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Typicality approach to the optical conductivity in thermal and many-body localized phases

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We study the frequency dependence of the optical conductivity $\text{Re}\,\sigma(\omega)$ of the Heisenberg spin-$\frac{1}{2}$ chain in the thermal and near the transition to the many-body localized phase induced by the strength of a random z-directed magnetic field. Using the method of dynamical quantum typicality, we calculate the real-time dynamics of the spin-current autocorrelation function and obtain the Fourier transform $\text{Re}\,\sigma(\omega)$ for system sizes much larger than accessible to standard exact-diagonalization approaches. We find that the low-frequency behavior of $\text{Re}\,\sigma(\omega)$ is well described by $\text{Re}\,\sigma(\omega) \approx \sigma_{\text{dc}} + a|\omega|^\alpha$, with $\alpha \approx 1$ in a wide range within the thermal phase and close to the transition. We particularly detail the decrease of σ_{dc} in the thermal phase as a function of increasing disorder for strong exchange anisotropies. We further find that the temperature dependence of σ_{dc} is consistent with the existence of a mobility edge.

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Introduction. Many-body localization (MBL) generalizes the concept of Anderson localization [1] to interacting systems. In a pioneering work [2], Basko, Aleiner, and Altshuler showed perturbatively that the Anderson insulator is stable to small interactions. Thus, an isolated quantum many-body system can undergo a dynamical phase transition from a thermal phase to an MBL phase where eigenstate thermalization [3–5] breaks down. Subsequent numerical works further revealed the richness of disordered many-body systems [6–9]. A characteristic property of MBL systems is a logarithmic growth of entanglement after a global quench [10,11], which has lead to a phenomenological understanding in terms of locally conserved quantities [12–14]. An exciting aspect of MBL is that it allows one to protect quantum orders at finite energy densities (both symmetry breaking and topological ones), which would melt in thermal phases [15–19]. On the experimental side, first observations of MBL in optical-lattice systems have been made by studying quantum quenches in disordered systems of interacting particles [20]. Furthermore, the I-V characteristics of amorphous iridium oxide reveal an insulating state where MBL might play a role [21].

In the ongoing discussion of MBL, a central model is the spin-$\frac{1}{2}$ XXZ chain with a spatially random z-directed magnetic field, being equivalent to interacting spinless fermions in a random on-site potential of strength W. Furthermore, the XXZ chain is a fundamental model for the study of transport and relaxation in low dimensions [22] and relevant to the physics of quasi-one-dimensional quantum magnets [23–28], cold atoms in optical lattices [29], and nanostructures [30], as well as to physical questions in a much broader context [31,32]. This model is also of paramount interest due to its remarkably rich dynamical phase diagram, manifest in the frequency- and temperature-dependent optical conductivity $\sigma(\omega,T)$. Despite integrability of the disorder-free XXZ chain, $W = 0$, the exact calculation of $\sigma(\omega,T)$ at $T \neq 0$ has been and continues to be a challenge to theory and is an important goal of new analytical and numerical techniques. While it has become clear that, for small particle-particle interactions $\Delta < 1$, $\sigma(\omega,T)$ features a nondissipative Drude contribution at $\omega = 0$ and any $T \geqslant 0$ [33–45], much less is known on the dynamics at $\omega \neq 0$. Yet, signatures of diffusion, e.g., with a well-behaving limit $\omega \to 0$, have been found only for strong $\Delta > 1$ and high T [46–48] as well as for $\Delta = 1$ and very low T [49–51].

Perturbations, such as spin-phonon coupling [52–54], dimerization [55,56], interactions between further neighbors [57,58] or different chains [24,25,59–64], break the integrability of the XXZ chain and therefore add another layer of complexity. In this context, improving numerical approaches is imperative to progress in understanding. Within the class of relevant perturbations, disorder plays a remarkable role since it goes along with MBL as a new dynamical state of matter. Early on, a numerical work based on Lanczos diagonalization [65] found that, at $\Delta = 1$ and $W = 1$, the low-ω optical conductivity at high T follows the power law $\text{Re}\,\sigma(\omega) \approx \sigma_{\text{dc}} + a|\omega|^\alpha$, with $\alpha \approx 1$, being different from Mott's law for the Anderson insulator $\alpha \approx 2$. Such α was also observed for small but finite Δ and in a wider range of W [66]. A more recent theoretical study [67] has suggested that $\alpha \to 1$ when approaching the MBL transition from the localized ($\sigma_{\text{dc}} = 0$) side, attributed to rare metallic regions, in contrast to $\alpha \approx 2$, due to rare resonant pairs deep in the localized phase.

In this Rapid Communication, we study the optical conductivity in disordered systems using complementary numerical methods, with a particular focus on dynamical quantum typicality (DQT) [43,44,68] (see also Refs. [69–80]). This method employs the fact a single pure state can exhibit properties identical to that of the complete statistical ensemble. This fact has been demonstrated in nontrivial phases of the disorder-free XXZ chain and allows to study the long-time

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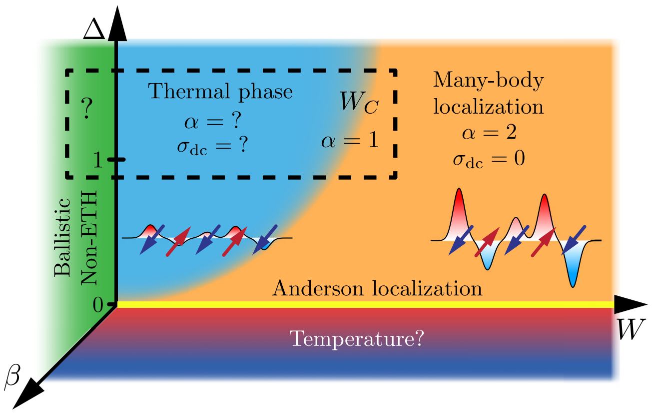

FIG. 1. Dynamical phase diagram (sketch) of disordered spin-$\frac{1}{2}$ XXZ chains. Issues studied in this Rapid Communication: Scaling of dc conductivity σ_{dc} and low-frequency exponent α for strong interactions $\Delta \geqslant 1$ and disorders $W \geqslant 0$ up to the MBL transition; temperature dependence and existence of mobility edge; typicality in finite systems with $W > 0$.

dynamics of quantum systems with Hilbert spaces being much larger than those accessible to standard exact-diagonalization (ED) approaches. While in localized phases it is clear that a single *eigenstate* cannot be a typical representative, i.e., the eigenstate thermalization hypothesis (ETH) [3–5] is not satisfied, we show for finite systems that DQT, which is *different* from ETH, works well, i.e., still the overwhelming majority of states drawn at random from a high-dimensional Hilbert space are typical.

To outline, we apply DQT to disordered XXZ chains and demonstrate that a single pure state can indeed represent the full statistical ensemble within the entire range from the thermal to the MBL phase. In particular, we find that $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a|\omega|^{\alpha}$ with $\alpha \approx 1$ in a wide range of parameters within the thermal phase and close to the transition. Moreover, we detail the dependence of σ_{dc} on W and connect to known results on either very small or very large W. Finally, we determine the T dependence of σ_{dc} down to low T in the thermal phase. We find that this dependence is consistent with the existence of an MBL mobility edge. Thus, our results provide for a comprehensive picture of dynamical phases in disordered XXZ chains, as illustrated in Fig. 1.

Model. We study the antiferromagnetic XXZ spin-$\frac{1}{2}$ chain with periodic boundary conditions, given by ($\hbar = 1$)

$$H = J \sum_{r=1}^{L} \left(S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z + B_r S_r^z \right), \qquad (1)$$

where $S_r^{x,y,z}$ are the components of spin-$\frac{1}{2}$ operators at site r. $J > 0$ is the exchange coupling constant, L the total number of sites, and Δ the anisotropy. The local magnetic fields B_r are drawn at random from a uniform distribution in the interval $[-W,W]$. Thus, translation invariance and integrability of the model are broken for any $W \neq 0$. Total magnetization S^z is strictly conserved for any value of W. This model has been studied extensively in the context of MBL at $\Delta = 1$ and several exact-diagonalization studies find an MBL phase at infinite temperatures for $W/J \gtrsim 3.5$ [6,9]. In this Rapid Communication, we study the grand-canonical ensemble $\langle S^z \rangle = 0$, taking into account all S^z sectors.

The spin-current operator $j = J \sum_r (S_r^x S_{r+1}^y - S_r^y S_{r+1}^x)$ follows from the continuity equation. We are interested in the autocorrelation function at inverse temperatures $\beta = 1/T$ ($k_B = 1$), $C(t) = \mathrm{Re}\,\langle j(t) j \rangle / L$, where the time argument of j has to be understood with respect to the Heisenberg picture, $j = j(0)$, and $C(0) = J^2/8$ at high temperatures $\beta \to 0$. From $C(t)$, we determine the optical conductivity via the Fourier transform

$$\mathrm{Re}\,\sigma(\omega) = \frac{1 - e^{-\beta\omega}}{\omega} \int_0^{t_{\max}} dt\, e^{i\omega t} C(t), \qquad (2)$$

where the cutoff time $t_{\max}$ has to be chosen much larger than the relaxation time τ, with $C(\tau)/C(0) = 1/e$ [63,64]. Note that, using the Jordan-Wigner transformation, H can be mapped onto interacting spinless fermions. In this picture, B_r is a discorded on-site chemical potential and j is the particle current.

Methods. We use the DQT method, which is most conveniently formulated in the time domain t and relies on the relation

$$C(t) = \mathrm{Re}\,\frac{\langle \Phi_\beta(t) | j | \varphi_\beta(t) \rangle}{L \langle \Phi_\beta(0) | \Phi_\beta(0) \rangle} + \epsilon, \qquad (3)$$

where $|\Phi_\beta(t)\rangle = e^{-\imath H t - \beta H/2} |\psi\rangle$, $|\varphi_\beta(t)\rangle = e^{-\imath H t}\, j\, e^{-\beta H/2}$ $|\psi\rangle$, and $|\psi\rangle$ is a *single* pure state drawn at random. Most important, the remainder ϵ scales inversely with the partition function, i.e., ϵ is exponentially small in the number of thermally occupied eigenstates [43,44,68]. The great advantage of Eq. (3) is that it can be evaluated without any diagonalization by using forward-iterator algorithms. Here, we employ a fourth-order Runge-Kutta iterator with a discrete time step $\delta t J = 0.01 \ll 1$. Using this iterator, together with sparse-matrix representations of operators, we can reach system sizes as large as $L = 30$. However, since we have to average over $N \gg 1$ disorder realizations (to obtain the algebraic mean), we consider $L \leqslant 26$.

To additionally corroborate our DQT results, we employ ED for $L = 14$ and the finite-temperature Lanczos method (FTLM), formulated in the frequency domain ω and yielding $\mathrm{Re}\,\sigma(\omega)$ with a frequency resolution $\delta\omega \propto 1/M$ [81], where $M \sim 400$ is the number of Lanczos steps used.

Results. We now present our DQT results, starting with the infinite-temperature limit $\beta \to 0$. If not stated otherwise, all DQT data are obtained from real-time data $tJ \leqslant 40$, where the autocorrelation function $C(t)$ decays fully to zero [82]. This finite-time window yields a frequency resolution $\delta\omega/J \approx 0.08$.

First, for medium disorder $W/J = 2$, we compare in Fig. 2 the optical conductivity $\mathrm{Re}\,\sigma(\omega)$, as obtained from DQT and FTLM for a system of size $L = 22$. The excellent agreement clearly shows that a single pure state, drawn at random from a high-dimensional Hilbert space, is a typical representative of the full statistical ensemble. This demonstration of typicality in disordered systems of finite size constitutes a first central result of our Rapid Communication and is the fundament for using DQT as an accurate numerical method, for this and other values of W [82].

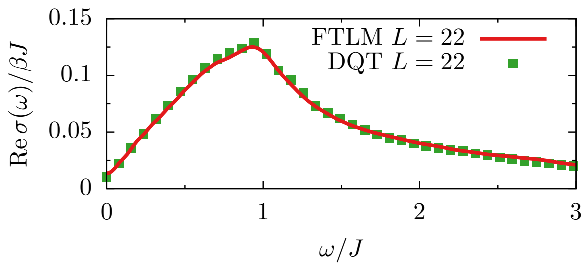

FIG. 2. Comparison of DQT ($tJ \leqslant 40$) and FTLM ($M = 400$): $\mathrm{Re}\,\sigma(\omega)$ at $\beta \to 0$, $\Delta = 1$, and $W/J = 2$ for $L = 22$ and $N = 200$. The excellent agreement clearly shows the validity of typicality. Such agreement is also found for other values of W (see Ref. [82]).

In Fig. 3 we summarize our optical-conductivity results $\mathrm{Re}\,\sigma(\omega)$ for $\Delta = 1.0$ (upper row) and $\Delta = 1.5$ (lower row) along the transition from small disorder $W/J = 0.5$ (left-hand side) to strong disorder $W/J = 4$ (right-hand side). Several comments are in order. First, while finite-size effects increase as W decreases, we find no significant L dependence for large $L \geqslant 22$ in the disorder range $0.5 \leqslant W/J \leqslant 4.0$, depicted in Fig. 3. Second, while averaging over disorder realizations is more important for larger W, statistical errors for $N = 200$ are already smaller than the symbol size used for each W shown. Third, despite the large difference in L, the overall agreement with ED data, depicted for $L = 14$ in Figs. 3(a)–3(d), proves again that typicality is remarkably well satisfied. Finally, it is evident from Fig. 3(a) that already at high T finite-size effects can be significant for $L = 14$.

As shown in Fig. 3, the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ has a well-defined value σ_{dc} at $\omega = 0$ and a maximum $\sigma_{\max} > \sigma_{\mathrm{dc}}$ located at $\omega_{\max} > 0$ for all W depicted. While σ_{dc} decreases fast as W increases, $\sigma_{\max}$ has a much weaker W dependence [see Fig. 4(b)]. In particular, the position $\omega_{\max}$ moves to higher frequencies and eventually saturates at large W [see Fig. 4(c)]. Most notably, for $\omega \ll \omega_{\max}$ the optical conductivity is well described by a power law, i.e., $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a|\omega|^{\alpha}$, where $\alpha \approx 1$. The exponent $\alpha = 1$ has been proposed in Ref. [67] at the MBL transition. We find this exponent also in a wide range of the thermal phase. This finding does not depend on the frequency resolution and the disorder average [see Figs. 3(d) and 3(h)], and can be substantiated by a log-log plot after subtracting σ_{dc} [see Fig. 4(a)]. We further checked that our finding is true for binary disorder [82]. Note that the above power law is different from Mott's law $\mathrm{Re}\,\sigma(\omega) \propto \omega^{\alpha}$ with $\alpha = 2$, valid for $W/\Delta \gg 1$ [67]. Moreover, it differs from a subdiffusive power law with $\sigma_{\mathrm{dc}} = 0$ and $\alpha < 1$ [83,84], in agreement with Ref. [85].

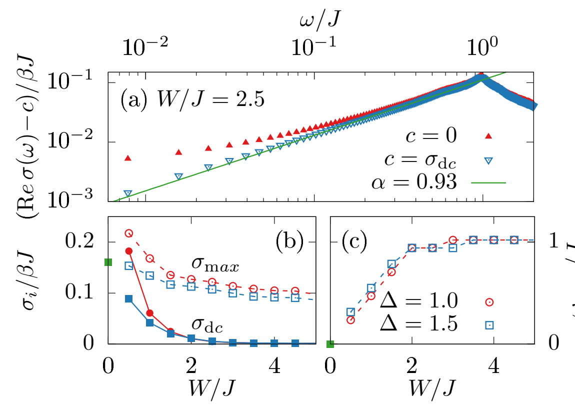

FIG. 4. (a) Log-log plot of $\mathrm{Re}\,\sigma(\omega) - c$, with $c = 0$ and $c = \sigma_{\mathrm{dc}}$, at $W = 2.5$, $\Delta = 1$, and $\beta \to 0$ ($\langle S^z \rangle = 0$, $L = 20$, $tJ \leqslant 400$, $N = 1000$) as well as a power-law fit with the exponent $\alpha = 0.93$ being close to 1. (b), (c) Disorder dependence of σ_{dc}, the maximum $\sigma_{\max}$, and its position $\omega_{\max}$ at $\Delta = 1.0, 1.5$ and $\beta \to 0$ ($\langle S^z \rangle = 0$, $L = 24$, $tJ \leqslant 40$, $N = 200$). For $W = 0$, also the $\Delta = 1.5$ result of, e.g., Ref. [47], is indicated (green square).

For $W \to 0$, Figs. 4(b) and 4(c) suggest $\omega_{\max} \to 0$ and $\sigma_{\mathrm{dc}} = \sigma_{\max}$ for $\Delta = 1.0$ and 1.5. On the one hand, this suggestion is in line with results at $W = 0$ for $\Delta = 1.5$ in Refs. [47,48,86]. On the other hand, for $\Delta = 1.0$, the complete form of $\mathrm{Re}\,\sigma(\omega)$ vs ω is still under scrutiny [49–51,57,87], including the existence of a finite σ_{dc}.

Next, we turn to lower temperatures $\beta \neq 0$, focusing on $\Delta = 1$ and $W = 2$, where σ_{dc} is already small but still nonzero

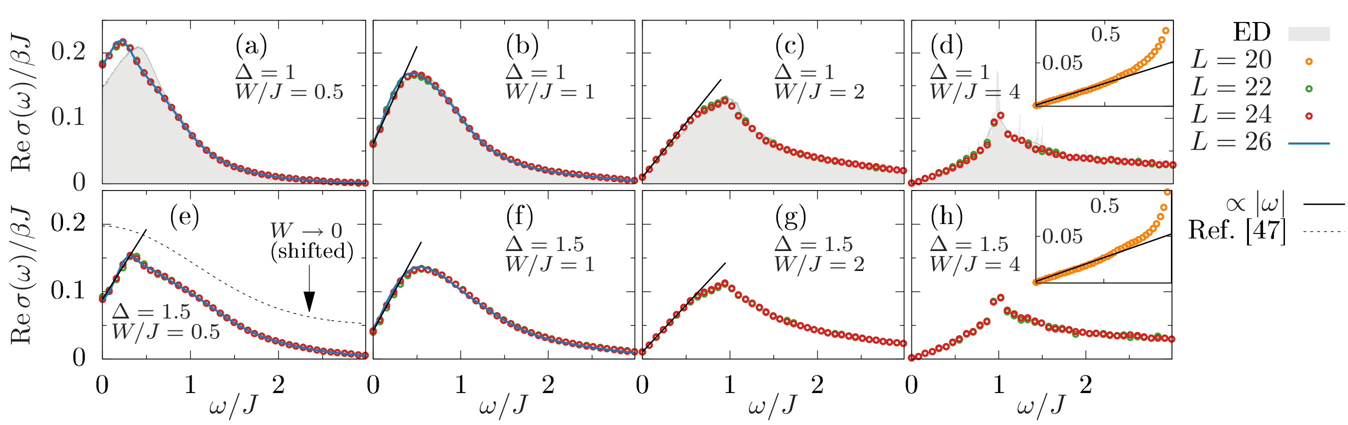

FIG. 3. $\mathrm{Re}\,\sigma(\omega)$ at $\beta \to 0$ for $\Delta = 1.0$ (upper row) and $\Delta = 1.5$ (lower row) in the transition from small $W/J = 0.5$ (left-hand side) to strong $W/J = 4$ (right-hand side) for the ensemble $\langle S^z \rangle = 0$, as obtained numerically for $L = 14$ using ED and $L > 14$ using DQT ($tJ \leqslant 40$; $L < 26$: $N = 200$; $L = 26$: $N = 20$). For $W = 4$, $L = 20$ data are shown for $N = 10\,000$ and $tJ \leqslant 120$ (insets), reducing statistical errors and increasing frequency resolution. In all cases (a)–(h), the low-ω behavior is well described by $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a|\omega|$ (lines). In (e) the perturbative result of Ref. [47] for $W \to 0$ is depicted [82].

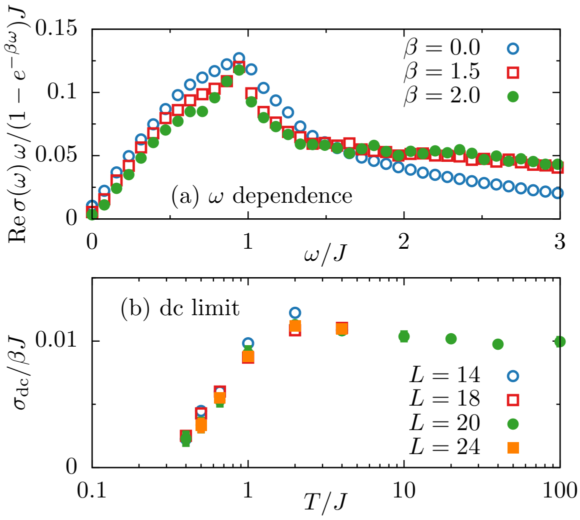

FIG. 5. (a) $\mathrm{Re}\,\sigma(\omega)$ at intermediate $W/J = 2$ and various $\beta J \leqslant 2$ for $\Delta = 1$ ($\langle S^z \rangle = 0$, $L = 24$, $tJ \leqslant 40$, $N = 1000$). (b) Temperature dependence of σ_{dc} for different $L \leqslant 24$. (Small error bars for the two largest $L = 20$ and 24 indicate the difference between $N = 500$ and 1000.) This temperature dependence is consistent with a mobility edge located at $E - E_{\mathrm{min}} \sim 2J$.

at $\beta = 0$. In Fig. 5(a) we depict our results for $\mathrm{Re}\,\sigma(\omega)\,\omega/(1 - e^{-\beta\omega})$, i.e., the mere Fourier transform of $C(t)$, for various $\beta J \leqslant 2$ and a single $L = 24$. Clearly, spectral weight at $\omega/J \gtrsim 2$ increases as β increases, while the overall structure at $\omega/J \sim 1$ only weakly depends on β. In Fig. 5(b) we show the temperature dependence of σ_{dc}, which is well converged for $L \geqslant 20$ and $N \geqslant 500$ in the entire temperature range depicted. Apparently, at high temperatures, $\sigma_{\mathrm{dc}}/\beta \approx$ const. For $T/J \lesssim 2$, however, $\sigma_{\mathrm{dc}}/\beta$ decreases rapidly as T decreases. This finding is a central result of our Rapid Communication. It is very suggestive of an interpretation in which extended states are frozen out below an energy scale of order $E - E_{\mathrm{min}} \sim 2J$. Speaking differently, this result points to the existence of a *mobility edge* in terms of E, where E_{min} refers to the lower bound of the spectrum. Similar results have been reported in Ref. [65] for smaller values of W.

Summary and conclusion. We studied the frequency dependence of the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ of the XXZ spin-$\frac{1}{2}$ chain in the transition from a thermal to a many-body localized phase induced by the strength of a spatially random magnetic field. To this end, we used numerical approaches to large system sizes, far beyond the applicability of standard ED, with a particular focus on DQT. In particular, we showed that the DQT approach represents a powerful tool to study dynamical responses of MBL systems. First, we demonstrated the validity of typicality in disordered systems. Then, we found that the low-frequency behavior of $\mathrm{Re}\,\sigma(\omega)$ is well described by $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a|\omega|^{\alpha}$, with a constant $\alpha \approx 1$ in a wide range of the thermal phase and close to the transition. We further detailed the decrease of σ_{dc} as a function of increasing disorder or decreasing temperature. We particularly found that the temperature dependence is consistent with the existence of a mobility edge.

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