

## Spin diffusion in a perturbed isotropic Heisenberg spin chain

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The isotropic Heisenberg chain represents a particular case of an integrable many-body system exhibiting superdiffusive spin transport at finite temperatures. Here, we show that this model has distinct properties also at finite magnetization  $m \neq 0$ , even upon introducing the SU(2) invariant perturbations. Specifically, we observe nonmonotonic dependence of the diffusion constant  $\mathcal{D}_0(\Delta)$  on the spin anisotropy  $\Delta$ , with a pronounced maximum at  $\Delta = 1$ . The latter dependence remains true also in the zero magnetization sector, with superdiffusion at  $\Delta = 1$  that is remarkably stable against isotropic perturbation (at least in finite-size systems), consistent with recent experiments with cold atoms.

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*Introduction.* The integrable quantum many-body lattice models and their anomalous finite-temperature  $T > 0$  transport properties have long been the subject of theoretical investigations [1]. In this context, the one-dimensional isotropic Heisenberg model has been paradigmatic. In spite of its exact solvability [2], understanding the plethora of anomalous transport properties continues to posit a challenge, especially concerning the observed anomalous superdiffusive spin transport at  $T > 0$  emerging at the junction of the gapless regime at  $\Delta < 1$ , implying finite spin stiffness  $D(T > 0) > 0$  [3–5] featuring ballistic spin transport [6–8], and gapped regime for  $\Delta > 1$  with vanishing  $D(T > 0) = 0$  and finite (dissipationless) diffusion constant  $\mathcal{D}_0 < \infty$  [9]. While postulated earlier [10], the superdiffusion of the isotropic  $\Delta = 1$  point with Kardar-Parisi-Zhang (KPZ) dynamical scaling exponent  $z = 3/2$  has been recently established both numerically [9,11–13] and analytically within the generalized hydrodynamics (GHD) [14–18]. It is worth noting that isotropic Heisenberg chains can be approximately realized in spin-chain materials [19,20] (possessing very large thermal conductivity owing to nearly conserved energy current [21]), as well as in cold-atom optical lattices [22–24].

The understanding of the effects of (even weak) integrability breaking perturbations (IBPs) remains particularly challenging [25–27]. In connection with the dc spin conductivity  $\sigma_0$  and related spin diffusion  $\mathcal{D}_0$ , the role of the uniform (preserving translational symmetry) perturbative term  $gH'$  has been addressed numerically within the easy-plane regime  $\Delta < 1$  [28–31]. It was proposed, via perturbation-theory arguments, that at high  $T$  and weak  $g \ll 1$  the dc conductivity scales as  $\propto 1/g^2$ , but in general exhibiting multiple relaxation times [31] related to the different conserved quantities involved in the current relaxation. On the other hand, in the easy-axis  $\Delta > 1$  regime, the role of IBPs is unusual [32,33] due to finite, anomalous/dissipationless diffusion even in the integrable model. The spin transport in the perturbed isotropic Heisenberg model seems to be even richer. In particular, due

to the SU(2) spin symmetry, the isotropic perturbations that preserve such symmetry are expected to have different (even singular) effect on spin transport [24,34,35], in contrast to anisotropic ones [30].

In this Letter, we show that the distinctive transport properties of the isotropic Heisenberg model are, at high  $T$ , not exclusive to the integrable (i.e., unperturbed) model or to vanishing magnetization density  $m = 0$ , but are instead seen also at finite  $m > 0$  and finite isotropic perturbation strengths. We present numerical evidence for the following: (i) In the  $m = 0$  sector for  $\Delta = 1$ , superdiffusive transport is extremely robust to the isotropic perturbations of even moderate strength  $g$ , exhibiting superdiffusive scaling of the diffusion constant  $\mathcal{D}_0 \sim L^\zeta$  with  $0 < \zeta < 1/2$  for system sizes up to  $L = 100$ . (ii) For isotropic perturbations at  $\Delta = 1$ , the diffusion constant  $\mathcal{D}_0(\Delta)$  features a peak at  $\Delta = 1$  in all magnetization sectors. In contrast, the anisotropic IBPs lead to a monotonic dependence  $\mathcal{D}_0(\Delta)$ . Away from  $\Delta \approx 1$  and  $m = 0$ , in both cases, the results appear close to the standard perturbation theory  $\mathcal{D}_0 \propto 1/g^2$  scaling, while for  $\Delta = 1$  the  $g$  dependence of our results is less conclusive. (iii) In the unperturbed isotropic spin chain, the high- $T$  spin stiffness, measured in the units of static spin susceptibility, reveals a roughly linear dependence  $D^*(m) \simeq 2|m|$  across a broad range of densities  $m \gtrsim 0.3$  that have gone unnoticed so far. This dependence eventually crosses over to the nonanalytic behavior  $D^*(m) \simeq m^2 \ln(1/|m|)$  at small  $m$ , which is hard to observe numerically. Finite magnetization results are obtained with the microcanonical Lanczos method (MCLM) on systems up to  $L = 36$  sites. However, the most challenging regime appears in the vicinity of critical point  $m = 0$ ,  $\Delta = 1$ . Here, we employ the time-evolving block decimation (TEBD) technique for boundary-driven open systems with up to  $L = 100$  sites to establish the nonequilibrium steady state (NESS).

*Model.* We study the  $S = 1/2$  XXZ Heisenberg spin chain with general anisotropy  $\Delta$  adding the IBP of the

strength  $g$ ,

$$H = J \sum_i [S_{i+1}^x S_i^x + S_{i+1}^y S_i^y + \Delta S_{i+1}^z S_i^z] + g J H'. \quad (1)$$

We deal with the IBPs, which (at least partly) conserve the translational symmetry of the model, and concentrate on the case of the staggered exchange,

$$H'_I = \sum_i (-1)^i (S_{i+1}^x S_i^x + S_{i+1}^y S_i^y + \Delta S_{i+1}^z S_i^z), \quad (2)$$

$$H'_{II} = \frac{1}{2} \sum_i (-1)^i (S_{i+1}^x S_i^x + S_{i+1}^y S_i^y). \quad (3)$$

The  $H'_I$  perturbation at  $\Delta = 1$  preserves the SU(2) symmetry and we will refer to it as the isotropic IBP. On the other hand, the  $H'_{II}$  perturbation breaks this symmetry. We consider Hamiltonians that conserve total magnetization, namely  $s_{\text{tot}}^z = mL$ , where  $|m| \leq 1/2$  is the magnetization density of the system, and the spin current operator is given by  $j_s = (J/2) \sum_i [1 + g(-1)^i] (i S_{i+1}^+ S_i^- + \text{H.c.})$ . We use  $J = 1$  as the unit of energy and analyze finite systems with  $L$  sites, either closed with periodic boundary conditions (PBCs) or open with boundary driving.

*Perturbed Heisenberg chain—finite magnetization.* We first consider the high- $T$  dynamical conductivity  $\tilde{\sigma}(\omega) = T \sigma(\omega)$  of a perturbed system with PBCs and fixed magnetization  $s_{\text{tot}}^z = mL$ , focusing here on the intermediate  $m = 1/4$ . We evaluate  $\tilde{\sigma}(\omega)$  using the MCLM [36–38] by employing a large number of Lanczos steps, i.e., here typically  $M_L = 20000$  for systems up to  $L = 36$  with  $N_{\text{st}} \lesssim 10^7$  basis states. This allows for frequency resolution  $\delta\omega \approx 10^{-3}$ , important to resolve also the large dc  $\tilde{\sigma}_0 = \tilde{\sigma}(\omega \rightarrow 0)$  emerging due to long relaxation times  $\tau \gg 1$ . Consequently, the dc diffusion constant can be extracted assuming the generalized Einstein relation,  $\mathcal{D}_0 = \tilde{\sigma}_0 / (T \chi_0)$ ,  $\chi_0 = (1/\pi) \int \sigma(\omega) d\omega = (1/4 - m^2)/T$ , which is valid in perturbed/normal systems [33]. Note that the diffusion  $\mathcal{D}_0$  is a well defined concept even at  $T \rightarrow \infty$ , unlike conductivity  $\sigma_0 = \sigma(\omega \rightarrow 0) \propto 1/T$ .

(I) Isotropic IBP: Results for the diffusion constant  $\mathcal{D}_0$  in the presence of  $H'_I$  perturbation at magnetization density  $m = 1/4$  as the function of the anisotropy  $\Delta$  are presented in Figs. 1(a) and 1(b). Most strikingly, as shown in Fig. 1(a),  $\mathcal{D}_0$  reveals a pronounced peak at isotropic point  $\Delta = 1$  with high value  $\mathcal{D}_0 \gg 1$  even at substantial  $g = 0.3$ . The results are reliable despite the very large  $\mathcal{D}_0$ , also implying a narrow peak in dynamical  $\tilde{\sigma}(\omega)$ , as evidenced by analyzing systems of different numerical complexity  $L = 24$ –36. Dependence on the perturbation strength  $g$  is quite consistent with expected standard  $\mathcal{D}_0 \propto 1/g^2$ ; see Fig. 1(b). In addition, in Figs. 1(c) and 1(d), we present the frequency  $\omega$  dependence of the integrated conductivity,  $I(\omega) = (1/\pi) \int_0^\omega \sigma(\omega') d\omega'$ , obtained with help of the exact diagonalization (ED) and MCLM. The diffusion constant can be alternatively extracted as the slope of the latter, i.e.,  $I(\omega \rightarrow 0) \propto \mathcal{D}_0 \omega$ . As evident from the presented results, although  $\mathcal{D}_0 = \tilde{\sigma}_0 / (T \chi_0)$  differ slightly from the slope of  $I(\omega)$ , the overall agreement is perfect. In Fig. 2 we present the variation of  $\mathcal{D}_0(\Delta)$  for a range of magnetization densities  $m = [0, 6]/28$ , at a moderate IBP strength  $g = 0.2$ , as obtained via MCLM in canonical ensembles at  $L = 28$ . The  $H'_I$  perturbation, in the vicinity of the isotropic point  $\Delta = 1$ ,

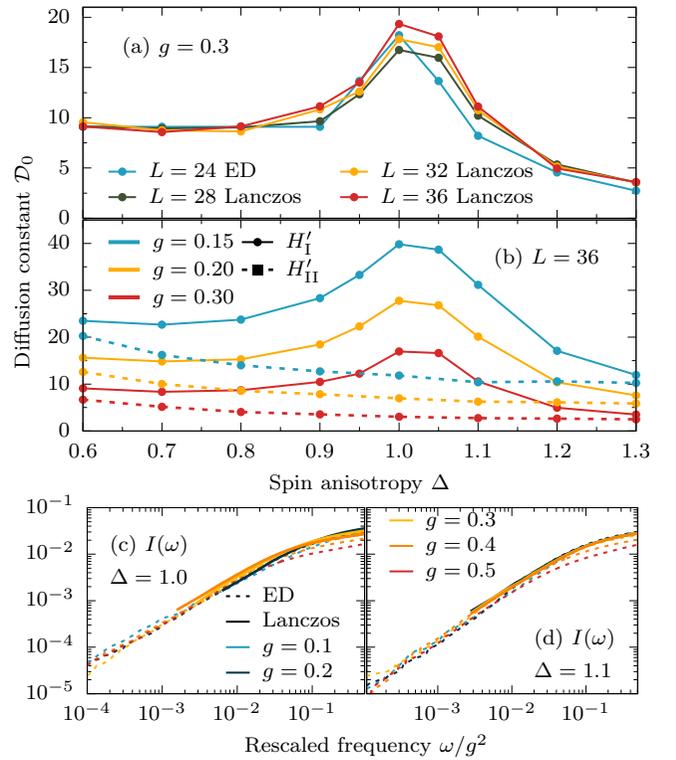


FIG. 1. Diffusion constant  $\mathcal{D}_0$  vs anisotropy  $\Delta$  at fixed magnetization density  $m = 1/4$  for  $H'_I$  perturbation at strength  $g = 0.3$ , as obtained for different system sizes via ED ( $L = 24$ ) and MCLM ( $L = 28$ –36). (b)  $\mathcal{D}_0$  vs  $\Delta$  for isotropic (full lines) and anisotropic (dashed lines)  $g = 0.15$ –0.3, obtained via MCLM for  $L = 36$ . (c), (d) Integrated optical conductivity  $I(\omega)$  for (c)  $\Delta = 1$  and (d)  $\Delta = 1.1$  as the function of the rescaled frequencies by the square of the perturbation strength  $\omega/g^2$ . Dashed (solid) line depicts  $L = 20$  ( $L = 36$ ) ED (MCLM) data.

reveals a striking variation of  $\mathcal{D}_0(m)$  with magnetization. Importantly, for all  $m > 0$  we observe a nonmonotonic  $\mathcal{D}_0(\Delta)$ , developing a peak around  $\Delta = 1$ .

(II) Anisotropic  $H'_{II}$  IBP: In Fig. 1(b) and Fig. 2 (inset), we display the effect of the anisotropic IBP  $H'_{II}$ , which behaves regularly in several respects: (i) Around  $\Delta \approx 1$ , the variation

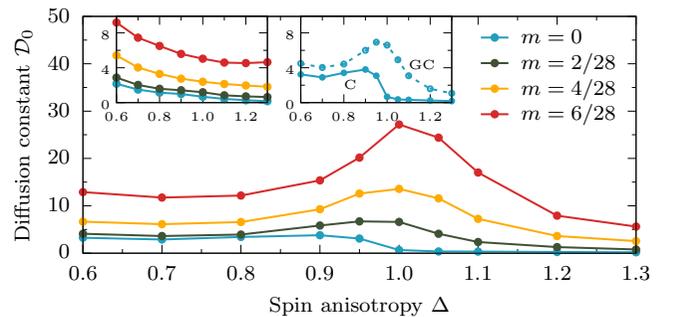


FIG. 2. Diffusion constant  $\mathcal{D}_0$  vs anisotropy  $\Delta$ , as calculated via MCLM in ensembles with magnetization densities  $m = [0, 6]/28$  and  $g = 0.2$  for  $H'_I$  (main panel) and  $H'_{II}$  (left inset) perturbation, respectively. Right inset: Comparison of canonical  $m = 0$  and grand canonical results.

with  $\Delta$  is smooth and monotonically decreasing without any specific feature at  $\Delta = 1$ . (ii)  $\mathcal{D}_0$  value is much smaller, at least at  $\Delta \approx 1$ . (iii) The scaling with  $\mathcal{D}_0 \propto 1/g^2$  can be accurately followed for all the considered values of  $g$ , Fig. 1(c). (iv) The above points are true for all considered magnetization sectors  $m$ ; see inset of Fig. 2.

*Perturbed Heisenberg chain—zero magnetization.* Our closed-system MCLM analysis indicates that the canonical  $m = 0$  results at accessible system sizes  $L \leq 28$  do not match with the corresponding grand canonical average (see inset of Fig. 2 and [39]). This remains true even for substantial  $g \approx 0.3$  and is most pronounced for isotropic IBPs. As a consequence, the analysis of the spin transport in the vicinity of  $m = 0$  and  $\Delta = 1$  requires special attention, and previous studies have already reported that this regime is particularly sensitive to finite size/time effects [34]. To achieve larger  $L$ , we study open Heisenberg chains via the TEBD technique for vectorized density matrices [40,41], where the spin current is driven via boundary Lindblad operators  $L_1 = \sqrt{1 + \mu}S_1^-$ ,  $L_2 = \sqrt{1 - \mu}S_1^+$ ,  $L_3 = \sqrt{1 - \mu}S_L^-$ ,  $L_4 = \sqrt{1 + \mu}S_L^+$  with a small spin bias  $\mu$ . In such setup, for diffusive systems, the magnetization profile in NESS is linear; while for superdiffusive, the same resembles  $\text{tr}(S_i^z \rho_{ss}^c) \approx \frac{\mu}{\pi} \arcsin(-1 + 2 \frac{i-1}{L-1})$  [9,39]. We extract the spin diffusion constant via  $\mathcal{D}_0 = -j_{ss}/\nabla s^c$ , where  $\nabla s^c$  is the magnetization gradient extracted from a finite fraction  $f$  of the central spin profile and  $j_{ss}$  is the NESS current [9,39].

(I) Isotropic IBP: For the isotropic  $H'_I$  IBP at  $\Delta = 1$ , an approximately linear bulk spin profile nonetheless retains some curvature reminiscent of the unperturbed profile for finite  $L$  [9,39]. This already indicates that for the isotropic IBP at  $\Delta = 1$ , at considered system sizes  $L \leq 100$ , there is still no restoration of normal diffusive transport. The diffusion constant is extracted using  $f = 0.2$ .

For the isotropic IBP at  $\Delta = 1$ , Fig. 3(a) presents the estimated system-size dependence of  $\mathcal{D}_0(L)$  by fitting  $\mathcal{D}_0 \sim L^\zeta$ , with exponent  $\zeta$  plotted in the inset. Recall that  $\zeta$  is related to the dynamical exponent  $z$  by  $\zeta = 2 - z$  [9,11]. In the unperturbed case  $g = 0$ , we get  $\zeta = 0.46$ , complying with the analytically expected KPZ superdiffusion with  $\zeta = 1/2$ . The surprising observation is that also for systems with isotropic IBPs, we find a robust signature of superdiffusion, albeit with a smaller exponent  $\zeta$ ,  $0.27 < \zeta < 0.37$  (but far away from the diffusive  $\zeta = 0$ ). Our results agree with previous numerical results [34,35] that reported  $z = 3/2$  scaling for isotropic IBPs from the short-time dynamics. Similarly, the recent finite size/time measurements in a cold-atom experiment [24] gave an estimate  $1.7 < z < 1.9$  in weakly perturbed systems. We note that we do not anticipate these intermediate  $0 < \zeta < 1/2$  exponents to match the true universal exponent  $\zeta$ ; they might be a transient effect, a consequence of finite systems (in our case) or times (in experimental setup), and the fraction  $f$  to estimate the bulk magnetization gradient. Curiously, the NESS current for the whole regime obeys  $j_{ss} \sim L^{-\gamma}$ ,  $\gamma \approx 0.5$ , consistent with KPZ scaling  $z = 3/2$ . While this aspect deserves further investigations, the main conclusion remains that superdiffusion is exceptionally robust against perturbations respecting the SU(2) symmetry, and the expected onset of diffusion would require much larger system sizes (in NESS formalism) and times (for closed systems).

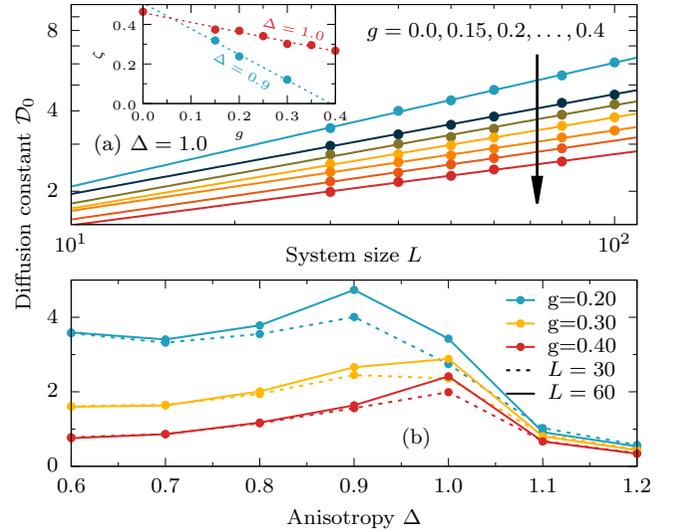


FIG. 3. (a) Scaling of NESS diffusion constant vs  $L$  for  $H'_I$  perturbation at various perturbation strengths  $g = 0.15-0.4$ , including the unperturbed result  $g = 0$ , fitted with the power laws  $\mathcal{D}_0 \propto L^\zeta$  with different  $\zeta = [0.24-0.5]$ . In the inset, fitted  $\zeta$  for different  $g$  are shown for  $\Delta = 1.0$  and  $\Delta = 0.9$ . (b) Diffusion constant  $\mathcal{D}_0$  vs  $\Delta$  for  $H'_I$  perturbation of different strength  $g = 0.15-0.4$ , obtained via NESS method for sizes  $L = 30, 60$ .

In Fig. 3(b) we display dependence  $\mathcal{D}_0(\Delta)$  for  $L = 30, 60$  and different strengths  $g = 0.2, 0.3, 0.4$  of  $H'_I$  perturbation. At stronger IBPs  $g = 0.3, 0.4$ , we observe a peak in the diffusion constant  $\mathcal{D}_0$  at  $\Delta = 1$ , similarly as in ED calculations at finite magnetization densities  $m > 0$ , Fig. 2 and [39]. Although at weaker strength  $g = 0.2$  the peak of  $\mathcal{D}_0(\Delta)$  moves inside the  $\Delta < 1$  regime, comparing the data for  $L = 30, 60$  makes it apparent that results are only well converged (with the system size) away from  $\Delta \approx 1$ . For this purpose, we repeat the system-size analysis also for  $\Delta = 0.9$ . Apparently, the  $H'_I$  perturbation promotes anomalous  $\mathcal{D}_0 \sim L^{\zeta_{0.9}}$  scaling also for  $\Delta = 0.9$ , but with  $\zeta_{0.9} < \zeta$ ; see inset of Fig. 3(a). This explains that with increasing  $L$ ,  $\mathcal{D}_0(\Delta = 0.9)$  grows slower than  $\mathcal{D}_0(\Delta = 1.0)$  and the  $\Delta \approx 0.9$  peak for  $g = 0.2$  is only a finite size effect, while we expect the true thermodynamic peak at  $\Delta = 1$ . Similarly, we believe that the  $\Delta < 1$  peak at canonical and grand canonical result for the closed system at  $m = 0$ , inset of Fig. 2, is likewise an artifact of small system sizes. To ensure ballistic scaling at  $g = 0$ ,  $\zeta_{0.9}$  could either cross over to  $\zeta_{0.9} \rightarrow 1$  at small  $g$  or show a discontinuous jump at  $g = 0$ .

(II) Anisotropic  $H'_{II}$  IBP: For the anisotropic IBP and  $\Delta = 1$ , NESS yields the linear magnetization profile, which is a characteristic of diffusive transport [9,39]. Far away from  $\Delta = 1$ , e.g., at  $\Delta = 0.5$ , we observe the expected IBP strength scaling  $\mathcal{D}_0 \propto 1/g^2$  [39]. For  $\Delta = 1.0$ , our results show normal  $1/L$  finite size corrections; however, we cannot access small enough IBP strengths  $g$ , and consequently large enough  $L$ , to reveal the anticipated  $\mathcal{D}_0 \propto 1/g^{2/3}$  scaling [30]; for  $g$  and  $L$  parameters considered, we see no asymptotic scaling with  $g$  yet [39].

*Spin stiffness at finite magnetization  $m > 0$ .* We finally discuss certain interesting properties of the unperturbed system at finite magnetization that have so far gone undetected. The

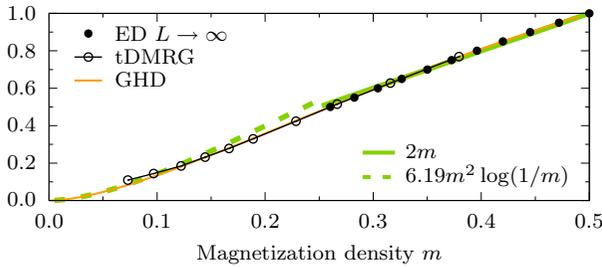


FIG. 4. (a) Normalized spin stiffness  $D^*$  vs magnetization density  $m$  obtained from (i) extrapolated  $L \rightarrow \infty$  ED data [39] (solid black points), (ii) tDMRG result Ref. [43] (open black points), and (iii) GHD exact calculation (orange line). Simple linear relation  $D^* = 2|m|$  (green solid line) at large magnetization and  $D^*(m) = 6.19m^2 \ln(1/|m|)$  (green dashed line) at small magnetization is also presented.

distinctive feature of the unperturbed ( $g = 0$ ) integrable spin chains at finite magnetization is the ballistic spin transport at  $T > 0$ , i.e., finite spin stiffness  $D$  in the spin conductivity  $\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{\text{reg}}(\omega)$ . In a system with PBCs and given  $s_{\text{tot}}^z$ , the  $D(T \gg 1)$  can be evaluated using ED by calculating all diagonal and degenerate matrix elements  $TD = \sum_{\epsilon_n = \epsilon_l} \langle n | j_s | l \rangle^2 / (2LN_{\text{st}})$ , with  $N_{\text{st}}$  as the number of many-body states. In the thermodynamic limit, the exact computation of  $D$  is possible using the GHD formalism [17,42]. We find it convenient to discuss the normalized spin stiffness  $D^* = D/\chi_0$ , with static spin susceptibility  $\chi_0 = (1/4 - m^2)/T$  providing the conductivity sum rule  $\chi_0 = \frac{1}{\pi} \int \sigma(\omega) d\omega$ .

We concentrate here on the most interesting isotropic point  $\Delta = 1$ , relegating the discussion of other regimes to [39]. In Fig. 4, we show (i) ED results, with extrapolations to  $L \rightarrow \infty$ , (ii) tDMRG results from Ref. [43], and (iii) GHD exact results [17,42], obtained as detailed in [39]. For large magnetizations, the observed approximate slope of  $2|m|$  can be, from the viewpoint of GHD, accurately captured by the contributions of magnons and two-magnon bound states [39]. Despite larger bound states becoming increasingly important at lower magnetization, it turns out, unexpectedly, that for  $m \gtrsim 0.3$ , contributions conspire to a nearly linear curve. As elaborated in [39], upon approaching close to half filling ( $m = 0$ ), the behavior crosses over to the theoretically established [14,17] anomalous nonanalytic scaling  $D^*(m) \sim m^2 \ln(1/|m|)$ , signaling the onset of superdiffusion at  $m = 0$ . Despite different order of limits ( $\lim_{L \rightarrow \infty} \lim_{\tau \rightarrow \infty}$ ), extrapolation of our ED results within the accessible range is found in good agreement with the tDMRG data and GHD. At lower magnetization densities, tDMRG values fall on top of the GHD curve until they also depart from it due to finite time limitations.

**Conclusions.** In this Letter, we show that the anomalous behavior of transport in the isotropic Heisenberg chain is not

limited to the unperturbed (i.e., integrable) model or to zero average magnetization  $m = 0$  (zero external magnetic field), but manifests itself over the entire range of  $m$  and at unexpectedly strong perturbations. For  $H'_I$  perturbation that is isotropic at  $\Delta = 1$ , we observe anomalously large diffusion constants at  $\Delta = 1$ , with nonmonotonic dependence of  $\mathcal{D}_0(\Delta)$  on  $\Delta$  for all magnetizations, and with the peak at  $\Delta = 1$  becoming more pronounced at larger  $m$ . By contrast, anisotropic  $H'_{II}$  perturbations yield much smaller diffusion constants  $\mathcal{D}_0(\Delta)$  with monotonic  $\Delta$  dependence around  $\Delta \approx 1$ . The observed behavior is quite unusual, especially considering that in the unperturbed isotropic chain  $\mathcal{D}_0$  becomes singular as  $m \rightarrow 0$ ; one would expect  $\mathcal{D}_0$  to decay with increasing  $m$ . At the same time, however, in the perturbed system  $\mathcal{D}_0$  is also affected by broadening effects associated with quasiparticles acquiring finite lifetimes and thus decay of finite stiffness (i.e., Drude peak) may play a more prominent role. We leave this aspect as an open problem for future work.

The most challenging to discern is the behavior of the perturbed Heisenberg chain at  $m = 0$  and  $\Delta = 1$ . Here, the anisotropic perturbation suppresses the superdiffusion and leads to finite  $\mathcal{D}_0$  well converged with system size. Contrarily, for the isotropic perturbation, even the largest open-system NESS results conform with a superdiffusive scaling with  $L$ ,  $\mathcal{D}_0 \sim L^\zeta$ , with exponent  $\zeta \in [0.25, 0.4]$  decreasing with increasing perturbation strength  $g$ . The intriguing conclusion of our findings is that for finite systems, certain features of the unperturbed KPZ superdiffusion with  $\zeta = 1/2$  remain fairly robust even for moderately strong isotropic perturbations. Moreover, dynamical exponents in the range  $z = 2 - \zeta \in [1.6, 1.75]$  are quite consistent with recent experiments on spin superdiffusion in cold-atom lattices, where the perturbation to the Heisenberg chain is added via the exchange between neighboring chains [24]. We repeat, however, that we do not claim these  $0 < \zeta < 1/2$  exponents to be universal, and they might be effected by transient effects.

We emphasize that similar dichotomy of anisotropic vs isotropic perturbations is also observed in other examples, e.g., the next-neighbor exchange, checked by us with MCLM in closed systems.

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