Spin transport in disordered long-range interacting spin chain

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Using a numerically exact technique we study spin transport and the evolution of spin-density excitation profiles in a disordered spin-chain with long-range interactions, decaying as a power-law, $r^{-\alpha}$ with distance and $\alpha < 2$. Our study confirms the prediction of recent theories that the system is delocalized in this parameters regime. Moreover we find that for $\alpha > 3/2$ the underlying transport is diffusive with a transient super-diffusive tail, similarly to the situation in clean long-range systems. We generalize the Griffiths picture to long-range systems and show that it captures the essential properties of the exact dynamics.

**Introduction.**—Many-body localization (MBL) extends the notion of Anderson localization to interacting systems [1]. For local interactions, its existence is well established theoretically [2, 3] and experimentally in one-dimensional systems [4–6] (see [7] for a recent review), but there is evidence of localization also in two-dimensional systems [8–13]. For long-range interactions the fate of MBL is less clear. Some studies suggest that the many-body localization is stable for $\alpha > 2d$ [14–17], and some claim that the system is delocalized for all $\alpha$ in the thermodynamic limit [17–19]. Finite size systems of size $L$ are claimed to exhibit an effective many-body-like localization transition at a critical disorder which scales with the system size (as a power-law for $\alpha < 2d$), and diverges in the thermodynamic limit [14, 16, 17, 19, 20].

Understanding the dynamics of disordered systems with long-range interactions is of great importance to a number of physical systems, such as nuclear spins [21], dipole-dipole interactions of vibrational modes [22–24], Frenkel excitons [25], nitrogen vacancy centers in diamond [26–30] and polarons [31]. Long range interactions are also common in atomic and molecular systems, where interactions can be dipolar [32–37], van der Waals like [32, 38], or even of variable range [39–42]. Some aspects of the dynamics in such systems were studied numerically in Ref. [43], analytically in Ref. [44] and experimentally in Ref. [45], however spin transport in such systems was not considered.

The delocalized phase of one-dimensional systems with local interactions, shows subdiffusive transport [46–50], accompanied by sublinear growth of the entanglement entropy [51–53] and intermediate statistics of eigenvalue spacing [54]. Anomalous transport is commonly explained by rare insulating regions, which effectively suppress transport in one-dimensional systems. This mechanism is known as the Griffith’s picture [48, 55, 56] (see Ref. [57] for a recent review and also Ref. [58] were rare regions were introduced externally). In dimensions higher than one the Griffiths picture predicts diffusion, since rare regions can be circumvented [56], however approximate numerical studies [8] as also recent experiments [10, 11] suggest that at least for short to intermediate times the relaxation and transport are anomalous. It is crucial to understand if this discrepancy follows from incompleteness of the Griffiths picture. While there are no efficient numerically exact methods to study the dynamics of two-dimensional interacting systems, some progress can be obtained for one-dimensional long-range interacting systems. While the Griffiths picture was not generalized to this setting, in analogy to the reasoning of higher dimensions [56], normal diffusive behavior is expected.

In a previous work we have shown that for clean systems with long-range interactions the local part of the Hamiltonian dictates the spreading of the bulk of a local spin excitation, while the long-range part of the Hamiltonian only introduces a weak perturbative effect, in the face of power-law tails of the excitation profile, with an exponent proportional to $\alpha$ [59]. The tails yield a superdiffusive signature of transport for all $\alpha$, if a sufficiently high moment of the excitation profile is considered [59].

A natural question which arises is whether the effect of long-range interactions in disordered systems goes beyond a perturbative correction as it happens for their clean counterparts. Moreover, if localization is destabilized by long-range interactions, what is the resulting nature of spin transport?

In this work we consider and answer these questions using a numerically exact matrix product state (MPS) method. The study of long-ranged interacting systems naturally requires large system sizes. In fact, we show that for $\alpha = 1.75$, finite size effects are pronounced even for a chain of 51 spins, which is currently considered as the state-of-the-art limit of exact diagonalization based techniques [60]. MPS techniques are therefore indispensable to obtain numerically exact results for chains with long-range interaction, albeit only up to some finite time. This limitation arises since the required numerical effort scales exponentially with the entanglement entropy of the state, which for generic systems is known to grow linearly with time [61]. We stress that our aim here is not to address the question of stability of the MBL phase in the presence of long-range interactions, but to study...
the dynamics in the delocalized phase. Moreover, since it is technically hard to distinguish between very slow transport and absence of transport, especially in a limited time-interval, our method is not well suited for such purpose.

Time-evolution of long-ranged systems can be conveniently obtained by the time-dependent variational principle (TDVP) applied to the manifold of MPS [62–64]. It was successfully utilized to study the dynamics of spin chains with local interactions in disordered or quasiperiodic potentials [65, 66]. For low bond dimensions and very far from the numerically exact limit this method was proposed as an inexpensive candidate to achieve accurate hydrodynamic description of transport [67], however it was shown to be unreliable for generic systems [68]. In this study, we use TDVP as a numerically exact method, and study the nature of transport in long-range-interacting disordered one-dimensional spin chain. We focus on parameter regimes in which the interaction is sufficiently long-ranged and all existing theories predict delocalization. Yet it is sufficiently short-ranged, such that the corresponding clean system as well as heat transport in disordered system [44] show asymptotic diffusive behavior. These restrictions correspond to $1<\alpha<2.0$, and without loss of generality we set $\alpha=1.75$ through this work.

**Model.**— We study transport properties of the one-dimensional long-ranged disordered Heisenberg model,

$$H = J \sum_{i=1}^{L-1} \sum_{j>i} L \left( \frac{1}{\alpha} \left( S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \right) + \sum_{i=1}^{L} h_i S_i^z,$$

where $h_i$ is uniformly distributed in the interval $[-W,W]$ and $S_i^{x,y,z}$ are the appropriate projections of the spin-1/2 operators on site $i$. In the following, we use $J=1$, which sets the time unit of the problem, and we set the power-law of the interaction to $\alpha=1.75$ as motivated above. To study the dynamical properties of this model we calculate two-point spin correlation function,

$$C_x(t) = \left\langle \hat{S}_{L/2+x}^z(t) \hat{S}_{L/2}^z(0) \right\rangle,$$

which amounts to the spreading of a spin-excitation as a function of time. Here the expectation value is calculated at infinite temperature, namely $\left\langle \hat{\mathcal{O}} \right\rangle = \text{Tr} \hat{\mathcal{O}}/\mathcal{N}$ where $\mathcal{N}$ is the Hilbert space dimension, which is a regime of interest for many cold-atoms experiments. It is convenient to characterize the spreading by the width of the excitation profile,

$$\sigma^2(t) = \sum_{x=-L/2}^{L/2} x^2 C_x(t)$$

which is analogous to the classical mean-square displacement (MSD). Typically the MSD scales as, $\sigma^2(t) \sim t^\gamma$, with $\gamma = 2$ ($\gamma = 1$) for ballistic (diffusive) transport and $0 < \gamma < 1$ corresponding to subdiffusive transport. We also define a time-dependent diffusion constant $D(t)$ as the time-derivative of $\sigma^2(t)$, which in the long-time limit converges to the linear-response diffusion constant (when the system is diffusive) [69–72].

**Method.**— The Hilbert-space dimension of a quantum lattice systems scales exponentially with the size of the system. Any wavefunction in the Hilbert space can be written as a matrix product state (MPS),

$$|\Psi[A]\rangle = \sum_{\{s_n\}=1}^{d} A^{s_1}(1)A^{s_2}(2)\ldots A^{s_N}(L) |s_1s_2\ldots s_L\rangle$$

where $d$ is the local Hilbert space dimension, $A^{s_i}(i) \in \mathbb{C}^{D_{s_i-1} \times D_{s_i}}$ are complex matrices and $D_0 = D_L = 1$, such that the product of matrices evaluates to a scalar coefficient for a given configuration $|s_1s_2\ldots s_L\rangle$. To be an exact representation of the wavefunction the dimension of the matrices, the bond dimension, must scale exponentially with the systems size. Typically one approximates the wavefunction by truncating the dimension of the matrices to a predetermined dimension with computationally tractable number of parameters. Exact results are obtained when the approximate dynamics are converged with respect to the bond dimension.

The time-dependent variational principle (TDVP) allows one to obtain a locally optimal (in time) evolution of the wavefunction on the manifold of MPS $\mathcal{M}_\chi$, with some fixed bond dimension $\chi$. It amounts to solving a tangent-space projected Schrödinger equation [64]:

$$\frac{d|\Psi[A]\rangle}{dt} = -i P_{\mathcal{M}} H |\Psi[A]\rangle,$$

where $P_{\mathcal{M}}$ is the tangent space projector to the manifold $\mathcal{M}_\chi$. Equation (5) is solved using a second-order Trotter-Suzuki decomposition of the projector. The Hamiltonian is approximated as a sum of exponentials, which can be efficiently represented as an MPO [73]. The number of exponentials is chosen such that the resulting couplings do not differ by more than 2% from the exact couplings for any pair of sites. Through this work we have used a bond-dimension of up to $\chi = 512$ and timestep of $dt = 0.1$ and verified that our results are convergent with respect to these numerical parameters (see [74]). We average over initial conditions and disorder realizations at the same time and use 1000 realizations unless stated otherwise. All calculations are performed using the TenPy library using a two-site version of the TDVP for MPS and exploiting that the Hamiltonian conserves the total magnetization [75].

**Results.**— Figure 1 shows the MSD (3) as a function of time for various disorder strengths and two system sizes. After a transient ballistic regime and within the available
timescales the width grows linearly with time, which is indicative of a diffusive transport. For the weakest disorder a slight departure from linear behavior is observed, which however seems to vanish when bond-dimension is increased (see 74). Convergence with respect to system size is achieved for all but the weakest disorder strength ($W = 2$). We attribute the finite size effects at weak disorder to the slowly decaying tail of the excitation profile, discussed below, which leads to slow convergence of the MSD with respect to the system size also in clean systems 59, 76. At strong disorder, oscillatory features emerge, with a period of the order the hopping rate. These oscillations are common in disordered systems, and typically correspond to oscillations of spin between nearby localization centers. Since oscillations lead to a noisy derivative and hence $D(t)$, we extract the diffusion constant from a linear fit of the MSD over a sliding window of times (see inset of Fig. 1). We note that the location of the window barely affects the extracted constant, suggesting convergence to its asymptotic value. The diffusion constant decreases with the disorder strength $W$, with a functional dependence well described by $D \sim W^{-1}$ (see inset in Fig. 1).

For transport that is not purely diffusive, the width of the spin excitation profile contains only partial information on transport, since in this case the asymptotic shape of the profile is not described by a Gaussian. To get a full picture of transport it is therefore pertinent to examine the evolution in time of the excitation profiles, which we do in in Fig. 2. Similarly to the clean case 59, 76, the tails of the excitation profile follow a power-law of $-2\alpha$ regardless of disorder strength, which suggests that the disorder cannot suppress the long-range hops of the spin. These tails are responsible for the divergence of the MSD (with system size) for $\alpha < 3/2$, indicating a transition to a super-diffusive transport (not shown, but see Fig. 4). While Fig. 1 suggests that transport is diffusive for $\alpha > 3/2$, the bulk of the excitation is not well described by a Gaussian, and a rescaling of the excitation profiles, anticipating diffusion (see bottom row of Fig. 2) leads to a good collapse of the tails but not of the bulk of the excitation. Good convergence in time of the behavior of the MSD suggests that while the MSD has approached its asymptotic form, one cannot say the same for the profiles. Similar finite-time behavior was observed in clean local systems (see Fig. 5 in Ref. [77]).

Since the exact numerical study of long-range systems is rather limited in time, it is beneficial to find a phenomenological model which reproduces the relevant dynamical features, and at the same time suggests an effective mechanism. For disordered local systems the Griffiths picture serves this purpose [48, 55, 56]. We generalize the Griffiths picture to long-range systems by introducing a finite probability for long jumps with a rate which decays as, $x^{-2\alpha}$, in accord with the long-range part of the Hamiltonian [78]. This reduces to the following

Figure 1. MSD as a function time for different disorder strengths ($W = 2 - 12$) and system sizes $L = 75$ (solid) and $L=51$ (dashed) at $\chi = 512$. The shaded area shows standard deviation obtained from a bootstrapping procedure. The inset shows the diffusion constant obtained from a linear fit over different time-windows against inverse disorder strength, with the black dotted line a linear fit of the diffusion constant for $t = 8 - 12$ as a function of disorder strength.

Figure 2. Magnetization profiles at different times on log-log scale (upper panels) and rescaled log-log scale (lower panel) for bond dimension $\chi = 512$ and different disorder strengths ($W = 2.0, 4.0$ and $6.0$ from left to right). The shaded area shows the standard deviation of the profile obtained from a bootstrapping procedure. Profiles are smoothed by a Gaussian filter with a standard deviation of 2.0. Black dotted line is a guide to the eye of a power-law, $x^{-2\alpha}$. 
the master equation,
\[ \frac{\partial P_n}{\partial t} = \sum_i W_{in} P_i - \left( \sum_j W_{nj} \right) P_n \]
\[ W_{ij} = \frac{e^{-h_{ij}}}{|i-j|^{\alpha}} \quad i \neq j \]

where \( h_{ij} \) is a symmetric matrix composed of independent random variables, which stand for the heights of the barriers. The precise shape of the distribution of the barrier heights is not important, as long as it is unbounded, guaranteeing the existence of very weak links. To be concrete, we take it to be the exponential distribution, \( p(h) = h_0^{-1} \exp[-h/h_0] \). We note in passing, that while the form of the transition matrix is similar to the power-law random banded matrices used to study Anderson localization with power-law hopping [79], there are crucial differences: (a) we are applying it to a classical problem, (b) \( W_{ij} \) has many-elements close to zero, and must satisfy, \( W_{ii} = -\sum_{i \neq j} W_{ij} \).

We numerically solve (6) for about 500 realizations of the transition rate matrix, \( W_{ij} \), with \( h_0 = 8 \) and a lattice size of \( L = 1000 \). At time \( t = 0 \) the walker is initiated at the origin, \( P_n(t=0) = \delta_{0n} \). In Fig. 3 we plot the probability to find a walker at site \( n \) for various time. The resulting probability distribution has a Gaussian form in the bulk, followed by a power-law tail, which can be better seen after the rescaling, \( \sqrt{t}P_n(n/\sqrt{t}) \) (similarly to the rescaling in Fig. 2). We obtain a perfect collapse of the bulk of the probability distribution computed at various times, while the power-law tail is monotonously decreasing with time, indicating a transient super-diffusive behavior. In Fig. 4 we calculate the time-dependent diffusion coefficient from,
\[ D(t) = \frac{1}{2} \frac{\partial \sigma^2}{\partial t} = \frac{1}{2} \sum_n n^2 P_n(t), \]

which converges to a finite diffusion constant. For \( \alpha = 3/2 \) the asymptotic diffusion constant diverges due to the presence of the power-law tail in \( P_n \sim n^{-2\alpha} \). For \( \alpha < 3/2 \) the system, therefore, becomes super-diffusive, similarly to what is observed in clean systems [59, 76] and analytically predicted for heat transport [44]. For \( \alpha > 3/2 \), after a transient super-diffusive behavior the system is diffusive with a diffusion constant which decreases with \( \alpha \).

Discussion.—In this work, using a numerically exact method, we studied transport in a disordered spin-chain with interactions between the spins decaying as \( x^{-\alpha} \) with distance. For clean systems and \( \alpha > d/2 \) the long-range interaction appears to be a perturbative effect which is manifested by power-law tails of the relevant excitation profile, while the dynamics of the bulk of the excitation is governed by the local interactions [59, 80]. Carrying over this analysis to long-range disordered systems suggests localization, since local interacting systems exhibit MBL at sufficiently strong disorder. Our study strongly suggests that such an analysis is not applicable in the disordered case. Even in the presence of the strongest studied disorder the system is delocalized in accord with existing theories of localization in long-range systems, predicting a critical disorder strength increasing as a power-law with system size [14–17]. The long-range part of the Hamiltonian thus destabilizes localization and leads to spreading of spin excitations. Interestingly, while for local disordered systems transport is subdiffusive in the delocalized phase, here we find diffusive transport with a diffusion constant as a function of time (see Eq. (3) for definition). Right panel. The asymptotic diffusion coefficient computed for various ranges of the hopping \( \alpha \). The black dashed lines are guides to the eye, indicating the asymptotic diffusion coefficient. The solid black line indicates divergence of the diffusion coefficient as \( \alpha \rightarrow 3/2 \).
constant that does not depend on the system size and seems to decrease with disorder as $W^{-1}$. This finding is not consistent with the prediction of $\kappa \sim W^{-3}$, which can be obtained from Ref. [44] for the heat conductivity by setting $\alpha = 1.75$ and the temperature to $T = W$. It also suggests that the scaling of the critical disorder strength with system size advocated by existing theories does not affect transport in the delocalized phase, at least far away from the critical point. The observed diffusive transport is consistent with a generalization of the Griffiths mechanism [56]. While for local one-dimensional systems rare-blocking regions effectively suppress transport, long-range interactions introduce and effective way to circumvent blocking regions. We have confirmed this picture by a numerical solution of a long-range random-barrier model (6). This model correctly reconstructs the phenomenology of the long-range interacting disordered spin-chain, and gives a prediction on the dependence of the diffusion constant on the range of the Hamiltonian (see right panel of Fig. 4). It is important to note, that since this model is classical, similarly to the standard Griffiths picture, it cannot capture the MBL transition even when it is present. Given the substantial computational cost of repeating our analysis for multiple $\alpha$’s, we leave the detailed analysis of the $\alpha$ dependence of the diffusion constant to future studies. While our study is inline with the generalized Griffiths picture it is possible that absence of anomalous transport in disordered long-range chains is related to the absence of localization. This concern is pertinent given previously observed inconsistencies of the Griffiths picture [8, 81] (cf. [82, 83], and see also the very recent [84]), suggesting that our understanding of the mechanism of anomalous transport in the vicinity of the MBL transition is far from being complete.

SUPPLEMENTARY MATERIAL

Convergence with respect to numerical parameters.—Numerical exactness of the dynamics generated by TDVP-MPS is obtained by converging with respect to the bond-dimension, $\chi$, as well as the time-step, $dt$. In Fig. 5, we provide comparisons of the mean-square displacement (MSD) from calculations with bond-dimensions up to $\chi = 512$. All results for the MSD reported in the main article are converged up to a deviation of 2% between the two largest bond dimensions. In order to check for convergence with the time-step it is sufficient to use a smaller bond dimension, since time-step errors are usually more severe at smaller bond dimension. Fig. 6 shows the relative deviation of the MSD at the MS at several time-steps from a reference calculation at time-step $dt = 0.005$. The large relative error initially is caused by an approximately constant error in absolute terms and that becomes negligible in relative terms after times larger than a few units of the hopping. A time-step of $dt = 0.1$ is thus

Figure 5. Convergence of $\sigma^2$ with respect to bond dimension. Upper panel: $\sigma^2$ at bond dimensions $\chi = 512$ (solid), $\chi = 256$ (dashed) and $\chi = 128$ (dotted). Lower panel: Relative error $\Delta \sigma^2$ compared to a reference calculation with bond dimension $\chi = 512$. The system size for both panels is $L = 51$ and a time-step of $dt = 0.1$ is used.

Figure 6. Convergence of $\sigma^2$ with respect to time-step. Relative error $\Delta \sigma^2$ compared to a reference calculation with time-step $dt = 0.005$ for $L = 51$, $\chi = 64$ at weak and strong disorder.
Figure 7. Convergence of the spin excitation profiles with respect to bond dimension for $L = 51$ and $dt = 0.1$ at various disorder strengths and times. Upper panels: Relative error $\Delta S_z$ between calculations with $\chi = 512$ and $\chi = 256$. Lower panels: Tails of spin excitation profiles with $\chi = 512$ (solid lines) and $\chi = 256$ (black dotted lines).

sufficient to obtain a converged MSD within the range of disorder strengths studied. Evaluating the spatial spin excitation profile in the tails at strong disorder becomes sensitive to numerical noise for small values of $C_x$ and is limited by a complex interplay of time-step errors and accumulation of numerical round-off errors. As shown in Fig. 7, the convergence of the tails of the spin excitation profile with respect to bond dimension is generally well controlled (<5%) up to times for which the MSD is converged as well.

The authors acknowledge fruitful discussions with Alexander Burin. This research was supported by the Israel Science Foundation (grants No. 527/19 and 218/19). BK acknowledges funding through the National Science Foundation Grant No. CHE-1464802.

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