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Real-time energy dynamics in spin- $\frac{1}{2}$ Heisenberg chains

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We study the real-time dynamics of the local energy density in the spin-1/2 XXZ chain starting from initial states with an inhomogeneous profile of bond energies. Numerical simulations of the dynamics of the initial states are carried out using the adaptive time-dependent density matrix renormalization group method. We analyze the time dependence of the spatial variance associated with the local energy density to classify the dynamics as either ballistic or diffusive. Our results are consistent with ballistic behavior both in the massless and the massive phase. We also study the same problem within Luttinger liquid theory and obtain that energy wave packets propagate with the sound velocity. We recover this behavior in our numerical simulations in the limit of very weakly perturbed initial states.

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I. INTRODUCTION

The understanding of transport properties of low-dimensional systems with strong correlations still poses viable challenges to theorists. These include, on the one hand, the fundamental problem of calculating transport coefficients for generic models such as the Heisenberg chain,^{1,2} and on the other hand, the theoretical modeling of experiments that typically require the treatment of spin or electronic degrees of freedom coupled to phonons, in particular, in the case of the thermal conductivity.^{3,4} Most theoretical work is focused on the linear-response regime, in which the properties of current-current autocorrelation functions determine transport properties (see Refs. 1 and 2 for a review).

More recently, the out-of-equilibrium properties of one-dimensional systems have evolved into an active field of research, one reason being recent advances in experiments with ultracold atoms.⁵ These have paved the way for studying the dynamics of quantum many-body systems that are driven far away from equilibrium in a controlled manner, with little or no coupling to external degrees of freedom. Much attention has been paid to the question of thermalization, typically studied in so-called quantum quenches (see Ref. 6 and references therein). While global quantum quenches in homogeneous systems usually do not induce any finite net currents (of either spin, energy, or particles), we will be particularly interested in setups that feature finite net currents. Such situations are realized in, for instance, the sudden expansion of particles in optical lattices after the removal of trapping potentials.⁷ Further examples are spin and/or particle currents induced by connecting two regions with opposite magnetizations or by letting two particle clouds collide (see, for instance, Refs. 8–11).

Theoretical work in this context ranges from the expansion dynamics of bosons and fermions in optical lattices^{12–18} over the dynamics of wave packets in spin chains,^{19–28} to the demonstration of signatures of spin-charge separation in such setups.^{29,30} In the aforementioned examples, nonequilibrium situations were studied with either finite spin or particle currents. In our work, we address the energy dynamics for a

model that is prototypical for systems with strong correlations, namely, the spin-1/2 XXZ chain:

$$H_{XXZ} = \sum_{i=1}^{L-1} h_i := J \sum_{i=1}^{L-1} \left[\frac{1}{2} (S_i^+ S_{i+1}^- + \text{H.c.}) + \Delta S_i^z S_{i+1}^z \right], \quad (1)$$

where S_i^μ and $\mu = x, y, z$ are the components of a spin-1/2 operator acting on site i and S_i^\pm are the corresponding lowering/raising operators. The global energy scale is set by the exchange coupling J , Δ is the exchange anisotropy in the z direction, and L denotes the number of sites. Equation (1) describes either interacting quantum spins or, via the Jordan-Wigner transformation,³¹ spinless fermions.

Specifically, we follow the time evolution of the local energy density $\langle h_i \rangle$ starting from initial states that are far away from the ground state of Eq. (1) and that feature an inhomogeneous profile in the local energy density (see Fig. 1 for a sketch). We emphasize that, in the main part of our work, we choose the initial conditions such that only finite energy currents exist, whereas the spin (particle) density is constant during the time evolution, hence all spin (particle) currents vanish. Obviously, an initial state with an inhomogeneous spin density profile leads to both finite spin and energy currents, and we revisit this case, previously studied in Refs. 20 and 28.

Our work is motivated by and closely related to a specific experiment on a spin-ladder material. Many low-dimensional quantum magnets are known to be very good thermal conductors with heat predominantly carried by magnetic excitations at elevated temperatures.^{32,33} Examples for materials that exhibit particularly large thermal conductivities are $(\text{Sr,La,Ca})_{14}\text{Cu}_{24}\text{O}_{41}$ (Refs. 34 and 35) and SrCuO_2 (Ref. 36). While these experiments are carried out under steady-state conditions and in the regime of small external perturbations, more recently, time-resolved measurements have been performed on $\text{La}_9\text{Ca}_5\text{Cu}_{24}\text{O}_{41}$ (Ref. 37). For this spin ladder material, two approaches have been implemented:

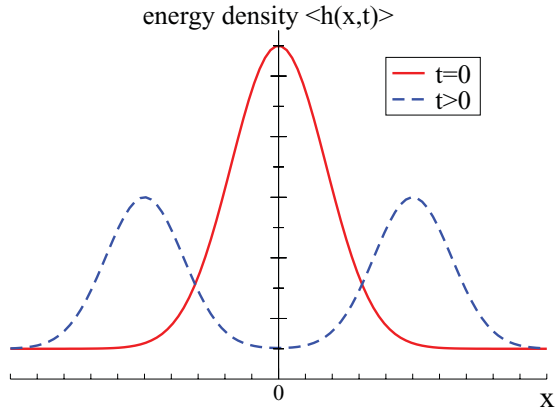


FIG. 1. (Color online) Sketch of our setup: we prepare initial states with an inhomogeneous distribution of local energies and then study the time evolution of the local energy density.

a time-of-flight measurement in which one side of the sample is heated up with a laser pulse and the time-dependent response is recorded on the other side. Second, a nonequilibrium local heat distribution was generated in the surface of the material by shining laser light on it. It is possible to record the heat dynamics via thermal imaging that uses the response of an excited thin fluorescent layer placed on top of the spin ladder material.

It is the latter case that we mimic in our work: the time evolution of local energy densities induced by inhomogeneous initial distributions. We utilize the time-dependent density matrix renormalization group (tDMRG)^{38–42} technique. It allows us to simulate the dynamics of pure states whereas in the experiment, temperature likely plays a role. Our work thus addresses qualitative aspects in the first place, while a direct comparison with experimental results is beyond the scope of this study. The goal is to demonstrate that in a spin-1/2 chain described by Eq. (1), the energy dynamics is ballistic, irrespective of how far from equilibrium the system is and also irrespective of the presence or absence of excitation gaps. To this end, we use the same approach as in Ref. 20. We classify the dynamics based on the behavior of the spatial variance $\sigma_E^2(t)$ of the local energy density. The ballistic case is $\sigma_E^2(t) \sim t^2$, whereas diffusion implies $\sigma_E^2 \sim t$. Our main result for the XXZ chain, based on numerical tDMRG simulations, is that energy propagates ballistically at sufficiently long times, independently of model parameters (such as Δ). One can then interpret the prefactor V_E in $\sigma_E^2(t) = V_E^2 t^2$ as a measure of the average velocity of excitations contributing to the expansion. The velocity V_E can be calculated analytically and exactly in noninteracting models, which (in the absence of impurities or disorder) typically have ballistic dynamics, and we consider two examples: (i) the noninteracting limit of the XXZ Hamiltonian ($\Delta = 0$), i.e., spinless fermions and (ii) the Luttinger liquid, which is the universal low-energy theory in the continuum limit of Eq. (1) for $|\Delta| < 1$. We show that our tDMRG results agree with the exactly known expansion velocity V_E in these two examples.

Our main result, namely, the numerical observation of $\sigma_E^2(t) \sim t^2$ independently of initial conditions or model parameters such as the exchange anisotropy Δ , is consistent with

the qualitative picture derived from linear-response theory. Within that theory, transport properties of the XXZ chain have intensely been studied in recent years, both the energy^{43–47} and the spin transport.^{1,2,47–62} Ballistic dynamics is associated with the existence of nonzero Drude weights. Since the total energy current of the anisotropic spin-1/2 chain is a conserved quantity for all Δ , the thermal conductivity $\kappa(\omega)$ diverges in the zero-frequency limit and is given by $\text{Re } \kappa(\omega) = D_E \delta(\omega)$, where D_E is the thermal Drude weight.^{43–46} This behavior is different from the spin conductivity $\sigma(\omega)$. This quantity takes the form $\text{Re } \sigma(\omega) = D_s \delta(\omega)$ only at the noninteracting point $\Delta = 0$, whereas for $0 < \Delta \leq 1$, many numerical studies^{1,2,60,61} indicate $D_s(T > 0) > 0$, with a finite weight at finite frequencies, though. Therefore, for $0 < \Delta \leq 1$, $\text{Re } \sigma(\omega) = D_s \delta(\omega) + \sigma_{\text{reg}}(\omega)$. Recent field-theoretical and numerical work suggests that the regular part $\sigma_{\text{reg}}(\omega)$ of $\sigma(\omega)$ in massless phases is consistent with diffusive behavior.^{54,56,62} A finite value of the current-current correlation function in the long time limit is associated with a finite Drude weight. Finite Drude weights can be traced back to the existence of conservation laws,^{43,60} and, in consequence, a potential relation between integrability⁶³ and ballistic behavior—in the sense of nonzero Drude weights—has been intensely discussed (see, e.g., Refs. 1, 2, 47, 60–62 and further references cited therein). Very recently, Prosen has presented results that provide a lower bound to the spin Drude weight that is non zero for $\Delta < 1$.⁶⁰ This is in qualitative agreement with earlier exact diagonalization studies.^{2,47,48} The particular point $\Delta = 1$ is still discussed controversially;^{47,49,52,54,59–61} first, no finite lower bound to the Drude weight is known,⁶⁰ and second, the qualitative results of exact diagonalization studies seem to depend on details of the extrapolation of finite-size data to the thermodynamic limit and the statistical ensemble that is considered.^{47,48,59}

Our approach that analyzes the time dependence of spatial variances, albeit restricted to the analysis of densities, is numerically easily tractable and is an alternative to the numerically cumbersome evaluation of current correlation functions. tDMRG has, for instance, been applied to evaluate current-current autocorrelation functions in the thermodynamic limit.⁵⁴ However, the accessible time scales are quite limited ($t \sim 10/J$), making an unambiguous interpretation of the results difficult and the approach is not applicable to nonequilibrium. Our approach allows us, at least in principle, to study the entire regime of weakly perturbed states to maximally excited ones. An earlier analysis of spin-density wave packets in various spin models has yielded the following picture (all based on the time-dependence of the spatial variance);²⁰ in massless phases, ballistic dynamics is seen, whereas in massive ones, examples of diffusive dynamics have been identified. It is important to stress that the observation of a variance that increases linear in time is a necessary condition for the validity of the diffusion equation.

Finally, to complete the survey of related literature, recent studies have addressed steady-state spin and energy transport in open systems coupled to baths with no restriction to the linear-response regime.^{28,61,64–66} These studies suggest spin transport to be ballistic in the gapless phase of the XXZ spin chain and to be diffusive in the gapped phase with a negative differential conductance at large driving strengths. The heat

current has been addressed in Ref. 64 where Fourier's law has been validated for the Ising model in a tilted field.

A byproduct of any tDMRG simulation is information on the time-evolution of the entanglement entropy. While this is not directly related to this article's chief case, it nevertheless provides valuable information on the numerical costs of tDMRG simulations. Qualitatively, speaking (see the discussion in Ref. 42 and references therein), the faster the entanglement growth is the shorter are the time scales that can be reached with tDMRG. We here show that the quenches studied in this work generate a mild logarithmic increase of entanglement, which is why this problem is very well suited for tDMRG. Such a behavior is typical for so-called local quenches.⁶⁷ This result might be useful for tDMRG practitioners.

This paper is organized as follows. First, we introduce the model and the quantities used in our analysis in Sec. II. Section III A reviews the framework of bosonization, which is applied in Sec. III B to give an analytical derivation of ballistic spin and energy dynamics in the low-energy case, valid in the massless phase of Eq. (1). Sections IV and V contain our numerical results. First, we study the energy dynamics in the absence of spin currents in Sec. IV. To this end, we generate an initial state consisting of a variable number of ferromagnetic bonds in the center of an antiferromagnetic chain. We calculate the time evolution of these states under Eq. (1) finding ballistic energy dynamics independent of the phase and the strength of the perturbation. To supplement these findings we derive an observable, which depends on the local currents, and whose expectation value is time-independent whenever $\sigma_E^2(t) \sim t^2$. The numerical calculation of this quantity indicates ballistic dynamics as well. Section V revisits the scenario of Ref. 20 where local spin and energy currents are present during the dynamics as we start from states with an inhomogeneous spin density. In that case, the energy density shows ballistic dynamics in the massless phase with a velocity matching the bosonization result in the limit of small perturbations. In the massive phase, we observe a different behavior of the two transport channels, i.e., ballistic energy dynamics while the spin dynamics looks diffusive.²⁰ Finally, we summarize our findings in Sec. VI. Additionally, we discuss the entanglement growth induced by coupling two regions with an opposite sign of the exchange coupling in the Appendix.

II. SETUP AND DEFINITIONS

A. Preparation of initial states and definition of spatial variance

In this work, we focus on spin-1/2 XXZ chains of a finite length L given by Eq. (1) where our goal is to study the dynamics of an inhomogeneous distribution of the local energy density originating from a local quench of system parameters. The inhomogeneous distributions are generated by preparing the system in the respective ground states of the following Hamiltonians that are perturbations of H_{XXZ} from Eq. (1). First,

$$H_{\text{init}}^J = \sum_{i=1}^{L-1} \frac{J_i}{J} h_i, \quad (2)$$

where h_i is defined in Eq. (1), and second,

$$H_{\text{init}}^B = H_{XXZ} - \sum_i B_i S_i^z, \quad (3)$$

where

$$B_i = B_0 e^{-\frac{(i-L/2)^2}{2\sigma_0^2}}. \quad (4)$$

In the first case, we quench site-dependent exchange couplings. In this scenario, we obtain initial states with large local energy densities. Typical initial states that are ground states of Eq. (2) are shown in Fig. 2. These states have b bonds with ferromagnetic $J_i < 0$ in the center while the rest has antiferromagnetic $J_i > 0$. We refer to this setup as the J_i quench.

In the second case, the dynamics is driven by an inhomogeneous spin density, enforced by an external magnetic field applied in the initial state. This allows us to generate smooth spatial perturbations of $\langle h_i \rangle$ with small differences in energy compared to the ground state of Eq. (1). We refer to this setup as the B_0 quench. A more detailed discussion of the initial states generated by a J_i quench will be given in Sec. IV A. The B_0 quench was introduced in detail in Ref. 20.

The definition of the local energy density from the Hamiltonian Eq. (1) is not unambiguous. For instance, it is always possible to add local terms to the Hamiltonian whose total contribution by summation over all lattice sites vanishes. However, this seeming ambiguity can be resolved up to constants by requiring that any block of adjacent lattice sites $\sum_{i=l}^m h_i$ is Hermitian and yet to have the same structure as the

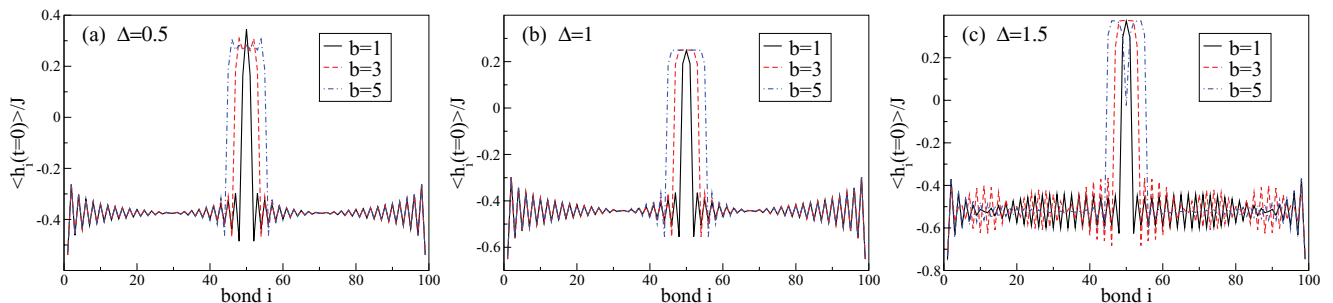


FIG. 2. (Color online) Profile of the local energy density $\langle h_i \rangle$ in the initial states induced by a J_i quench for $b = 1, 3, 5$ [compare Eq. (30)] for (a) $\Delta = 0.5$, (b) $\Delta = 1$, and (c) $\Delta = 1.5$. In all cases, the system forms a region with ferromagnetic nearest-neighbor spin correlations in the middle of the chain. In the regions with antiferromagnetic $J_i > 0$, the local energy density oscillates, reflecting the antiferromagnetic nearest-neighbor correlations.

total Hamiltonian H . These details seem to be rather specific, yet for the definition of the appropriate local energy density within the Luttinger liquid description, see below, these formal considerations are important. For the XXZ chain the local energy density is therefore determined by the bond energies $\langle h_i \rangle$.

To classify the dynamics of a density e_i we study its spatial variance

$$\sigma_E^2(t) = \sum_{i=1}^{L-1} (i - \mu)^2 e_i(t), \quad (5)$$

where μ is the first moment of e_i . The e_i are the normalized distribution linked to the energy density via

$$e_i = \delta E^{-1} \langle \tilde{h}_i \rangle \quad (6)$$

where $\langle \tilde{h}_i \rangle = \langle h_i \rangle - \langle h_i \rangle_0$ denotes the expectation value of h_i in the initial state shifted by the ground state expectation value $\langle h_i \rangle_0 = \langle \psi_0 | h_i | \psi_0 \rangle$.

$$\delta E := E_{\text{init}} - E_0 = \sum_i \langle \tilde{h}_i \rangle \quad (7)$$

is the energy difference between the initial state $|\psi_{\text{init}}\rangle$ [i.e., the ground state of either H_{init}^J or H_{init}^B] and the ground state $|\psi_0\rangle$ of Eq. (1), both energies measured with respect to the unperturbed Hamiltonian from Eq. (1):

$$E_0 = \langle \psi_0 | H_{XXZ} | \psi_0 \rangle, \quad E_{\text{init}} = \langle \psi_{\text{init}} | H_{XXZ} | \psi_{\text{init}} \rangle. \quad (8)$$

On physical grounds, the energy density should be normalized by the amount of energy transported by the propagating perturbation. This is well approximated by the energy difference δE between the initial state and the ground state of Eq. (1), as we have verified in many examples. In some cases, though, the propagating energy is, on a quantitative level, better described by estimating the area under the perturbations, as δE may also contain contributions from static deviations from the ground state bond energies in the background. Nevertheless, δE does not depend on the overall zero of energy and is an obvious measure of how far the system is driven away from the ground state. This, all together, justifies our definition of the e_i .

To remove static contributions depending only on the initial distribution $e_i(t=0)$, we subtract $\sigma_E^2(t=0)$ and study $\delta\sigma_E^2(t) := \sigma_E^2(t) - \sigma_E^2(0)$. $\delta\sigma_E^2(t) \sim (V_E t)^2$ is expected to grow quadratically in time in the case of ballistic behavior, where V_E has the dimensions of a velocity. For diffusive behavior, we expect, from the fundamental solution of the diffusion equation,⁶⁹ that $\delta\sigma_E^2(t) \sim Dt$ grows linearly in time, where D is the diffusion constant (see, e.g., the discussion in Ref. 20). Within linear response theory the diffusion constant can be related to transport coefficients via Einstein relations, see, e.g., Ref. 70. To be clear, the observation of $\delta\sigma_E^2 \sim t^2$ or $\delta\sigma_E^2 \sim t$ is a necessary condition for the respective type of dynamics and time-dependent crossovers are possible.

B. Spatial variance in the noninteracting case

For pedagogical reasons and to guide the ensuing discussion, we next calculate the spatial variance in the noninteracting limit of Eq. (1), i.e., at $\Delta = 0$. Using the

Jordan-Wigner transformation, we can write the Hamiltonian as

$$H = \frac{J}{2} \sum_i (S_i^+ S_{i+1}^- + \text{H.c.}) = -\frac{J}{2} \sum_i (c_i^\dagger c_{i+1} + \text{H.c.}), \quad (9)$$

where c_i^\dagger creates a spinless fermion on site i . A subsequent Fourier transformation diagonalizes the Hamiltonian:

$$H = \sum_k \epsilon_k c_k^\dagger c_k. \quad (10)$$

Since we will compare with numerical results on systems with open boundary conditions, we obtain

$$\epsilon_k = -J \cos(k), \quad k = \frac{\pi n}{L+1}, \quad n = 1, \dots, L. \quad (11)$$

Next, we compute

$$\delta\sigma_E^2(t) = \sum_i e_i(t)(i - i_0)^2 - \sum_i e_i(t=0)(i - i_0)^2$$

with e_i from Eq. (6) and $h_i = -J(c_i^\dagger c_{i+1} + \text{H.c.})/2$. By expressing $c_i^{(\dagger)}$ through their Fourier transform and by plugging in the time evolution of $c_k^{(\dagger)}$, we finally obtain, after straightforward calculations:

$$\delta\sigma_E^2(t) = V_E^2 t^2, \quad (12)$$

i.e., ballistic dynamics independently of the initial state. Terms linear in t will be absent if in the initial state, the density is symmetric with respect to its first moment, i.e., $e_{\mu+\delta} = e_{\mu-\delta}$ and if the wave packet has no finite center-of-mass momentum at $t=0$ already. In the remainder of the paper, we will work under these two additional assumptions that are valid for all initial states considered in our work. The prefactor V_E^2 is given by

$$V_E^2 = \frac{1}{\delta E} \sum_k \epsilon_k v_k^2 \delta n_k, \quad (13)$$

where $v_k = \partial\epsilon_k/\partial k$ and

$$\delta n_k = n_k^{\text{init}} - n_k$$

is the difference between the momentum distribution function (MDF) in the initial state and the one in the ground state of Eq. (1). Since we use open boundary conditions, we compute n_k from

$$n_k = \langle c_k^\dagger c_k \rangle := \frac{2}{L+1} \sum_{r,r'} \sin(kr) \sin(kr') \langle c_r^\dagger c_{r'} \rangle. \quad (14)$$

We can also express δE via δn_k :

$$\delta E = \sum_k \epsilon_k \delta n_k.$$

The expression (13) suggests that V_E is the average velocity of excitations contributing to the propagation of the wave packet. Characteristic for ballistic dynamics, V_E^2 is fully determined by the initial conditions through δn_k .

For completeness, we mention that an analogous calculation can be done for the spatial variance σ_S of the spin density. This quantity is defined as

$$\sigma_S^2(t) := \frac{1}{\mathcal{N}} \sum_{i=1}^L (i - \mu)^2 \langle S_i^z(t) + 1/2 \rangle. \quad (15)$$

The normalization constant \mathcal{N} measures the number of propagating particles. The spin density is, in terms of spinless fermions,

$$S_i^z = c_i^\dagger c_i - 1/2 = n_i - 1/2.$$

The result for the spatial variance of the spin density is

$$\delta\sigma_S^2(t) = \sigma_S^2(t) - \sigma_S^2(0) = V_S^2 t^2 \quad (16)$$

with

$$V_S^2 = \frac{1}{\mathcal{N}} \sum_k v_k^2 \delta n_k. \quad (17)$$

Although we started from the Hamiltonian for $\Delta = 0$, we stress that Eqs. (12), (16), (13), and (17) are valid for any dispersion relation ϵ_k , irrespective of the presence of a gap, provided that k has the meaning of a momentum.

C. Energy current

Another aspect worth noting is that the time-evolving state carries a nonzero energy current, a situation that usually does not appear in the case of a global quench. From the equation of continuity for the energy density, one can derive the well-known expression for the local energy current operator,⁴³

$$j_i^E = J^2 \tilde{S}_{i-1} \cdot (\tilde{S}_i \times \tilde{S}_{i+1}), \quad (18)$$

where $\tilde{S} = (S^x, S^y, \Delta S^z)$. With periodic boundary conditions, the total current $J_E = \sum_i j_i^E$ is a conserved quantity, i.e., $[H, J_E] = 0$ (see Ref. 43). On a system with open boundary conditions such as the ones that are well suited for DMRG, this property is lost, yet the dynamical conductivity still has a quasi-Drude peak at very low frequencies, reminiscent of the true Drude peak $\text{Re}\kappa(\omega) = D_E \delta(\omega)$ of a system with periodic boundary conditions.⁶⁸ The latter form is recovered on a system with open boundary conditions as $L \rightarrow \infty$ (see Ref. 68), showing that ballistic dynamics due to the existence of globally conserved currents can still be probed on systems with open boundary conditions.

To connect the local energy currents to the spatial variance of the time-dependent density one can rewrite the time derivative of $\sigma_E^2(t)$ using the equation of continuity, assuming no current flow to sites at the boundary (this assumption is justified in our examples as long as we restrict ourselves to times before reflections occur at the boundary in our simulations):

$$\begin{aligned} \partial_t \sigma_E^2(t) &\sim \sum_{r=1}^L (r - \mu)^2 \partial_t \langle h_r(t) \rangle \\ &= -\langle j_1^E \rangle + \sum_{r=1}^L (2r - 2\mu + 1) \langle j_r^E(t) \rangle. \end{aligned} \quad (19)$$

If $\sigma_E^2(t) = V_E^2 t + b$ and $\mu \neq \mu(t)$, then using $\langle J_E \rangle = 0$ leads to

$$\sum_{r=1}^L r \partial_t \langle j_r^E(t) \rangle \sim \frac{1}{2} \partial_t^2 \sigma_E^2(t) = V_E^2 = \text{const}. \quad (20)$$

If we interpret this equation as an operator equation, then we see that we can define a quantity J_E^* via

$$J_E^* = \sum_{r=1}^L r \partial_t j_r^E. \quad (21)$$

If for a given initial state and over a certain time window, $\langle J_E^*(t) \rangle = \text{const}$, then we have identified a regime with ballistic dynamics, $\delta\sigma_E^2(t) \sim t^2$. If $\langle J_E^*(t) \rangle = \text{const}$ holds for all times and initial states, then J_E^* is a conserved quantity, $[H, J_E^*] = 0$. This is the case at $\Delta = 0$, the noninteracting limit of Eq. (1), where $\langle J_E^* \rangle = V_E^2 \delta E$ from Eq. (13).

We emphasize that we have here identified an operator that connects the phenomenological observation of a quadratic increase of $\sigma_E^2(t)$ to the local energy currents. In ballistic regimes, its expectation value becomes stationary.

For completeness, we mention an analogous result in the diffusive regime where $\sigma_E^2 \sim t$. Then, expectation values of the operator

$$J_E^D = \sum_{r=1}^L (r - \mu) j_r^E(t) \quad (22)$$

are time independent. Obviously, similar expressions can be written down for the spatial variance associated with the spin density.

III. PROPAGATING ENERGY AND SPIN WAVE PACKETS IN A LUTTINGER LIQUID

In the gapless phase, i.e., for $|\Delta| < 1$, the low-energy and low-momentum properties of the XXZ chain can be described by an effective Luttinger liquid theory.⁷¹ In the following, we want to analyze the energy density and the spin dynamics of the XXZ chain in this exactly solvable hydrodynamic limit. Specifically, we show that at least asymptotically for large times, the spatial variance always grows quadratically both in the case of spin and energy dynamics. In addition, we work out the precise dependence of the prefactor in front of the t^2 increase of the spatial variance on system parameters. Since our DMRG results to be presented in Secs. IV and V show that $\sigma_E^2(t) \sim t^2$ at any Δ , we did not investigate the influence of marginally relevant perturbations at $\Delta = 1$ on the wave-packet dynamics. In passing, we mention that in the massive phase, where the appropriate low-energy theory is the sine-Gordon model, the expansion velocity could also be derived at the Luther-Emery point (this case was studied in, e.g., Refs. 25 and 26).

A. Bosonization of the anisotropic spin-1/2 chain

The Hamiltonian (1) can be mapped onto a system of interacting spinless fermions via the Jordan-Wigner transformation.³¹ Within a hydrodynamic description in terms

of a linearized fermionic dispersion relation, the Hamiltonian can be represented in terms of a Luttinger liquid theory (LL),

$$H_{LL} = \frac{u}{4} \int \frac{dx}{2\pi} \left[K(\rho_L - \rho_R)^2 + \frac{1}{K}(\rho_L + \rho_R)^2 \right], \quad (23)$$

using the notation of Ref. 72. The sum of the two left- and right-moving densities $\rho_L(x) + \rho_R(x)$ of the spinless Jordan-Wigner fermions is proportional to the continuum approximation of the local magnetization S_i^z up to a constant. The sound velocity u can be related to the parameters of the XXZ chain in Eq. (1) via the group velocity⁷³

$$u = v_g = J \frac{\pi \sin(\nu)}{2\nu}, \quad (24)$$

with $\cos \nu = \Delta$. Similarly, the Luttinger parameter K is given by the relation $K = \pi/[2(1 - \nu)]$. In the noninteracting case, $\Delta = 0$, we have $K = 1$ and $u = J$.

B. Ballistic dynamics in the gapless phase

Within the Luttinger liquid description for $\Delta < 1$, an initially inhomogeneous local energy density profile always propagates ballistically independently of the details of the perturbation as can be seen from general arguments. For the effective low-energy Hamiltonian, the probability distribution $e(x, t)$ associated with the local energy density is given by

$$e(x, t) = \mathcal{E}^{-1} \langle \psi_{\text{init}} | \hat{h}(x, t) | \psi_{\text{init}} \rangle, \quad (25)$$

where $|\psi_{\text{init}}\rangle$ is the initial state,

$$\begin{aligned} \hat{h}(x) = & u(K + K^{-1})/(8\pi) \sum_{\eta} \partial_x \varphi_{\eta}^{\dagger}(x) \partial_x \varphi_{\eta}(x) \\ & - u(K - K^{-1})/(8\pi) [\partial_x \varphi_L^{\dagger}(x) \partial_x \varphi_R^{\dagger}(x) \\ & + \partial_x \varphi_R(x) \partial_x \varphi_L(x)] \end{aligned} \quad (26)$$

and

$$\mathcal{E} = \int dx \langle \psi_{\text{init}} | \hat{h}(x, t = 0) | \psi_{\text{init}} \rangle. \quad (27)$$

For the exact definition of the fields $\varphi_{\eta}^{(\dagger)}$, see, e.g., Ref. 72. The local energy density operator consists of decoupled left- and right-moving contributions in the basis in which the Hamiltonian for the time evolution is diagonal. This allows for a separation of $e(x, t)$ into left- and right-moving contributions, which both propagate with the sound velocity v_g : $e(x, t) = e_L(x + v_g t, t = 0) + e_R(x - v_g t, t = 0)$.

Assuming an $L \leftrightarrow R$ symmetry in the initial state, i.e., a state with zero total momentum, one obtains for the variance from Eq. (5):

$$\delta\sigma_E^2(t) = \sigma_E^2(t) - \sigma_E^2(t = 0) = (V_E t)^2 \quad (28)$$

for all times t with $V_E = v_g = u$. This result can also be obtained from evaluating Eq. (13) in the continuum limit.

In the case of an initial $L \leftrightarrow R$ asymmetry in the initial state, we get $\delta\sigma_E^2(t) \rightarrow (v_g t)^2$ for $t \rightarrow \infty$, but the short-time behavior may differ. Thus within the validity of a Luttinger liquid description the energy transport is always ballistic for all initial conditions. This is evident from a physical point of view as all excitations propagate with exactly the same velocity v_g , the left movers to the left and the right movers

to the right. Note that the applicability of a Luttinger liquid description is manifestly restricted to cases in which the initial energy density profile is a smooth one in the sense that the associated excitations do not feel the nonlinearity of the fermionic dispersion relation. Thus, the time-evolution starting from initial profiles such as the ones shown in Fig. 2 is beyond the scope of this low-energy theory.

In analogy to the above arguments, the dynamics of spin-density wave packets is also ballistic in the XXZ chain for $\Delta < 1$ in the Luttinger liquid limit. In the bosonic theory, the spin density is proportional to $\rho_L(x) + \rho_R(x)$ up to a constant, see Sec. III A. The associated probability distribution $\rho(x, t) = \mathcal{Q}^{-1} \langle \rho_L + \rho_R \rangle / 2\pi$, with $\mathcal{Q} = \int dx \langle \rho_L + \rho_R \rangle / 2\pi$, can again be separated into a left- and a right-moving contribution, i.e.,

$$\rho(x, t) = \rho_L(x + v_g t, t = 0) + \rho_R(x - v_g t, t = 0). \quad (29)$$

Thus similar to the case of the energy dynamics, one finds ballistic behavior for $|\Delta| < 1$ consistent with the numerical results of Ref. 20.

IV. DMRG RESULTS FOR THE J_i QUENCH

Now we turn to the numerical simulations. Using the adaptive time-dependent DMRG³⁸⁻⁴² method, we can access the real-time dynamics of initial bond-energy distributions. Within this approach, we can probe the microscopic dynamics including the time dependence of bond energies or the entanglement entropy starting from various initial states in an essentially exact manner without limitations in the range of parameters. We discuss the pure energy dynamics in the absence of spin currents induced by the J_i quench in this section. We detail the construction of initial states and their specific features, then move on to the analysis of the time evolution of the bond energies. We calculate the spatial variance and the related quantity J_E^* and discuss the emergent velocities of the energy dynamics. Within the numerical accuracy of our simulations we find a quadratic increase of $\sigma_E^2(t)$ in all cases studied. However, it seems that for a J_i quench a large number of different velocities contribute as opposed to the Luttinger liquid theory result, the latter valid at low energies. Our study of the energy current during the time evolution and the time evolution of the expectation value $\langle J_E^*(t) \rangle$, defined in Eq. (21), gives additional insights into short-time dynamics and further validates the conclusion of ballistic energy dynamics.

A. Initial states

Let us first describe the typical shape of initial states induced by a J_i quench on a few bonds in the middle of the spin chain. To be specific, in the Hamiltonian (2), we set

$$J_i = \begin{cases} J, & i < L/2 - b, \\ -J, & \text{for } L/2 - b \leq i \leq L/2 + b, \\ J, & i > L/2 + b, \end{cases} \quad (30)$$

which provides us with initial states with an inhomogeneous energy density profile with a width of $2b$ of the ferromagnetic region. Outside this ferromagnetic region, we obtain antiferromagnetic nearest-neighbor correlations.

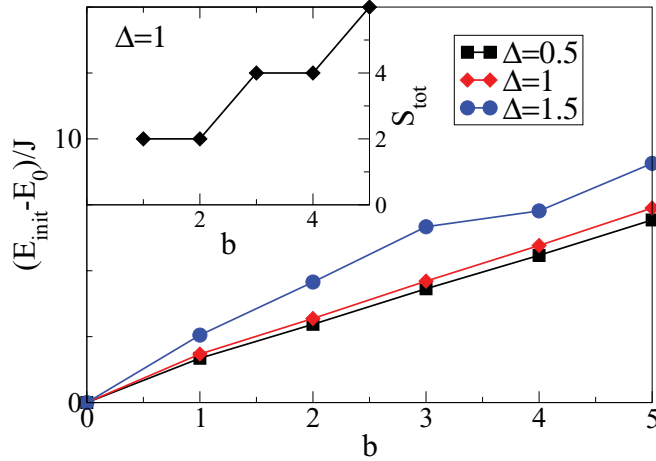


FIG. 3. (Color online) Energy difference δE between the initial state and the ground state for the J_i quench as a function of b for $\Delta = 0.5, 1, 1.5$. The inset shows the hierarchy of states with increasing total spin, which appear as initial states when the total spin is a good quantum number, i.e., at $\Delta = 1$.

Figure 2 shows the profile of the local energy density of XXZ chains with $L = 100$ sites with (a) $\Delta = 0.5$, (b) $\Delta = 1$, and (c) $\Delta = 1.5$, induced by a sign change of J_i on $b = 1, 3, 5$ bonds [compare Eq. (30)], obtained using DMRG with $m = 200$ states exploiting the $U(1)$ symmetry to ensure zero global magnetization $S_{\text{tot}}^z = \sum_i \langle S_i^z \rangle = 0$ and, in consequence, $\langle S_i^z \rangle = 0$. In all cases shown in Fig. 2, the system forms a region with ferromagnetic nearest-neighbor correlations in the middle of the chain. Note that for $\Delta \neq 1$, $\langle h_i \rangle$ is the sum of the nearest-neighbor transverse and longitudinal spin correlations, the latter weighted with Δ . In the regions with antiferromagnetic $J_i > 0$, the local energy density oscillates, reflecting the antiferromagnetic nearest-neighbor correlations. Figure 3 shows the energy difference δE . As a function of b , the energy difference δE increases linearly once the smallest possible ferromagnetic region has been established. The minimum energy difference $\delta E = E_{\text{init}} - E_0$ is of the order of $2J$, i.e., initial states that are only weak perturbations of the respective ground state cannot be generated using a J_i quench.

At the isotropic point $\Delta = 1$, we can explain the dependence of the initial state on the width b in a transparent manner. The ground-state energy per site for the antiferromagnetic ground state is known from the Bethe Ansatz to be $\lim_{L \rightarrow \infty} E_0(L)/L = -\ln(2) + 1/4$,⁷⁴ while for the ferromagnetic ground state, $E_0/(L - 1) = 1/4$, excluding the boundary sites, which gives rise to a very small system-size dependence. By growing the ferromagnetic region symmetrically with respect to the center of the chain and taking $E_0(L)$ from the unperturbed ground state with open boundaries, we obtain states with an energy that increases as

$$\delta E(b) = (2b - 1)[E_0/(L - 1) - 0.25] + \delta E^0, \quad (31)$$

for our finite system size (δE^0 is simply an offset). Equation (31) exactly reproduces the data for $\Delta = 1$ shown in Fig. 3.

Furthermore, at $\Delta = 1$, the total spin

$$S_{\text{tot}}^2 = \sum_i \vec{S}_i \cdot \sum_j \vec{S}_j \quad (32)$$

is a conserved quantity. Since the ground-state calculation only respects the conservation of magnetization ($S_{\text{tot}}^z = 0$), we obtain a hierarchy of states with $S > 0$. This can be easily understood by considering the block structure of the initial state. Taking, e.g., a total of $L = 100$ spins and assuming a ferromagnetic region of only two spins (i.e., $b = 1$), the two ferromagnetic spins are fully polarized with a total spin of $S = 1$, while each of the antiferromagnetic blocks has 49 spins and therefore a total spin of $S = 1/2$. Thus the total spin of the whole chain is $S_{\text{tot}} = 2$. Increasing the width of the ferromagnetic region by one, i.e., to $b = 2$, we have $S = 2$ in the middle, and the antiferromagnetic blocks are of even length, both having $S = 0$ in their ground state. This pattern repeats itself upon increasing the length $2b$ of the ferromagnetic region.

B. Time evolution of bond energies after a J_i quench

Now we focus on the time evolution of the local energy density induced by the aforementioned perturbation. At time $t = 0^+$, we set all $J_i = J$ and then evolve under the dynamics of Eq. (1). The DMRG simulations are carried out using a Krylov-space based algorithm^{75,76} with a time step of typically $0.25J$ and by enforcing a fixed discarded weight. We restrict the discussion to times smaller than the time needed for the fastest excitation to reach the boundary.

1. J_i quench: qualitative features

Figure 4 shows the time evolution of the bond energies $\langle h_i(t) \rangle$ as a contour plot for $\Delta = 0.5, 1, 1.5$ at $b = 1$. Despite the different ground states for the selected values of anisotropy, all features of the dynamics such as two distinct rays starting at the edges of the block of ferromagnetic correlations, are similar. The solid white lines for $\Delta = 0.5$ and $\Delta = 1$ indicate an excitation spreading out from the center of the ferromagnetic region with the group velocity given by Eq. (24) (these lines are parallel to the outer rays visible in the figure, i.e., the fastest propagating particles). Note that Eq. (24) holds only in the gapless phase ($|\Delta| \leq 1$). Besides the outer rays that define a light-cone structure, Fig. 4 unveils the presence of more such rays inside the light cone. Since our particular initial states have a sharp edge in real space, there ought to be many excitations with different momenta k contributing to the expansion.

2. J_i quench: spatial variance

Our main evidence for ballistic dynamics in both phases is based on the analysis of the spatial variance, shown in Fig. 5. Fitting a power law (straight lines) to the data, i.e., $\sigma_E^2(t) - \sigma_E^2(0) = \alpha t^\beta$ yields a quadratic increase with $\beta \approx 2$, classifying the dynamics as ballistic.

In order to estimate uncertainties in the fitting parameter α , we compare this to the results of fitting a pure parabola $\sigma_E^2(t) - \sigma_E^2(0) = V_E^2 t^2$ to the data. Typically, V_E^2 deviates from α by about 10% while the exponent of the power-law fit is

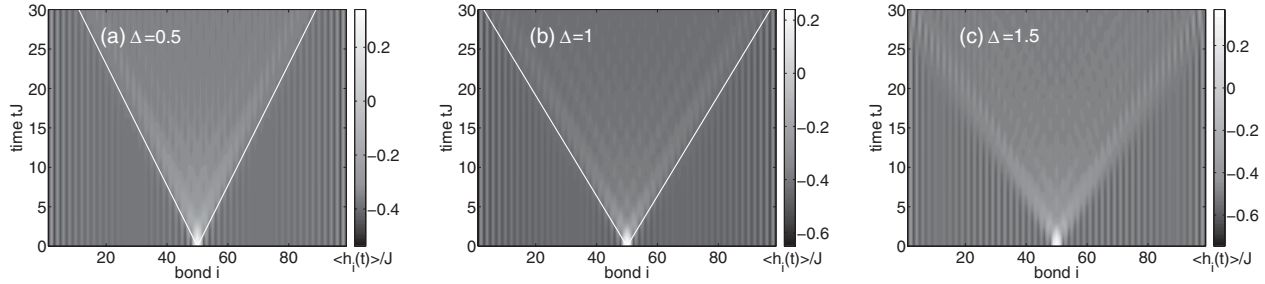


FIG. 4. Time evolution of the bond energy distribution starting from initial states with $b = 1$ from Fig. 2 for (a) $\Delta = 0.5$, (b) $\Delta = 1$, and (c) $\Delta = 1.5$. Despite the different ground-state phases, for the selected values of the exchange anisotropy Δ , main features of the dynamics such as two distinct rays extending from the edges of the perturbation are similar. The solid white lines for $\Delta = 0.5$ and $\Delta = 1$ indicate the propagation of a single excitation starting in the middle of the chain at time $t = 0$ moving with the group velocity v_g from Eq. (24). This is also the velocity in the outer rays.

usually different from 2 by 5%. As an example, for $\Delta = 0.5$ and $b = 1$, we obtain $\beta = 2.03$ and $\alpha = 0.53$ versus $V_E^2 = 0.6J^2$. The main reason for the deviation of β from two is, in fact, that the short-time dynamics is not well described by a power law at all over a b -dependent time window. We shall see later, in Sec. IV C, that the ballistic dynamics sets in

only after the block of ferromagnetically correlated bonds has fully “melted.” Indeed, by excluding several time steps at the beginning of the evolution from the power-law fit, we observe that $\beta \rightarrow 2$ and $\alpha \rightarrow V_E^2$. Therefore we will present results for V_E^2 , obtained by fitting $\sigma_E^2(t) - \sigma_E^2(0) = V_E^2 t^2$ to our tDMRG data.

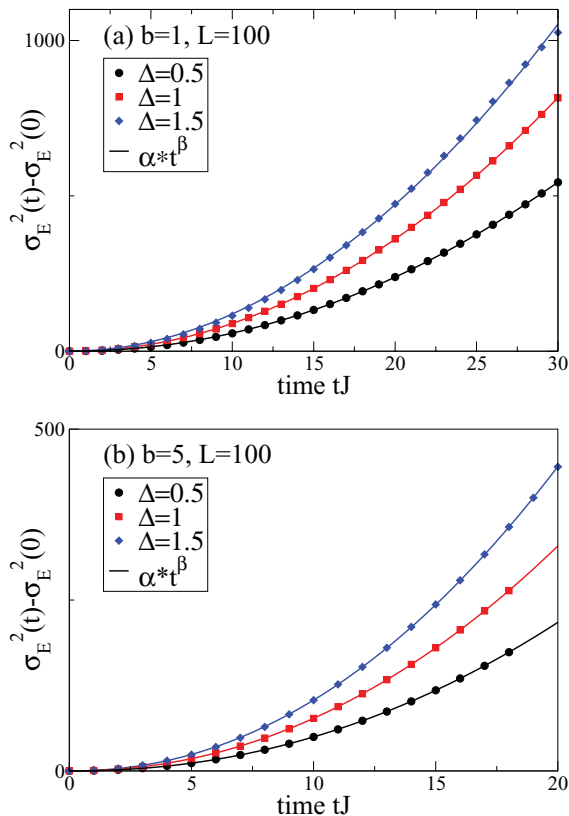


FIG. 5. (Color online) Spatial variance of the evolving energy distribution for (a) $b = 1$, (b) $b = 5$, and $\Delta = 0.5, 1, 1.5$. Fitting a power law (straight lines) to $\sigma_E^2(t) - \sigma_E^2(0) = \alpha t^\beta$ yields a quadratic increase with sufficient accuracy, classifying the dynamics as ballistic. For instance, we find $\alpha = 0.53$, $\beta = 2.03$ for $\Delta = 0.5$ and $b = 1$ [black circles in (a)]. We do not find any qualitative difference between the massless ($|\Delta| \leq 1$) and the massive ($\Delta > 1$) phases. The deviations between the fit and the tDMRG data in the $\Delta = 1.5$ curves at the largest times simulated are due to the boundaries.

3. Exploiting $SU(2)$ symmetry at $\Delta = 1$ for the J_i quench

Before proceeding to the discussion of the expansion velocity V_E^2 , we wish to discuss the long-time limit, which can be accessed in the case of $\Delta = 1$. Since our perturbation is proportional to the operators for the local energy density, global symmetries of the unperturbed Hamiltonian are respected by the initial states of the type in Eq. (30). Therefore, at $\Delta = 1$, we can exploit the conservation of total spin S , a non-Abelian symmetry. This can be used to push the simulations to much longer times, since we can perform the time evolution in an $SU(2)$ invariant basis.⁷⁷ The number of states needed to ensure a given accuracy is reduced substantially compared to a simulation that only respects $U(1)$ symmetry. Therefore we can work with larger system sizes and study the long-time dynamics of the energy density. As we can reach longer times, we can also analyze and discuss finite-size effects for $\Delta = 1$ here. Figure 6 shows our result for the time evolution respecting $SU(2)$ symmetry (blue triangles) for a system of $L = 200$ sites and $\Delta = 1$, $b = 1$ compared to the result from Fig. 5 for $L = 100$ sites (red squares). We still find a quadratic increase of $\sigma_E^2(t)$ and thus ballistic dynamics for times up to $t \sim 60/J$ and in addition, the prefactor does not depend on the system size. Both simulations were carried out keeping the discarded weight below 10^{-4} , which requires at most $m = 900$ states using only $U(1)$ symmetry on $L = 100$ sites versus a maximum of $m = 400$ using $SU(2)$ for $L = 200$ sites.

4. Expansion velocity

The results for V_E^2 are collected in Fig. 7 and plotted as a function of δE for $\Delta = 0, 0.5, 1, 1.5$. In the noninteracting case, $\Delta = 0$, V_E^2 is constant for $b \geq 2$, while at $b = 1$ (the smallest possible δE), $V_E^2 = 0.5J^2$. For all $\Delta > 0$, V_E^2 slightly decreases with δE and V_E^2 is much smaller than v_g^2 given by Eq. (24), suggesting that indeed, many velocities contribute during the expansion of the energy wave packet.

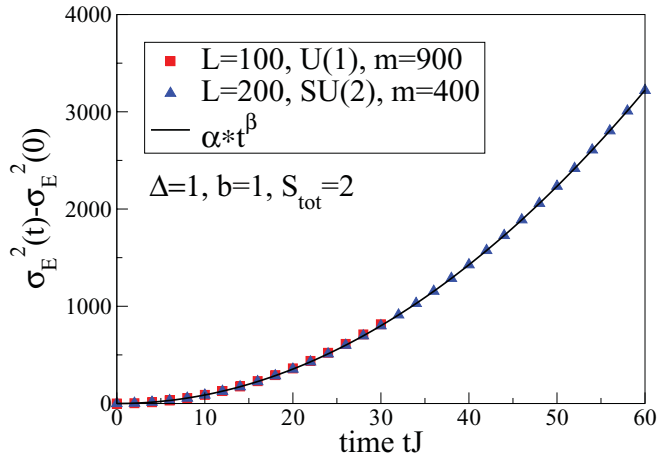


FIG. 6. (Color online) Long-time evolution exploiting the conservation of total spin S_{tot} at $\Delta = 1$ for $L = 200$ sites using an initial state with $b = 1$. For comparison, we plot the result for $L = 100$ sites using only $U(1)$ symmetry. Fixing the discarded weight to 10^{-4} , we need less than half the number of states. Furthermore, we find that the spatial variance is very robust against finite-size effects.

Intuitively, one might associate the decrease of V_E^2 , which is a measure of the average velocity of propagating excitations contributing to the expansion, to band curvature: the higher δE , the more excitations with velocities smaller than v_g are expected to factor in.

It is instructive to consider the noninteracting limit first by comparing the numerical results obtained from a time evolution with exact diagonalization to the analytical (and also exact result) from Eq. (13). To that end, we need to compute the MDF [see Eq. (14)] of the initial state. Our results for $\Delta = 0$, which are shown in Fig. 8, unveil a peculiar property: the J_i quench always induces changes at all k , i.e., the system is not just weakly perturbed in the vicinity of k_F . This is not surprising since our initial states have sharp edges in real space (compare Fig. 2). Moreover, the J_i quench changes the MDF in

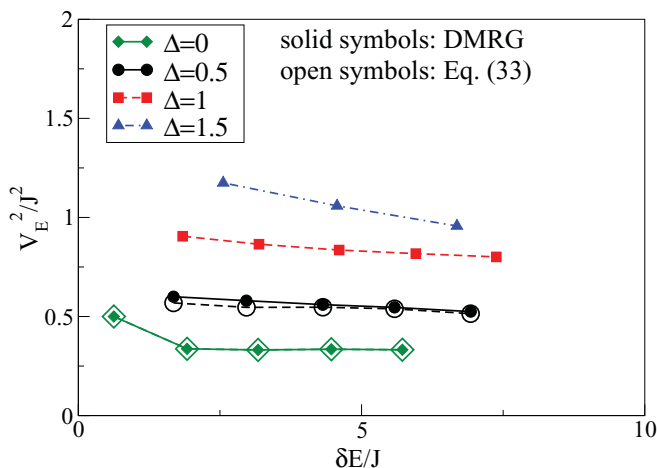


FIG. 7. (Color online) Prefactors V_E^2 of the fits $\sigma_E^2 - \sigma_E^2(0) = V_E^2 t^2$ as functions of δE for $\Delta = 0, 0.5, 1, 1.5$ and J_i quenches with $b = 1, 2, 3, 4, 5$ (for $\Delta = 1.5$, we show $b = 1, 2, 3$ only). For $\Delta > 0$, V_E^2 decreases slightly with b , while $V_E^2 < v_g^2$. At $\Delta = 0$, V_E^2 is roughly constant for $b > 2$.

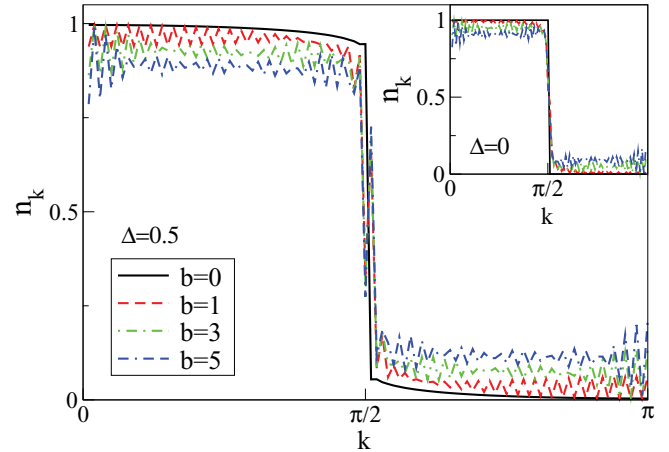


FIG. 8. (Color online) MDF of the initial states generated by a J_i quench at $\Delta = 0.5$ and $\Delta = 0$ (inset) with $b = 1, 3, 5$. For comparison, we include the MDF of the ground state (solid black line).

such a way that $\delta n_k(b) = n_k^{\text{init}}(b) - n_k$ is point symmetric with respect to $k_F = \pi/2$, where k_F is the Fermi wave vector. As Fig. 7 shows, V_E^2 as extracted from fits to $\delta \sigma_E^2$ (solid symbols) and V_E^2 from Eq. (13) (open symbols) perfectly agree with each other, as expected.

The MDF of initial states for the interacting systems are also such that $\delta n_k \neq 0$ at all momenta and we may therefore conclude that the observation $V_E < v_g$ is due to the fact that the J_i quench induces many excitations with velocities smaller than v_g (compare the data shown for $\Delta = 0.5$ shown in Fig. 8). Of course, Eq. (13) is not directly applicable to the interacting case since, first, it does not account for the correct eigenstates at $\Delta \neq 0$ and second, in general, $\langle h_i \rangle \neq \langle J(S_i^+ S_{i+1}^- + \text{H.c.})/2 \rangle$. Nevertheless, by numerically calculating δn_k for the interacting system and by using the renormalized velocity in Eq. (13) instead of J [i.e., $J \rightarrow v_g(\Delta)$], we obtain an estimate for V_E^2 from

$$V_E^2 \approx \frac{v_g^2}{\delta E} \sum_k \cos(k) \sin^2(k) \delta n_k. \quad (33)$$

This reproduces the qualitative trend of the tDMRG results for V_E^2 as we exemplify for $\Delta = 0.5$ in Fig. 7.

To summarize, the overall picture for the time evolution of the bond energies after a J_i quench is that energy propagates ballistically with an expansion velocity V_E that is approximately given by Eq. (33). Combined with the observation that on a finite system, a J_i quench induces changes in the MDF at all momenta k , we conclude that many excitations contribute to the wave-packet dynamics, resulting in $V_E < v_g$, both in the noninteracting and in the interacting case.

C. Energy currents

To conclude the discussion of the J_i quenches we present our results for the local energy currents at $\Delta = 1$ in Fig. 9. By comparison with Fig. 4(b), we see that the local current is the strongest in the vicinity of the wave packet. The energy current in each half of the system becomes a constant after a few time steps, i.e., $J_{L/2}^E := \sum_{i=1}^{L/2-1} j_i^E$ reaches a constant value. We

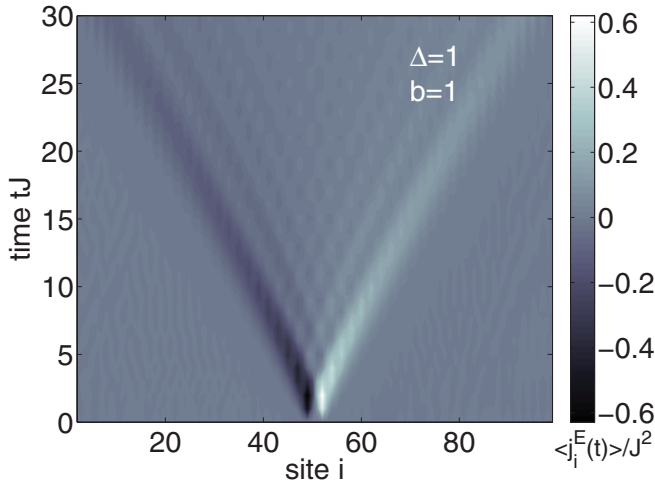


FIG. 9. (Color online) Real-time evolution of the local energy current, Eq. (18), at $\Delta = 1$ for a J_i quench with $b = 1$.

plot the absolute value of $\langle J_{L/2}^E \rangle$ for $\Delta = 0.5, 1, 1.5$ for $b = 1$ in Fig. 10(a). The qualitative behavior is independent of Δ : as soon as the initial perturbation has split up into two wave packets, we have prepared each half of the chain in a state with a constant, global current $\langle J_{L/2}^E \rangle = \text{const}$. For a system with periodic boundary conditions, the total current $J_E = \sum_i j_i^E$ is a conserved quantity.⁴³ Since the effect of boundaries only factors in once these are reached by the fastest excitations, we directly probe the conservation of a global current with our setup, after some initial transient dynamics. Therefore we can link the phenomenological observation of ballistic wave-packet dynamics to the existence of a conservation law in the system.

While the currents $\langle J_{L/2}^E \rangle$ clearly undergo some transient dynamics [see Fig. 10(a)], we have derived a quantity in Sec. II, called J_E^* , whose expectation value is stationary if $\sigma_E^2 \sim t^2$. We now numerically evaluate $\langle J_E^*(t) \rangle$ from Eq. (21), which provides an independent probe of ballistic dynamics. Figure 10(b) shows our results for $\Delta = 1$ and J_i quenches with $b = 1, 2, 3, 4, 5$. It turns out that $\langle J_E^*(t) \rangle$ is indeed constant at sufficiently large times, consistent with the observation of $\delta\sigma_E^2 \sim t^2$. In Sec. IV B, we have noted that $\delta\sigma_E^2 \not\sim t^2$ at short times $t \lesssim b/J$. This renders $\langle J_E^*(t) \rangle$ a time-dependent quantity over the same time window. Clearly, the time window over which $\langle J_E^*(t) \rangle \neq \text{const}$ depends on b [see Fig. 10(b)], which suggests that the deviation of ballistic dynamics is associated to the “melting” process of the region with ferromagnetic correlations. We have carefully checked that these observations are robust against errors in the calculation of time derivatives in Eq. (21) induced by the finite time step. Since $\langle J_E^*(t) \rangle$ is time dependent (at least at short times), we conclude that J_E^* is not a conserved quantity in the interacting case. Finally, within our numerical accuracy and as an additional consistency check, we find that $\langle J_E^* \rangle / \delta E = \alpha$ in the stationary state as expected from the discussion in Sec. II C.

To summarize, $\langle J_E^*(t) \rangle = \text{const}$ whenever $\delta\sigma_E^2 \sim t^2$ but $\langle J_E^* \rangle$ is very sensitive to the initial transient dynamics in the energy dynamics and becomes constant after a time $\approx bJ$. Furthermore, our setup serves to prepare each half of the system in a state with a finite global energy current $\langle J_{L/2}^E \rangle$

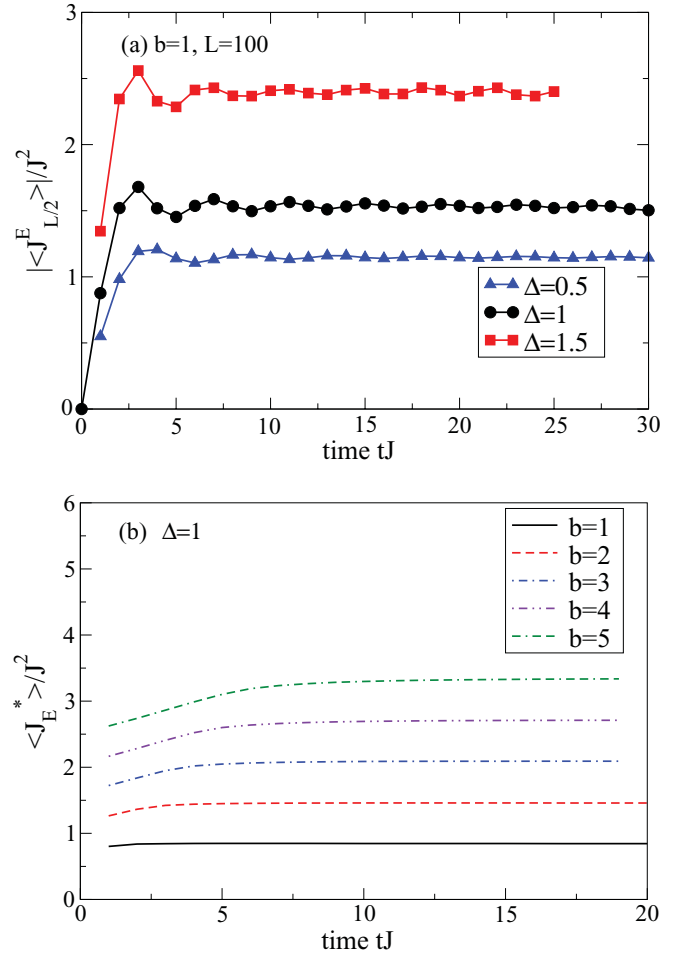


FIG. 10. (Color online) (a) Absolute value of the current in each half of the system. A constant value is reached after $t \approx 5/J$. (b) The quantity $\langle J_E^*(t) \rangle$ from Eq. (21) derived from a pure quadratic increase of the spatial variance for $\Delta = 1$ and $b = 1, 2, 3, 4, 5$. This quantity is constant, as expected from the discussion in Sec. IV C, except for the initial transient dynamics at $t < b/J$.

that, after some transient dynamics, does not decay since the global energy current operator is a conserved quantity.

V. COUPLED SPIN AND ENERGY DYNAMICS

After focusing on the energy dynamics in the absence of spin/particle currents we now revisit the case of spin dynamics starting from states with $\langle S_i^z(t=0) \rangle \neq 0$. Thus during the time evolution, the local spin and energy currents are both nonzero. In Ref. 20, the dynamics of the magnetization was studied, where the inhomogeneous spin-density profile was induced by a Gaussian magnetic field in the initial state. We take the initial state to be the ground state of Eq. (3) in the sector with zero global magnetization, i.e., $S_{\text{tot}}^z = \sum_i \langle S_i^z \rangle = 0$. Such a perturbation naturally also results in an inhomogeneous energy density in the initial state, which is coupled to the spin dynamics during the time evolution.²⁸

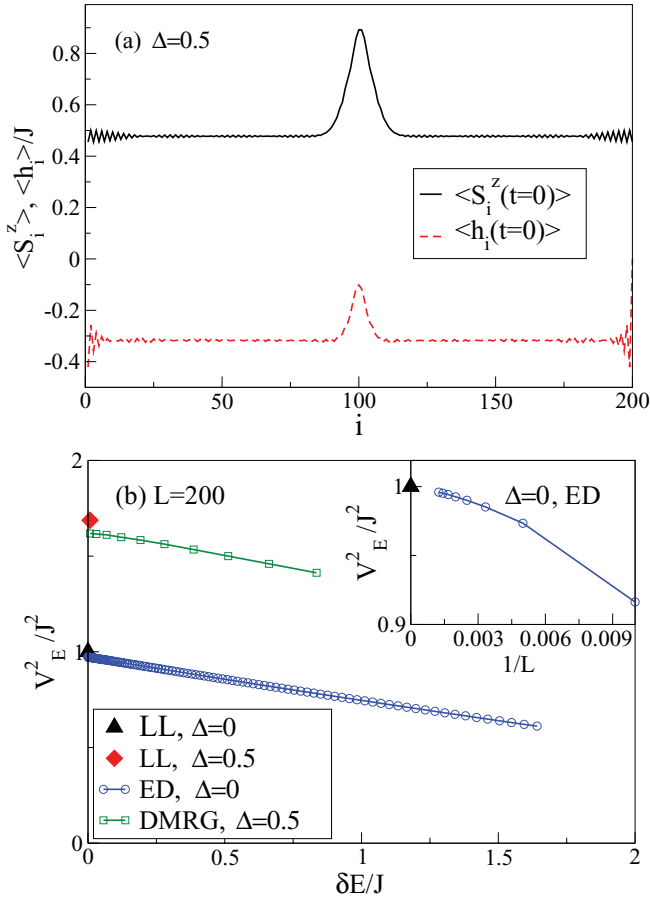


FIG. 11. (Color online) (a) Magnetization (solid black line) and energy density (dashed red line) in the initial state, for a B_0 quench with $B_0 = J$ and $\sigma_0 = 5$ for $\Delta = 0.5$ on a lattice of $L = 200$ sites. (b) Prefactor V_E^2 of $\delta\sigma_E^2(t) = V_E^2 t^2$ for the energy dynamics after a B_0 quench in the massless phase of the XXZ chain, compared to the group velocity [Eq. (24)] for $\Delta = 0, 0.5$ and $L = 200$. On this system size and in the limit of small perturbations, V_E^2 is approximately 5% smaller than the prediction from the Luttinger liquid theory for both Δ . For $\Delta = 0$, finite-size scaling of $V_E^2(\delta E \rightarrow 0)$ using $L = 100, 200, \dots, 800$ yields $V_E^2 \rightarrow v_g^2$ as shown in the inset.

A. Massless phase

In Fig. 11(a), we compare the initial magnetization (black solid line) and the local bond energies (dashed red line) induced by a Gaussian magnetic field with $B_0 = J$ and $\sigma_0 = 5$ at $\Delta = 0.5$ finding qualitatively the same pattern; both the spin and the energy density follow the shape of the magnetic field, resulting in a smooth perturbation with small oscillations in the background away from the wave packet.

For the time evolution of the bond energies at $0 < \Delta \leq 1$, we perform an analysis of their spatial variance analogous to the discussion of the J_i quench, finding ballistic dynamics in the massless phase. Since with a B_0 quench, initial states with very small δE can be produced, we next connect our numerical results to the predictions of LL theory, valid in the limit $\delta E \ll J$ (compare Sec. III).

Since we enforce zero global magnetization, we draw magnetization from the background into the peak.¹⁴ Therefore one has to carefully estimate the contributions to δE that

do not contribute to the time dependence of bond energies yet change the background density n_{bg} . The latter, in turn, affects the expected group velocity and we thus expect to recover the LL result derived for the half-filled case, i.e., propagation with v_g from Eq. (24), in the limit of large systems where $n_{bg} \rightarrow 1/2$. Furthermore, B_0 quenches induce $2k_F$ oscillations in the spin and energy density.²⁰ To account for this, we use coarse graining, i.e., averaging the energy density over neighboring sites, and we take the sum only over the area of the peak when estimating δE . We obtain $\delta E^{\text{peak}} := \sum_{L/2-x}^{L/2+x} (\langle h_i \rangle - \langle h_i \rangle_0)$, where $\langle h_i \rangle_0$ denotes the ground-state expectation value. From this quantity we calculate the velocity via $V_E^2 \rightarrow V_E^2 \cdot \delta E / \delta E^{\text{peak}}$, which is shown in Fig. 11(b). Note that while δE^{peak} is the correct normalization to obtain the correct velocities, we label our initial states via δE . At $\Delta = 0$ (blue circles), V_E^2 decreases linearly as a function of δE . Next we compare the result from the low-energy theory from Sec. III (solid symbols at $\delta E = 0$) to our tDMRG data. For both $\Delta = 0$ and $\Delta = 0.5$, V_E^2 for $L = 200$ sites is approximately 5% smaller than v_g^2 from Eq. (24), which is mainly due to the deviation of the background density from half filling. While it is hard to get results for larger systems than $L \sim 200$ in the interacting case, we can solve the $\Delta = 0$ case numerically exactly in terms of free spinless fermions, allowing us to go to sufficiently large L to observe $V_E^2(L) \rightarrow v_g^2$ as $L \rightarrow \infty$. The inset of Fig. 11(b) shows the finite-size scaling of $V_E^2(L)$ for $\Delta = 0$ using $L = 100, 200, \dots, 800$, which yields $V_E^2 \rightarrow v_g^2$ in the limit $L \rightarrow \infty$, taking first $\delta E \rightarrow 0$ for each system size. We thus, in principle, have numerical access to the dynamics in the low-energy limit well described by Luttinger liquid theory using a B_0 quench.

B. Massive phase

In Ref. 20, examples of a linear increase of the spatial variance of the magnetization $\sigma_S^2(t)$, defined in Eq. (16), were found in the massive phase, which were interpreted as an indication of diffusive dynamics. We now demonstrate that while the spin dynamics may behave diffusively, i.e., $\delta\sigma_S^2 \sim t$ over a certain time window, the energy dynamics in the same quench is still ballistic, i.e., $\delta\sigma_E^2 \sim t^2$.

In Fig. 12, we show the full time evolution of the bond energies for a Gaussian magnetic field with $B_0 = 1.5J$ and $\sigma_0 = 5$ on a chain of $L = 200$ sites at $\Delta = 1.5$. It consists of two rays propagating with opposite velocities. In Fig. 13, we compare the spatial variance of the magnetization $\sigma_S^2(t)$ to the one of the bond energies $\sigma_E^2(t)$ calculated in the same time evolved state. The main panel of Fig. 13 shows $\sigma_E^2(t) - \sigma_E^2(0)$, which is very well described by a power-law fit with an exponent $\beta = 2.03$ on the accessible time scales. The inset of Fig. 13 displays the data for $\delta\sigma_S^2(t) = \sigma_S^2(t) - \sigma_S^2(0)$ taken from Ref. 20. The spatial variance of the energy density is quadratic in time, even at times $t \gtrsim 12/J$ where the spatial variance of the magnetization increases only linearly. This example reflects the qualitative difference between spin and energy transport in the massive phase of the XXZ model at zero global magnetization. The conservation of the global energy current is consistent with the observation of ballistically propagating energy wave packets, while spin clearly does not propagate ballistically. Our result, obtained in the nonequilibrium case with a

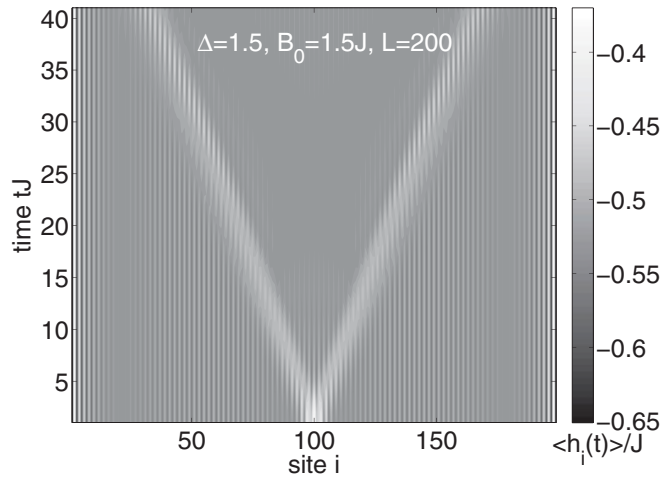


FIG. 12. (Color online) Time-dependent bond energies for the dynamics induced by a B_0 quench with $B_0 = 1.5J$, $\sigma_0 = 5$ on a chain of $L = 200$ sites at $\Delta = 1.5$. In this case, both local spin and local energy densities are perturbed and the corresponding local currents are nonzero.

zero-temperature background density, is consistent with the picture established from both linear-response theory^{51,55} and steady-state simulations.^{28,61,64}

Very recently, Jesenko and Žnidarič have also studied the time evolution of spin and energy densities induced by a B_0 quench.²⁸ They concentrate their analysis on the velocity of the fastest wave fronts, contrasting energy against spin dynamics. Based on the presence of these rays of fast propagating particles, they claim that the wave packet dynamics still has ballistic features. However, their analysis neglects the influence of slower excitations that also contribute to the dynamics of the wave packet, which is captured by the variance, and it ignores the decay of the intensity in the outer rays that we typically observe whenever $\delta\sigma_S^2 \sim t$.²⁰ The latter is, if at all, weak in a ballistic expansion characterized by

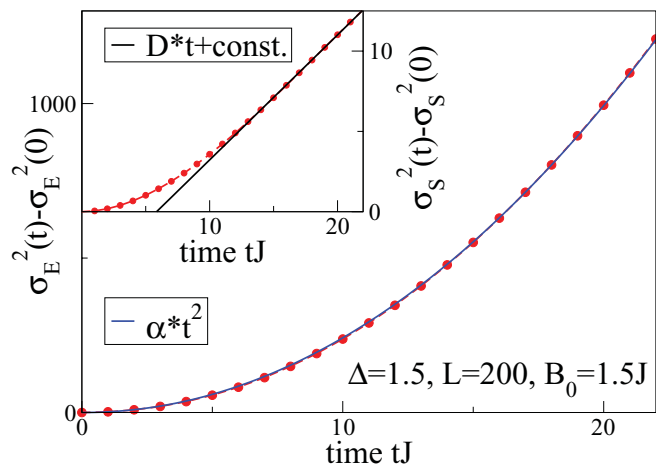


FIG. 13. (Color online) Spatial variance of the energy density (main panel) and the spin density (inset), induced by a B_0 quench with $B_0/J = 1.5$ and $\sigma_0 = 5$ [compare Eq. (3)] at $\Delta = 1.5$. In this case, both local spin and local energy densities are non zero during the time evolution. The inset was reproduced from Ref. 20.

$\delta\sigma_S^2 \sim t^2$. Therefore, while the analysis of Ref. 28 unveils interesting details of the time evolution of densities during a B_0 quench, we maintain that the variance is a useful quantity to identify candidate parameter sets for spin diffusion in, e.g., the nonequilibrium regime. Final proof of diffusive behavior then needs to be established by either demonstrating the validity of the diffusion equation or by computing correlation functions, see, e.g., Refs. 55 and 61. For instance, in Ref. 28, Jesenko and Žnidarič analyze the steady-state currents in the $\Delta > 1$ regime at finite temperature and obtain diffusive behavior.

VI. SUMMARY

We studied the real-time energy dynamics in XXZ spin-1/2 chains at zero temperature in two different scenarios. First, we investigated the energy dynamics in the absence of spin currents induced by a local sign change in the exchange interactions. The spatial variance behaves as $\delta\sigma_E^2(t) \propto t^2$ for all Δ , consistent with ballistic dynamics. In the gapless regime, the velocity of the fastest excitation present in the dynamics is the group velocity v_g of spinons, yet our particular quench also involves excitations with much smaller velocities resulting in expansion velocities $V_E < v_g$. Furthermore, the ballistic dynamics can be related to properties of energy currents. While the total current vanishes in our setup, i.e., $\langle J_E \rangle := \sum_i \langle j_i^E \rangle = 0$, the current in each half of the chain $\langle J_{L/2}^E \rangle > 0$ takes a constant value, after some transient dynamics. Therefore, in each half of the system, we prepared a state with a conserved global current, allowing us to make a direct connection to the predictions of linear-response theory where the existence of ballistic dynamics is directly linked to conservation laws that prohibit currents from decaying.⁴³ Moreover, we identified an observable J_E^* built from local currents whose expectation value $\langle J_E^*(t) \rangle$ is time independent if $\delta\sigma_E^2 \propto t^2$ and vice versa. This carries over to other types of transport as well and, in fact, the analysis of the time dependence of $\langle J_E^* \rangle$ can be used as an independent means to identify ballistic regimes, or to unveil the absence thereof.

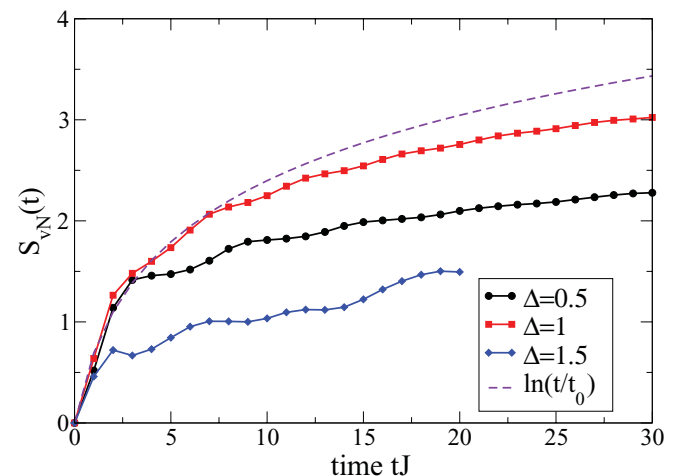


FIG. 14. (Color online) Time dependence of the von Neumann entropy S_{VN} for a bipartition that cuts the system across the central bond during the time evolution starting from a ferromagnetic region coupled to an antiferromagnetic one at $\Delta = 0.5, 1, 1.5$

In the second part, we studied the energy dynamics induced by quenching a Gaussian magnetic field, with two main results. These quenches allow us to access the regime of weakly perturbed initial states and in that limit, we recover the predictions from Luttinger liquid theory for the wave-packet dynamics. Their variance simply grows as $\delta\sigma_E^2 = v_g^2 t^2$. In the massive phase, a very interesting phenomenon occurs, since the energy dynamics is ballistic on time scales over which the spin dynamics behaves diffusively although both are driven by the same perturbation. This resembles the picture established from linear-response theory,⁴³ there applied to the finite-temperature case, in the nonequilibrium setup studied here. While our numerical results cover spin chains on real-space lattices and initial states far from equilibrium, the extension of our work to a finite temperature of the background will be crucial to tackle the most important open questions.

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APPENDIX: ENTANGLEMENT GROWTH

Here, we want to study the growth of entanglement across a junction separating regions in a spin chain with ferromagnetic correlations from ones with antiferromagnetic ones.

To that end, we take initial states inspired by Ref. 19 where one half of the system has a positive and the other one a negative J . We obtain this configuration as a variation of J_i -quench choosing:

$$J_i = \begin{cases} J, & i < L/2, \\ 0, & \text{for } i = L/2, \\ -J, & i > L/2, \end{cases} \quad (\text{A1})$$

in Eq. (2). We then perform the time evolution under the antiferromagnetic Hamiltonian [Eq. (1)]. As a measure of the entanglement we calculate the von Neumann entropy

$$S_{vN} = -\text{Tr}(\rho_A \ln \rho_A) \quad (\text{A2})$$

of the reduced density matrix $\rho_A = \text{Tr}_B \rho$, where $\rho = |\psi(t)\rangle\langle\psi(t)|$ and $|\psi(t)\rangle$ is the time-evolved wave function, for a bipartition in which we cut the chain into two halves of length $L/2$ across the central link. Our results are plotted in Fig. 14. We observe that the von Neumann entropy grows at most logarithmically (purple dashed line), in agreement with Ref. 21. The overall largest values of $S_{vN}(t)$ are found at the critical point $\Delta = 1$ (red squares). This behavior is very similar to the observations made in Ref. 19 for spin dynamics starting from a state with all spins pointing up (down) in the left (right) half.

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