Maximal Speed for Macroscopic Particle Transport in the Bose-Hubbard Model

Jérémy Faupin,[1,*] Marius Lemm,[2,†] and Israel Michael Sigal[3,‡]
[1]*Institut Elie Cartan de Lorraine, Université de Lorraine, 57045 Metz Cedex 1, France*
[2]*Department of Mathematics, University of Tübingen, 72076 Tübingen, Germany*
[3]*Department of Mathematics, University of Toronto, Toronto, M5S 2E4 Ontario, Canada*

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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.

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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 nonrelativistic condensed-matter systems similarly display an *effective "light" cone* which provides a system-dependent 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 ten 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 (ASTLOs)*. 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 spacetime estimates. We are able to flexibly design ASTLOs that capture the key dynamical information about the localization of particles in spacetime 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

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

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

We assume that $J^\Lambda_{x,y} = J^\Lambda_{y,x}$ and we let $V_x: \{0, 1, 2, \dots\} \to \mathbb{R}$ 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

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

where $|\cdots|$ denotes the Euclidean distance. Our bounds will involve the constant $\kappa_J^{(p)}$ for some $p \geq 2$ 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}.

Suppose that Λ is a box in $\mathbb{Z}^d$ and we have the decay bound $|J^\Lambda_{xy}| \lesssim (|x-y|+1)^{-\alpha}$ for some exponent $\alpha \geq d+3$. Then we can take $p = \alpha - d - 1$ as $\kappa_J^{(\alpha-d-1)}$ is upper-bounded 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.,

$$J^\Lambda_{x,y} = J\delta_{x\sim_\Lambda y}, \qquad V_x(n_x) = \frac{U}{2} n_x(n_x - 1), \qquad (3)$$

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

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

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

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

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 $P_{\bar{N}_S < c}$, $P_{\bar{N}_{S^c} \geq c}$, etc., for the associated spectral projectors of $\bar{N}_S$, where $S^c = \Lambda \backslash S$.

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) and let $p \geq 2$. 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

$$\psi_t = e^{-itH} P_{\bar{N}_{X^c} \leq \eta} \phi. \qquad (6)$$

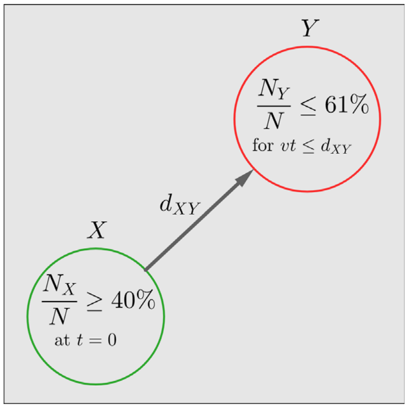

FIG. 1. As shown in Theorem 1, the transport of 1% of the particles from X to Y takes time proportional to d_{XY}. A macroscopic cloud of particles moves at most at speed $v_{\max}$.

Then we have the decay estimate

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

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

To interpret the result, see Fig. 1 and consider an initial state ϕ so that $P_{\bar{N}_{X^c} \leq \eta}\phi = \phi$, meaning the fraction of particles outside of X is at most η (say, $\eta = 0.6$ and so at most 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

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

[see (7)]. For finite-range hopping, we can take $p \geq 2$ arbitrarily large and so 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 us, for the first time, to consider the important class of *Mott states*

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

[A common choice is $\nu_x \equiv \nu$ with $\nu - 1 < (\mu/U) < \nu$ 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 $d_{XY} \geq vt$ even if X grows with system size. The constant 2 can be replaced by any number > 1. (vi) It is an open question 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], Fig. 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. 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 raise the particle number on the outer annulus above ξN for any $\xi > \eta$.

ASTLOs: Definition and basic properties.—The overarching idea behind our approach is to construct special adiabatic spacetime localization observables (ASTLOs) [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 semi-interval $[0, \infty)$; see Fig. 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 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 $v't$ away 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 $\mathbb{A}_t$ are useful because, in addition to decreasing quasimonotonically 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

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

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

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

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 $\mathcal{C}_{\eta,\xi}$. In words, these are smooth (infinitely differentiable) and nonnegative 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 $f' \equiv f^{(1)}$ denoting the first derivative,

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

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 $f \in \mathcal{C}_{\eta,\xi}$ implies that $\Phi(t)$ is an approximate spectral projector in the sense that

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

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

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

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

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

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

$D\Phi(t)$ is called the Heisenberg derivative of $\Phi(t)$. Here and in the following, we may assume without loss of generality that ψ_0 lies in the domain of the unbounded operator H by using a standard approximation argument.

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

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

we can now formulate the key technical result.

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

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

Here $\mathbb{A}_t'$, $\tilde{\mathbb{A}}_t$, and $\tilde{\mathbb{A}}_t'$ 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 the Supplemental Material (SM) [48]. A key ingredient in the proof is the bound

$$\| [J, |x|] \| \leq \kappa_J^{(1)} \equiv v_{\max} \tag{20}$$

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 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 $f \in \mathcal{C}_{\eta,\xi}$ and $\chi \in \mathcal{C}_{1/2,1}$. 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 $t \leq (s/\epsilon v)$, we obtain

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

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

$$\int_0^t \langle f'(\mathbb{A}_r)\mathbb{A}_r'\rangle_r dr \le Cs^{1-p}\int_0^t \langle \tilde{f}'(\tilde{\mathbb{A}}_r)\tilde{\mathbb{A}}_r'\rangle_r dr + Cts^{1-p} \le Cts^{1-p} \quad (21)$$

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

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 $t \ge r \ge 0$,

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

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

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 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 quasimonotonic 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 ASTLOs 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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[*]jeremy.faupin@univ-lorraine.fr
[†]marius.lemm@uni-tuebingen.de
[‡]im.sigal@utoronto.ca

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[48] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.128.150602 for the proof of Theorem 2, which includes Refs. [49,50], the statement and proof of Lemma 14 concerning system size-independent bounds on $\kappa_J^{(\alpha-d-1)}$, and a remark on the form of dependency of the constant $C_{\kappa_J^{(p)},\xi-\eta}$ on $\xi-\eta$.

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