Scaling of Diffusion Constants in the Spin-1/2 XX Ladder

R. Steinigeweg,1 F. Heidrich-Meisner,2 J. Gemmer,3 K. Michielsen,4 and H. De Raedt5

1Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany
2Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany
3Department of Physics, University of Osnabrück, D-49069 Osnabrück, Germany
4Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany and RWTH Aachen University, D-52056 Aachen, Germany
5Department of Applied Physics, Zernike Institute for Advanced Materials, University of Groningen, NL-9747AG Groningen, The Netherlands

(Dated: June 12, 2014)

We study the dynamics of spin currents in the XX spin-1/2 ladder at finite temperature. Within the framework of linear response theory, we numerically calculate autocorrelation functions for quantum systems larger than what is accessible with exact diagonalization using the concept of dynamical quantum typicality. We show that spin Drude weights vanish exponentially fast with increasing system size. As a main result, we unveil qualitatively different dependencies of the spin diffusion coefficient on the rung-interaction strength, resulting from a crossover from exponential to Gaussian dissipation as the rung coupling increases. This behavior is also derived analytically. We further discuss the relation of our results to experiments with cold atomic gases.

PACS numbers: 05.60.Gg, 71.27.+a, 75.10.Jm

Introduction. The theoretical understanding of transport properties of interacting quantum many-body systems is paramount in characterizing states of matter. Strongly interacting one-dimensional (1D) systems may exhibit either diffusive or ballistic transport properties at finite temperatures [1, 2], the latter being due to local conservation laws in integrable models [1, 3, 8]. These unusual properties have been speculated to be related to the observation of huge magnetic thermal conductivities in 1D quantum magnets [3, 11] and may have potential applications in signal propagation in artificial 1D systems on surfaces [12] or for spintronics applications [13, 14]. Generic non-integrable 1D systems are believed to exhibit no ballistic dynamics [15, 18] and presumably diffusive transport (see Refs. 19–22 for possible exceptions or corrections).

More recently, it has become possible to address qualitative aspects of mass transport in experiments with ultra-cold quantum gases in optical lattices [23–25], based on the realization of Bose- and Fermi-Hubbard models in these systems [26]. Studies that utilized the so-called sudden expansion, i.e., the release of a trapped gas of atoms into an empty optical lattice, support the picture that mass transport in two-dimensional Hubbard models is diffusive for both bosons and fermions [23, 24], while experiments with strongly interacting bosons in 1D have clearly shown ballistic transport properties [25]. Bosons in 1D subject to infinitely strong interactions, called hard-core bosons, are integrable via the exact mapping to non-interacting fermions [27] and thus Ref. 24 establishes an unambiguous experimental realization of ballistic dynamics in an integrable 1D system, rendering this a suitable starting point for future studies. Moreover, hard-core bosons are equivalent to spin-1/2 XX models, establishing a direct connection to research on the transport properties of quantum magnets.

An important question is the effect of integrability breaking on transport properties. In quantum gas experiments, a straightforward way to break integrability is to induce an inter-chain coupling and indeed, experimental results for sudden expansions in the 1D-2D crossover of interacting bosons indicate a rapid emergence of diffusive-like behavior upon increasing the inter-chain coupling [24].

As an alternative to the dimensional crossover, one can consider two coupled chains, i.e., a ladder, which can easily be realized in optical lattices using superlattices [28]. This system, in particular, is accessible to state-of-the-art numerical methods. First studies of the dynamics of hard-core bosons on a ladder geometry in the sudden expansion [29] or for wave-packet dynamics [30] indicate diffusive dynamics for sufficiently large inter-chain coupling, yet a systematic and quantitative analysis of ballistic and diffusive contributions based on linear response theory is lacking.

In this Letter, we address precisely this question using the spin-1/2 XX ladder. By exploiting the concept of dynamical quantum typicality [31–33], we are able to study ladders with up to $N \leq 36$ spins, larger than what can be accessed with exact diagonalization. In addition, we can reach the long time scales as required to detect and analyze ballistic contributions [34]. In the high-temperature limit, we first demonstrate the absence of ballistic contributions and then compute the diffusion constant as a function of the inter-chain coupling. As a main result, we identify three regimes characterized by qualitatively different time dependencies of current autocorrelation functions. Finally, we discuss a possible experiment...
Jordan-Wigner transformation maps hard-core bosons to the case of spin-1/2 operators at site \((i,k)\), \(J_{\parallel} > 0\) is the antiferromagnetic exchange coupling constant along the legs, and \(J_z = r J_{\parallel} > 0\) is the strength of the rung interaction. While the XX ladder splits into two integrable XX chains of free Jordan-Wigner fermions for \(r = 0\), it simplifies to a set of uncoupled dimers for \(r \to \infty\). In the case of \(r \neq 0\), the XX ladder is non-integrable and the Jordan-Wigner transformation maps hard-core bosons to interacting fermions \([23]\). In general, the model in Eq. (1) preserves the total magnetization \(S^z\) and is invariant under periodic boundary conditions. We do not restrict ourselves to a certain \(S^z\) sector and take into account the full Hilbert space with \(d = 2^N\) states, which corresponds to \(\langle S^z \rangle = 0\) \([30]\).

The longitudinal spin current is defined via the continuity equation and has the well-known form

\[
\dot{\psi} = J_{\parallel} \sum_{i=1}^{N/2} \sum_{k=1}^{2} \left( S_{i,k}^x S_{i+1,k}^x + S_{i,k}^y S_{i+1,k}^y - S_{i,k}^y S_{i+1,k}^x - S_{i,k}^x S_{i+1,k}^y \right) .
\]

The spin current commutes with the Hamiltonian only at \(r = 0\). Within the framework of linear response theory, we are interested in the autocorrelation function at the inverse temperatures \(\beta = 1/T\) (\(k_B = 1\)),

\[
C(t) = \text{Re} \frac{\langle \psi(t)| \dot{\psi}(t) \rangle}{N \langle \psi|\psi \rangle},
\]

where the time argument of \(\dot{\psi}\) has to be understood w.r.t. the Heisenberg picture, \(\dot{\psi} = \dot{\psi}(0)\), and \(C(0) = J_{\parallel}^2/8\) in the high-temperature limit \(\beta \to 0\). From this autocorrelation we obtain the two central quantities

\[
\overline{C} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} dt C(t), \quad D = \frac{1}{\chi} \int_{0}^{t_2} dt C(t)
\]

with \(t_2 > t_1\) and \(t_2 \to \infty\). The first quantity \(\overline{C}\) is the spin Drude weight, which, being the non-decaying part of \(C(t)\), signals ballistic transport \([1]\). The second quantity \(D\) is the spin-diffusion constant and well-defined for a vanishing \(\overline{C}\) [and a sufficiently fast decay of \(C(t)\)]. The prefactor \(\chi\) is the static susceptibility (per spin) and \(\chi = 1/4\) as \(\beta \to 0\). The numerical calculation of the two quantities in Eq. (4) is feasible by choosing finite but sufficiently long times \(t_1\) and \(t_2\), where \(C(t)\) has already decayed to its final value, and \(t_2 \gg t_1\).

Numerical method. Our numerical method relies on replacing the trace \(\text{Tr}\{\phi\} = \sum_n \langle n| \phi |n \rangle\) in Eq. (3) by a scalar product involving a single pure state \(|\psi\rangle\). More precisely, following the concept of quantum typicality, we draw \(|\psi\rangle\) at random according to a probability distribution that is invariant under all possible unitary transformations in Hilbert space (Haar measure). Using a so-constructed \(|\psi\rangle\) and abbreviating \(|\psi_\beta\rangle = e^{-\beta H/2}|\psi\rangle\), the autocorrelation function in Eq. (5) is approximated by \([31, 35]\)

\[
C(t) \approx \text{Re} \frac{\langle \psi_\beta| \dot{\psi}(t)| \psi_\beta \rangle}{N \langle \psi_\beta|\psi_\beta \rangle},
\]

the approximation becoming more accurate as the dimension of the Hilbert space increases \([34, 37]\).

The salient feature of Eq. (5) is that it can be calculated numerically without diagonalization of the Hamiltonian. To this end one has to introduce two pure states: The first reads \(|\Phi_\beta(t)\rangle = e^{-i H t - \beta H/2}|\psi\rangle\) and the second is \(|\varphi_\beta(t)\rangle = e^{-i H t } e^{-\beta H/2}|\psi\rangle\). Then,

\[
\langle \psi_\beta| \dot{\psi}(t) |\psi_\beta \rangle = \langle \Phi_\beta(t)|\dot{\Phi}_\beta(t) \rangle.
\]

The dependence of the two states on \(t\) and \(\beta\) is calculated numerically by a massively parallel implementation of a Suzuki-Trotter product formula or Chebyshev polynomial algorithm. This allows us to study quantum systems with as many as \(N = 36\) spins [Hilbert-space dimension \(d = O(10^{11})\)], although we do not exploit symmetries of Eqs. (1) and (2) at present \([34]\).

Results. We begin with high temperatures \(\beta \to 0\) and an intermediate rung interaction strength \(r = 1\). In Fig. (a) we summarize our numerical results for the spin-current autocorrelation function \(C(t)\) for different system sizes \(N = 20, 24, 28,\) and 36. Clearly, \(C(t)\) rapidly decays towards zero for all \(N\), with almost no finite-size effects visible in the lin-log plot. Particularly, for all \(N\) depicted, there is no signature of a dissipationless contribution of \(C(t)\) for times \(t J_{\parallel} \leq 50\). To illustrate the existence of such a contribution, Fig. (b) shows a semi-log plot of \(C(t)\) up to times \(t J_{\parallel} \leq 400\). Although a dissipationless contribution becomes visible, it amounts to only 1% of the initial value \(C(0)\) for \(N = 20\) and systematically decreases further when system size is increased. Already for \(N = 28\), it takes a tiny value \(\ll 1\%\). Note that we do not determine \(\overline{C}\) for larger \(N\) since, for such \(N\), the computational effort is unreasonably high for the long times \(t J_{\parallel} > 400\) required.

In Fig. we provide a detailed finite-size analysis of the non-decaying contribution, based on system sizes where this contribution can be extracted from the long-time window \([t_1, 2 J_{\parallel}] = [300, 400]\), see Fig. (b) as well as
the definition of $C$ in Eq. (4). Our usage of a log-lin plot unveils an exponential decrease with system size, over more than two orders of magnitude. Certainly, this kind of decrease may be expected for a highly non-integrable model \[35\] but we observe this scaling for various rung couplings $r = 0.25$, $0.5$, $0.75$, and $1$. What is more, the exponent turns out to be practically independent of $r$ while the amplitude scales roughly $\propto 1/r$. Based on these results, we conclude that, for $r > 0$, the Drude weight vanishes in the thermodynamic limit. Compared to earlier studies of transport in gapped 1D spin systems \[13\], we resolve a particularly clean exponential and fast decay of the Drude weight.

Since the Drude weight vanishes, the central quantity of interest is the diffusion constant. In fact, we are able to calculate the diffusion constant even quantitatively using large systems, due to the tiny non-decaying contribution for such systems. Still, we have to choose a finite time $t_2$ for the evaluation of $D$ in Eq. (3). In praxis, we determine the decay time $\tau$, where $C(\tau)/C(0) = 1/e$, and calculate $D$ for $t_2 = 5.5\tau \gg \tau$. For instance, from the data shown for $r = 1$ in Fig. 1(c), we get $t_2 J_{||} \approx 28$ and therefore, a reasonable choice of $t_2$ with little finite-size effects for large $N$. Note that we cannot choose extremely long $t_2$, which would artificially blow up tiny non-decaying contributions or include other finite-size effects.\[30\]

In Fig. 3 we depict the resulting quantitative values of the diffusion constant as a function of the rung coupling $r$. Values for different $N$ illustrate little finite-size effects for all $r$. The log-log plot clearly unveils several regimes with a power-law dependence of $D$ on $r$. More precisely, we observe three qualitatively different regimes: (i) $r \ll 1$: $D \propto 1/r^2$, (ii) $1 \leq r \lesssim 2$: $D \propto 1/r$, and (iii) $r \gg 1$: $D = \text{const}$. Note that in the XXZ chain similar regimes appear as a function of the exchange anisotropy \[30\].

To gain insight into the origin of the scaling of $D$ with $r$, we consider the time dependence of the spin-current autocorrelation function $C(t)$ in more detail. In Fig. (a) we show $C(t)$ for a weak rung coupling $r = 0.25$. Evidently, the time dependence of $C(t)$ is well described by a simple exponential relaxation. Due to this exponential relaxation and the scaling $D \propto 1/r^2$ in Fig. 3, the weak $r \ll 1$ regime turns out to be a conventional perturbative regime \[38\], \[39\]. For $r > 1$ the behavior changes qualitatively. In Fig. (b) we depict $C(t)$ for a corresponding strong rung coupling $r = 1.5$. Here the exponential relaxation turns into a Gaussian decay. This kind of decay, and particularly the scaling $D \propto 1/r$ in Fig. 3 is in line with the generic behavior suggested in Refs. \[38\] and \[39\] for the case of strong perturbations. In fact, according to Ref. \[39\], one expects at high temperatures $\beta \to 0$

$$C(t) = C(0) e^{-r^2 \gamma t^2}, \quad \gamma = \frac{\text{Tr}\{i[j, H_{||}]^2\}}{\text{Tr}\{j^2\}} = \frac{1}{4} \quad (7)$$

and therefore, $D = C(0) \sqrt{\pi/(2r\chi \sqrt{\gamma})} \approx 0.89/r$. The prediction of Eq. (7) is in good agreement with the numerical data for $C(t)$ at $r = 1.5$ in Fig. (b). However, it does not incorporate possible revivals of $C(t)$ that occur in our case because of the band-like spectrum that emerges in the limit of strong rung dimers for $r \to \infty$. In Fig. (b) we illustrate the onset of such revivals for a large rung coupling $r = 4$. These revivals explain the
FIG. 3. (color online) Spin-diffusion constant $D$ versus the coupling ratio $r = J_\perp / J_\parallel$ for high temperatures $\beta \to 0$. There are apparently three scaling regimes: (i) $r \ll 1$: $D \propto 1/r^2$, (ii) $1 \lesssim r \lesssim 2$: $D \propto 1/r$, and (iii) $r \gg 1$: $D = \text{const}$. The $1/r$ curve indicated is given in Eq. (4) and below.

third regime with $D = \text{const}$ as shown in Fig. 3 in analogy to the spin-1/2 XXZ chain, where similar revivals appear close to the trivial Ising limit $\beta J = 0$. The identification of these three regimes characterized by a qualitatively different decay of current autocorrelations is a main result of this Letter.

Finally, we describe an experiment with cold quantum gases, in which our results for the diffusion constant could be verified. XX spin models can be realized with a single-component Bose gas in an optical lattice in the limit of infinitely strong repulsive on-site interactions, see, e.g., Refs. 24 and 40. In order to probe diffusion, one would desire a homogeneous background density with half a particle per site, which could be accomplished by using a box trap [41] instead of harmonic trapping potentials.

The basic idea to measure $D$ is to induce a local perturbation in the density, by, e.g., superimposing a dimple trap using methods along the lines of [42], and then to monitor the time evolution of the density profile as a function of position. From such information, one can extract the diffusion constant from the time dependence of the variance, as demonstrated numerically for 1D spin systems.

The qualitative dependence of $D$ on $r$ depends on temperature (see, e.g., Ref. 44 for a theory of diffusion in 1D gapped quantum magnets at low $T$) and therefore, it is necessary to put the gas at sufficiently high temperatures to be able to observe our qualitative predictions. This can be done by subjecting the gas to heating. We checked that the qualitative decay of $C(t)$ does not change down to $T/J_\parallel \sim 2$ and hence it is reasonable to expect no qualitative changes in the $r$ dependence of $D$ either. Similarly, small deviations from $\langle S^z \rangle = 0$ do not seem to change the picture qualitatively.

**Conclusion.** We studied the dynamics of spin currents in the spin-1/2 XX ladder at finite temperature. Within the framework of linear response theory, we numerically calculated autocorrelation functions for large quantum systems by exploiting the concept of dynamical quantum typicality. We showed that spin Drude weights vanish exponentially fast with increasing system size. We further found qualitatively different dependencies of the spin diffusion coefficient on the rung-interaction strength, resulting from a crossover from exponential to Gaussian dissipation at intermediate coupling strengths, which we also derived analytically.

We thank U. Schneider for helpful discussions. F. H.-M. acknowledges support from the DFG through FOR 912 via grant HE-5242/2-2. The authors gratefully acknowledge the computing time granted by the JARA-HPC Vergabegremium and provided on the JARA-HPC Partition part of the supercomputer JUQUEEN at Forschungszentrurn Jülich.

FIG. 4. (color online) Spin-current autocorrelation function $C(t)$ for high temperatures $\beta \to 0$ and qualitatively different regimes of the coupling ratio $r = J_\perp / J_\parallel$. (a) Weak-$r$ regime: The decay curve of $C(t)$ is exponential and thus supports the expectation $D \propto 1/r^2$ from conventional perturbation theory. (b) Strong-$r$ regime: The decay curve agrees with the Gaussian prediction in Eq. (4) and is in line with the generic behavior $D \propto 1/r$ suggested in Refs. 39 and 38. However, for large $r$, revivals occur due to the simple structure of the spectrum in the rung-dimer limit of $r \to \infty$, resulting in $D = \text{const}$. In (b) $C(t)$ is shown for a finite temperature $\beta J_\parallel = 0.5$ also.

* r.steinigeweg@tu-bs.de

[1] X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B 55, 11029 (1997).
[2] F. Heidrich-Meisner, A. Honecker, and W. Brenig, Eur. J. Phys. Special Topics 151, 135 (2007).
[3] M. Žnidarič, Phys. Rev. Lett. 106, 220601 (2011).
[4] R. Steinigeweg and W. Brenig, Phys. Rev. Lett. 107, 250602 (2011).
[5] A. Rosch and N. Andrei, Phys. Rev. Lett. 85, 1092 (2000).
See supplemental material.
FIG. S1. (color online) Spin-current autocorrelation function $C(t)$ in the XX ladder for (a) $\langle S^z \rangle = 0$, (b) $S^z = 0$ for a strong rung coupling $r = J_\perp / J_\parallel = 1.5$ in the high-temperature limit $\beta \to 0$. (c) The resulting time-dependent diffusion coefficient, as extracted from $C(t)$ depicted in (a), (b). Although finite-size results for $\langle S^z \rangle = 0$ and $S^z = 0$ differ from each other, they seem to converge to the same value in the thermodynamic limit. Apparently, the convergence of $\langle S^z \rangle = 0$ is much faster in time and there are no finite-size effects up to times $t J_\parallel \sim 10$ comparing $N = 28$ and $N = 34$. Hence, our choice of $t_2 J_\parallel = 8.3$ for extracting $D$ from $D(t)$ is reasonable.

FIG. S2. (color online) Spin-current autocorrelation function $C(t)$ in the XX ladder for rung couplings (a) $r = 0.25$, (b) $r = 1.5$, (c) $r = 4$ in the high-temperature limit $\beta \to 0$ and $\langle S^z \rangle = 0$, $S^z = 0$, $S^z = 1$. In all cases, $N = 34$. Apparently, the cases of half filling $S^z = 0$ and almost half filling $S^z = 1$ are practically identical for finite $N$ already. No significant difference to $\langle S^z \rangle = 0$ is visible for $r = 0.25$, while differences for larger $r$ are finite-size effects, as illustrated in Fig. S1.
FIG. S3. (color online) Spin-current autocorrelation function $C(t)$ in the XX ladder for rung couplings (a) $r = 0.5$, (b) $r = 1.5$, (c) $r = 4$ and different temperatures $\beta J_{\parallel} \leq 1$. In all cases, $\langle S^z \rangle = 0$ and $N = 28$. Apparently, $C(t)$ is qualitatively the same for temperatures down to $\beta J_{\parallel} \sim 0.5$. 