macroscopic particle transport in the BH model for general initial states. We obtain an explicit bound (4) on the maximal speed that is independent of the particle number and easily computable from the hopping parameters of the Hamiltonian. In particular, our result is the first to provide a thermodynamically stable ballistic particle propagation bound on the prototypical Mott states (9) which resolves a longstanding open problem. See Theorem 1 below for the formal statement. Our result is a new kind of macroscopic-type Lieb-Robinson bound for particle transport. It remains to be seen if the method can be adapted to propagation of other physical characteristics, e.g., entanglement.

Our main idea is to control the time evolution by means of a new class of observables which we call *adiabatic spacetime localization observables (ASTLO)*. The construction is inspired by the method of propagation observables developed in [41–47] and thereby connects these developments to the study of many-body lattice gases for the first time.

Let us explain the conceptual idea that makes our ASTLOs an effective tool. Monotonic quantities, such as entropy, have long played a central role in studying dynamics. The main limiting factors for using these quantities is that they are global and there exist only few of them.

ASTLOs widely expand this framework. They are monotonic up to self-similar terms and small error terms as summarized in (19) below. The self-similar terms can be made much smaller because self-similarity allows for iterative bootstrapping. In effect, this makes the expectation values of ASTLOs approximately monotonic (i.e., monotonic up to small error terms), which leads to our space-time estimates. We are able to flexibly design AST-LOs that capture the key dynamical information about the localization of particles in space-time precisely because we have relaxed the monotonicity condition. We believe that this insight can be used to design and utilize analogs of ASTLOs for many other problems in quantum dynamics.

These techniques are fully analytical, rigorous, and robust. Accordingly, the proof applies to a wide variety of BH type models with rather long-ranged hopping and on general lattices.

SETTING AND MAIN RESULT

We consider a finite connected subset Λ of a lattice $\mathcal{L} \subset \mathbb{R}^d$. For example, $\mathcal{L} = \mathbb{Z}^d$ and Λ is a discrete box. We shall prove bounds that are independent of the number of sites in Λ and which therefore extend to the infinite-volume limit.

We consider a system of bosons on Λ described by the generalized Bose-Hubbard model Hamiltonian

$$H_{\Lambda} = -\sum_{x,y\in\Lambda} J_{xy}^{\Lambda} b_x^{\dagger} b_y + \sum_{x\in\Lambda} V_x(n_x) - \mu \sum_{x\in\Lambda} n_x.$$
(1)

acting on the bosonic Fock space \mathcal{F} .

We assume that $J_{x,y}^{\Lambda} = J_{y,x}^{\Lambda}$ and we let V_x : {0,1,2,...} $\rightarrow \mathbb{R}$ be an arbitrary local potential. We allow for long-ranged hopping in the BH Hamiltonian. The hopping range is quantified by an integer parameter p and the quantity

$$\kappa_J^{(p)} = \max_{x \in \Lambda} \sum_{y \in \Lambda} |J_{xy}^{\Lambda}| |x - y|^p \tag{2}$$

where $|\cdot|$ denotes the Euclidean distance. Our bounds will involve the constant $\kappa_J^{(p)}$ for some $p \ge 2$ and to have a well-defined infinite-volume limit, we assume that $\kappa_J^{(p)}$ is upper-bounded independently of the system size. This is our main assumption on the hopping elements J_{xy} .



FIG. 1. As shown in Theorem 1, the transport of 1% of the particles from X to Y takes time proportional to d_{XY} . A macroscopic cloud of particles moves at most at speed v_{max} .

Suppose that Λ is a box in \mathbb{Z}^d and we have the decay bound $|J_{xy}^{\Lambda}| \leq (|x-y|+1)^{-\alpha}$ for some exponent $\alpha \geq d+3$. Then we can take $p = \alpha - d - 1$ as $\kappa_J^{(\alpha-d-1)}$ is upperbounded independently of the system size [48, Lemma 14]. As another example, the standard BH Hamiltonian involves nearest-neighbor hopping and quadratic on-site interaction [28, eq. (65)], i.e.,

$$J_{x,y}^{\Lambda} = J\delta_{x \sim \Lambda y}, \qquad V_x(n_x) = V(n_x) = \frac{U}{2}n_x(n_x - 1).$$
(3)

where $x \sim_{\Lambda} y$ means x and y are nearest neighbors in Λ . In this case, $\kappa_J^{(p)} = \kappa_J^{(1)} = 2dJ$ assuming the lattice embedding is such that nearest neighbors have Euclidean distance 1.

We will show that the *maximal propagation speed* is given by

$$v_{\max} \equiv \kappa_J^{(1)} = \max_{x \in \Lambda} \sum_{y \in \Lambda} |J_{xy}^{\Lambda}| |x - y|.$$
(4)

Our main result controls the macroscopic change of local particle numbers outside of an effective light cone with slope determined by v_{max} . To formulate it precisely, we define for a given subset $S \subset \Lambda$, the local particle numbers

$$N_S = \sum_{x \in S} n_x, \qquad \bar{N}_S = \frac{N_S}{N_\Lambda}.$$
 (5)

We recall that the total particle number $N_{\Lambda} = \sum_{x \in \Lambda} n_x$ is conserved by H_{Λ} . For $c \in \mathbb{R}$ and $S \subset \Lambda$, we write $P_{\overline{N}_S \leq c}$, $P_{\overline{N}_S c \geq c}$, etc., for the associated spectral projectors of \overline{N}_S , where $S^c = \Lambda \setminus S$.

Given a set $S \subset \Lambda$, we write $R_{\min}(S)$ for the radius of the smallest Euclidean ball B so that $S \subseteq B$. We write $\langle A \rangle_{\psi} = \langle \psi, A \psi \rangle$ for the expectation value of an observable A in state ψ . Given two subsets of the lattice $X, Y \subset \Lambda$, we write d_{XY} for their Euclidean distance. **Theorem 1** (Main result). Consider the Hamiltonian H_{Λ} given by (1) with the hopping matrix J_{xy}^{Λ} satisfying $\kappa_J^{(p)} < \infty$ for some $p \geq 2$. Fix numbers $v > v_{\max}$ and $0 \leq \eta < \xi \leq 1$.

Let X and Y be disjoint subsets of Λ and let ϕ be any normalized state. Consider the time-evolved state

$$\psi_t = e^{-itH} P_{\bar{N}_{X^c} < \eta} \phi. \tag{6}$$

Then we have the decay estimate

$$\langle P_{\bar{N}_Y \ge \xi} \rangle_{\psi_t} \le C_{\kappa_J^{(p)}, \xi - \eta} \, d_{XY}^{1-p}, \tag{7}$$

whenever $d_{XY} \ge vt + 2R_{\min}(X)$.

To interpret the result, see Figure 1 and consider an initial state ϕ so that $P_{\bar{N}_{Xc} \leq \eta} \phi = \phi$, meaning the fraction of particles outside of a ball X is at most η (say, $\eta = 0.6$ and so at least 60% of all particles are outside of X). Then (7) shows that the time it takes to raise the fraction of particles inside Y to $\xi > \eta$ (say, to 61% of all particles) is at least proportional to the distance d_{XY} . In short, moving $(\xi - \eta)N$ particles from X to Y takes time proportional to d_{XY} . This proves that macroscopic many-body transport is at most ballistic.

A few remarks on Theorem 1 are in order. (i) The notation $C_{\kappa_J^{(p)},\xi-\eta}$ means that the constant depends on the values of $\kappa_J^{(p)}$ and $\xi-\eta$. It also depends on $v-v_{\max}$, but importantly neither on t nor d_{XY} . (ii) The left-hand side of (7) vanishes at t = 0. We prove that it remains small as long as one stays outside of an effective light cone

$$d_{XY} \ge vt + 2R_{\min}(X) \tag{8}$$

(see (7)). For finite-range hopping, the decay outside of the effective light cone is faster than any polynomial. (iii) The maximal speed v_{max} from (4) is independent of particle number and of the observables X and Y. It only depends on model parameters similarly to the Lieb-Robinson velocity. (iv) The result applies to a broad class of initial states including ones that can have positive local particle density. This allows, for the first time, to consider the important class of *Mott states*

$$\phi = \bigotimes_{x \in \Lambda} (a_x^{\dagger})^{\nu_x} |0\rangle, \qquad \nu_x \in \{0, 1, 2, \ldots\}.$$
(9)

(A common choice is $\nu_x \equiv \nu$ with $\nu - 1 < \frac{\mu}{U} < \nu$ which gives a Mott insulating ground state of (3) in the limit $U \gg J$.) (v) The term $2R_{\min}(X)$ in the condition following (8) plays no role when X is a fixed bounded set. Moreover, if $d_{0Y} = d_{XY} + R_{\min}(X)$ (e.g., if X has symmetry) then (8) can be relaxed to $d_{XY} \ge vt$ even if X grows with system size. The constant 2 can be replaced by any number > 1. (vi) It is an open queston if Theorem 1 can be extended to include the case p = 1. We mention that a well-known experimental setup which encapsulates the zero-temperature phase diagram of the Bose-Hubbard model places the bosons in a large radial trap generated by a radially decreasing local chemical potential. In this setup, the ground state is comprised of concentric annuli which alternate between Mott insulating phases (of different densities) and superfluid phases [28, Figure 13]. Now consider two such Mott phases separated by a superfluid annulus of width w such that the Mott phase on the smaller annulus contains at least $(1-\eta)N$ particles and the Mott phase on the larger annulus contains at most ξN for some $\eta < \xi$. If we turn off the trap at time t = 0, then our result predicts that it will require a time proportional to w/v_{max} to equilibrate the particle densities between the two Mott phases.

ASTLOS: DEFINITION AND BASIC PROPERTIES

The overarching idea behind our approach is to construct special adiabatic spacetime localization observables (ASTLO) (see (11) below) which are quasimonotonic along quantum trajectories. An important ingredient to make ASTLOs work is to use smooth, slowly varying (adiabatic) cutoff functions instead of sharp ones because this makes the time derivative comparatively small.

Given $v > v_{\max}$, let $\epsilon \in (0, \frac{1}{2})$ be small enough such that $v' = (1 - \epsilon)v > v_{\max}$ still. We define the smeared out light cone indicator as

$$\chi_t(|x|) = \chi\left(\frac{|x| - R_{\min}(X) - v't}{\epsilon d_{XY}}\right),\tag{10}$$

where χ is a smoothed out indicator function of the semiinterval $[0, \infty)$; see Figure S1 in [48]. (A precise definition will be given below.) By translation, we may assume that $X \subset \Lambda$ is contained in $B_{R_{\min}(X)}$, the Euclidean ball of radius $R_{\min}(X)$ centered at 0.

We consider $s = \epsilon d_{XY}$ as the large adiabatic parameter that makes $\chi_t(x)$ slowly varying. The associated adiabatic spacetime localization operator (ASTLO) is then the Fock space operator \mathbb{A}_t given by the (normalized) second quantization of χ_t , i.e.,

$$\mathbb{A}_t = \frac{1}{N_\Lambda} \sum_{x \in \Lambda} \chi_t(|x|) n_x. \tag{11}$$

Physically, the first-order ASTLO \mathbb{A}_t can be thought of as a smeared-out localized relative number operator. It measures how many particles are at least distance v'taway from the ball $B_{R_{\min}(X)}$, but it only fully counts the particles whose distance from the light cone is at least of order ϵd_{XY} . Conversely, the particles whose distance from the light cone is positive but $\ll \epsilon d_{XY}$ contribute almost nothing to \mathbb{A}_t . The ASTLOS A_t are useful because, in addition to decreasing quasi-monotonically along quantum trajectories, they satisfy the following two somewhat competing properties: (I) They are closely connected to the more sharply varying local particle numbers N_{X^c} and N_Y . (II) Their adiabatic nature leads to a slow time evolution (small commutators).

Let us explain point (I) further. We begin by noting that local particle number operators and ASTLOs are sums of n_x 's and thus commute. Then $x \in X \subset B_{R_{\min}(X)}$ implies $\chi_0(|x|) = 0$ and so we have the operator inequality

$$\bar{N}_{X^c} \ge \mathbb{A}_0. \tag{12}$$

Since X contains the origin, we have for any $y \in Y$ that $|y| \ge d_{XY}$. The assumption $d_{XY} \ge vt + 2R_{\min}(X)$ and our choice of ϵ then imply that $\chi_t(|y|) = 1$. Hence, we obtain the second operator inequality

$$\bar{N}_Y \le \mathbb{A}_t \tag{13}$$

which clarifies point (I) above.

SKETCH OF PROOF OF THEOREM 1

To treat positive densities, we introduce an augmented ASTLO by taking a monotonic function of the operator \mathbb{A}_t via the spectral theorem. Let f be a monotonic smooth cutoff function that goes from 0 to 1 between η and ξ . To be precise, f belongs to the following class of cutoff functions $C_{\eta,\xi}$. In words, these are smooth (infinitely differentiable) and non-negative functions which interpolate smoothly between 0 and 1 on the interval $[\eta, \xi]$ and are identically zero to its left and identically 1 to its right. Formally, with $f^{(1)} \equiv f^{(1)}$ denoting the first derivative,

$$\mathcal{C}_{\eta,\xi} = \Big\{ f \in C^{\infty}(\mathbb{R}) : f, f' \ge 0, \sqrt{f'} \in C^{\infty}(\mathbb{R}), f = 0 \text{ on} \\ (-\infty, \eta), f = 1 \text{ on } (\xi, \infty), \operatorname{supp} f' \subset (\eta, \xi) \Big\}.$$

We emphasize that the class of cutoff functions is independent of the adiabatic parameter $s = \epsilon d_{XY}$ and of time t. Now we define the approximate spectral projector for the ASTLO via the spectral theorem as

$$\Phi(t) = f(\mathbb{A}_t) = \sum_{\lambda \in \operatorname{spec}\mathbb{A}_t} f(\lambda) P_{\lambda}(\mathbb{A}_t).$$

with $P_{\lambda}(\mathbb{A}_t)$ the projector onto the λ -eigenspace of \mathbb{A}_t .

The fact that $f \in C_{\eta,\xi}$ implies that $\Phi(t)$ is an approximate spectral projector in the sense that

$$P_{\bar{N}_{X^c} \le \eta} \Phi(0) = 0, \qquad P_{\bar{N}_Y \ge \xi} = P_{\bar{N}_Y \ge \xi} \Phi(t).$$
 (14)

We denote $\langle A \rangle_t = \langle A \rangle_{\psi_t}$. The above relations (14) give

$$\langle \Phi(0) \rangle_0 = 0, \qquad \langle P_{\bar{N}_Y \ge \xi} \rangle_t \le \langle \Phi(t) \rangle_t.$$
 (15)

As anticipated, we see that the task reduces to controlling the dynamical growth of the function $t \mapsto \langle \Phi(t) \rangle_t$ governed by the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \Phi(t) \right\rangle_t = \left\langle D\Phi(t) \right\rangle_t, \tag{16}$$

where
$$D\Phi(t) = \frac{\partial}{\partial t}\Phi(t) + i[H, \Phi(t)].$$
 (17)

 $D\Phi(t)$ is called the Heisenberg derivative of $\Phi(t)$.

Reverting from $\Phi(t)$ to $f(\mathbb{A}_t)$ and introducing the notation

$$\chi_t'(|x|) = \chi'\left(\frac{|x| - R_{\min}(X) - v't}{s}\right),\qquad(18)$$

we can now formulate the key technical result.

Theorem 2 (Bound on the Heisenberg derivative). Let $f \in C_{\eta,\xi}$ and $\chi \in C_{1/2,1}$. Then, there exists a constant C > 0 and cutoff functions $\tilde{f} \in C_{\eta,\xi}$ and $\tilde{\chi} \in C_{1/2,1}$ such that for all t and all sufficiently large s,

$$Df(\mathbb{A}_t) \leq -\frac{v' - v_{\max}}{s} f'(\mathbb{A}_t) \mathbb{A}'_t + \frac{C}{s^2} \tilde{f}'(\tilde{\mathbb{A}}_t) \tilde{\mathbb{A}}'_t + \frac{C}{s^p}.$$
(19)

Here \mathbb{A}'_t , \mathbb{A}_t and \mathbb{A}'_t are mutually commuting, positive operators defined in the natural way: namely, by replacing χ_t by respectively χ'_t , $\tilde{\chi}_t$ and $\tilde{\chi}'_t$ in (11), while replacing ϵd_{XY} by s.

The proof of Theorem 2 is lengthy and deferred to [48]. A key ingredient in the proof is the bound

$$\|[J, |x|]\| \le \kappa_1 \equiv v_{\max} \tag{20}$$

(uniformly in Λ) where $Jf(x) = \sum_{y} J_{xy} f_{y}$ is an operator on the one-particle space $\ell^{2}(\Lambda)$. The bound (20) follows from Lemma 5 in the SM and the Schur test; it is where formula (4) for v_{max} arises in our argument.

Proof of Theorem 1. The key idea is to iterate (19). We fix $f \in C_{\eta,\xi}$ and $\chi \in C_{1/2,1}$. We use $s = \epsilon d_{XY}$, take the expectation of (19) and integrate over time. Using (16), $\langle \Phi(t) \rangle_t \geq 0$ and, by (15), $\langle \Phi(0) \rangle_0 = 0$, as well as $v' - v_{\max} = \epsilon v > 0$ and $t \leq \frac{s}{\epsilon v}$, we obtain

$$\int_0^t \langle f'(\mathbb{A}_r) \mathbb{A}'_r \rangle_r \mathrm{d}r \le C s^{-1} \int_0^t \langle \tilde{f}'(\tilde{\mathbb{A}}_r) \tilde{\mathbb{A}}'_r \rangle_r \mathrm{d}r + C t s^{1-p}.$$

Since this holds for any $f \in C_{\eta,\xi}$, we can iterate. It follows that there exist $\tilde{f} \in C_{\eta,\xi}$ and $\tilde{\chi} \in C_{1/2,1}$ so that

$$\int_{0}^{t} \langle f'(\mathbb{A}_{r})\mathbb{A}_{r}' \rangle_{r} \mathrm{d}r \leq Cs^{1-p} \int_{0}^{t} \langle \tilde{f}'(\tilde{\mathbb{A}}_{r})\tilde{\mathbb{A}}_{r}' \rangle_{r} \mathrm{d}r + Cts^{1-p} \\\leq Cts^{1-p} \tag{21}$$

where the second estimate uses that $\|\tilde{f}'(\tilde{\mathbb{A}}_r)\| \leq \|\tilde{f}'\|_{\infty} \leq C$ by the functional calculus and that $\langle \tilde{\mathbb{A}}'_r \rangle_r \leq C$

which in turn follows from the Cauchy-Schwarz inequality $\langle b_x^{\dagger} b_y \rangle_r \leq \langle n_x \rangle_r + \langle n_y \rangle_r$.

Integrating the expectation of (19) over time and using $\langle \Phi(t) \rangle_t = \langle \Phi(r) \rangle_r + \int_r^t \langle D\Phi(r) \rangle_r dr$ and (21), we obtain, for any $t \ge r \ge 0$,

$$\langle \Phi(t) \rangle_t \le \langle \Phi(r) \rangle_r + C(t-r)s^{-p},$$
 (22)

showing the essential monotonicity of $\langle \Phi(t) \rangle_t$ under the evolution. Setting here r = 0 and using (15) gives the desired bound $\langle P_{\bar{N}_Y > \xi} \rangle_t \leq Cts^{-p}$.

CONCLUSIONS

We have resolved a longstanding open problem in the area of quantum lattice gases by providing the first derivation of a maximal speed for macroscopic particle transport in the Bose-Hubbard model. Our result is a new kind of macroscopic-type Lieb-Robinson bound for particle transport. It complements other recent results [37–40] which hold for special initial states and are otherwise closer to the original formulation of the Lieb-Robinson bound.

Our result could be used to control the temporal rate of change of the expected local particle fraction $\frac{N_U}{N}$ inside a region U for suitable initial states. This would open the door to a finer investigation of the dynamical behavior of the local particle fraction.

The central physical idea underpinning our proof is to engineer the ASTLOs, adiabatic and quasi-monotonic spacetime observables whose support dynamically tracks and controls the surplus of particles outside the effective light cone. The analytical method that we use is quite robust. For example, it applies without significant change to a wide variety of BH type models with different hoppings and different lattice structures.

Regarding broader extensions, we note that our AST-LOs here are specifically designed to track particle transport and thereby naturally give rise to the commutator [J, x]. To control propagation of other physical quantities, e.g. entanglement, one would use adapted observables which have to satisfy the appropriate analog of (20) uniformly in Λ . This change would also affect the value of the maximal speed bound (but not its existence).

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Supplemental Material: Maximal speed for macroscopic particle transport in the Bose-Hubbard model

This appendix provides the complete proof of Theorem 2. In the following, c, C > 0 stand for generic positive constants whose value may change from line to line and which may implicitly depend on parameters such as $\|\chi'\|_{\infty}$ or on $\kappa_J^{(1)}, \ldots, \kappa_J^{(p)}$ defined in (2). Note that all $\kappa_J^{(q)} < \infty, q = 1, \ldots, p$, by an assumption of Theorem 2.



FIG. S1. Example of a cutoff function $\chi \in C_{1/2,1}$.

Recall the definition of the set of cutoff functions, where we write $f^{(1)} \equiv f'$ for the first derivative from now on,

$$\mathcal{C}_{\eta,\xi} = \left\{ f \in C^{\infty}(\mathbb{R}) : f, f^{(1)} \ge 0, \sqrt{f^{(1)}} \in C^{\infty}(\mathbb{R}), f = 0 \text{ on } (-\infty,\eta), f = 1 \text{ on } (\xi,\infty), \text{supp } f^{(1)} \subset (\eta,\xi) \right\}.$$
(S1)

An example of a cutoff function lying in $C_{1/2,1}$ is shown in Figure S1. For $\chi \in C_{1/2,1}$, we write $\chi_{t,s}$ for (10) with the variable s replacing ϵd_{XY} , that is,

$$\chi_{t,s}(|x|) = \chi\left(\frac{|x| - R_{\min}(X) - v't}{s}\right),\tag{S2}$$

and we define $\tilde{\chi}_{t,s}$ and $\chi'_{t,s}$ analogously; see eq. (18). We also consider the generalized ASTLO

$$\mathbb{A}_{t,s} = \frac{1}{N} \mathrm{d}\Gamma(\chi_{t,s}) \tag{S3}$$

Fix $f \in \mathcal{C}_{\eta,\xi}$. We shall consider the time evolution of the observable

$$\Phi_s(t) = f(\mathbb{A}_{t,s}). \tag{S4}$$

The operators $\mathbb{A}'_{t,s}$, $\mathbb{A}_{t,s}$ and $\mathbb{A}'_{t,s}$ are defined analogously as explained after Theorem 2.

In the remainder of this section, we prove Theorem 2 through various expansions in the small parameter s^{-1} .

TOOLBOX AND DEFINITIONS

In this section, we prepare the proof of Theorem 2 by recalling some mathematical tools used in the rigorous Schrödinger equation theory.

Commutator expansions with error estimates

We review relevant commutator expansions with error estimates. These results were first derived in [46] and then improved in [47, 50, 51]. We denote $ad_A H = [A, H]$ and write ad_A^k for the k-fold iteration of this map. We introduce the weighted norms $||f||_m = \int_{\mathbb{R}} (1 + x^2)^{m/2} |f(x)| dx$.

Lemma 3. Let $f \in C^{\infty}(\mathbb{R})$ be bounded, with $\sum_{k=0}^{M+2} \|f^{(k)}\|_{k-M-1} < \infty$, for some $M \ge 1$. Let A be a bounded self-adjoint operator and let B be a bounded operator. Then

$$[B, f(A)] = \sum_{k=1}^{M-1} \frac{(-1)^{k-1}}{k!} \mathrm{ad}_A^k(B) f^{(k)}(A) + \mathrm{Rem}_M,$$
(S5)

where
$$\operatorname{Rem}_{M}(A, f) = (-1)^{M-1} \int_{\mathbb{R}^{2}} (z - A)^{-1} B_{M}(H) (z - A)^{-n} d\widetilde{f}(z).$$
 (S6)

There exists a constant C > 0 such that we have the error estimate

$$\|\operatorname{Rem}_{M}\| \le C \|\operatorname{ad}_{A}^{M}(B)\| \sum_{k=0}^{M+2} \|f^{(k)}\|_{k-M-1}.$$
(S7)

Here and in the following, we use the convention that for M = 1, the sum on the right-hand side of (S5) is omitted.

Proof of Lemma 3. We only sketch the proof and refer to [50] for the details. The proof of Lemma 3 relies on the Helffer-Sjöstrand formula for a function f of a self-adjoint operator A and its derivatives, i.e.

$$f^{(k)}(A) = k! \int_{\mathbb{R}^2} \mathrm{d}\tilde{f}(z)(z-A)^{-k-1}, \quad \mathrm{d}\tilde{f}(z) = -\frac{1}{2\pi} \partial_{\bar{z}} \bar{f}(z) \mathrm{d}x \mathrm{d}y, \tag{S8}$$

where z = x + iy and \tilde{f} is an almost analytic extension of f. We quote the following result from [50].

Lemma 4 (Lemma B.2 in [50]). Let $M \ge 0$ and $f \in C^{M+2}(\mathbb{R})$ with $\sum_{k=0}^{M+1} \|f^{(k)}\|_{k-1} < \infty$. Then there exists an almost analytic extension $\tilde{f} : \mathbb{C} \to \mathbb{C}$ of f satisfying

$$\int_{\mathbb{R}^2} |d\tilde{f}(z)| |\mathrm{Im}(z)|^{-M-1} \le C \sum_{k=0}^{M+2} ||f^{(k)}||_{k-M-1}$$
(S9)

and (S8) holds for all self-adjoint operators A. The integral in (S8) converges in norm sense and is bounded uniformly in A.

The almost analytic extension \tilde{f} can be defined in an explicit manner, see e.g. [50, (B.5)].

Using (B.14)-(B.15) and the remark following (B.18) of [50], we have

$$[B, f(A)] = \sum_{k=1}^{M-1} \frac{(-1)^{k-1}}{k!} \operatorname{ad}_{A}^{k}(B) f^{(k)}(H) + \operatorname{Rem}_{M}.$$
(S10)

We recall the convention that for M = 1, the sum on the right-hand side is omitted. Since the operator B_M is bounded, we can control the remainder via (S9), i.e.,

$$\|\operatorname{Rem}_{M}\| \le \|\operatorname{ad}_{A}^{M}(B)\| \int_{\mathbb{R}^{2}} \|z - A\|^{-M-1} |d\widetilde{f}(z)|$$
 (S11)

$$\leq \|\mathrm{ad}_{A}^{M}(B)\| \int_{\mathbb{R}^{2}} |\mathrm{Im}z|^{-M-1} |d\widetilde{f}(z)| \tag{S12}$$

$$\leq C \| \mathrm{ad}_{A}^{M}(B) \| \sum_{k=0}^{M+2} \| f^{(k)} \|_{k-M-1},$$
(S13)

as desired.

Basic properties of second quantization

We begin by introducing some standard notation. Let us consider a one-particle operator $A : \ell^2(\Lambda) \to \ell^2(\Lambda)$, i.e., a $|\Lambda| \times |\Lambda|$ matrix A acting as

$$Af(x) = \sum_{y \in \Lambda} A_{xy} f_y, \qquad f \in \ell^2(\Lambda).$$

We write $d\Gamma(A)$ for its lift to the Fock space defined by

$$d\Gamma(A) = \sum_{x,y \in \Lambda} b_x^{\dagger} A_{xy} b_y.$$
(S14)

We note that $d\Gamma$ is a linear map.

For instance, we can express the hopping term in the Hamiltonian (1) as

$$T = \sum_{x,y \in \Lambda} J_{xy} b_x^{\dagger} b_y = \mathrm{d}\Gamma(J), \text{ where we set } Jf(x) = \sum_y J_{xy} f_y.$$
(S15)

It is convenient to abuse notation and to identify a function $F : \Lambda \to \mathbb{C}$ with the multiplication operator that acts diagonally on $f \in \ell^2(\Lambda)$ via Ff(x) = F(x)f(x). Then

$$d\Gamma(F) = \sum_{x \in \Lambda} F(x) b_x^{\dagger} b_x = \sum_{x \in \Lambda} F(x) n_x.$$
(S16)

For instance, we can rewrite Definitions (5) and (11) as

$$N_U = \mathrm{d}\Gamma(\mathbb{1}_U), \qquad \mathbb{A}_t = \frac{1}{N_A} \mathrm{d}\Gamma(\chi_t)$$

The canonical commutation relations for b_x and b_x^{\dagger} imply the following standard relation.

$$[\mathrm{d}\Gamma(A),\mathrm{d}\Gamma(B)] = \mathrm{d}\Gamma([A,B]). \tag{S17}$$

In particular, for functions $F, G : \Lambda \to \mathbb{C}$, we have that $d\Gamma(F)$ and $d\Gamma(G)$ commute.

Another general property of the second quantization is that it is monotonic with respect to the partial order on Hermitian operators. That is, for Hermitian $|\Lambda| \times |\Lambda|$ matrices A and B, we have

$$A \le B \implies \mathrm{d}\Gamma(A) \le \mathrm{d}\Gamma(B).$$
 (S18)

To verify (S18), we diagonalize $B - A = U \operatorname{diag}(\lambda_1, \ldots, \lambda_{|\Lambda|}) U^{-1}$ and exchange the order of summation to obtain

$$\mathrm{d}\Gamma(B) - \mathrm{d}\Gamma(A) = \sum_{j} \lambda_{j} C_{j}^{\dagger} C_{j}, \quad \text{with } C_{j} = \sum_{y} \overline{U_{yj}} b_{y}.$$

The following special case of an iterated commutator will be useful.

Lemma 5. Let $k \geq 1$ and $F : \Lambda \to \mathbb{C}$. We have

$$\mathrm{ad}_{\mathrm{d}\Gamma(F)}^{k}(H) = \mathrm{ad}_{\mathrm{d}\Gamma(F)}^{k}(T) = \mathrm{d}\Gamma(\mathrm{ad}_{F}^{k}(J)) \tag{S19}$$

where $\operatorname{ad}_{F}^{k}(J)$ is the $|\Lambda| \times |\Lambda|$ matrix with the matrix entries

$$\left(\mathrm{ad}_{F}^{k}(J)\right)_{xy} = J_{xy}(F(x) - F(y))^{k}, \qquad x, y \in \Lambda.$$
(S20)

Proof. The first relation in (S19) follows from the fact that $d\Gamma(F)$ commutes with H - T since both are linear combinations of the commuting opeators n_x . The second relation in (S19) follows from the fact that $T = d\Gamma(J)$ and the identity (S17). Finally, (S20) holds by a straightforward induction.

In particular, Lemma 5 implies that the total particle number N_{Λ} is conserved:

$$[H_{\Lambda}, N_{\Lambda}] = 0. \tag{S21}$$



FIG. S2. The derivative $h = \chi'$ of the cutoff function χ shown in Figure S1. Note that h is an admissible function in $\mathcal{A}_{1/2,1}$.

Admissible functions

For an interval $I \subset \mathbb{R}$, we write $C_c^{\infty}(I)$ for the class of smooth functions with compact support in I. For the proof of Theorem 2, we introduce the following useful function class.

Definition 6. Let $\xi, \eta \in [0, 1]$ with $\eta < \xi$. We introduce the class of admissible functions

$$\mathcal{A}_{\eta,\xi} = \left\{ h \in C_c^{\infty}((\eta,\xi)) : h \ge 0, \sqrt{h} \in C^{\infty}(\mathbb{R}) \right\}$$

The following lemma shows that the elements of $C_{\eta,\xi}$ from (S1) can be seen as antiderivatives of admissible functions up to a multiplicative constant.

Lemma 7. If $h \in \mathcal{A}_{\eta,\xi}$, then there exists $f \in \mathcal{C}_{\eta,\xi}$ so that

$$h(r) = f^{(1)}(r) \int_{\mathbb{R}} h(\tilde{r}) \mathrm{d}\tilde{r}$$

Proof. The lemma follows by setting

$$f(r) = \frac{\int_{-\infty}^{r} h(\tilde{r}) \mathrm{d}\tilde{r}}{\int_{\mathbb{R}} h(\tilde{r}) \mathrm{d}\tilde{r}}.$$

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Evolution of the propagation observables

In this section, we calculate the Heisenberg derivative $D\Phi_s(t)$ defined in (17). For the first term in $D\Phi_s(t)$, cf. (17), we have

$$\frac{\partial}{\partial t}\Phi_s(t) = -\frac{v'}{s}f'(\mathbb{A}_{ts})\mathbb{A}'_{ts}.$$
(S22)

with

$$\mathbb{A}'_{t,s} = \frac{1}{N} \mathrm{d}\Gamma(\chi'_{t,s}), \quad \text{where } \chi'_{t,s} \text{ is defined in (18).}$$
(S23)

Indeed, to verify (S22), we note that $\mathbb{A}_{t,s}$ and $\mathbb{A}'_{t,s}$ commute and are both diagonal in the basis of Mott states (9). On a given Mott state, (S22) then holds by the chain rule.

The main work is thus to consider the commutator $i[H, \Phi_s(t)]$ in (17). Central objects in the argument are the multiple commutators:

$$B_k = \operatorname{ad}_{\mathbb{A}_t}^k(iH), \qquad k \ge 1.$$

We set $u_1 = \sqrt{f^{(1)}}$ which by $f \in C_{\eta,\xi}$ satisfies $u_1 \ge 0$ and $u_1 \in C_c^{\infty}((\eta,\xi))$. Furthermore, for $k \ge 2$, we let $u_k \in C_c^{\infty}(\mathbb{R}_+)$ be s.t. $f^{(k)} \prec u_k$, where we introduced the notation

$$g_1 \prec g_2 \quad \stackrel{\text{def}}{\longleftrightarrow} \quad g_2 = 1 \text{ on supp } g_1.$$
 (S24)

With these definitions, we have

Lemma 8. Assume $f \in \mathcal{C}_{\eta,\xi}$. Let $\operatorname{Re} A = \frac{i}{2}(A + A^{\dagger})$. Then we have

$$i[H, \Phi_s(t)] = u_1 B_1 u_1 + S + R,$$
(S25)

$$S = \sum_{k=2}^{p-1} \frac{(-1)^{k-1}}{k!} u_k \operatorname{Re} \left(B_k f^{(k)} \right) u_k$$

$$+ \sum_{k=1}^{p-1} \frac{(-1)^{k-1}}{k!} \sum_{j=1}^{p-k-1} \operatorname{Re} \left(u_k^{(j)}(\mathbb{A}_{t,s}) B_{k+j} g_k u_k \right),$$
(S26)

$$R = \operatorname{Re}\left(\operatorname{Rem}_{p}(\mathbb{A}_{t,s}, f) + \sum_{k=1}^{p-1} \frac{(-1)^{k-1}}{k!} \operatorname{Rem}_{p-k}(B_{k}, u_{k})^{\dagger} g_{k} u_{k}\right),$$
(S27)

where $f^{(1)} \equiv f^{(1)}$ and $\operatorname{Rem}_p(A, f)$ is defined in (S6).

Proof of Lemma 8. The assumption $f \in C_{\eta,\xi}$ implies $f^{(1)} \in C_c^{\infty}(\mathbb{R}_+)$. Hence we can apply Lemma 3 to $i[H, \Phi_s(t)] = i[H, f(\mathbb{A}_{t,s})]$ to obtain, for $p \geq 2$

$$i[H, \Phi_s(t)] = \sum_{k=1}^{p-1} \frac{(-1)^{k-1}}{k!} B_k f^{(k)}(\mathbb{A}_{t,s}) + \operatorname{Rem}_p(\mathbb{A}_{t,s}, f).$$

Next, we symmetrize this expression up to another commutator.

Defining $g_k = f^{(k)}$ for $k \ge 1$, where $f^{(1)} \equiv f^{(1)}$ and recalling $f^{(k)} \prec u_k$, so that $f^{(k)} = f^{(k)}u_k^2$, we write

$$f^{(k)} = g_k u_k^2, \qquad k \ge 1.$$

In the following, for the sake of readability, we often suppress the argument $\mathbb{A}_{t,s}$ from the notation. We have

$$B_k f^{(k)} = u_k B_k g_k u_k + [B_k, u_k] g_k u_k, \qquad k \ge 1.$$

The commutator $[B_k, u_k] \equiv [B_k, u_k(\mathbb{A}_{t,s})]$ can be further expanded via the adjoint version of Lemma 3,

$$[B_k, u_k] = \sum_{j=1}^{p-1-k} \frac{1}{j!} u_k^{(j)} B_{k+j} + \operatorname{Rem}_{p-k} (B_k, u_k)^{\dagger}.$$

Combining these commutator expansions, we obtain

$$i[H, \Phi_s(t)] = (I) + (II) + (III),$$
 (S28)

$$(\mathbf{I}) = u_1 B_1 u_1, \tag{S29}$$

$$(\mathrm{II}) = \sum_{k=2}^{p-1} \frac{(-1)^{k-1}}{k!} u_k B_k g_k u_k + \sum_{k=1}^{p-1} \frac{(-1)^{k-1}}{k!} \sum_{j=1}^{p-k-1} \frac{1}{j!} u_k^{(j)} B_{k+j} g_k u_k,$$
(S30)

(III) =
$$\operatorname{Rem}_p(\mathbb{A}_{t,s}, f) + \sum_{k=1}^{p-1} \frac{(-1)^{k-1}}{k!} \operatorname{Rem}_{p-k}(B_k, u_k)^{\dagger} g_k u_k.$$
 (S31)

Since $i[H, \Phi_s(t)]$ is self-adjoint, we have that $i[H, \Phi_s(t)] = (I) + \operatorname{Re}((II)) + \operatorname{Re}((III))$, which gives (S25).

PROOF OF THEOREM 2

In the next subsections, we consider the symmetrized expansion (S25) and estimate the three terms on the r.h.s. in reverse order, starting with the norm bound on the remainder term R which is the easiest.

Controlling the remainder term R

We first show that the remainder term R in (S25) is small as $s \to \infty$.

Lemma 9. There exists a constant C > 0 such that

$$||R|| \le Cs^{-p}\kappa_J^{(p)}, \qquad s \ge 1$$

Proof of Lemma 9. By the remainder estimate (S7), we have

$$\|\operatorname{Rem}_p(\mathbb{A}_{t,s}, f)\| \le \|\operatorname{ad}_{\mathbb{A}_{t,s}}^p(H)\| \sum_{k=0}^{p+2} \|f^{(k)}\|_{k-p-1} \le C \|B_p\|.$$

Similarly, using that $g_k \prec u_k$ and that $\|g_k(\mathbb{A}_{t,s})\| \leq \|g_k\|_{\infty}$ by the functional calculus,

$$\|\operatorname{Rem}_{p-k}(B_k, u_k)^{\dagger} g_k u_k\| \leq \|\operatorname{Rem}_{p-k}(B_k, u_k)\| \|g_k\|_{\infty}$$
$$\leq \sum_{l=0}^{p-k+2} \|u_k^{(l)}\|_{l-p+k-1} \|B_p\| \leq C \|B_p\|, \quad k \geq 1.$$

We see that it remains to prove

$$\|B_p\| \le s^{-p} \kappa_J^{(p)}. \tag{S32}$$

We recall that $\mathbb{A}_{t,s} = N^{-1} d\Gamma(\chi_{t,s})$ and use Lemma 5 with $F = \chi_{t,s}(|\cdot|)$ to write

$$B_p = \operatorname{ad}_{\mathbb{A}_{t,s}}^p(iH) = \frac{1}{N} i d\Gamma(\operatorname{ad}_{\chi_{t,s}}^p(J))$$
$$= i \frac{1}{N} \sum_{x,y \in \Lambda} (\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^p J_{xy} b_x^{\dagger} b_y.$$
(S33)

Denote $\tilde{B}_k = i^{k-1}B_k = i^k \operatorname{ad}_{\mathbb{A}_{t,s}}^k(H)$. By applying the operator Cauchy-Schwarz inequality to the self-adjoint operators $i^p(\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^p J_{xy} b_x^{\dagger} b_y$ and the symmetry $J_{yx} = J_{xy}$, we obtain

$$\tilde{B}_{p} \leq \frac{1}{N} \sum_{x,y \in \Lambda} |\chi_{t,s}(|x|) - \chi_{t,s}(|y|)|^{p} |J_{xy}| n_{x}$$
(S34)

Finally the mean-value theorem implies

$$|\chi_{t,s}(|x|) - \chi_{t,s}(|y|)| \le s^{-1} ||x| - |y|| ||\chi'_{t,s}||_{\infty} \le s^{-1}C|x - y|$$

and so $\tilde{B}_p \leq s^{-p} C \kappa_J^{(p)}$. This proves (S32) and hence Lemma 9.

Estimating the symmetrized subleading term S

The argument used to prove Lemma 9 can be refined if we replace the application of the mean-value theorem by iterated Taylor expansion. This is precisely what is needed for the subleading term S in (S25).

We recall that we assume that χ belongs to the following space of cutoff functions

$$\mathcal{C}_{1/2,1} = \left\{ \chi \in C^{\infty}(\mathbb{R}_{+}) : \chi, \chi' \ge 0, \ \sqrt{\chi'} \in C^{\infty}(\mathbb{R}_{+}), \ \operatorname{supp} \chi' \subset (\frac{1}{2}, 1), \\ \chi(r) = 0 \text{ for } r \le \frac{1}{2}, \ \chi(r) = 1 \text{ for } r \ge 1 \right\}.$$
(S35)

Proposition 10. There exist a constant C > 0 and functions $\tilde{\chi} \in \mathcal{C}_{1/2,1}$, $h \in \mathcal{A}_{\eta,\xi}$ such that

$$S \le h(\tilde{\mathbb{A}}_{t,s})\tilde{\mathbb{A}}_{t,s}^{(1)} + Cs^{-p}, \tag{S36}$$

where, recall, the operators $\tilde{\mathbb{A}}_{t,s}$ and $\tilde{\mathbb{A}}'_{t,s}$ are defined in Theorem 2.

In the remainder of this subsection, we prove Proposition 10 in three separate steps. We begin by setting up convenient notation for Taylor expansions. Fix $1 \le k \le p$. We can use Lemma 5 with $F = \chi_{t,s}$ to write

$$B_k = \mathrm{ad}_{\mathbb{A}_{t,s}}^k(iH) = i\frac{1}{N}\mathrm{d}\Gamma(\mathrm{ad}_{\chi_{t,s}}^k(J))$$
(S37)

Therefore the main object we aim to control is the iterated commutator

$$(\mathrm{ad}_{\chi_{t,s}}^k(J))_{xy} = (\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^k J_{xy}.$$
(S38)

By Taylor's theorem with Lagrange remainder, we have the option to expand for any $L \ge 0$

$$\chi_{t,s}(|x|) - \chi_{t,s}(|y|) = \sum_{\ell=1}^{L-1} \frac{\chi_{t,s}^{(\ell)}(|x|)}{\ell!} (|x| - |y|)^{\ell} + R_L$$
$$= \sum_{\ell=1}^{L-1} s^{-\ell} \frac{(\chi^{(\ell)})_{t,s}(|x|)}{\ell!} (|x| - |y|)^{\ell} + R_L,$$

with the remainder bound $|R_L| \leq s^{-L} \frac{\|\chi^{(L)}\|_{\infty}}{L!} ||x| - |y||^L \leq s^{-L}C|x-y|^L$. It is convenient to introduce the notation

$$\chi_{t,s}(|x|) - \chi_{t,s}(|y|) = \sum_{\ell=1}^{L} \mathcal{T}_{\ell}^{(L)},$$
with $\mathcal{T}_{l}^{(L)} = \begin{cases} s^{-\ell} \frac{(\chi^{(\ell)})_{t,s}(|x|)}{\ell!} (|x| - |y|)^{\ell}, & \text{for } 1 \le \ell \le L - 1 \\ R_{L}, & \text{for } \ell = L. \end{cases}$
(S39)

We note that all terms in the expansion satisfy a bound of the form

$$\mathcal{T}_{\ell}^{(L)}| \le Cs^{-\ell}|x-y|^{\ell}, \qquad 1 \le \ell \le L,$$
(S40)

where the constant C only depends on ℓ and $\chi_{t,s}$.

Step 1: Symmetrically preserving support information. We introduce localizing functions on the left and right side of the Hermitian matrix $i^k(\operatorname{ad}_{\chi_{t,s}}^k(J))$. This symmetric sandwiching is needed for proving an operator inequality of the form (S36).

Lemma 11. There exist constants c, C > 0 and a function $\tilde{\chi} \in C_{1/2,1}$ such that

$$i^{k}(\mathrm{ad}_{\chi_{t,s}}^{k}(J)) = c\sqrt{\tilde{\chi}_{t,s}'}i^{k}(\mathrm{ad}_{\chi_{t,s}}^{k}(J))\sqrt{\tilde{\chi}_{t,s}'} + \mathcal{R},$$
(S41)

where \mathcal{R} is a Hermitian matrix satisfying the norm bound

$$\|\mathcal{R}\| \le C\kappa_J^{(p)} s^{-p}. \tag{S42}$$

Proof of Lemma 11. Recall (S24). We choose $\tilde{u} \in C_c^{\infty}(\frac{1}{2}, 2)$ with $\tilde{u} \ge 0$, such that

$$\chi^{(1)}, \chi^{(2)}, \dots, \chi^{(p)} \prec \tilde{u}.$$
 (S43)

Then we define $\tilde{\chi} \in \mathcal{C}_{1/2,1}$ by

$$\tilde{\chi}(r) = \frac{1}{c} \int_{-\infty}^{r} \tilde{u}(r')^2 \mathrm{d}r', \qquad c = \int_{\mathbb{R}} \tilde{u}(\rho)^2 \mathrm{d}\rho.$$
(S44)

(Compare the proof of Lemma 7.) We have $\sqrt{c\tilde{\chi}'} = \tilde{u}$ and hence also $\sqrt{c\tilde{\chi}'_{t,s}} = \tilde{u}_{t,s}$.

The matrix \mathcal{R} can now be written as

$$\mathcal{R} = i^k \mathrm{ad}_{\chi_{t,s}}^k(J) - i^k \tilde{u}_{t,s} \mathrm{ad}_{\chi_{t,s}}^k(J) \tilde{u}_{t,s}.$$

We note that \mathcal{R} is automatically Hermitian as the difference of two Hermitian matrices and so it suffices to prove the norm bound (S42). For this, we consider a fixed (x, y)-matrix element \mathcal{R}_{xy} which by (S38) reads

$$\mathcal{R}_{xy} = i^k (\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^k (1 - \tilde{u}_{t,s}(|x|)\tilde{u}_{t,s}(|y|)) J_{xy}.$$

We decompose

$$1 - \tilde{u}_{t,s}(|x|)\tilde{u}_{t,s}(|y|) = 1 - \tilde{u}_{t,s}(|x|) + \tilde{u}_{t,s}(|x|)(\tilde{u}_{t,s}(|x|) - \tilde{u}_{t,s}(|y|)).$$

We first consider the term $1 - \tilde{u}_{t,s}(|x|)$ and employ a Taylor expansion of order L = p - k + 1 to obtain

$$(1 - \tilde{u}_{t,s}(|x|))(\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^{k} = (1 - \tilde{u}_{t,s}(|x|)) \left(\sum_{\ell=1}^{p-k+1} \mathcal{T}_{\ell}^{(p-k+1)}\right) (\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^{k-1} = (1 - \tilde{u}_{t,s}(|x|))R_{p-k+1}(\chi_{t,s}(|x|) - \chi_{t,s}(|y|))^{k-1}$$

where we used $(1 - \tilde{u})\chi^{(\ell)} = 0$ for all $1 \le \ell \le p$.

By (S40), we can bound the absolute value of this expression by

$$Cs^{-p}|x-y|^{-p}.$$

Taylor expanding around the point y instead yields the same bound, albeit with a potentially different constant C, on the second term $\tilde{u}_{t,s}(|x|)(\tilde{u}_{t,s}(|x|) - \tilde{u}_{t,s}(|y|))$.

By the Schur test and the fact that \mathcal{R} is Hermitian, we obtain the norm bound

$$\|\mathcal{R}\| \le \sup_{x \in \Lambda} \sum_{y \in \Lambda} |R_{xy}| \le Cs^{-p} \sup_{x} \sum_{y \in \Lambda} |x - y|^{-p} |J_{xy}| = Cs^{-p} \kappa_J^{(p)}$$
(S45)

and Lemma 11 is proved.

Step 2: Bound on the iterated commutator. In this step, we prove

Lemma 12. There exist constants c, C > 0 and a function $\tilde{\chi} \in C_{1/2,1}$ such that for every $1 \leq k \leq p$, the iterated commutators are bounded as

$$\pm \tilde{B}_k \equiv \pm i^k \mathrm{ad}^k_{\mathbb{A}_{t,s}}(H) \le s^{-k} c \tilde{\mathbb{A}}^{(1)}_{t,s} + C s^{-p}.$$
(S46)

where, recall, the operator $\tilde{\mathbb{A}}'_{t,s}$ is defined in Theorem 2 and is given by (cf. (18))

$$\tilde{\mathbb{A}}_{t,s}^{(1)} = \frac{1}{N} \mathrm{d}\Gamma(\tilde{\chi}_{t,s}'), \qquad \tilde{\chi}_{t,s}'(|x|) = \quad \tilde{\chi}'\left(\frac{|x| - R_{\min}(X) - vt}{s}\right).$$
(S47)

Proof of Lemma 12. We observe that it suffices to prove the operator inequalities

$$\pm i^{k} \mathrm{ad}_{\chi_{t,s}}^{k}(J) \le s^{-k} c \tilde{\chi}_{t,s}' + C s^{-p}.$$
(S48)

Indeed, assuming (S48), the monotonicity and linearity of second quantization $d\Gamma(\cdot)$, see (S18), give

$$\pm \tilde{B}_k = \frac{1}{N} \mathrm{d}\Gamma(\pm i^k \mathrm{ad}_{\chi_{t,s}}^k(J)) \le s^{-k} \frac{c}{N} \mathrm{d}\Gamma(\tilde{\chi}'_{t,s}) + \frac{C}{N} s^{-p} \mathrm{d}\Gamma(\mathbb{1})$$
$$\le s^{-k} c \tilde{\mathbb{A}}_{t,s}^{(1)} + C s^{-p}.$$

the last step used that $d\Gamma(1) = N$.

$$\|\mathrm{ad}_{\mathbf{Y}_{t,s}}^k(J)\| \le Cs^{-k}.\tag{S49}$$

This will imply the modified claim (S48). Indeed, together Lemma 11 and (S49) give

$$\begin{split} \pm i^k(\mathrm{ad}_{\chi_{t,s}}^k(J)) = & c\sqrt{\tilde{\chi}_{t,s}'}i^k(\pm \mathrm{ad}_{\chi_{t,s}}^k(J))\sqrt{\tilde{\chi}_{t,s}'} + \mathcal{R} \\ \leq & c\|\mathrm{ad}_{\chi_{t,s}}^k(J)\|\tilde{\chi}_{t,s}' + \|\mathcal{R}\| \\ \leq & c\tilde{\chi}_{t,s}' + Cs^{-p}\kappa_J^{(p)} \end{split}$$

up to a change of the constant c > 0.

We now prove (S49). We shall use (S39) but need to be careful when expanding $(\chi_{t,s}(x) - \chi_{t,s}(y))^k$ because we can only control overall polynomial powers up to order $|x - y|^p$ through $\kappa_J^{(p)}$. Therefore, we iteratively expand only as far as necessary to get the desired error s^{-p} .

The iterative Taylor expansion reads

$$(\chi_{t,s}(x) - \chi_{t,s}(y))^k = \sum_{\ell_1=1}^{p-k+1} \mathcal{T}_{\ell_1}^{(p-k+1)} \sum_{\ell_2=1}^{p-k+2-\ell_1} \mathcal{T}_{\ell_2}^{p-k+2-\ell_1}$$
$$\times \sum_{\ell_3=1}^{p-k+3-\ell_1-\ell_2} \mathcal{T}_{\ell_3}^{(p-k+2-\ell_1-\ell_2)} \dots \sum_{\ell_k=1}^{p-\ell_1-\dots-\ell_{k-1}} \mathcal{T}_{\ell_k}^{(p-\ell_1-\dots-\ell_{k-1})}$$

where $\mathcal{T}_{\ell}^{(L)}$ are defined after (S39) and with the usual convention that empty sums equal zero. As can be seen from the last term, the orders of the Taylor expansions are chosen so that any admissible tuple (ℓ_1, \ldots, ℓ_k) satisfies $k \leq \ell_1 + \ldots + \ell_k \leq p$.

The estimate (S40) implies

$$\mathcal{T}_{\ell_1}^{(p-k+1)} \mathcal{T}_{\ell_2}^{(p-k+2-\ell_1)} \dots \mathcal{T}_{\ell_k}^{(p-\ell_1-\dots-\ell_{k-1})} \le Cs^{-\ell_1-\dots-\ell_k} |x-y|^{\ell_1+\dots+\ell_k}.$$

By the Schur test,

$$\begin{aligned} \|\mathrm{ad}_{\chi_{t,s}}^{k}(J)\| &\leq C \sup_{x \in \Lambda} \sum_{y \in \Lambda} |J_{xy}| \sum_{\ell_{1}, \dots, \ell_{k}} s^{-\ell_{1} - \dots - \ell_{k}} |x - y|^{\ell_{1} + \dots + \ell_{k}} \\ &\leq C \sum_{p=k}^{p} s^{-p} \kappa_{J}^{(p)} \leq C s^{-k}, \end{aligned}$$

where $\sum_{\ell_1,...,\ell_k} = \sum_{\ell_1=1}^{p-k} \sum_{\ell_2=1}^{p-k+1-\ell_1} \sum_{\ell_3=1}^{p-k+2-\ell_1-\ell_2} \dots \sum_{\ell_k=1}^{p+1-\ell_1-\dots-\ell_{k-1}}$, which yields (S49) and hence Lemma 12.

Step 3: Addressing asymmetry and concluding Proposition 10

While Lemma 12 goes in the right direction, it is not so obvious how to use it to obtain an operator inequality for S because in (S26), B_k does not appear in the symmetric form $C^{\dagger}B_kC$.

In our specific situation, the asymmetry can be addressed by combining the following two technical observations.

- (i) Any operator inequality $A \leq B$ with B > 0 can be rephrased as the norm bound $||B^{-1/2}AB^{-1/2}|| \leq 1$ and in our situation the target observable $\tilde{\mathbb{A}}'_{t,s} = N^{-1} \mathrm{d}\Gamma(\tilde{\chi}'_{t,s}) \geq 0$ is positive semidefinite and can thus be made positive definite by a limiting procedure.
- (ii) The target observable $\tilde{\mathbb{A}}'_{t,s}$ commutes with the source of the asymmetry, $g_k = g_k(\mathbb{A}_{t,s})$ and the latter is uniformly bounded by the functional calculus, $\|g_k(\mathbb{A}_{t,s})\| \leq \|g_k\|_{\infty} \leq c$.

The details are as follows.

Proof of Proposition 10. Recall (S24). Fix $1 \le k \le p$ and find $v \in C_c^{\infty}((\eta, \xi))$ with $v \ge 0$ so that

$$\left\{u_k^{(j)}\right\}_{\substack{2 \le k \le p-1\\ 0 \le j \le p-1}} \prec v$$

We claim that

$$S \le c\tilde{\mathbb{A}}_{t,s}^{(1)} + Cs^{-p}.$$
(S50)

This will be sufficient to conclude the lemma. Indeed, it implies

$$S = v(\mathbb{A}_{t,s})Sv(\mathbb{A}_{t,s}) \le v(\mathbb{A}_{t,s})(c\tilde{\mathbb{A}}_{t,s}^{(1)} + Cs^{-p})v(\mathbb{A}_{t,s})$$
$$\le c \ h(\mathbb{A}_{t,s})\tilde{\mathbb{A}}_{t,s}^{(1)} + Cs^{-p}.$$

where we defined the admissible function $h = v^2 \in \mathcal{A}_{\eta,\xi}$.

It remains to prove the claim (S50). A generic term contributing to S is of the form

$$\operatorname{Re}\left(w_1(\mathbb{A}_{t,s})B_kw_2(\mathbb{A}_{t,s})\right),$$

where w_1, w_2 are real-valued functions. (For example, $w_1 = u_k$ and $w_2 = g_k u_k$ gives $u_k (B_k g_k + g_k B_k^{\dagger}) u_k$.) In the following, we shall again suppress the argument $\mathbb{A}_{t,s}$ from the notation.

Let $\varepsilon > 0$. We claim that

$$\operatorname{Re}\left(w_{1}B_{k}w_{2}\right) \leq \frac{1}{2}cs^{-k}(\tilde{\mathbb{A}}_{k}'+\varepsilon) + Cs^{-p}$$
(S51)

with the constant C > 0 as in Lemma 12 and c > 0 to be determined. This implies (S50) by sending $\epsilon \to 0$.

We would like to derive (S51) via Lemma 12. As mentioned before, the main challenge is to address the asymmetry due to $w_1 \neq w_2$.

We will derive (S51) from

$$\operatorname{Re}\left(w_1 B_k w_2\right) \le \frac{1}{2} c s^{-k} (\tilde{\mathbb{A}}'_k + \varepsilon) + C s^{-p} w_1 w_2 \tag{S52}$$

by using that $||w_1(\mathbb{A}_{t,s})|| ||w_2(\mathbb{A}_{t,s})|| \le ||w_1||_{\infty} ||w_2||_{\infty} \le c$ thanks to the functional calculus.

Since $\tilde{\mathbb{A}}'_k + \varepsilon > 0$ and $w_1 w_2 = w_2 w_1$, the claim (S52) is equivalent to the norm bound

$$\|D\operatorname{Re}(w_1(B_k - Cs^{-p})w_2)D\| \le 2cs^{-k},$$
(S53)

where $D = \frac{1}{\sqrt{\tilde{\mathbb{A}}'_{t,s} + \epsilon}}$. To estimate the left-hand side we use the commutativity

$$[D, w_j(\mathbb{A}_{t,s})] = 0, \qquad j = 1, 2, \tag{S54}$$

by the functional calculus and $[\tilde{\mathbb{A}}'_{t,s}, \mathbb{A}_{t,s}] = N^{-1} d\Gamma([\tilde{\chi}'_{t,s}, \chi_{t,s}]) = 0$. This allows us to pull out the norms of w_1 and w_2 . Using this, the estimate $\|w_1(\mathbb{A}_{t,s})\| \|w_2(\mathbb{A}_{t,s})\| \le \|w_1\|_{\infty} \|w_2\|_{\infty} \le c$ and the relation $\|A^{\dagger}\| = \|A\|$, we obtain

$$\|D\operatorname{Re}(w_{1}(B_{k}-Cs^{-p})w_{2})D\| \\ \leq \|D(B_{k}-Cs^{-p})D\| \|w_{1}(\mathbb{A}_{t,s})\| \|w_{2}(\mathbb{A}_{t,s})\| \\ \leq c \|D(B_{k}-Cs^{-p})D\|.$$

Since $k \leq p$, the triangle inequality and Lemma 12 give, up to changing the constant c, the inequality

$$\left\| D(B_k - Cs^{-p})D \right\| \le cs^{-k}$$

which proves (S53) and therefore (S52).

Estimating the main term $iu_1B_1u_1$

We can estimate the leading term term $iu_1B_1u_1$ in a more refined way compared to S by using that the first derivative has a sign, $\chi' \geq 0$. This fact allows to reproduce $\mathbb{A}_{t,s}^{(1)}$ exactly at lowest order (in favor of the $\tilde{\mathbb{A}}_{t,s}^{(1)}$ that appeared above for higher orders) as asserted in Theorem 2.

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Lemma 13. Let $\tilde{\chi} \in \mathcal{C}_{1/2,1}$ be given by Lemma 11. There exists a constant C > 0 such that

$$(\mathbf{I}) \le \kappa_J^{(1)} s^{-1} \mathbb{A}_{t,s}^{(1)} + C s^{-2} \tilde{\mathbb{A}}_{t,s}^{(1)} + C s^{-p}, \qquad p \ge 3.$$
(S55)

Proof of Lemma 13. Since $u_1 = u_1^{\dagger}$ appears symmetrically and $d\Gamma(\cdot)$ is monotonic, it suffices to prove the operator inequality

$$iad_{\chi_{t,s}}(J) \le \kappa_J^{(1)} s^{-1} \chi'_{t,s} + C s^{-2} \tilde{\chi}'_{t,s} + C s^{-p}$$
 (S56)

By applying Lemma 11 with k = 1, there exist constants c, C > 0 and $\tilde{\chi} \in \mathcal{C}_{1/2,1}$ such that

$$iad_{\chi_{t,s}}(J) = c\sqrt{\tilde{\chi}'_{t,s}}iad_{\chi_{t,s}}(J)\sqrt{\tilde{\chi}'_{t,s}} + \mathcal{R}$$
(S57)

where the remainder \mathcal{R} is Hermitian with norm controlled by $||\mathcal{R}|| \leq Cs^{-p}$ (see (S45)) and can thus be ignored in the following. Moreover, the construction in the proof of Lemma 11 satisfies the relation

$$c\tilde{\chi}'_{t,s} = 1,$$
 on supp χ_s

as can be seen from (S43) and (S44).

Combining this with (S57), we see that (S56) is implied by the operator inequality

$$iad_{\chi_{t,s}}(J) \le \kappa_J^{(1)} s^{-1} \chi'_{t,s} + C s^{-2}$$
 (S58)

Similarly to Step 3 in the proof of Proposition 10, we rephrase the claimed operator inequality (S58) as the following norm bound,

$$\|M'_{iad_{\chi_{t,s}}}(J)M'\| \le 1$$
, where $M' = 1/\sqrt{\kappa_J^{(1)}s^{-1}\chi'_{t,s} + Cs^{-2}}$. (S59)

We shall prove (S59) via the Schur test. We first consider the matrix elements

$$|i(\mathrm{ad}_{\chi_{t,s}}(J))_{xy}| = |\chi_{t,s}(|x|) - \chi_{t,s}(|y|)||J_{xy}|.$$

We consider a mixture of the Taylor expansions around x and around y. This can in fact be extended to any order; see [40, Lemma 2.2].

Without loss of generality, assume $|x| \ge |y|$. By monotonicity, we have $\chi_{t,s}(|x|) \ge \chi_{t,s}(|y|)$ and by (S39)

$$\begin{aligned} |\chi_{t,s}(|x|) - \chi_{t,s}(|y|)| &= \chi_{t,s}(|x|) - \chi_{t,s}(|y|) = \chi'_{t,s}(|x|) \frac{|x| - |y|}{s} + R_2^{(2)} \\ &\leq \chi'_{t,s}(|x|) \frac{|x - y|}{s} + Cs^{-2}|x - y|^2. \end{aligned}$$

Since $\chi \in \mathcal{C}_{1/2,1}$, we have $u = \sqrt{\chi'} \in C^{\infty}(\mathbb{R})$ and so

$$\chi'_{t,s}(|x|) \le u_{t,s}(|x|)u_{t,s}(|y|) + Cs^{-1}|x-y|$$

We have shown that for $|x| \ge |y|$,

$$|\chi_{t,s}(|x|) - \chi_{t,s}(|y|)| \le s^{-1} \sqrt{\chi'_{t,s}(|x|)\chi'_{t,s}(|y|)} |x - y| + Cs^{-2} |x - y|^2.$$

The same estimate holds if $|x| \ge |y|$ by interchanging the roles of x and y in the above argument.

Hence, we can bound the matrix elements appearing in (S59) by

$$\begin{split} & \left| \left(M' i \operatorname{ad}_{\chi_{t,s}}(J) M' \right)_{xy} \right| \\ \leq & M' \left(\sqrt{\chi'_{t,s}(|x|) \chi'_{t,s}(|y|)} \frac{|x-y|}{s} + Cs^{-2} |x-y|^3 \right) |J_{xy}| M' \\ \leq & |J_{xy}| \frac{|x-y|}{c} + |J_{xy}| |x-y|^3. \end{split}$$

Applying the Schur test and recalling the Definition (2) of $\kappa_{I}^{(p)}$ proves (S59) and thus Lemma 13.

Conclusion of the proof of Theorem 2

Proof. We apply estimates of R, S and $u_1 i B_1 u_1$ given in Lemma 9, Propositions 10 and Lemma 13 to the r.h.s. of the expansion (S25) to obtain

$$D\Phi_{s}(t) \leq \frac{\kappa_{J}^{(1)} - v'}{s} f^{(1)}(\mathbb{A}_{t,s}) \mathbb{A}_{t,s}^{(1)} + Cs^{-2}h(\mathbb{A}_{t,s})\tilde{\mathbb{A}}_{t,s}' + Cs^{-M}$$
(S60)

By Lemma 7, there exists $\tilde{f} \in \mathcal{C}_{\eta,\xi}$ such that

 $h = C\tilde{f}^{(1)}.$

Recall (S24). We can find $\hat{\chi} \in \mathcal{C}_{\eta,\xi}$ satisfying

 $\chi, \tilde\chi \prec \hat\chi$

and so, by monotonicity of \tilde{f} ,

$$C\tilde{f}^{(1)}(\mathbb{A}_{t,s})\tilde{\mathbb{A}}^{(1)}_{t,s} \leq C\tilde{f}^{(1)}(\hat{\mathbb{A}}_{t,s})\hat{\mathbb{A}}^{(1)}_{t,s}$$

Finally, we rename $\hat{\chi}$ as $\tilde{\chi}$ again to avoid confusion with the Fourier transform. This proves Theorem 2.

SYSTEM SIZE-INDEPENDENT UPPER BOUNDS ON $\kappa_I^{(p)}$

Suppose that Λ is a box in \mathbb{Z}^d of sidelength L, i.e.,

$$\Lambda \equiv \Lambda_L = \{ y = (y_1, \dots, y_d) : 0 \le y_j \le L - 1 \}.$$

Recall the definition

$$\kappa_J^{(p)}(L) = \max_{x \in \Lambda_L} \sum_{y \in \Lambda_L} |J_{xy}^{\Lambda}| |x - y|^p$$

where we have made the *L*-dependence of $\kappa_{L}^{(p)}(L)$ explicit in the notation.

Lemma 14. Suppose that $|J_{xy}^{\Lambda}| \leq C(|x-y|+1)^{-\alpha}$ for $\alpha \geq d+2$. Then, there exists a constant $c_d > 0$ such that

$$\kappa_J^{(\alpha-d-1)}(L) \le c_d, \quad \text{for all } L \ge 1.$$
 (S61)

Since the boxes are parametrized by their sidelength L, this proves that $\kappa_J^{(\alpha-d-1)}(L)$ is upper-bounded independently of system size under the decay assumption $|J_{xy}^{\Lambda}| \leq C(1+|x-y|)^{-\alpha}$ for $\alpha \geq d+2$, as was asserted in the main text.

Proof. By the decay assumption, we have

$$\kappa_J^{(\alpha-d-1)}(L) = \max_{x \in \Lambda_L} \sum_{y \in \Lambda_L} |J_{xy}^{\Lambda}| |x-y|^{\alpha-d-1} \leq C \max_{x \in \Lambda_L} \sum_{y \in \Lambda_L} (|x-y|+1)^{-\alpha} |x-y|^{\alpha-d-1} \leq C \sum_{y \in \mathbb{Z}^d} (|y|+1)^{-\alpha} |y|^{\alpha-d-1}.$$

In the last step, we extended the sum to all of \mathbb{Z}^d at which point it becomes independent of x and L.

The last sum is easily seen to be finite by power counting. To make this precise, we use that $|y|^{\alpha-d-1} \leq (|y|+1)^{\alpha-d-1}$ and use a standard integral comparison,

$$\sum_{y \in \mathbb{Z}^d} (|y|+1)^{-\alpha} |y|^{\alpha-d-1} \le \sum_{y \in \mathbb{Z}^d} (|y|+1)^{-d-1} \le C \int_{\mathbb{R}^d} (|y|+1)^{-d-1} < \infty.$$

Since this finite upper bound is independent of L, Lemma 14 is proved.

REMARK ON PARAMETER DEPENDENCIES

It is in principle possible to obtain the dependence of implicit constants on the parameters η, ξ in Theorems 1 and 2. This could be used, to widen the scope of our result to situations of mesoscopic particle transport, i.e., propagation of a total of $\propto N^{\delta}$ particles with $0 < \delta < 1$.

For this, one simply takes $\eta = \eta_0 N^{\delta-1}$ and $\xi = \xi_0 N^{\delta-1}$. In that case, the distance d_{XY} in (7) will be accompanied by a factor $N^{\delta-1}$. This means that the final estimate is useful on sufficiently large scales compared to the total particle number.

While we do not track the precise dependence of the constants η, ξ for the sake of simplicity, we explain here how this can be done in principle. The key observation is that ξ, η can be removed from the function classes $\mathcal{A}_{\eta,\xi}$ and $\mathcal{C}_{\eta,\xi}$ by an affine change of variables

$$a(r) = (2\xi - 2\eta)r + 2\eta - \xi$$

which sends $[\frac{1}{2}, 1] \rightarrow [\eta, \xi]$. We have

$$\mathcal{A}_{\eta,\xi} = \left\{ h \in C^{\infty}(\mathbb{R}) : h(r) = h_1(a(r)) \text{ with } h_1 \in \mathcal{A}_{\frac{1}{2},1} \right\},$$
$$\mathcal{C}_{\eta,\xi} = \left\{ f \in C^{\infty}(\mathbb{R}) : f(r) = f_1(a(r)) \text{ with } f_1 \in \mathcal{C}_{\frac{1}{2},1} \right\}$$

In particular, for $h \in \mathcal{A}_{\eta,\xi}$ it holds that

$$|h^{(k)}(r)| = 2^k (\xi - \eta)^k |h_1^{(k)}(a(r))|$$

where $h_1 \in \mathcal{A}_{\frac{1}{2},1}$ does not explicitly depend on η, ξ . An analogous statement holds for $f \in \mathcal{C}_{\eta,\xi}$. We see that each derivative is naturally accompanied by a factor $\xi - \eta$ in addition to the factor s^{-1} that arose for each derivative taken in the proof of Theorem 2 given in the preceding sections.