Modified Matthiessen's rule: More scattering leads to less resistance

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We study the breaking of integrability by a finite density of dilute impurities, specifically the emerging diffusive transport. Provided the distance between impurities (localized perturbations) is large, one would expect the scattering rates to be additive, and therefore, the resistivity to be proportional to the number of impurities (the so-called Matthiessen's rule). We show that this is, in general, not the case. If transport is anomalous in the original integrable system without impurities, the diffusion constant in the nonintegrable system at low impurity density has a nontrivial power-law dependence on the impurity density, with the power being determined by the dynamical scaling exponent of anomalous transport. We also find a regime at high impurity density in which, counterintuitively, adding more impurities to an already diffusive system increases transport rather than decreases it.

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I. INTRODUCTION

A kinetic Drude model of transport [1,2] has been proved again and again to be a rather useful picture despite its "cartoonish" simplicity (or, perhaps, precisely because of it). The electric current J (or a current of any other conserved quantity) is given by $J = nev$, where $en = eN/V$ is the density of the conserved charge and v is a "characteristic velocity." The Drude model explains finite conductivity σ as being due to rare scattering events that perturb an otherwise ballistic motion of electrons. With τ being the scattering, i.e., the relaxation time, the velocity an electron initially at rest will reach in time τ under a uniform acceleration eE/m is $v = eE\tau/m$, resulting in $J = \frac{ne^2\tau}{m}E$. In other words, in the Drude model the conductivity depends on the single parameter τ as $\sigma = \frac{ne^2\tau}{m}$. While the above is not much more than a dimensional analysis, the question one has to answer for a particular situation is what determines v, or, equivalently, τ; for example, does it actually correspond to a velocity of any real excitation? Nevertheless, it does highlight the crucial role played by a characteristic time (velocity) in such a ballistic picture.

Now imagine a material in which several different types of scatterings can occur, each characterized by its own scattering time τ_k. Provided scattering events are separated, one would argue that they are independent, and therefore, one can just add the individual scattering rates to obtain the total rate $1/\tau$ as

$$\frac{1}{\tau} = \sum_k \frac{1}{\tau_k}. \tag{1}$$

The above additivity principle, being equivalent to saying that in Fermi's golden rule we have to add probabilities instead of amplitudes, means that if we have K impurities each causing scattering with rate $1/\tau_0$, we will have $\tau = \tau_0/K$. Therefore, the conductivity will scale as

$$\sigma \propto \frac{1}{K}, \tag{2}$$

or, equivalently, resistivity will be linearly proportional to the number of impurities K.

Matthiessen's rule [1–4], Eqs. (1) and (2), can be, for instance, observed in metals at low temperatures where the phonon scattering is negligible and impurities dominate, resulting in the resistivity being proportional to the concentration of impurities. Matthiessen's rule is rather natural—it predicts that if one adds twice as many impurities to a clean metal, the resistivity will be twice as large. We will show that this textbook fact is, in fact, not correct if the clean material without impurities is not ballistic. In such a case the rule has to be modified to

$$\sigma \propto \frac{1}{K^{2-z}}, \tag{3}$$

where z is the dynamical (transport) exponent of the clean system (e.g., a ballistic system has $z = 1$, diffusive $z = 2$, subdiffusive $z > 2$). Therefore, resistivity is, in general, not proportional to K. Interestingly, for $z > 2$ one can even have a regime where adding more impurities will actually increase conductivity.

We note that while violations of Matthiessen's rule have been observed before [5,6], e.g., due to nonisotropic scattering, they are rather small. Here we present a mechanism for a complete and conceptually new breakdown of the rule. The idea was already put forward recently in Ref. [7], where it was demonstrated for the isotropic Heisenberg model at high temperature which is superdiffusive with $z = 3/2$. In the present work we shall verify the modified rule for a continuous set of anomalous transport coefficients z.

The type of model that we address is sketched in Fig. 1; the main result that we verify is in Eq. (8), with the supporting data in Fig. 5 below.

II. FIBONACCI MODEL

We would like to study transport in a model with anomalous transport to which local perturbations (impurities) are

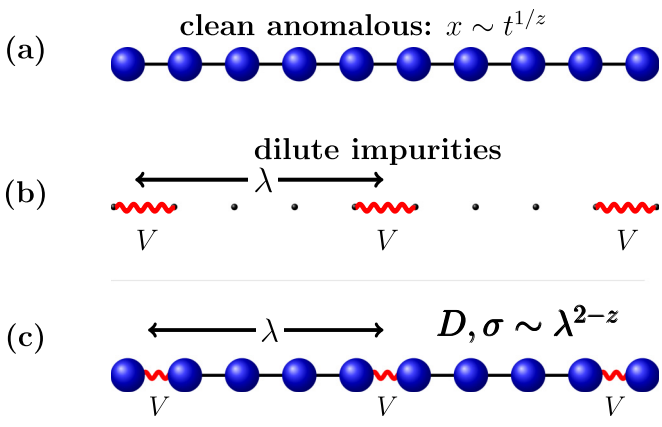

FIG. 1. We study transport in the system shown in (c), which has dilute integrability-breaking impurities (red wiggles). It is obtained by taking (a) an integrable system with anomalous transport and adding (b) interaction at every λth bond. As shown in (c), this results in diffusive transport with the diffusion constant D and the conductivity σ scaling as λ^{2-z} with distance λ between impurities (the additivity-based Matthiessen's rule predicts $D, \sigma \sim \lambda$).

added. We are, in particular, interested in the limit where the distance λ between impurities is large (see Fig. 1). While the limit $\lambda \gg 1$ represents a rather special type of perturbation, which will allow for simple theory, it is very much the relevant limit for high-purity materials. For instance, in cuprates researchers have studied [8–10] the influence of diagonal or off-diagonal disorder with concentrations $1/\lambda \approx 10^{-2}$–$10^{-4}$ on heat conductivity. We remark that we are interested in the thermodynamic limit (TDL) while keeping λ fixed, i.e., a finite density of impurities that will always result in normal diffusive (Ohmic) transport as opposed to, for instance, the case of a single impurity [11–13], which, while it changes an integrable system to a chaotic one according to standard criteria, does not modify the system's transport [12]. We also do not focus on details of how the broken integrability leads to finite diffusion constants (see, e.g., Refs. [14–24]).

We study a one-dimensional interacting Fibonacci model. Taking a one-dimensional spin-1/2 chain will allow for an efficient numerical assessment of spin transport at an infinite temperature. The Fibonacci model, which in its noninteracting version with $V_j \equiv 0$ will serve as our unperturbed clean model, is described by the Hamiltonian

$$H = \sum_{j=1}^{L-1} \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + V_j \sigma_j^z \sigma_{j+1}^z + \sum_{j=1}^{L} h_j \sigma_j^z. \quad (4)$$

The on-site fields are given by the Fibonacci potential of amplitude h, $h_j = h\{2f(\beta j) - 1\}$, where $\beta = (\sqrt{5}-1)/2$ and $f(x) = [x+\beta] - [x]$, with $[x]$ being an integer part of x. For instance, the beginning of the sequence is $h_j = h(+1, -1, +1, +1, -1, \ldots)$. Because $f(x)$ is periodic and β is irrational, the on-site potential is quasiperiodic. In the noninteracting model in which all interactions V_j are zero this allows for nontrivial transport properties that are intermediate between the ballistic transport one would have for a periodic potential and localization for random h_j. Namely, the noninteracting Fibonacci model is critical [25–28] for any h and displays a continuously varying anomalous transport [29], going from ballistic ($z = 1$) at $h = 0$ to localized ($z = \infty$) in the limit $h \to \infty$. Due to its interesting physical and mathematical [30] properties the noninteracting Fibonacci model has been much studied [25–29], including for transport [31,32], and has been realized in experiments [33,34].

The interacting Fibonacci model is less understood [31,35–38]. We shall focus on a particular case of dilute interactions; that is, we will have nonzero interaction equal to $V_j = 1$ at every λth site (see Fig. 1). For such perturbation transport will always be diffusive in the TDL; as long as one has average $\lambda \gg 1$, none of our results, like Eq. (8), should depend on the precise form of a localized perturbation and the fact that perturbed sites are exactly λ sites apart. While we shall use spin language and calculate the spin diffusion constant D, we could equivalently use the Jordan-Wigner transformation and use the language of spinless fermions and speak about conductivity σ (σ and D are trivially proportional to each other).

Because we want to study spin transport in the limit of large λ, it is crucial to have access to sufficiently large systems such that $L \gg \lambda \gg 1$. To achieve that we will use an explicit nonequilibrium driving setting where the driving is effectively accounted for by boundary Lindblad operators. The evolution of the system's density operator $\rho(t)$ is therefore described by the Lindblad master equation [39,40],

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = i[\rho, H] + \sum_k 2L_k \rho L_k^\dagger - \{\rho, L_k^\dagger L_k\}. \quad (5)$$

To force a nonzero current through the system and effectively describe driving we use four Lindblad operators L_k acting on the boundary spins, $L_1 = \sqrt{(1+\mu)}\,\sigma_1^+$, $L_2 = \sqrt{(1-\mu)}\,\sigma_1^-$ and $L_3 = \sqrt{(1-\mu)}\,\sigma_L^+$, $L_4 = \sqrt{(1+\mu)}\,\sigma_L^-$. After a long time the solution of the Lindblad equation converges to a nonequilibrium steady state (NESS) ρ_∞. If the driving parameter is $\mu = 0$, the steady state is a trivial $\rho_\infty \propto \mathbb{1}$ as such driving represents equilibrium driving at infinite temperature. For finite μ, however, there will be a nonzero magnetization gradient and a current in the NESS. Specifically, we are interested in the NESS expectation value of the local spin, $z_k = \mathrm{tr}(\rho_\infty \sigma_k^z)$, and of the spin current $J = 2\mathrm{tr}[\rho_\infty(\sigma_k^x \sigma_{k+1}^y - \sigma_k^y \sigma_{k+1}^x)]$. Due to the continuity equation the current J is independent of the site k. We will use $\mu = 0.1$, which is in the linear regime in which z_k and J are proportional to μ. Such driving has been used many times [41] in the last decade to study transport and is quite efficient, sometimes enabling numerical calculation of the NESS ρ_∞ for systems with $L \sim 10^3$. For more numerical details see the Appendix.

The main object of our study is the scaling of the NESS current J with system size L and λ. Let us first recall the definition of the dynamical scaling exponent z. In a closed setting, that is, without reservoirs, we have the scaling relation between distance and time $x \sim t^{1/z}$; for example, the variance of a localized disturbance will grow as $(\delta x)^2 \sim t^{2/z}$ with time. For instance, if one deals with diffusive transport, one will have $z = 2$; if one has ballistic transport, then $z = 1$. In a nonequilibrium situation in which one explicitly drives the system the scaling exponent z will be, instead, reflected in the

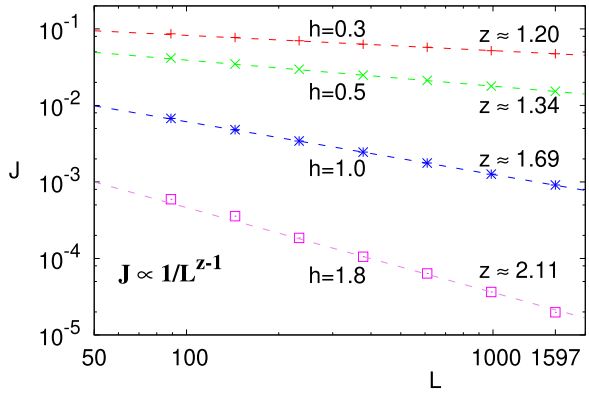

FIG. 2. Anomalous transport in the noninteracting Fibonacci model, Eq. (4), with $V_j \equiv 0$. Dashed lines are $\sim 1/L^{z-1}$ with the best fitting powers z.

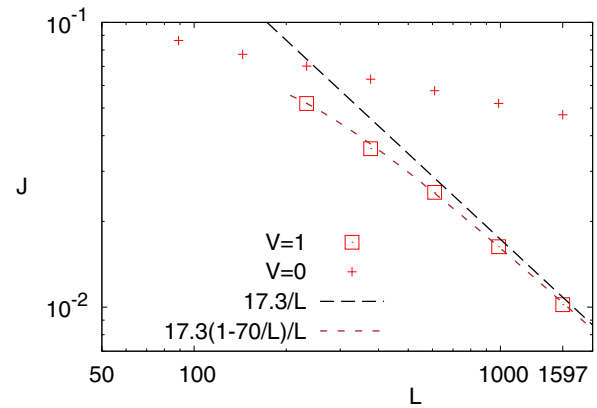

FIG. 3. Scaling of the NESS current J with system size L in the Fibonacci model with $\lambda = 128$ and $h = 0.3$. While the noninteracting model is superdiffusive with $z \approx 1.2$ (red pluses, the same data as in Fig. 2), the interacting one (squares) is diffusive with $J \propto 1/L$. Dashed black and brown curves are the best-fitting leading and subleading asymptotics.

scaling of the steady-state current J with system size (see, e.g., the review in Ref. [41]). In the linear response regime, where the current is proportional to the driving potential difference μ, one has

$$J \propto \frac{\mu}{L^{z-1}}. \tag{6}$$

The power of the algebraic scaling of current with L therefore defines the transport type. In the case of diffusion where $z = 2$ the proportionality coefficient D is the diffusion constant,

$$J = D\frac{2\mu}{L}. \tag{7}$$

To check the modified Matthiessen's rule we need the dynamical scaling exponent z of the clean noninteracting model with all $V_j \equiv 0$. This has been studied many times, beginning with Ref. [29]; here for completeness we numerically calculate z using the same Lindblad NESS driving that we then use for the interacting case. In Fig. 2 we show these data. Because the model is noninteracting, we can, in fact, avoid going through the matrix product operator (MPO) ansatz and time-dependent density matrix renormalization group (tDMRG) to obtain ρ_∞ and numerically treat very large systems ($L > 10^4$) more directly [42]. However, we show only systems up to $L = 1597$ as this is the largest size that we will be able to simulate in the interacting model. Dynamical exponents z obtained from a boundary-driven Lindblad setting reported in Fig. 2 are within 5% of the exponents obtained from unitary dynamics [43] in Ref. [36].

III. MODIFIED MATTHIESSEN'S RULE

We now study the interacting model for different values of h and distances λ between sites with interaction $V_j = 1$. Expectedly, in all cases studied, transport is diffusive in the TDL. An example of data demonstrating that is shown in Fig. 3. We can see that for sufficiently large L one gets diffusive scaling $J \sim 1/L$. From the brown dashed curve that overlaps with numerical points we can also see that a relative finite-size correction behaves as $\sim 1/L$, as is expected theoretically for diffusive boundary-driven systems [44]. For the large $\lambda = 128$ shown, the correction $\approx 70/L$ is also rather large; one needs $L > 700$ in order to be within 10% of the asymptotic $J \sim 17.3/L$. The diffusion constant can be read from the prefactor and is therefore equal to $D \approx 17.3/(2\mu) \approx 86$.

Let us derive the theoretical prediction for the scaling of the diffusion constant (or, equivalently, of conductivity) with λ. In Fig. 4 we show the NESS magnetization profile and the current for one set of parameters. The NESS current is, apart from noisy fluctuations due to finite MPO size χ homogeneous. The size of the fluctuations is one way of estimating the error of J (about 5% in this case; see Table I). More telling is the spin profile. We can see that in between the sites with scattering the profile is reminiscent of one in an anomalous model. The jump in the magnetization (i.e., in the driving potential) across a segment with resistance R is JR. The total

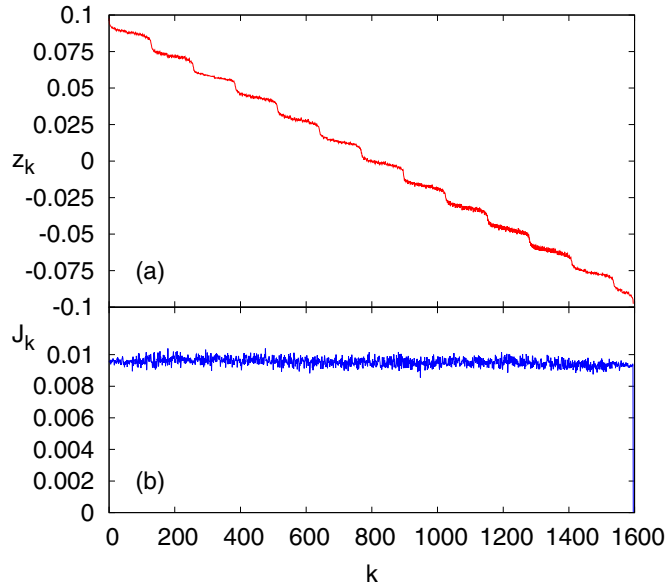

FIG. 4. NESS expectation value of (a) local spin and (b) local spin current for $L = 1597$, $\lambda = 128$, and $h = 0.3$. In (a) we can see a repeating pattern of noninteracting sections of length λ separated by bonds with impurities.

TABLE I. MPO size χ, convergence times t_∞ to the NESS, and the estimated error of the steady-state current J for a couple of system sizes L, distances between impurities λ, and on-site fields h. Not all L used in Fig. 5 are shown.

h	λ	L	χ	t_∞	Error J (%)
0.3	8	233	100	7×10^2	1
		610	100	2×10^3	3
	128	610	100	5×10^3	5
		1597	100	4×10^3	5
0.5	32	233	80	3×10^2	2
		610	50	7×10^2	7
	128	610	200	8×10^2	4
		1597	100	2×10^3	13
1.0	8	233	150	8×10^2	3
		610	200	2×10^3	2
	32	144	100	1×10^3	6
		233	200	2×10^3	10
1.8	8	233	100	1×10^4	10
		610	100	5×10^3	7
	32	233	200	5×10^3	10
		987	100	1×10^4	20

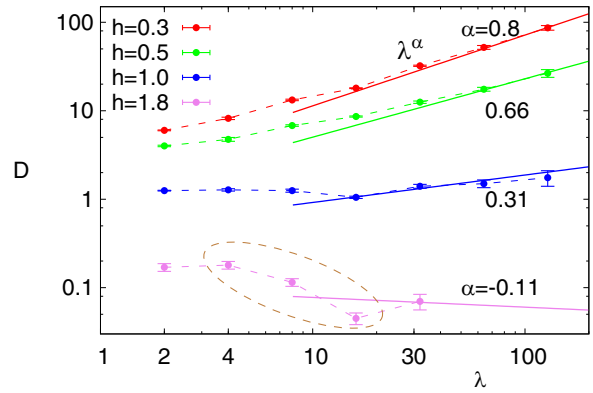

FIG. 5. Dependence of the spin diffusion constant D on the distance λ between impurities. Straight lines are $\sim\lambda^\alpha$, with powers α being equal to theoretical $\alpha = 2 - z$, with z from Fig. 2. The modified Matthiessen's rule (8) holds for large $\lambda > 30$, whereas for small λ and large $h = 1.8$ (circled points), where the rule is not expected to hold, one has a regime where more impurities produce larger D ("more is less": more scattering at smaller λ causes less resistance).

jump in magnetization across the whole chain, which is 2μ in our case, is simply a sum of jumps at the impurity sites and jumps across the noninteracting segments. For a localized perturbation, in our case a single bond, we can assume that it has a finite resistance R_0. The jump in magnetization at each site with perturbation will therefore scale as $\sim JR_0$ and will in the TDL go to zero for all systems with $z > 1$ because $J \sim 1/L^{z-1}$. Therefore, in the TDL all magnetization drop occurs in the scattering-free noninteracting segments of length λ. There are $K = L/\lambda$ such segments, so that in each magnetization will change by $\Delta z = 2\mu/K$. Looking at a noninteracting segment of length λ that is described by the scaling exponent z, we can conclude that the current should be $J = \Delta z/\lambda^{z-1}$. This brings us to the final result [7] that in the TDL one has $J \sim 2\mu\lambda/(L\lambda^{z-1})$, giving diffusion constant scaling for large λ,

$$D \propto \frac{1}{\lambda^{z-2}}. \tag{8}$$

This is the modified Matthiessen's rule. Only for the ballistic clean model does one recover the standard scaling $D \sim \lambda \sim 1/K$ from Eq. (2). Because the derivation is completely general, with the only ingredient being a defining relation of anomalous transport in a clean model, Eq. (6), it is expected to hold in the limit $\lambda \to \infty$ for any system that has anomalous transport and to which one adds dilute impurities at average linear distance λ.

A relevant question is, How common are such anomalous systems in which the rule has to be modified? One might argue that it is rather special; typically, one expects to have either a ballistic transport ($z = 1$) in integrable models [45], like in homogeneous free fermions, or a diffusive one ($z = 2$) in the case of generic interacting systems. While the Fibonacci potential is clearly special, one can note that in noninteracting models one can, in general, engineer the system's properties [46]. Recently, it has become clear that anomalous transport, however, is not limited to only noninteracting quantum systems. Specifically, superdiffusive $z = 3/2$ behavior can be found in interacting systems like the isotropic Heisenberg model [47] relevant for real materials [8–10], as well as in other integrable isotropic [48] systems [49–54], including classical ones [55–57]. Another case, which is not completely resolved, is a possible more generic superdiffusion emerging from effective theories at low temperature [54,58,59]. Anomalous transport can also be engineered in stochastic models [60].

What is the crux that leads to the modified rule in which the resistivity is not simply proportional to the number of impurities? It is the clean sections without impurities that for large λ and in the TDL cannot be neglected. While the extensive number of scattering sites causes diffusive scaling of current $J \sim 1/L$, the anomalous parts in between determine the value of D. If one were to just add resistances of all K scattering sites and K anomalous segments, one would get a total chain resistance $KR_0 + K\lambda^{z-1} = L\lambda^{z-2}(R_0/\lambda^{z-1} + 1)$, so that for $z > 1$ and large λ one could neglect the scattering term with R_0. Because the clean sections are subballistic, they are not negligible; in fact, they dominate over scattering on impurities. We can say that in a way additivity still holds if we understand it correctly: it should be applied to the anomalous parts instead of only summing up the scattering rates on impurities. We can also see that having large λ while keeping the scattering sections at a fixed length (fixed R_0) is crucial. If we were also to increase the length of the scattering sections with L, we would recover the original Matthiessen's rule where $D \sim \lambda$.

Let us now verify whether the modified Matthiessen's rule (8) indeed holds for any value of z, not just $z = 3/2$, which was already checked in Ref. [7]. Creating plots like in Fig. 3, we calculate D for a range of λ and four different values of the on-site field amplitude h, thereby tuning the value of z in the noninteracting clean model without impurities. Results are shown in Fig. 5. We can see that for all superdiffusive cases, $h = 0.3, 0.5, 1.0$, and for large enough λ (about $\lambda > 30$) we

indeed get the modified scaling $D \sim \lambda^{2-z}$ with theoretical z from Fig. 2. Unfortunately, for subdiffusive $h = 1.8$, where we would expect D to decrease with λ at a sufficiently large λ, the numerics gets very hard, and we could not get sufficiently precise results at larger λ (errors are large, and we have data for only $\lambda \leqslant 32$, which is likely not yet in the true asymptotic regime of large λ; see the Appendix). Nevertheless, data for $h = 1.8$ in Fig. 5 are compatible with the expected asymptotic $D \sim 1/\lambda^{0.1}$.

There is, however, one other interesting behavior visible at smaller λ, where the modified Matthiessen's rule (8) does not yet hold. For $h \leqslant 1.0$ we can see (Fig. 5) that for such small λ (say,$\lambda = 4$–10) we have the expected behavior: putting more impurities in our system, i.e., decreasing λ, the diffusion constant decreases. Heuristically, we can explain this decrease in diffusion as being due to increased scattering. However, for $h = 1.8$ and $\lambda \approx 4$–16 the diffusion constant instead increases as we decrease λ (a small effect of a similar kind is visible also for $h = 1.0$). For instance, at $\lambda = 16$ we have diffusion constant $D \approx 0.05$; adding, then, twice as many impurities, resulting in $\lambda = 8$, we would expect that D would decrease, but instead, it increases to $D \approx 0.12$. In this regime more scattering results in less resistivity. We could argue that this is, indeed, in line with Eq. (8) for subdiffusive clean systems with $z > 2$; however, we stress that the rule is not yet expected to hold at such small λ. Also, the decrease in D is much larger than would be predicted by Eq. (8). It is true, however, that the origin of this effect could be similar to that for the modified Matthiessen's rule, but with a more complicated dependence on λ because λ is not yet asymptotic. We also note that the effect is similar in spirit to various noise (dephasing) assisted enhancements of transport observed in, e.g., Refs. [32,61–63].

IV. CONCLUSION

We studied how transport coefficients like conductivity or the diffusion constant depend on the concentration of localized integrability-breaking perturbations: impurities. The standard textbook argument would suggest that in the limit of dilute impurities the diffusion constant will be inversely proportional to the number of impurities, also known as Matthiessen's rule. We have demonstrated that this rule is, in fact, true only in a special case when a system without impurities is a ballistic conductor. In the generic situation of anomalous transport the scaling instead has to be modified, so that the diffusion constant has a nontrivial power-law dependence on the impurity density, with the power being given by the dynamical exponent. This modified rule has been verified for spin transport at infinite temperature in the interacting Fibonacci model. We also found an interesting nonasymptotic regime in which adding more impurities can increase the diffusion constant.

What we were not able to fully check is the case of subdiffusion. Our numerical results are for a specific type of impurities—interaction on every λth bond—and for a particular conserved charge (spin). We expect the modified Matthiessen's rule to hold in general also if one were to start with a clean anomalous nonintegrable system.

ACKNOWLEDGMENT

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APPENDIX: NUMERICAL DETAILS

The numerical method used to obtain the NESS ρ_∞ of the Lindblad equation is the same one that we used in our previous works. Here we briefly repeat the essentials (for more details, see, e.g., the references cited in Refs. [21,47,64]) and give the representative parameters used.

The density operator $\rho(t)$ is expanded in the basis of products of Pauli matrices $\sigma^\alpha = \sigma_1^{\alpha_1} \cdots \sigma_L^{\alpha_L}$ as

$$\rho(t) = \sum_\alpha c_\alpha(t)\sigma^\alpha, \tag{A1}$$

where $\sigma_k^{\alpha_k} \in \{\sigma_k^x, \sigma_k^y, \sigma_k^z, \mathbb{1}_k\}$. Expansion coefficients are written in terms of the product of $(\chi \times \chi)$-dimensional matrices M (MPO),

$$c_\alpha = \left\langle M_1^{(\alpha_1)} \cdots M_L^{(\alpha_L)} \right\rangle. \tag{A2}$$

The time-dependent solution $\rho(t)$ is then obtained as $\rho(t) = e^{\mathcal{L}t}\rho(0)$ by evolving matrices M in time using small Trotter-Suzuki time steps of length $\Delta t = 0.05$, using standard procedures as in, e.g., pure-state tDMRG [65]. Note that because the local operator basis is of size 4, as opposed to 2 for a pure-state evolution of qubit chains, the complexity of simulating $\rho(t)$ in an L-site qubit chain is the same as simulating pure states in a ladder of length L (or a spin-3/2 chain of length L). The NESS is, in our case, always unique, so one can start with an arbitrary initial $\rho(0)$, eventually converging to the NESS after a long time. The crucial parameter is the matrix size χ. Namely, the larger χ is, the smaller truncation errors are; however, the complexity of each step grows as $\sim\chi^3$, and therefore, simulations get very slow at larger χ. Even if we start with a product initial density operator which requires only $\chi = 1$, evolution will cause the necessary χ to quickly grow with time. Therefore, we simply keep the matrix size constant and equal to χ from the very beginning. Because the Lindbladian propagator is not unitary, the orthogonality of the Schmidt eigenvectors is not preserved. To remedy that we reorthogonalize our MPO representation of $\rho(t)$ every few steps (typically, 10–20 steps, when we also calculate the expectation values of the magnetization and the local current).

The required convergence time t_∞ until the NESS is reached as well as the necessary χ for a given precision greatly varies with the potential strength h and with system size L. Some representative numbers can be found in Table I. In particular, in line with previous studies of the Heisenberg model with random fields [64], computational complexity rapidly increases with growing h. For h large enough that the clean noninteracting system is subdiffusive (e.g., $h = 1.8$, where $z \approx 2.11 > 2$), the convergence time and the estimated errors at fixed χ, say, $\chi = 100$, rapidly increase. This means that we unfortunately could not reliably probe the case of large z and therefore a regime of negative powers $2 - z$. Solving a boundary-driven Lindblad equation with an MPO ansatz is therefore a very good method at small h but becomes less efficient at larger on-site fields [64].

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