


Long-Range Free Fermions: Lieb-Robinson Bound, Clustering Properties, and Topological Phases

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 (Received 17 October 2022; revised 12 January 2023; accepted 1 February 2023; published 17 February 2023)

We consider free fermions living on lattices in arbitrary dimensions, where hopping amplitudes follow a power-law decay with respect to the distance. We focus on the regime where this power is larger than the spatial dimension (i.e., where the single particle energies are guaranteed to be bounded) for which we provide a comprehensive series of fundamental constraints on their equilibrium and nonequilibrium properties. First, we derive a Lieb-Robinson bound which is optimal in the spatial tail. This bound then implies a clustering property with essentially the same power law for the Green's function, whenever its variable lies outside the energy spectrum. The widely believed (but yet unproven in this regime) clustering property for the ground-state correlation function follows as a corollary among other implications. Finally, we discuss the impact of these results on topological phases in long-range free-fermion systems: they justify the equivalence between Hamiltonian and state-based definitions and the extension of the short-range phase classification to systems with decay power larger than the spatial dimension. Additionally, we argue that all the short-range topological phases are unified whenever this power is allowed to be smaller.

DOI: [10.1103/PhysRevLett.130.070401](https://doi.org/10.1103/PhysRevLett.130.070401)

Introduction.—Locality is a central concept in quantum many-body physics [1]. One of the most important implications of locality, which explicitly means the Hamiltonian is a sum of local terms, is the Lieb-Robinson bound that claims a “soft” light cone for correlation propagation [2–4]. Further assuming an energy gap in the Hamiltonian, locality implies that the ground-state correlation functions should decay exponentially [5,6]. This so-called clustering property gives a partial justification for studying phases of quantum matter [7] by focusing on short-range correlated many-body states, which typically obey entanglement area laws [8,9] and admit efficient representations based on tensor networks [10].

The past couple of years have witnessed a series of breakthroughs on generalizing the above locality-related results to those “not-so-local” quantum many-body systems with power-law decaying interactions [11–21], commonly dubbed long-range systems [22]. This topic is of both fundamental and practical importance as long-range interactions appear ubiquitously in nature and quantum simulators [23–27]. In particular, the problem of finding

Lieb-Robinson bounds with optimal light-cone behaviors has recently been solved for both interacting [20] and noninteracting (free-fermion) [18] long-range systems. In contrast, other results such as clustering properties and phase classifications remain to be improved or explored, even on the noninteracting level [28]. We note that, despite their simplicity, free fermions can already accommodate various topological phases [29–31], whose long-range generalizations have been considered in various specific models [32–37] and may be realized effectively in spin systems such as atomic arrays [38,39] and nitrogen-vacancy (NV) centers [40]. Also, long-range models appear naturally in the context of fermionic Gaussian projected entangled pair states [41–43].

In this Letter, we report some essential progress on long-range free fermions, focusing on universal and rigorous results both in and out of equilibrium. First, we derive a new Lieb-Robinson bound as the noninteracting counterpart of that in Ref. [12], which is optimal in the spatial tail but not in the light cone. This bound implies an (almost) optimal clustering property for Green's functions, leading to a widely believed ground-state clustering property among other applications. The latter result justifies the equivalence between state and Hamiltonian formalisms for long-range free-fermion topological phases. In addition, we argue that the topological classification of short-range phases remains applicable to long-range phases if the decay power is larger than the spatial dimension, and collapses otherwise.

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Setup.—For simplicity, we focus on free fermions living on a d -dimensional hypercubic lattice $\Lambda \subset \mathbb{Z}^d$ with particle number conservation, where possible internal states (e.g., spin) per site form a set I . The generalization to the cases without number conservation and other lattices is straightforward (see Supplemental Material [44]). Denoting \hat{c}_{rs}^\dagger (\hat{c}_{rs}) as the creation (annihilation) operator of a fermion with internal state $s \in I$ at site $\mathbf{r} \in \Lambda$, we know that the Hamiltonian generally reads

$$\hat{H} = \sum_{\substack{\mathbf{r}, \mathbf{r}' \in \Lambda \\ s, s' \in I}} H_{rs, r's'} \hat{c}_{rs}^\dagger \hat{c}_{r's'}, \quad (1)$$

where H is a $|\Lambda||I| \times |\Lambda||I|$ Hermitian matrix. We assume the hopping amplitudes follow a power-law decay. This means for any $|I| \times |I|$ block $[H_{rr'}]_{ss'} \equiv H_{rs, r's'}$, or equivalently $H_{rr'} \equiv P_r H P_{r'}$ with P_r being the projector onto site \mathbf{r} , there exist two positive $\mathcal{O}(1)$ constants [46] J and α such that

$$\|H_{rr'}\| \leq \frac{J}{(|\mathbf{r} - \mathbf{r}'| + 1)^\alpha}, \quad (2)$$

where $\|\cdot\|$ is the operator norm and $|\mathbf{r} - \mathbf{r}'|$ is the distance between \mathbf{r} and \mathbf{r}' . We call such a long-range system satisfying Eq. (2) α decaying to highlight the explicit exponent.

Several comments are in order. First, given a fixed α , one can equivalently replace $|\mathbf{r} - \mathbf{r}'| + 1$ by $|\mathbf{r} - \mathbf{r}'|$ in Eq. (2) with $\mathbf{r} \neq \mathbf{r}'$ specified. While both are commonly used conventions, we prefer Eq. (2) as we need not exclude $\mathbf{r} = \mathbf{r}'$. Second, one can check that $\alpha > d$ is necessary and sufficient for any α -decaying Hamiltonian to have bounded single particle energies, i.e., $\|H\| < \infty$, so that the total energy is extensive. Our results are mostly obtained in this thermodynamically stable regime [19]. Third, the Bloch Hamiltonian of a long-range periodic system is not analytic or even continuous (if $\alpha < d$) in the wave vector \mathbf{k} , in stark contrast to the short-range case of finite-range or exponentially decaying hopping.

Lieb-Robinson bound.—For free fermions it suffices to consider individual single particles. Our first main result concerns how fast an initially localized particle propagates under the time evolution governed by \hat{H} :

Theorem 1: Lieb-Robinson bound.—For any α -decaying Hamiltonian H with $\alpha > d$, there exists an $\mathcal{O}(1)$ constant t_c depending only on α and d such that for any $t > t_c$

$$\|P_{\mathbf{r}} e^{-iHt} P_{\mathbf{r}'}\| \leq \frac{K(t)}{(|\mathbf{r} - \mathbf{r}'| + 1)^\alpha}, \quad (3)$$

where $K(t)$ grows polynomially fast in time and $K(t) \propto t^{\alpha(\alpha+1)/(\alpha-d)}$ for large t .

Equation (3) essentially gives an upper bound on the wave function amplitude on site \mathbf{r} at time t of a single-particle state initially localized at \mathbf{r}' . It thus constrains the

spreading of the wave function in this “continuous-time quantum walk” [47].

This bound (3) appears to be rather similar to the bound in Ref. [12] for interacting long-range systems, but a crucial difference here is that in our (free) case it holds for the whole $\alpha > d$ regime while the interacting case requires $\alpha > 2d$, as we will explain for the derivation in the next paragraph. As is also the case in Ref. [12], the time scaling of $K(t)$ in Eq. (3) is far from optimal. Indeed, the light cone $t \propto |\mathbf{r} - \mathbf{r}'|^{(\alpha-d)/(\alpha+1)}$ is linear only in the short-range limit $\alpha \rightarrow \infty$, while optimally it would be linear already for $\alpha > d + 1$ [18]. On the other hand, the spatial tail of Eq. (3) is optimal. To see this, we only have to consider $\hat{H} = J/(|\mathbf{r} - \mathbf{r}'| + 1)^\alpha \times (\hat{c}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}'} + \text{H.c.})$. Then we have $\|P_{\mathbf{r}} e^{-iHt} P_{\mathbf{r}'}\| \geq 2t / [\pi(|\mathbf{r} - \mathbf{r}'| + 1)^\alpha]$ at a large distance, i.e., $\pi(|\mathbf{r} - \mathbf{r}'| + 1)^\alpha / (2J) > t$. It is also worthwhile to compare this bound (3) to the free-fermion bound in Ref. [18], which is optimal in the light cone but not in the tail.

Let us outline the proof of Theorem 1. It is instructive to first recall that a direct Taylor expansion of e^{-iHt} gives a bound like Eq. (3) but with $K(t) \propto e^{\lambda t}$ [6]. To tighten this exponential dependence, the basic idea is to separate the Hamiltonian into the short-range and long-range parts, i.e., $H = H_{\text{sr}} + H_{\text{lr}}$, where the short-range part is determined $[H_{\text{sr}}]_{rs, r's'} = H_{rs, r's'}$ for $|\mathbf{r} - \mathbf{r}'| \leq \chi$ (χ : cutoff parameter) but otherwise $[H_{\text{sr}}]_{rs, r's'} = 0$. We can then work in the interaction picture with respect to the former:

$$e^{-iHt} = e^{-iH_{\text{sr}}t} T e^{-i \int_0^t dt' H_{\text{lr}}^{(I)}(t')}, \quad (4)$$

where T denotes the time ordering and $H_{\text{lr}}^{(I)}(t) = e^{iH_{\text{sr}}t} H_{\text{lr}} e^{-iH_{\text{sr}}t}$. By Taylor expansion in the interaction picture, we can also obtain an exponential factor but with a modified coefficient λ_χ , which can be made sufficiently small by properly choosing χ . While so far the procedure largely follows Ref. [12], a crucial difference here is that we further perform a *coarse graining* of the lattice Λ into $\tilde{\Lambda}$ at the same scale χ (see Fig. 1). This helps us get rid of a factor χ^d in λ_χ compared to the interacting case, making it proportional to $\chi^{-(\alpha-d)}$ rather than $\chi^{-(\alpha-2d)}$. Therefore, $\alpha > d$ is enough for suppressing $\lambda_\chi t$ by choosing a sufficiently large χ .

To further illustrate how and why the coarse graining works, we first write down the Taylor-expansion bound on the left-hand side of Eq. (3) in the interaction picture (4) [48]:

$$\begin{aligned} \|P_{\mathbf{r}} e^{-iHt} P_{\mathbf{r}'}\| &\leq \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \\ &\times \|P_{\mathbf{r}} e^{-iH_{\text{sr}}(t-t_n)} \prod_{m=1}^n \tilde{H}_{\text{lr}} e^{-iH_{\text{sr}}(t_m-t_{m-1})} P_{\mathbf{r}'}\|, \end{aligned} \quad (5)$$

where $t_0 \equiv 0$. Instead of inserting $\mathbb{1} = \sum_{\mathbf{r} \in \Lambda} P_{\mathbf{r}}$ ($\mathbb{1}$: identity) as is essentially the strategy used in Ref. [12], we insert

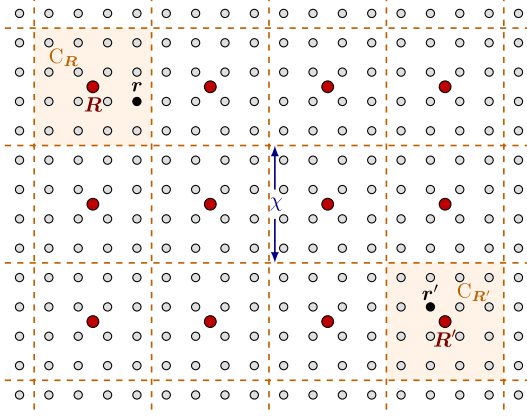


FIG. 1. Coarse graining of a square lattice Λ (gray circles) into $\tilde{\Lambda}$ (red circles) with a rescaling χ . Here, C_R denotes all the sites in Λ , including r , that are coarse grained into $R \in \tilde{\Lambda}$. The coarse-grained projector is thus defined as $P_R \equiv \sum_{r \in C_R} P_r$. Note that no periodicity of the Hamiltonian is assumed.

the coarse-grained decomposition $\mathbb{1} = \sum_{R \in \tilde{\Lambda}} P_R$ (see Fig. 1) so that each integrand in Eq. (5) can be upper bounded by

$$\sum_{\{R_j \in \tilde{\Lambda}\}_{j=1}^{2n}} \|P_R e^{-iH_{sr}(t-t_n)} P_{R_{2n}}\| \prod_{m=1}^n \|P_{R_{2m}} H_{lr} P_{R_{2m-1}}\| \times \|P_{R_{2m-1}} e^{-iH_{sr}(t_m-t_{m-1})} P_{R_{2m-2}}\|, \quad (6)$$

where $R_0 \equiv R'$ and R, R' are determined such that they include r, r' respectively. Obviously, except for the two boundary factors, the bulk product is always smaller than the refined decomposition (to each lattice site). In fact, it turns out to be smaller by a factor χ^{-nd} which leads to the qualitative improvement of λ_χ discussed above. This is because each $\|P_{R_{2m}} H_{lr} P_{R_{2m-1}}\|$ is roughly smaller than the corresponding sum of $\|P_{r_{2m}} H_{lr} P_{r_{2m-1}}\|$ by a factor χ^d ($r_m \in \Lambda$ is a site coarse grained into $R_m \in \tilde{\Lambda}$), while $\|P_{R_{2m-1}} e^{-iH_{sr}(t_m-t_{m-1})} P_{R_{2m-2}}\|$ differs from $\|P_{r_{2m-1}} e^{-iH_{sr}(t_m-t_{m-1})} P_{r_{2m-2}}\|$ by mostly an $\mathcal{O}(1)$ factor [44]. Note that in the interacting case this improvement is canceled by a factor of χ^d from (the interacting counterpart of) each $\|P_{R_{2m-1}} e^{-iH_{sr}(t_m-t_{m-1})} P_{R_{2m-2}}\|$, accounting for the size of support of P_R . It is the single-particle nature of free systems that allows us not to “pay the price.”

Clustering properties.—We move on to introduce the second main result—the clustering property of the Green’s function (or resolvent [49])

$$G(z) \equiv (z - H)^{-1}. \quad (7)$$

We assume z is outside the spectrum of H and we define $\Delta(z) \equiv \|G(z)\|^{-1}$ as the distance of z to such spectrum. Precisely speaking, we have

Theorem 2: Clustering property of the Green’s function.—For an α -decaying Hamiltonian H with $\alpha > d$ and $z \in \mathbb{C}$ that is not an eigenvalue of H , the Green’s function (7) satisfies

$$\|G_{rr'}(z)\| \leq \frac{\text{poly}[\log(|r - r'| + 1)]}{(|r - r'| + 1)^\alpha}, \quad (8)$$

where $G_{rr'} = P_r G(z) P_{r'}$ and $\text{poly}(\cdot)$ means a polynomially large function with $|r - r'|$ -independent coefficients, which nevertheless depend on $\Delta(z)$ and diverge for $\Delta(z) \rightarrow 0$.

Here, the condition $\Delta(z) \neq 0$ is absolutely necessary since otherwise even short-range hopping ($\alpha \rightarrow \infty$) can generate long-range correlations and interactions, manifesting as, for instance, Friedel oscillations [50] and Ruderman-Kittel-Kasuya-Yosida interactions [51] in the presence of impurities. The short-range counterpart of Theorem 2 has been considered in Ref. [52].

A direct corollary of Theorem 2 is the clustering property of ground-state correlation functions. In the case of free fermions, it is natural to consider the covariance matrix

$$C_{rs,r's'} \equiv \langle \Psi_0 | \hat{c}_{r's'}^\dagger \hat{c}_{rs} | \Psi_0 \rangle, \quad (9)$$

where $|\Psi_0\rangle$ is the ground state of \hat{H} . Without loss of generality, we may assume the Fermi energy, which lies in a band gap, to be zero, so that [53,54]

$$2C = \mathbb{1} - \text{sgn}H. \quad (10)$$

Thanks to Wick’s theorem, any correlation functions can be obtained from the covariance matrix (9), so it suffices to consider the clustering properties for the latter, i.e., a bound on $\|C_{rr'}\|$ with $C_{rr'} \equiv P_r C P_{r'}$. Note that

$$C = \oint_{\ell_{<}} \frac{dz}{2\pi i} G(z), \quad (11)$$

where $\ell_{<}$ is a closed loop that encompasses all the bands on the negative real axis, i.e., below the Fermi energy. Since the length of $\ell_{<}$ is bounded by a constant (due to the finiteness of $\|H\|$) while $\|G_{rr'}(z)\|$ satisfies Eq. (8) $\forall z \in \ell_{<}$, we know that $\|C_{rr'}\|$ also satisfies Eq. (8). Moreover, Theorem 2 has broader implications. For example, it implies that any bound state outside the spectrum induced by an impurity supported on $\mathcal{O}(1)$ sites has an algebraically decaying profile in real space, with essentially the same exponent α . This can be seen from $\psi_b = G(E_b) V \psi_b$, where ψ_b is the wave function of the bound state with eigenenergy E_b and V is the impurity potential [55]. We will again exploit Theorem 2 when discussing topological phases in the next section.

Finally, let us sketch out the proof of Theorem 2 [44]. Similar to Refs. [5,6,18,56,57] concerning ground-state correlations, the main idea is to construct an analytic filter

function $f_\sigma(t)$ such that it decays rapidly for large t and its Fourier transform $\mathfrak{F}[f_\sigma](\omega) \equiv \int_{-\infty}^{\infty} (dt/2\pi) f_\sigma(t) e^{-i\omega t}$ (also analytic) well approximates $(z - \omega)^{-1}$ if ω is away from z by a few σ 's, a control parameter to be determined later. Via Eq. (7) and up to some error terms involving σ , such a filter enables us to express $G_{r'r'}(z)$ as

$$P_r \mathfrak{F}[f_\sigma](H) P_{r'} = \int_{-\infty}^{\infty} \frac{dt}{2\pi} f_\sigma(t) P_r e^{-iHt} P_{r'}, \quad (12)$$

which can be bounded by the Lieb-Robinson bound (3) (and the trivial bound $\|P_r e^{-iHt} P_{r'}\| \leq 1$ for late times). The desired bound (8) is obtained by choosing an appropriate σ , which turns out to be proportional to $\Delta(z)$ and sublogarithmically suppressed by $|r - r'|$.

Topological phases.—Free-fermion topological phases are defined in terms of equivalence classes under continuous deformations of gapped quadratic Hamiltonians or alternatively of free-fermion (Gaussian) states. In the short-range case these two approaches can be readily seen to be equivalent [58]. In the long-range case, given an α decaying free-fermion state, it is easy to construct a parent Hamiltonian that is also α decaying by taking $H = \mathbb{1} - 2C$ [cf. Eq. (10)]. It follows that a continuous deformation of a state implies that of the parent Hamiltonian.

According to the clustering properties proven above, we know that the converse is also true if $\alpha > d$. Given a continuous path of gapped α -decaying Hamiltonians H_λ parametrized by $\lambda \in [0, 1]$, their ground states will also be (almost) α decaying due to the clustering property of ground-state correlations. It can be further shown that they define a continuous path in the space of states by using the clustering property of the Green's function. Indeed, we have

$$C_{\lambda'} - C_\lambda = \oint_{\ell_{<}} \frac{dz}{2\pi i} G_\lambda(z) (H_{\lambda'} - H_\lambda) G_{\lambda'}(z), \quad (13)$$

where $\ell_{<}$ encircles the lower bands of both H_λ and $H_{\lambda'}$, which is always possible given a minimal gap during the deformation. Because of Theorem 2, we have that $\|G_\lambda(z)\| \leq \max_r \sum_{r'} \|G_{\lambda, r'r'}(z)\|$ is bounded along $\ell_{<}$, implying that C_λ depends continuously on H_λ .

This analysis justifies the equivalence of considering free-fermion states and gapped quadratic Hamiltonians for $\alpha > d$. In this case we can also say something more about the structure of existing phases. One can show that every long-range gapped Hamiltonian with $\alpha > d$ is continuously connected to a short-range one, implying that there are no new phases unique to long-range Hamiltonians. To see this, consider the Hamiltonians defined by $H_{\kappa, r'r'} = e^{-\kappa|r-r'|} H_{r'r'}$ which constitute a continuous path with respect to κ and can be shown to be gapped for sufficiently small but finite κ [44]. This path connects the long-range

Hamiltonian at $\kappa = 0$ to a short-range one (i.e., exponentially decaying) at finite κ .

Furthermore, there should be no unification of short-range phases in the regime $\alpha > d$, since for translation-invariant systems the Bloch Hamiltonians $h(\mathbf{k})$ remain continuous in \mathbf{k} and all the short-range topological invariants remain well defined and robust under continuous deformations of the Hamiltonian. For disordered systems, the index theorem of Ref. [59] shows that topological invariants must remain equal to a fixed integer along any path H_λ provided that C changes continuously with respect to H , which we have shown above to be true.

Remarkably, the threshold $\alpha = d$, above which the short-range paradigm persists, is optimal, i.e., cannot be improved to be smaller. This is because if we allow $\alpha < d$ then all the *short-range* topological phases are expected to be unified (up to a 0D topological invariant such as the fermion number parity). Without loss of generality, we focus on translation-invariant representatives described by Bloch Hamiltonians. The argument is based on the well known result that all the short-range topological phases can be obtained by perturbing a Dirac Hamiltonian with a mass term [31]

$$h(\mathbf{k}) = \sum_{\mu=1}^d \sin k_\mu \Gamma_\mu - \left(\sum_{\mu=1}^d \cos k_\mu - m \right) \Gamma_0, \quad (14)$$

where $\{\Gamma_\mu\}_{\mu=0, \dots, d}$ are Hermitian Dirac matrices satisfying $\{\Gamma_\mu, \Gamma_\nu\} = 2\delta_{\mu\nu}$. Decreasing m from $m > d$ to $m \in (d-2, d)$, there is a single band crossing at $\mathbf{k} = \mathbf{0}$, giving rise to a transition from a trivial phase to a topological phase with unit topological number [60]. Let us take, for instance, the topological Bloch Hamiltonian $h_{\text{topo}}(\mathbf{k})$ defined by choosing $m = d-1$. We can show that $h_{\text{topo}}(\mathbf{k})$ is connected to the trivial Hamiltonian $h_0(\mathbf{k}) = \Gamma_0$ through a continuous path of long-range gapped Hamiltonians, provided that α is not constrained to be larger than d . To this end, we consider a linear interpolation from $h_0(\mathbf{k})$ to $h_{fD}(\mathbf{k})$ and then from $h_{fD}(\mathbf{k})$ to $h_{\text{topo}}(\mathbf{k})$, where $h_{fD}(\mathbf{k})$ is the *gapped* flattened Dirac Hamiltonian

$$h_{fD}(\mathbf{k}) = \sum_{\mu=1}^d \frac{\sin k_\mu}{\sqrt{\sum_{\mu=1}^d \sin^2 k_\mu}} \Gamma_\mu. \quad (15)$$

One can see that $h(\mathbf{k})^2 > 0$ during the whole deformation, meaning that the gap does not close [44]. Furthermore $h_{fD}(\mathbf{k})$ is (almost) d decaying in real space [44], while $h_0(\mathbf{k})$ and $h_{\text{topo}}(\mathbf{k})$ are local, so the Hamiltonian is at most as nonlocal as d decaying during the deformation. Numerical analysis suggests that also the ground state covariance matrix C remains always d decaying along such path, as shown in Fig. 2.

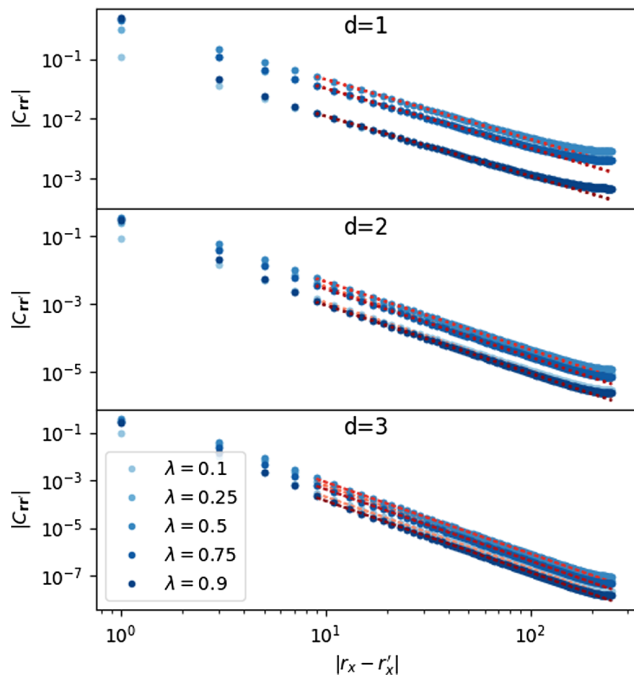


FIG. 2. Decay rates of $\|C_{rr'}\|$ for the ground states of the Hamiltonians h_λ defined by $h_\lambda = (1 - 2\lambda)h_0 + 2\lambda h_{fD}$ for $\lambda \in [0, 0.5]$ and $h_\lambda = 2(1 - \lambda)h_{fD} + (2\lambda - 1)h_{\text{topo}}$ for $\lambda \in [0.5, 1]$ in dimensions $d = 1, 2, 3$. The red dashed lines are a fit of the long distance behavior of the data with $\|C_{rr'}\| \propto |r - r'|^{-d}$, implying the ill-definedness of conventional topological numbers. The numerical calculations are performed on finite hypercubic lattices of side $L = 500$ with antiperiodic boundary conditions [61]. In all cases the odd sites along the x axis are plotted, as this is the subset of sites in the lattice that shows the slowest decay.

Summary and outlook.—We have derived a tight (in the sense of spatial tail) Lieb-Robinson bound for α -decaying free-fermion systems with $\alpha > d$. This bound allows us to prove an (almost) optimal clustering property for the Green’s function, which implies the clustering property for the ground-state correlations in gapped systems. These results justify the equivalence between state and Hamiltonian-based definitions of topological phases in long-range free-fermion systems. In addition, we argue that all the short-range topological phases are connected within the space of α -decaying systems with $\alpha < d$.

A relevant open problem is how to further improve the Lieb-Robinson bound to be consistent with the optimal light cone [18]. Also, one still has to examine the validity of bulk-edge correspondence [62] and prove the clustering properties for topological edge modes localized at sharp edges, where our local-impurity argument does not apply. Improving the entanglement area law [13,63] for long-range free fermions could be yet another direction of future study. One may also consider whether our progress can facilitate the long-range generalization of the clustering properties for short-range Anderson localized systems [64,65].

Z. G. is supported by the Max-Planck-Harvard Research Center for Quantum Optics (MPHQ). T. G. is supported by the Deutsche Forschungs-gemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy—EXC-2111–39081486. J. I. C. acknowledges support by the EU Horizon 2020 program through the ERC Advanced Grant QENOCOBA No. 742102.

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