Real-time broadening of non-equilibrium density profiles and the role of the specific initial-state realization

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The real-time broadening of density profiles starting from non-equilibrium states is at the center of transport in condensed-matter systems and dynamics in ultracold atomic gases. Initial profiles close to equilibrium are expected to evolve according to linear response, e.g., as given by the current correlator evaluated exactly at equilibrium. Significantly off equilibrium, linear response is expected to break down and even a description in terms of canonical ensembles is questionable. We unveil that single pure states with density profiles of maximum amplitude yield a broadening in perfect agreement with linear response, if the structure of these states involves randomness in terms of decoherent off-diagonal density-matrix elements. While these states allow for spin diffusion in the XXZ spin-1/2 chain at large exchange anisotropies, coherences yield entirely different behavior.

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I. INTRODUCTION

The mere existence of equilibration and thermalization is a key issue in many areas of modern many-body physics. While this question has a long and fertile history, it has experienced an upsurge of interest in recent years [1] due to the advent of cold atomic gases [2] as well as to the discovery of new states of matter such as many-body localized phases [3]. In particular, the theoretical understanding has seen substantial progress by the fascinating concepts of eigenstate thermalization [4–6] and typicality of pure quantum states [7–14] as well as by the invention of powerful numerical methods such as density-matrix renormalization group [15]. Much less is known on the route to equilibrium as such [16] and still the derivation of the conventional laws of (exponential) relaxation and (diffusive) transport on the basis of truly microscopic principles is a challenge to theory [17].

In strictly isolated systems any coupling to heat baths or particle reservoirs and any driving by external forces is absent. In such systems, the only possibility to induce a non-equilibrium process is the preparation of a proper initial state. While different ways of preparation can be chosen, a sudden quench of the Hamiltonian is a common preparation scheme [18]. However, once a specific state is selected, a crucial question is: To what extent is this state a non-equilibrium state? To answer this question, it is natural to measure the observable one is interested in. If the expectation value is far from equilibrium, the state should be also. If this value is close to equilibrium, the state should be correspondingly. Moreover, only in the latter case, the resulting dynamics of the expectation value and linear response theory are expected to agree with each other. While this line of reasoning is certainly intuitive, it neglects internal degrees of freedom of the initial state. In particular, the measurement of a single observable cannot detect if the underlying state is pure or mixed, entangled or non-entangled, etc. Therefore, an intriguing question is: Do such internal details play any role for the dynamics of an expectation value?

In this paper, we investigate exactly this question for the anisotropic spin-1/2 Heisenberg chain. Dynamics in this integrable many-body model has been under active scrutiny in various theoretical works and, in particular, spin dynamics constitutes a demanding problem resolved only partially despite much effort [19–40], even within the linear response regime and at high temperatures. While it has become clear that quasi-local conservation laws [25, 26] necessarily lead to ballistic behavior below the isotropic point, numerical studies [36–39] have reported signatures of diffusion above this point, in agreement with perturbation theory [39] and classical simulations [40].

To investigate spin transport, we first introduce a class of pure initial states. These initial states feature identical density profiles, where a maximum δ peak is located in the middle of the chain and lies on top of a homogeneous background, similar to [38]. For a subclass with internal randomness we then show analytically that the resulting non-equilibrium dynamics can be related to equilibrium correlation functions via the concept of typicality. This relation is verified in addition by large-scale numerical simulations. These numerical simulations also unveil the existence of remarkably clean diffusion for large exchange anisotropies, as one of our central findings. Eventually, we demonstrate that entirely different behavior emerges without any randomness in the initial state.

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II. MODEL AND OBSERVABLES

The Hamiltonian of the XXZ spin-1/2 chain with periodic boundary conditions reads

\[ H = J \sum_{r=1}^{L} (S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z) , \]  

(1)

where \( S_r^x, S_r^y, S_r^z \) are spin-1/2 operators at site \( r \), \( L \) is the number of sites, \( J > 0 \) is the antiferromagnetic exchange coupling constant, and \( (\Delta - 1) \) is the anisotropy. For all parameters, this model is integrable in terms of the Bethe Ansatz and the total magnetization \( S^z = \sum_r S_r^z \) is a strictly conserved quantity. We take into account all particle interactions of strength \( \Delta \) and total particle number \( N = S^z + L/2 \), i.e., \( \langle N \rangle = L/2 \) (see Appendix A for the half-filling case \( N = L/2 \)).

We are interested in the non-equilibrium dynamics of the local occupation numbers \( n_r = S_r^z + 1/2 \). Specifically, we consider the expectation values \( p_r(t) = \text{tr} \rho(t) \) for the density matrix \( \rho(t) \) at time \( t \). In this way, we study the time-dependent broadening of density profiles for a given initial state \( \rho(0) \). In this paper, we focus on pure states \( \rho(0) = |\psi(0)\rangle \langle \psi(0)| \).

III. INITIAL STATES

Obviously, it is possible to choose many different initial states \( |\psi(0)\rangle \) and the resulting dynamics can depend on details of the specific choice. A frequently used preparation scheme is a quantum quench, i.e., \( |\psi(0)\rangle \) is the eigenstate of another Hamiltonian. In this paper, however, we proceed in a different way.

To introduce our class of initial states, let \( |\varphi_k\rangle \) be the common eigenbasis of all \( n_r \), i.e., the Ising basis. Then, this class reads

\[ |\psi(0)\rangle \propto n_{L/2} |\Phi\rangle , \quad |\Phi\rangle = \sum_{k=1}^{2^L} c_k |\varphi_k\rangle , \]  

(2)

where \( c_k \) are complex coefficients and \( n_{L/2} \) projects onto Ising states with a particle in the middle of the chain. By construction, \( p_{L/2}(0) = 1 \) is maximum.

In the above class, a particular state is the one where all \( c_k \) are the same. It yields \( p_{r \neq L/2}(0) = p_{\text{eq.}} = 1/2 \) and still \( p_{L/2}(0) = 1 \). Hence, its density profile has a \( \delta \) peak on top of a homogeneous background. However, exactly this density profile also results when the \( c_k \) are drawn at random according to the unitary invariant Haar measure [11] (where real and imaginary part of the \( c_k \) are drawn from a Gaussian distribution with zero mean, as done in our numerical simulations performed below). In other words, it is impossible to distinguish the two states with equal and random coefficients by a measurement of their initial density profiles \( p_r(0) \) [41]. Only at times \( t > 0 \), their density profiles \( p_r(t) \) can be different, if these density profiles differ at all. Note that similar \( p_r(0) \) have been studied in Ref. [38].

Because our initial states are pure and have maximum \( p_{L/2}(0) = 1 \) as well, these states have to be considered as far-from-equilibrium states. Thus, it is natural to expect that the resulting dynamics of \( p_r(t) \) cannot be described by linear response theory. However, such an expectation turns out to be wrong for the case of random \( c_k \). In this case, \( |\Phi\rangle \) is a typical state [7–14], i.e., a trace \( \text{tr} |\Phi\rangle \langle \Phi| \) can be approximated by the expectation value \( \langle \Phi | \bullet | \Phi \rangle \) with high accuracy in large Hilbert spaces. Using this fact and exact math (see Appendix B for more details), we find the relation

\[ p_r(t) - p_{\text{eq.}} = 2 \langle (n_{L/2} - p_{\text{eq.}})(n_r(t) - p_{\text{eq.}}) \rangle , \]  

(3)

where \( \langle \bullet | \rangle = \text{tr} |\bullet\rangle \langle \bullet| \). This relation is a first main result of our paper. It unveils that the expectation value \( p_r(t) \) of a far-from-equilibrium state is directly connected to an equilibrium correlation function. It is important to note that such a relation cannot be derived for the other case of equal \( c_k \) (see also Appendix C for the specific type of randomness).

Due to the above relation, it is also possible to connect our non-equilibrium dynamics to the Kubo formula. To this end, one has to define the spatial variance

\[ \sigma(t)^2 = \sum_{r=1}^{L} r^2 \delta p_r(t) - \left[ \sum_{r=1}^{L} r \delta p_r(t) \right]^2 \]  

(4)

with \( \delta p_r(t) = 2(p_r(t) - p_{\text{eq.}}) \) and \( \sum_{r=1}^{L} \delta p_r(t) = 1 \). Then, following Ref. [42], it is straightforward to show that the time derivative of this variance

\[ \frac{d}{dt} \sigma(t)^2 = 2 D(t) \]  

(5)

is given by the time-dependent diffusion coefficient

\[ D(t) = \frac{4}{L} \int_0^t dt' \langle j(t')j \rangle , \]  

(6)

where \( j = \sum_{r=1}^{L} S_r^x S_{r+1}^x - S_r^y S_{r+1}^y \) is the well-known spin current. For \( \Delta = 0 \), \( [j, H] = 0 \) leads to \( D(t) \propto t \) such that \( \sigma(t) \propto t^2 \) scales ballistically. The partial conservation of \( j \) for \( \Delta < 1 \) [19–31] also excludes diffusive scaling \( \sigma(t)^2 \propto t \) in this \( \Delta \) regime. In fact, signatures of diffusion at high temperatures have been found only in the regime of large anisotropies \( \Delta > 1 \) [36–39]. Note that \( \sigma(t)^2 \propto t \) is merely a necessary and no sufficient criterion for diffusion since, by definition, the variance yields no information beyond the width of the distribution \( \delta p_r(t) \). This is why we study the full space dependence. For a recent numerical survey of Eq. (5), see [45].
IV. NUMERICAL METHOD AND RESULTS

Numerically, the time evolution of a pure state $|\psi(t)\rangle$ can be calculated by the method of full exact diagonalization. But this method is restricted to $L \sim 20$ sites, even if symmetries such as the translation invariance of $H$ are taken into account. Thus, we proceed differently and rely on a forward propagation of $|\psi(t)\rangle$ in real time. Such a propagation can be done by the use of fourth-order Runge-Kutta [14, 30, 31] or more sophisticated schemes such as Trotter decompositions or Chebyshev polynomials [43, 44]. Here, we use a massively parallelized implementation of a Chebyshev-polynomial algorithm. In this way, we can treat system sizes as large as $L = 36$. For such $L$, we can guarantee that the initial $\delta$ peak is located sufficiently far from the boundary of the chain. Otherwise, we would have to deal with trivial finite-size effects and also Eq. (5) would not hold [42].

Next, we turn to our numerical results, starting with a typical initial state $|\psi(0)\rangle$, i.e., the case of random $c_k$. For a single realization of this state, we summarize in Fig. 1 the resulting expectation value $p_r(t)$ in a 2D time-space density plot for different anisotropies $\Delta = 1.5$, 1.0, 0.5 and a large system with $L = 36$ sites. Several comments are in order. First, for all values of $\Delta$ shown, the initial $\delta$ peak monotonously broadens as a function of time and the non-equilibrium density profiles have the irreversible tendency to equilibrate. Such equilibration is non-trivial in view of our isolated and integrable model. Second, for times below the maximum $tJ = 20$ depicted, the spatial extension of the density profiles is still smaller than the length of the chain. Thus, unwanted boundary effects do not emerge for such times. Third, the broadening of the density profiles is faster for smaller values of $\Delta$ because the scattering due to particle interactions decreases as $\Delta$ decreases. Moreover, for the small $\Delta = 0.5$ in Fig. 1 (c), the width of the density profile clearly increases linearly as a function of time. This linear increase is the expected ballistic dynamics arising from partial conservation of the spin current. In contrast, for the larger $\Delta = 1.5$ and 1.0 in Figs. 1 (a) and (b), the width of the density profiles does not increase linearly and is rather reminiscent of a square-root behavior. However, such a conclusion is not possible on the basis of a density plot.

To gain insight into the dynamics at $\Delta = 1.5$, we depict in Fig. 2 (a) the site dependence of the expectation values $p_r(t)$ at fixed times $tJ = 0, 5, 10$ and 20. Conveniently, we subtract the equilibrium value $p_{eq}$ and use a semi-log plot to visualize also the tails of the density profiles. As illustrated by fits, the site dependence can be described by Gaussians (with $\sigma(t)$ as the only fit parameter)

$$p_r(t) - p_{eq} = \frac{1}{2}\sqrt{2\pi \sigma(t)} \exp\left[-\frac{(r/L/2)^2}{2\sigma(t)^2}\right]$$

and, remarkably, over several orders of magnitude. Such a pronounced Gaussian form of the density profiles is a second main result of our paper and has, to best of our knowledge, not been reported in the literature yet. This result unveils that the standard deviation $\sigma(t)$ is not just a width but also the only parameter required to describe the full site dependence. Furthermore, the Gaussian form is one of the clearest signatures of diffusion so far. Still, diffusion requires that $\sigma(t)$ scales as $\sigma(t) \propto \sqrt{t}$.

To further judge on diffusion, we show in Fig. 2 (b) the standard deviation $\sigma(t)$, as resulting from the Gaussian...
fits in Fig. 2 (a). We further depict linear-response results for \( \sigma(t) \) in Eq. (5) and the underlying \( D(t) \) in Eq. (6), as calculated in Ref. [31] for \( L = 34 \sim 36 \). On the one hand, the excellent agreement shows the very high accuracy of the typicality relation in Eq. (3). On the other hand, this agreement demonstrates that the known linear-response result \( \sigma(t) \propto \sqrt{t} \), resulting from \( D(t) \approx \text{const.} \) at such \( t \) [31, 38, 39], also holds for our non-equilibrium density dynamics. Hence, together with the Gaussian form, we can conclude that diffusion exists.

An analogous analysis for the isotropic point \( \Delta = 1.0 \) in Fig. 3 (a) shows that simple Gaussians are not able to describe the tails of the density profiles accurately. This is why the standard deviation \( \sigma(t) \) of corresponding fits slightly deviates from the linear-response result in Fig. 3 (b). But these deviations disappear if \( \sigma(t) \) is calculated exactly according to Eq. (4). Most notably, however, the time dependence of \( \sigma(t) \) is inconsistent with diffusion, as can be seen easiest from the non-constant \( D(t) \). In fact, \( \sigma(t) \) points to superdiffusion [37, 40], contrary to [46].

Now, we turn to the untypical initial state \( |\psi(0)\rangle \), i.e., the case of equal \( c_k \). Recall that for this state we obtain the same initial density profile but the relations in Eqs. (3) and (5) do not need to hold. In Fig. 4 we summarize the resulting expectation values \( p_r(t) \) in a 2D time-space density plot again. Compared to Fig. 1, the broadening turns out to be clearly different. The dynamics is frozen for \( \Delta = 1.5 \) in Fig. 4 (a) and features pronounced jets for \( \Delta = 0.5 \) in Fig. 4 (c). In particular, we do not find obvious indications of equilibration, at least for all times considered. These observations constitute a third main result of our paper. This result suggests that the lack of internal randomness in the initial condition is essential for the observation of non-equilibrium dynamics beyond linear response theory.

Finally, let us briefly mention another property of the untypical initial state \( |\psi(0)\rangle \), which could be responsible for the special dynamics found. This property is the lack of entanglement. In fact, it is easy to see that \( |\psi(0)\rangle \) can be written as the product state

\[
|\psi(0)\rangle \propto \ldots (|\uparrow\rangle + |\downarrow\rangle) \otimes |\uparrow\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle) \ldots
\]

with a spin-up state \( |\uparrow\rangle \) in the middle of the chain and a spin-up/spin-down superposition \( |\uparrow\rangle + |\downarrow\rangle \) at all other sites. By definition, such a product state is not entangled at all. In clear contrast, the typical initial state cannot be written as a product state.

V. CONCLUSIONS

In this paper, we have investigated the real-time broadening of non-equilibrium density profiles in the spin-1/2 XXZ chain. First, we have introduced a class of pure initial states with identical density profiles where a maximum \( \delta \) peak is located in the middle of the chain. Then, we have shown for a subclass with internal randomness that the resulting non-equilibrium dynamics can be connected to equilibrium correlation functions via the concept of typicality. This analytical result has been also verified by large-scale numerical simulations. These numerical simulations have further unveiled the existence of diffusion for large exchange anisotropies, as one of our key results. Finally, we have demonstrated that entirely different behavior emerges without any randomness in the initial state. Promising future directions of research include the identification of typical and untypical initial
states in non-integrable models, in many-body localized phases, and at low temperatures as well as a systematic analysis of the role of entanglement.

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Appendix A: Half-Filling Sector

To demonstrate that our results do not depend on our specific choice of \( \langle S^z \rangle = 0 \), we do the calculation in, e.g., Fig. 4 again for the half-filling sector \( S^z = 0 \). We depict the corresponding results in Fig. 5. It is clearly visible that the real-time broadening of the expectation values \( \langle n_r(t) \rangle \) is practically the same, apart from minor details related to \( p_{eq} \approx 1/2 \) in the half-filling case.

Appendix B: Typicality Approximation

Here, we provide details on the calculation leading to the relation in Eq. (3) of the main text. By carrying out the multiplication of the two brackets in the correlation function

\[
C(t) = 2 \langle (n_{L/2} - p_{eq})(n_r(t) - p_{eq}) \rangle + p_{eq}
\]

and applying \( \langle n_r(t) \rangle = p_{eq} \), we obtain

\[
C(t) = 2 \langle n_{L/2} n_r(t) \rangle = 2 \frac{\text{tr}[n_{L/2} n_r(t)]}{2L}.
\]

Using \( n_{L/2}^2 = n_{L/2} \) and a cyclic permutation in the trace, we get

\[
C(t) = 2 \frac{\text{tr}[n_{L/2} n_r(t) n_{L/2}]}{2L}.
\]

Exploiting typicality of the pure state \( |\Phi\rangle \), the correlation function can be rewritten as

\[
C(t) = 2 \frac{\langle |\Phi\rangle n_{L/2} n_r(t) n_{L/2} |\Phi\rangle}{\langle |\Phi\rangle |\Phi\rangle} + \epsilon
\]

with the small error \( \epsilon \propto 2^{-L/2} \). Due to \( n_{L/2} = n_{L/2} \), this expression becomes

\[
C(t) = 2 \frac{\langle n_{L/2} |\Phi\rangle n_r(t) n_{L/2} |\Phi\rangle}{\langle |\Phi\rangle |\Phi\rangle} + \epsilon
\]

and, due to \( n_r(t) = e^{iHt} n_r e^{-iHt} \), it reads

\[
C(t) = \frac{\langle e^{-iHt} n_{L/2} |\Phi\rangle n_r |e^{-iHt} n_{L/2} \rangle}{\langle |\Phi\rangle |\Phi\rangle} + \epsilon,
\]

where we have moved in addition the factor 2 from the front to the denominator. Finally, due to the definition of \( \langle |\psi(0)\rangle \), we can write

\[
C(t) = \langle |\psi(t)\rangle |n_r |\psi(t)\rangle + \epsilon = p_r(t) + \epsilon.
\]

Therefore, comparing Eqs. (B1) and (B7) and skipping the small error \( \epsilon \) for clarity yields

\[
p_r(t) - p_{eq} = 2 \langle (n_{L/2} - p_{eq})(n_r(t) - p_{eq}) \rangle.
\]
Appendix C: Specific Type of Randomness

As stated in the main text, the relations in Eqs. (3) and (5) have to be understood for typical states |Φ⟩ of uniform distribution [0, 2π]. This randomized product state has still ⟨ψ|^↑⟩ = 1/2 and ⟨ψ|L−1⟩ = 1. It involves only 2(L − 1) random numbers, in contrast to the state from the Haar measure with 2L random numbers. In Fig. 6 (c) we depict the resulting dynamics of the expectation values p_r(t). Compared to the two other random cases in Figs. 6 (a) and (b), the dynamical behavior turns out to be very different. This difference suggests again that the lack of entanglement could be the source of untypical dynamics.

Appendix D: Finite-Size Effects

Eventually, we show that our numerical results for the real-time broadening of the expectation values p_r(t) are free of significant finite-size effects. To this end, we redo the tJ = 10 calculations in Figs. 2 (a) and 3 (a) for a smaller but still large system size L = 30. In Fig. 7 we depict the results of these calculations, together with the previous L = 36 data. It is clearly visible that finite-size effects are negligibly small and are not responsible for the non-Gaussian tails at the isotropic point Δ = 1.0.
[21] X. Zotos, Phys. Rev. Lett. 82, 1764 (1999).
[22] J. Benz, T. Fukui, A. Klümper, and C. Scheeren, J. Phys. Soc. Jpn. 74, 181 (2005).
[23] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Phys. Rev. B 68, 134436 (2003).
[24] S. Fujimoto and N. Kawakami, Phys. Rev. Lett. 90, 197202 (2003).
[25] T. Prosen, Phys. Rev. Lett. 106, 217206 (2011).
[26] T. Prosen and E. Ilievski, Phys. Rev. Lett. 111, 057203 (2013).
[27] J. Herbrych, P. Prelovšek, and X. Zotos, Phys. Rev. B 84, 155125 (2011).
[28] C. Karrasch, J. H. Bardarson, and J. E. Moore, Phys. Rev. Lett. 108, 227206 (2012).
[29] C. Karrasch, J. Hauschild, S. Langer, and F. Heidrich-Meisner, Phys. Rev. B 87, 245128 (2013).
[30] R. Steinigeweg, J. Gemmer, and W. Brenig, Phys. Rev. Lett. 112, 120601 (2014).
[31] R. Steinigeweg, J. Gemmer, and W. Brenig, Phys. Rev. B 91, 104404 (2015).
[32] J. M. P. Carmelo, T. Prosen, and D. K. Campbell, Phys. Rev. B 92, 165133 (2015).
[33] D. Gobert, C. Kollath, U. Schollwöck, and G. Schütz, Phys. Rev. E 71, 036102 (2005).
[34] J. Sirker, R. G. Pereira, and I. Affleck, Phys. Rev. Lett. 103, 216602 (2009); Phys. Rev. B 83, 035115 (2011).
[35] S. Grossjohann and W. Brenig, Phys. Rev. B 81, 012404 (2010).
[36] P. Prelovšek, S. El Shawish, X. Zotos, and M. Long, Phys. Rev. B 70, 205129 (2004).
[37] M. ˇZnidarič, Phys. Rev. Lett. 106, 220601 (2011).
[38] C. Karrasch, J. E. Moore, and F. Heidrich-Meisner, Phys. Rev. B 89, 075139 (2014).
[39] R. Steinigeweg and W. Brenig, Phys. Rev. Lett. 107, 250602 (2011).
[40] R. Steinigeweg, EPL (Europhys. Lett.) 97, 67001 (2012).
[41] Strictly speaking, by drawing $c_k$ at random, it is possible to get the outcome $c_k = \text{const.}$ for all $k = 1, \ldots, 2^L$.
[42] R. Steinigeweg, H. Wichterich, and J. Gemmer, EPL (Europhys. Lett.) 88, 10004 (2009).
[43] R. Steinigeweg, F. Heidrich-Meisner, J. Gemmer, K. Michielsen, and H. De Raedt, Phys. Rev. B 90, 094417 (2014).
[44] F. Jin, R. Steinigeweg, F. Heidrich-Meisner, K. Michielsen, and H. De Raedt, Phys. Rev. B 92, 205103 (2015).
[45] C. Karrasch, T. Prosen, and F. Heidrich-Meisner, arXiv:1611.04832 (2016).
[46] I. Khait, S. Gazit, N. Y. Yao, and A. Auerbach, Phys. Rev. B 93, 224205 (2016).
[47] M. Stephan and J. Docter, J. Large-Scale Res. Facil. A1, 1 (2015).