Transport in Out-of-Equilibrium *XXZ* Chains: Exact Profiles of Charges and Currents

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We consider the nonequilibrium time evolution of piecewise homogeneous states in the XXZ spin-$1/2$ chain, a paradigmatic example of an interacting integrable model. The initial state can be thought of as the result of joining chains with different global properties. Through dephasing, at late times, the state becomes locally equivalent to a stationary state which explicitly depends on position and time. We propose a kinetic theory of elementary excitations and derive a continuity equation which fully characterizes the thermodynamics of the model. We restrict ourselves to the gapless phase and consider cases where the chains are prepared: (1) at different temperatures, (2) in the ground state of two different models, and (3) in the "domain wall" state. We find excellent agreement (any discrepancy is within the numerical error) between theoretical predictions and numerical simulations of time evolution based on time-evolving block decimation algorithms. As a corollary, we unveil an exact expression for the expectation values of the charge currents in a generic stationary state.

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During the last decade, the study of nonequilibrium dynamics in quantum many-body systems has experienced a golden age. The experimental possibility for investigating almost purely unitary time evolution [1] sparked off a diffuse theoretical excitement [2–7]. The challenge was to understand in which sense unitarily evolving systems can relax to stationary states, and, if this happens, how to determine the stationary values of the observables. The main focus has been on translationally invariant systems. There, a clear theoretical construction has been developed: while the full system can not relax, in the thermodynamic limit, finite subsystems can, as the rest of the system acts as an unusual bath. It was argued that the stationary values of local observables are determined by local and quasilocal conservation laws [2,4,8]. It is convenient to distinguish between generic models, where the Hamiltonian is the only local conserved quantity, and integrable models, where the number of local charges scales with the systems's size. It was conjectured that, in the former case, stationary values of local observables are described by Gibbs ensembles [9] while, in the latter, by so-called generalized Gibbs ensembles (GGEs) [10]. Importantly, traces of the underlying integrability remain even in the presence of small integrability-breaking perturbations: at intermediate times, the expectation values of local observables approach quasistationary plateaux retaining infinite memory of the initial state [11–14].

In the absence of translational invariance, the situation gets more complicated. In this context, a variety of different settings have been considered, which can be cast into two main classes. The first consists of dynamics governed by translationally invariant Hamiltonians on inhomogeneous states. Relevant examples are the sudden junction of two chains at different temperatures [15–22], with different magnetizations [23,24], or with other different global properties [25,26]. In the second class, we include dynamics where the Hamiltonian features a localized defect [27–30]. In both cases, a nonequilibrium steady state (NESS) emerges: around the junction of the chains in the first class of problems [22,31,32] and close to the defect in the second [27,30]. The characterization of the transport properties of the NESS have attracted tremendous attention; however, the NESS is just the tip of the iceberg. In the limit of large time t and large distance x from the inhomogeneity, the state becomes locally equivalent to a nontrivial stationary state, which, in integrable models, turns out to depend only on the "ray" $\zeta = x/t$ [23,26,30]. We will refer to the latter as a locally quasistationary state (LQSS) [30]. We note that ray-dependent profiles of specific observables emerge naturally in hydrodynamical approaches [33], which have also been applied in more generic systems [34]. Even though these problems have been under scrutiny for a long time, exact analytic results have been obtained only in noninteracting models and conformal field theories, the role of interaction remaining elusive until now.

In this Letter, we study transport phenomena in interacting integrable models, focusing on the first class of protocols. We propose a "kinetic theory" of the elementary excitations and obtain a continuity equation whose solution gives the exact LQSS characterizing the state of the system at late times. Solving the continuity equation gives us full access to the state and, in particular, to the expectation values of charge densities and related currents in the entire light cone. To illustrate our ideas, we use the paradigmatic example of the XXZ model.

The model.—We consider the XXZ spin-$1/2$ chain described by the Hamiltonian

$$\boldsymbol{H} = J\sum_{\ell=1}^{L}(\boldsymbol{s}^x_\ell \boldsymbol{s}^x_{\ell+1} + \boldsymbol{s}^y_\ell \boldsymbol{s}^y_{\ell+1} + \Delta \boldsymbol{s}^z_\ell \boldsymbol{s}^z_{\ell+1}), \quad (1)$$

where L is the chain's length, bold symbols indicate quantum operators, and $\{\boldsymbol{s}^\alpha_\ell\}$ are spins $1/2$. We consider $|\Delta| \leq 1$, parametrize the anisotropy as $\Delta = \cos(\gamma)$, and set $J = 1$. The model is solved by the Bethe ansatz [35]: every eigenstate $|\{\lambda_i\}\rangle$ is parametrized by a set of N complex "rapidities" $\{\lambda_i\}$ fulfilling the Bethe equations

$$\left(\frac{\sinh(\lambda_j + i\frac{\gamma}{2})}{\sinh(\lambda_j - i\frac{\gamma}{2})}\right)^L = \prod_{l\neq j}^{N}\left(\frac{\sinh(\lambda_j - \lambda_l + i\gamma)}{\sinh(\lambda_j - \lambda_l - i\gamma)}\right). \quad (2)$$

Following the "string hypothesis" [36], as $L \to \infty$ the solutions to (2) are organized in different types of "string" patterns, composed by a set of rapidities with the same real part and equidistant imaginary parts. The different string types are interpreted as different species of quasiparticles with real rapidities. In the thermodynamic limit $L \to \infty$ with N/L fixed, the thermodynamic Bethe ansatz (TBA) formalism applies; a thermodynamic state is parametrized by "particles" and "holes" distributions $\{\rho_k, \rho^h_k\}$, one for each species of quasiparticles. These distributions, usually called "root densities," are connected to one another through the thermodynamic version of (2), reported in [37]. The number of species is finite when γ is a rational multiple of π, which is the case considered in this Letter. The expectation value of the density $\boldsymbol{q}$ of a conserved charge $\boldsymbol{Q}$ in the stationary state $|\rho\rangle$ reads as [40]

$$\langle\rho|\boldsymbol{q}|\rho\rangle = \sum_k \int d\mu q_k(\mu)\rho_k(\mu), \quad (3)$$

where $q_k(\mu)$ is the single-particle eigenvalue of the charge and is independent of the state. If $|\rho\rangle$ is invariant under spin-flip $\prod_j \sigma^x_j$, it is completely characterized by the expectation values of the local and quasilocal charges obtained from the unitary representations of the transfer matrix [4,7]. We indicate these charges by $\boldsymbol{Q}^{(s)}_n$, with n, $2s \in \mathbb{N}$, and the single-particle eigenvalues by $q^{(s)}_{n,k}(\mu)$. The charges have an increasing typical range as a function of n and $q^{(s)}_{n,k}(\mu) = -(\sin\gamma/2)\partial_\mu q^{(s)}_{n-1,k}(\mu)$; in particular, $\boldsymbol{Q}^{(1/2)}_n$ are local [40] and $\boldsymbol{Q}^{(1/2)}_1 = \boldsymbol{H} - \Delta L/4$. We refer the reader to the Supplemental Material [37] and to the specific literature [4,36,40] for further details. A case without spin-flip invariance is discussed in Example 3.

Locally quasistationary state.—In integrable models, the information about an inhomogeneity spreads linearly in time because of stable quasiparticle excitations [41]. These contribute to the emergence of nontrivial behavior along the rays $\zeta = x/t$. Dephasing mechanisms [5] are also active in the inhomogeneous case, so at sufficiently late times, the dynamics are expected to slow down with an emergent time scale proportional to x. Thus, we assume that, for given ζ, the expectation values of observables can be eventually described by a stationary state $\boldsymbol{\rho}^{\rm LQSS}_\zeta$

$$\langle\mathcal{O}\rangle_{x,t} \equiv \langle\Psi_t|\mathcal{O}_x|\Psi_t\rangle = \mathrm{tr}(\boldsymbol{\rho}^{\rm LQSS}_\zeta \mathcal{O}_x) + o(t^{-\epsilon}). \quad (4)$$

Here, $\mathcal{O}_x$ acts nontrivially only around x. The state $\boldsymbol{\rho}^{\rm LQSS}_\zeta$ is the LQSS introduced in [30]; determining it exactly is our main goal.

Kinetic theory.—Being stationary (for given ζ), $\boldsymbol{\rho}^{\rm LQSS}_\zeta$ is characterized by a set of root densities $\{\rho_{\zeta,j}, \rho^h_{\zeta,j}\}$

$$\mathrm{tr}(\boldsymbol{\rho}^{\rm LQSS}_\zeta \mathcal{O}) = \langle\rho_\zeta|\mathcal{O}|\rho_\zeta\rangle. \quad (5)$$

In particular, the charges can be written as in (3).

Since the root densities are fixed by the expectation values of the charges [7], the full LQSS can be obtained by determining how their expectation values vary in time. We assume that the change is induced by the motion of elementary excitations and that the late time regime is characterized by a "dynamical equilibrium," where the thermodynamic state varies only slightly even though a macroscopic number of quasiparticles is moving. The nature of quasiparticle excitations remains well defined while moving through the system; on the other hand, the excitation energy $\varepsilon_{\zeta,k}(\lambda)$ and the momentum $p_{\zeta,k}(\lambda)$ depend on the macrostate [41], so the "mild" inhomogeneity of the LQSS modifies the propagation velocity $v_{\zeta,k}(\lambda) = \partial_\lambda\varepsilon_{\zeta,k}(\lambda)/\partial_\lambda p_{\zeta,k}(\lambda)$. This leads to

$$\langle\boldsymbol{q}\rangle_{x,t+\delta t} - \langle\boldsymbol{q}\rangle_{x,t} = \int d\tilde{x}(\underset{\tilde{x}\to x,t}{\Delta^{\boldsymbol{q}}} - \underset{x\to\tilde{x},t}{\Delta^{\boldsymbol{q}}}), \quad (6)$$

where $\underset{\tilde{x}\to x,t}{\Delta^{\boldsymbol{q}}}$ is the charge density $\boldsymbol{q}$ carried from $\tilde{x}$ to x by the quasiparticles in the time interval $[t, t+\delta t]$. For given $\tilde{x} - x$ and δt, only excitations with velocity $v = (x - \tilde{x})/\delta t$ contribute to $\underset{\tilde{x}\to x,t}{\Delta^{\boldsymbol{q}}}$, namely,

$$\underset{\tilde{x}\to x,t}{\Delta^{\boldsymbol{q}}} \equiv \sum_k \int d\lambda \delta(x - \tilde{x} - v_{\tilde{\zeta},k}(\lambda)\delta t)c^{\boldsymbol{q}}_k(\lambda|\tilde{\zeta}). \quad (7)$$

Here, $c^{\boldsymbol{q}}_k(\lambda|\zeta)d\lambda$ is the charge density transported by excitations with string type k and rapidity $\in [\lambda, \lambda + d\lambda]$. This quantity depends on ζ through $\boldsymbol{\rho}^{\rm LQSS}_\zeta$ and will be expressed in terms of the root densities $\rho_{\zeta,j}$ before long. Plugging (7) into (6) gives

$$\partial_t\langle\boldsymbol{q}\rangle_{x,t} = -\sum_k \int d\lambda \partial_x[v_{\zeta,k}(\lambda)c^{\boldsymbol{q}}_k(\lambda|\zeta)]. \quad (8)$$

By virtue of (3), we then find

$$\sum_k \int d\lambda[q_k(\lambda)\partial_t\rho_{\zeta,k}(\lambda) + \partial_x(v_{\zeta,k}(\lambda)c^{\boldsymbol{q}}_k(\lambda|\zeta))] = 0. \quad (9)$$

The next step is to fix the form of $c_k^{\boldsymbol{q}}(\lambda|\zeta)$ in terms of the root densities. To this aim, it is convenient to consider an auxiliary toy problem as follows. Let a macroscopic subsystem A be described by $|\rho\rangle_A$ with all the root densities equal to zero except for $\rho_k(\lambda)$, with $\lambda \in [\bar{\lambda}, \bar{\lambda}+\epsilon]$ and ϵ some small parameter. Then, let us release the subsystem in the vacuum (for which $\rho_j(\lambda) = 0$), namely in an infinite bath of spins up $|\Psi_0\rangle = |\rho\rangle_A \otimes |\uparrow \cdots \uparrow\rangle_B$. After a sufficiently long time, it is reasonable to expect local relaxation to the vacuum. From (3), it follows that the total charge density Δq flowed out of the subsystem reads $\Delta q = \int_{\bar{\lambda}}^{\bar{\lambda}+\epsilon} d\lambda q_k(\lambda)\rho_k(\lambda)$. Crucially, we interpret this expression as the charge density $c_k^{\boldsymbol{q}}(\lambda)\epsilon$ associated with the quasiparticles of species k and rapidity $\lambda \in [\bar{\lambda}, \bar{\lambda}+\epsilon]$ going out of the subsystem [42]

$$c_k^{\boldsymbol{q}}(\lambda) = q_k(\lambda)\rho_k(\lambda). \tag{10}$$

Let us go back to the expression (9) and take (10) as the transported charge density; we find

$$\sum_k \int d\lambda q_k(\lambda)[\partial_t \rho_{\zeta,k}(\lambda) + \partial_x(v_{\zeta,k}(\lambda)\rho_{\zeta,k}(\lambda))] = 0. \tag{11}$$

Since $q_k(\lambda)$ is independent of ζ, (11) is a continuity equation for the charge density and holds for any local and quasilocal charge $\boldsymbol{Q}_n^{(s)}$. Using the completeness of the set $\{q_{n,k}^{(s)}(\lambda)\}$, we have

$$\boxed{\partial_t \rho_{\zeta,k}(\lambda) + \partial_x(v_{\zeta,k}(\lambda)\rho_{\zeta,k}(\lambda)) = 0.} \tag{12}$$

This is our main result: the root densities $\rho_{\zeta,k}(\lambda)$, characterizing the state, obey a continuity equation with a ζ-dependent velocity, a remarkable effect of the interaction that induces a state-dependent dressing on the elementary excitations. *A priori*, one would expect the physical picture based on a kinetic theory of excitations to be only approximately correct. In fact, we will provide evidence that (12) exactly describes the dynamics at late times t and large distances x along the ray $\zeta = x/t$.

Charge currents.—In a spin chain, the current $\boldsymbol{j}_\ell[\boldsymbol{Q}]$ of a charge $\boldsymbol{Q} = \sum_\ell \boldsymbol{q}_\ell$ is defined through the following continuity equation:

$$\boldsymbol{j}_{\ell+1}[\boldsymbol{Q}] - \boldsymbol{j}_\ell[\boldsymbol{Q}] = i[\boldsymbol{q}_\ell, \boldsymbol{H}]. \tag{13}$$

Imposing $\mathrm{tr}(\boldsymbol{j}_\ell[\boldsymbol{Q}]) = 0$, this determines $\boldsymbol{j}_\ell[\boldsymbol{Q}]$ up to operators with zero expectation value in any translationally invariant state. In the infinite time limit along the ray $\zeta = x/t$, the time-evolving state becomes homogeneous, so the expectation values of the currents are independent of their particular definitions. From (11), it follows:

$$\langle \rho | \boldsymbol{j}_\ell[\boldsymbol{Q}] | \rho \rangle \sim \sum_k \int d\lambda q_k(\lambda) v_k(\lambda) \rho_k(\lambda), \tag{14}$$

where $|\rho\rangle$ is an arbitrary stationary state and the equivalence is up to a state-independent constant.

We now provide several compelling consistency checks for the validity of (14) and, in turn, of (11).

Check 1: Conservation of the energy current. In the XXZ model, the energy current is equal to the second charge, namely: $\boldsymbol{j}_{1,\ell}^{(1/2)} \sim \boldsymbol{q}_{2,\ell}^{(1/2)}$, where we introduced the notation $\boldsymbol{j}_{n,\ell}^{(s)} \equiv \boldsymbol{j}_\ell[\boldsymbol{Q}_n^{(s)}]$. Using some TBA identities, one can easily show that this relation is satisfied by (14) [37].

Check 2: Current(s) at equilibrium vs numerics. Figure 1 shows the expectation value of the current $\boldsymbol{j}_{2,\ell}^{(1/2)}$ in thermal states with inverse temperature $\beta \in [0, 5]$ and for different values of Δ. The prediction (14) is checked against numerical data obtained using an algorithm based on the matrix product density operator (MPDO) representation of a mixed state [37]. The agreement is unquestionably perfect: the discrepancies are smaller than the MPDO accuracy.

Check 3: Comparison with other results. Reference [22] independently obtained an expression for the currents in integrable quantum field theories with diagonal scattering. In [37], it is shown that this is equivalent to (14).

Determining the LQSS.—We now turn to our main goal: the determination of the LQSS evolving from an inhomogeneous state. We consider the time evolution of $|\psi_0\rangle^L \otimes |\psi_0\rangle^R$ under the Hamiltonian (1) at sufficiently long times. The dynamics is described by (12), which, using some TBA identities [37], can be recast in the form

$$[\zeta - v_{\zeta,k}(\lambda)]\partial_\zeta \vartheta_{\zeta,k}(\lambda)\rho_{\zeta,k}^t(\lambda) = 0, \tag{15}$$

where $\vartheta_{\zeta,k}(\lambda) \equiv \rho_{\zeta,k}(\lambda)/[\rho_{\zeta,k}(\lambda) + \rho_{\zeta,k}^h(\lambda)]$. Since $\rho_{\zeta,k}(\lambda) + \rho_{\zeta,k}^h(\lambda) > 0$, the solution $\vartheta_{\zeta,k}(\lambda)$ is a piecewise constant function of ζ. If, for any λ, $v_{\zeta,k}(\lambda) = \zeta$ has a unique solution [43], we find

$$\vartheta_{\zeta,k}(\lambda) = \theta_H(v_{\zeta,k}(\lambda) - \zeta)(\vartheta_k^L(\lambda) - \vartheta_k^R(\lambda)) + \vartheta_k^R(\lambda). \tag{16}$$

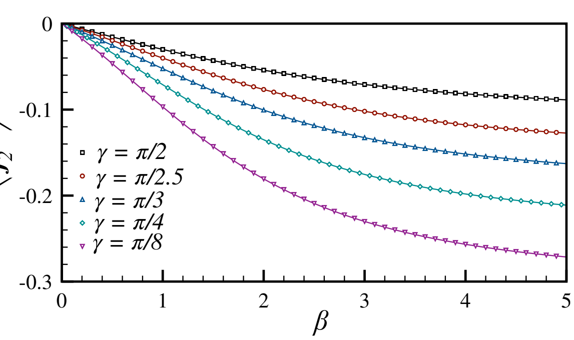

FIG. 1. Thermal expectation value of $\boldsymbol{j}_2^{(1/2)}$ for a wide range of temperatures and different anisotropies $\Delta = \cos(\gamma)$. Full lines are MPDO data (error $< 10^{-6}$) in a system of length $L = 50$. Symbols are the prediction (14).

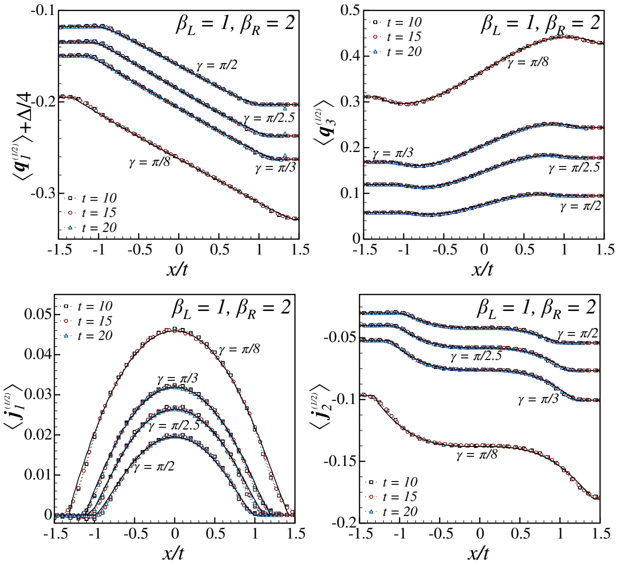

FIG. 2. Profiles of charge densities and currents for three different values of $\Delta = \cos(\gamma)$. A 60-site chain has been initially prepared in two halves at inverse temperatures $\beta_L = 1$ and $\beta_R = 2$. Symbols denote MPDO data; full black lines are the predictions based on (16). The tiny ripples in the predictions are numerical artifacts.

Here, $\theta_H(x)$ is the step function which is nonzero and equal to 1 only if $x > 0$. The functions $\vartheta_k^L(\lambda)$ and $\vartheta_k^R(\lambda)$ are the boundary conditions: due to the Lieb-Robinson bounds [44,45], there exists a maximal velocity $v_{\max}$ such that observables on rays $|\zeta| > v_{\max}$ never receive information about the inhomogeneity; as a result, $\vartheta_k^L(\lambda)$ and $\vartheta_k^R(\lambda)$ describe the stationary states emerging independently in the two, left and right, bulk parts of the system (see, also, Fig. 3).

As $v_{\zeta,k}(\lambda)$ depends on $\vartheta_{\zeta,k}(\lambda)$, (16) is only an implicit representation of the solution. In practice, one can solve the problem by iteration, starting from an initial $\vartheta_{\zeta,k}^{(0)}(\lambda)$, computing the excitation velocities, and iterating again until convergence is reached. The procedure is numerically very efficient and converges after few iterations.

Example 1: Two temperatures. Let us consider the transport problem *par excellence*: two chains prepared at different temperatures and then joined together [16].

In Fig. 2, we report the rescaled profiles of a number of charges and currents for different times $t = 10$, 15, 20 and interactions Δ. The rescaled numerical data are in excellent agreement with the analytical predictions. This strongly suggests that the solution of (12) fully characterizes the state of the system at late times.

We note that, at the edges of the light cone, the predictions are not smooth, as the profiles are exactly flat outside the light cone. This is an infinite-time property, and indeed, the numerical data are smooth at any time. Moreover, contrary to the noninteracting case, the velocities also depend on the temperatures [41], as revealed by the slight asymmetry of all the curves reported in Fig. 2.

We mention that the conjecture put forward in [21] for the energy current $\boldsymbol{j}_{1,\ell}^{(1/2)}$ at $\zeta = 0$ is only in fair agreement with our results [37].

Example 2: Global quench. We now study the dynamics after joining together two globally different pure states which are not stationary. This is a genuine global quench with nontrivial time evolution also outside the light cone. As an initial state, we take the tensor product between the Néel state $|\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ and the Bell state $\otimes_j (|\uparrow\uparrow\rangle_j - |\downarrow\downarrow\rangle_j/\sqrt{2})$. As explained before, the two boundary conditions ϑ^L, ϑ^R are the GGEs corresponding to the quenches $e^{-iHt}|\text{Néel}\rangle$ and $e^{-iHt}|\text{Bell}\rangle$ (see the bottom panel of Fig. 3). Relaxation is slower than in the first example, and the comparison with the time-evolving block decimation (TEBD) data shown in Fig. 3 is jeopardized by the smallness of the time reached, a consequence of the linear increase of the entropy both inside and outside the light cone. Nevertheless, the agreement is fairly good.

Example 3: Domain wall. If the initial state is not spin-flip invariant, the set $\{\boldsymbol{Q}_{n,\ell}^{(s)}\}$ is generally not sufficient to fix the state. First of all, one has to include the total spin along z, $\boldsymbol{S}^z$, but also quasilocal charges coming from nonunitary representations of the transfer matrix [4] might play some role. Nonetheless, for a domain-wall initial state [24] $|\uparrow\ldots\uparrow\rangle \otimes |\downarrow\ldots\downarrow\rangle$, the comparison with numerics provides strong evidence that the expectation values of $\boldsymbol{q}_{n,\ell}^{(s)}$, $\boldsymbol{s}_\ell^z$, and the corresponding currents, can be obtained from the root densities solving the continuity equation (12). The left boundary condition is $\vartheta_j^L(\lambda) = 0$, while $\vartheta_j^R(\lambda)$ corresponds to the state $\propto e^{\mu S^z}$ in the limit $\mu \to \infty$. Figure 4 shows the

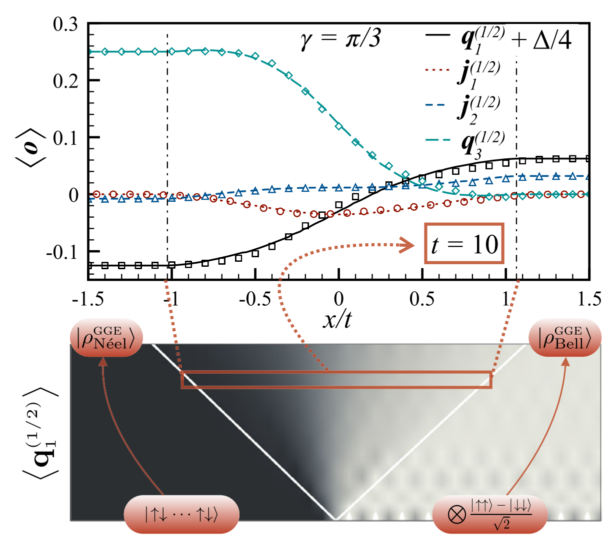

FIG. 3. Top: Profiles of different charge densities and currents for the quench of Example 2 with $\Delta = \cos(\pi/3)$. Predictions of Eq. (16) (lines) are compared with TEBD data at time $t = 10$ (symbols) obtained in a 100-site chain. Spatial oscillations in the TEBD data were smoothed out by taking a local spacial average. The vertical dotted-dashed lines represent the light-cone edges. Bottom: Space-time density plot of $\langle \boldsymbol{q}_1^{(1/2)} \rangle$.

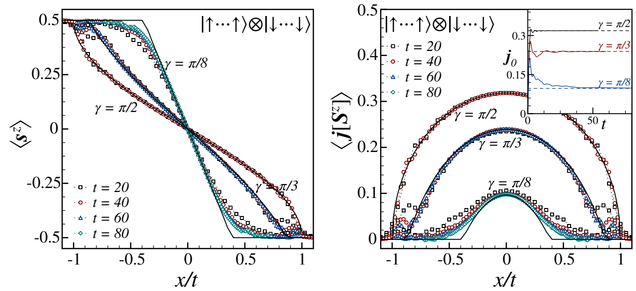

FIG. 4. Profiles of magnetization s^z_ℓ and spin current $\boldsymbol{j}_\ell[\boldsymbol{S}^z]$ evolving from a "domain-wall" state for three different values of $\Delta = \cos(\gamma)$. Symbols are numerical data for a 120-site chain; full black lines are the predictions based on (16). The inset shows the approach of $\boldsymbol{j}_0[\boldsymbol{S}^z]$ (full colored lines) to the prediction (dashed lines).

only two measured quantities exhibiting a nontrivial behavior. Remarkably, the effective velocities of quasiparticles shrink to zero in the limit $\Delta \to 1$. A more careful analysis will be carried out in a future work.

Conclusions.—Using a "kinetic theory" of quasiparticle excitations, we derived a continuity equation [cf. (12)] describing the late time dynamics of the *XXZ* spin-1/2 chain after joining together two macroscopically different homogeneous states. We provided compelling evidence that equation (12) is, in actual fact, the exact continuity equation fulfilled by the conserved charges of the model for late times and large distances. We tested the predictions for the late-time dynamics against TEBD numerical simulations and we have found excellent agreement. Our construction is sufficiently generic to be applicable to other interacting integrable models. In addition, the continuity equation can also be applied when integrability is broken by some localized inhomogeneity [19]: the solution of the late-time dynamics along the rays originating from the inhomogeneity is reduced to the determination of a few boundary conditions.

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Note added.—Recently, Ref. [22] appeared, where the same problem is independently studied for quantum field theories with diagonal scattering and a generalized hydrodynamical description is developed. In this framework, the authors derive an equation analogous to (12).

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