Density dynamics in translationally invariant spin-$\frac{1}{2}$ chains at high temperatures: A current-autocorrelation approach to finite time and length scales

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We investigate transport in several translationally invariant spin-$\frac{1}{2}$ chains in the limit of high temperatures. We concretely consider spin transport in the anisotropic Heisenberg chain, the pure Heisenberg chain within an alternating field, and energy transport in an Ising chain which is exposed to a tilted field. Our approach is essentially based on a connection between the evolution of the variance of an inhomogeneous nonequilibrium density and the current-autocorrelation function at finite times. Although this relationship is not restricted to the case of diffusive transport, it allows to extract a quantitative value for the diffusion constant in that case. By means of numerically exact diagonalization we indeed observe diffusive behavior in the considered spin chains for a range of model parameters and confirm the diffusion coefficients which were obtained for these systems from nonequilibrium bath scenarios.

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I. INTRODUCTION

Although transport in low-dimensional quantum systems has intensively been investigated theoretically in the past years, there still is an ongoing interest in understanding the transport phenomena in such systems, including their temperature and length-scale dependence.[1–31] Those works have often addressed a qualitative classification of the occurring transport types into ballistic or normal diffusive behavior and, in particular cases, the crucial mechanisms which are responsible for the emergence of diffusion have been studied. In this context the role of nonintegrability and quantum chaos is frequently discussed as an at least necessary condition.[9,10,21,28,30] Significant theoretical attention has been devoted to spin-$\frac{1}{2}$ chains,[1–23] e.g., to the prominent anisotropic Heisenberg chain (XXZ model).[1–19] Most controversial question appears whether or not the (finite temperature) transport in the pure Heisenberg chain is ballistic.[1–12]

Even though there certainly is a large variety of different methods for the investigation of transport in quantum systems, we concentrate here on two of the main approaches in detail which are also most relevant in the context of the present work. The first approach may be classified as a direct one since it is rather close to an experimental measurement setup: within the theory of open quantum systems[32] the model of interest is coupled locally, e.g., at both ends of a spin chain, to reservoirs of the transported quantity, e.g., at different temperature or chemical potential.[3,13,16,20–22,24,31,33] Due to the coupling to reservoirs, a stationary nonequilibrium state eventually results for which all relevant expectation values such as the current and the spatial-density profile of the transport quantity can be evaluated. Here, a vanishing profile corresponds to ballistic behavior, whereas normal diffusive dynamics is associated with a strictly linear profile, according to Fourier's law, respectively, Fick's law, see, e.g., Ref. 13. In the latter case a finite conductivity is simply given by the ratio of the current and the spatial-density gradient of the transported quantity. This conductivity can be also understood in terms of a diffusion coefficient since transport is driven by a gradient within the considered model and not by an external force.[34] One may therefore directly compare with the diffusion constant of a corresponding closed scenario, where transport is not induced by the coupling to baths but by an initially inhomogeneous nonequilibrium density.[31,34]

In order to simulate the influence of the baths the Liouville-von Neumann equation for the coherent evolution of the density matrix is routinely extended by an incoherent damping term, see, e.g., Ref. 33. The derivation of such a dynamical equation from a microscopic bath model is highly nontrivial and involves a combination of various subtle approximation schemes, e.g., improper approximations may eventually lead to a mathematically correct but physically irrelevant quantum master equation (QME).[33] One often intends to derive a proper QME of the Lindblad form[35] because its special structure allows to apply the numerically efficient method of stochastic unraveling,[36,37] e.g., spin-$\frac{1}{2}$ chains with about 16 sites become numerically tractable.[16] However, a recently suggested matrix-product operator ansatz has been shown to significantly increase this number of available sites up to several dozens,[13] i.e., finite-size effects are drastically reduced and the extracted conductivity may be interpreted as a pure bulk property of the model, if it does not depend crucially on the concrete form and strength of the bath coupling, of course.[31]

Another approach for the investigation of transport in quantum systems is the Green-Kubo formula (KF) which was originally derived for electrical conductance by the use of linear-response theory.[38,39] In that case the (frequency-dependent) electrical field is an external force which perturbs the system and the resulting current of charge through the system is the response to this external perturbation. The KF as such gives the (frequency-dependent) conductivity as the linear-response coefficient in terms of a current-autocorrelation function. The same approach is also used in the context of gradient-driven transport phenomena, e.g., for transport of energy or heat. In that case the current is driven by a much more complicated mechanism,[25,27,40–44] especially since it cannot be treated as a perturbation to the system. Nevertheless, simply by the replacement of the electrical current, e.g.,

by the energy current,[40] the KF is used for gradient-driven transport, too. But a rigorous justification of this replacement remains still a conceptual problem, see Ref. 25 or the overview paper Ref. 41 (and the comprehensive literature which is cited therein).

However, the KF is nowadays a standard method for the investigation of transport in spin chains,[1,2,4–8,15,20,23] not least due to its direct computability, once a finite piece of the considered system has been exactly diagonalized. As far as numerics is concerned, exact diagonalization is restricted to spin-$\frac{1}{2}$ chains with at most 24 sites. But another difficulty arises, if the KF is evaluated on the basis of a finite piece: one often distinguishes between ballistic and normal diffusive transport by the notion of the Drude weight, essentially the conductivity's singular contribution at zero frequency, see the review, Ref. 7, for example. Whenever it is finite, the long-time behavior is expected to be ballistic, and whenever it vanishes, the dc conductivity as the zero-frequency limit of the conductivity's regular nonsingular part determines the long-time behavior. Since for any finite system the conductivity exclusively consists of delta peaks at different frequencies, there apparently are only singular contributions and it therefore is a difficult question how to extract and extrapolate the dc conductivity from a finite system.[25] Moreover, the quantitative comparison of the resulting dc conductivity (due to a possibly hypothetic external force) with a diffusion constant (from nonequilibrium bath scenarios) is hardly possible without the detailed knowledge about an Einstein relation between both quantities.

In the present paper we do not intend to further discuss the above-mentioned conceptual and methodological problems which may come along with the KF. Instead we will present a different but in a sense related approach which particularly is not concerned with the most of those problems. To this end we will first introduce a "typical" inhomogeneous nonequilibrium density in Sec. II and then connect the evolution of the variance of this density to a current-autocorrelation function at finite times.[34] Remarkably, in the special limit of infinitely long times this connection will be shown to yield a generalized Einstein relation which relates the diffusion constant to the dc conductivity, i.e., as evaluated by the KF. Moreover, we will demonstrate that the great advantage of the connection is given by its direct applicability at finite times and for finite systems as well. In this context we will suggest another concept for the analysis of data which is available from current-autocorrelation functions.

By the use of the suggested concept we will investigate in Secs. III–V transport in several translationally invariant spin-$\frac{1}{2}$ chains in the special limit of high temperatures. We will concretely consider spin transport in the anisotropic Heisenberg chain, the pure Heisenberg chain within an alternating field, and energy transport in an Ising chain which is exposed to a tilted field. By means of numerically exact diagonalization we indeed observe strong indications for diffusive behavior in the considered spin chains for a range of model parameters and, what is more, we are able to quantitatively confirm the diffusion constants which were found for these systems from nonequilibrium bath scenarios in Refs. 13, 16, 21, and 22. Finally, we will close in Sec. VI with a summary and a conclusion.

II. CONNECTION BETWEEN VARIANCE AND CURRENT-AUTOCORRELATION FUNCTION

In this section we are going to introduce our approach to density-driven transport in translationally invariant quantum systems. To this end Sec. II A first presents the pertinent definitions and exclusively describes the general theory which eventually yields the basic Eq. (13) for the time-dependent diffusion constant $\mathcal{D}(t)$. In the following Sec. II B we then motivate to evaluate $\mathcal{D}(t)$ for finite times t and particularly illustrate the concept which will be used for the concrete spin chains in the subsequent sections. Thus, the reader which is not primarily interested in the theoretical details may directly continue with Sec. II B.

A. Diffusion constant

In the present paper we will investigate translationally invariant, one-dimensional quantum spin systems which are described by a respective Hamiltonian $\hat{H}$. In those quantum systems we will consider an overall conserved transport quantity $\hat{X}$, i.e., $[\hat{H},\hat{X}]=0$. This transport quantity and the Hamiltonian as well are decomposable into N formally identical addends $\hat{x}_\mu$, respectively, $\hat{h}_\mu$ corresponding to different positions, i.e.,

$$\hat{X}=\sum_{\mu=1}^{N}\hat{x}_\mu,\quad \hat{H}=\sum_{\mu=1}^{N}\hat{h}_\mu. \tag{1}$$

Thus, $\hat{x}_\mu$ is a local density of the transported quantity $\hat{X}$. Note that the $\hat{x}_\mu$ may be defined on the positions of the $\hat{h}_\mu$, in between, or both. The above decomposition is further done in such a way that Heisenberg's equation of motion for the local densities $\hat{x}_\mu$ reads

$$\frac{d}{dt}\hat{x}_\mu=\imath[\hat{H},\hat{x}_\mu]=\underbrace{\imath[\hat{h}_{\mu^-},\hat{x}_\mu]}_{\equiv\hat{j}_{(\mu-1)}}+\underbrace{\imath[\hat{h}_{\mu^+},\hat{x}_\mu]}_{\equiv-\hat{j}_\mu}, \tag{2}$$

where $\hat{h}_{\mu^-}$ and $\hat{h}_{\mu^+}$ represent those local addends of the Hamiltonian $\hat{H}$ which are located directly on the left-hand side, respectively, right-hand side of $\hat{x}_\mu$. This apparently implies a kind of locality. However, such a description can always be at least approximately enforced, if only interactions are reasonably short ranged. For all quantum systems in the following Secs. III–V the description will be even exact because interactions between nearest neighbors are taken into account solely. As routinely done, the comparison with a continuity equation suggests the definition of a local current $\hat{j}_\mu$ according to the scheme in Eq. (2), see Ref. 25, for example. This definition is consistent, if

$$\underbrace{\imath[\hat{h}_{\mu^+},\hat{x}_\mu]}_{-\hat{j}_\mu}+\underbrace{\imath[\hat{h}_{(\mu+1)^-},\hat{x}_{(\mu+1)}]}_{\hat{j}_\mu}=0, \tag{3}$$

where the latter holds, if $\hat{X}$ is globally preserved. The total current $\hat{J}$ is given by

$$\hat{J} = \sum_{\mu=1}^{N} \hat{j}_\mu. \tag{4}$$

Once the above decomposition has been established, we can define a certain class of initial states $\rho(0)$ which corresponds to some inhomogeneous, nonequilibrium density. To those ends let

$$\hat{d}_\mu \equiv \hat{x}_\mu - \langle \hat{x}_\mu \rangle \tag{5}$$

denote the deviation of the local densities $\hat{x}_\mu$ from their equilibrium average $\langle \hat{x}_\mu \rangle = \mathrm{Tr}\{\hat{x}_\mu \rho_{\mathrm{eq}}\}$, where ρ_{eq} is any stationary equilibrium state, i.e., $[\hat{H}, \rho_{\mathrm{eq}}] = 0$. Then the initial state $\rho(0)$ reads

$$\rho(0) \equiv \rho_{\mathrm{eq}} + \sum_{\mu=1}^{N} \frac{\delta_\mu}{\epsilon^2} \rho_{\mathrm{eq}}^{1/2} \hat{d}_\mu \rho_{\mathrm{eq}}^{1/2} \tag{6}$$

with some realization for the numbers δ_μ. The factor ϵ^2 is concretely given by

$$\epsilon^2 \equiv \frac{1}{N}(\langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2) \tag{7}$$

and therefore quantifies the equilibrium fluctuations of the transported quantity $\hat{X}$.

For the special initial state $\rho(0)$ we now consider the actual expectation values

$$d_\mu(t) \equiv \mathrm{Tr}\{\hat{d}_\mu(t)\rho(0)\}. \tag{8}$$

It follows that

$$\sum_{\mu=1}^{N} d_\mu(t) = \sum_{\mu=1}^{N} \delta_\mu \equiv \delta, \tag{9}$$

i.e., the sum δ of the numbers δ_μ in Eq. (6) determines the sum of the actual expectation values $d_\mu(t)$.

Of particular interest is the spatial variance $W^2(t)$ of the $d_\mu(t)$. It is given by

$$W^2(t) \equiv \sum_{\mu=1}^{N} \frac{d_\mu(t)}{\delta} \mu^2 - \left[\sum_{\mu=1}^{N} \frac{d_\mu(t)}{\delta} \mu \right]^2. \tag{10}$$

If the dynamics of the $d_\mu(t)$ was indeed generated by a discrete diffusion equation of the form

$$\frac{d}{dt} d_\mu(t) = \mathcal{D}(t)[d_{\mu-1}(t) - 2d_\mu(t) + d_{\mu+1}(t)], \tag{11}$$

then the evolution of this variance would read

$$\frac{d}{dt} W^2(t) = 2\mathcal{D}(t), \tag{12}$$

as long as the $d_\mu(t)$ vanish at the ends of a chain (open boundary conditions) or are reasonably concentrated at a sector of a ring (closed boundary conditions). Even though Eq. (11) implies Eq. (12), the inverse direction generally is not true, of course.

However, in Ref. 29 a connection of the form (12) has recently been found directly from Eq. (10), i.e., by first applying Heisenberg's equation of motion to Eq. (10) and subsequently manipulating the resulting equations. The time-dependent diffusion constant $\mathcal{D}(t)$ reads

$$\mathcal{D}(t) = \frac{1}{N\epsilon^2} \int_0^t dt' C(t') \tag{13}$$

and is essentially given in terms of a time integral over the current-autocorrelation function

$$C(t) \equiv \mathrm{Tr}\{\hat{J}(t)\rho_{\mathrm{eq}}^{1/2} \hat{J} \rho_{\mathrm{eq}}^{1/2}\}, \tag{14}$$

i.e., $C(t) = \langle \hat{J}(t)\hat{J} \rangle$ in the limit of high temperatures ($T \to \infty$). This limit will be considered throughout this work.

Strictly speaking, the above diffusion constant $\mathcal{D}(t)$ is restricted to the special initial state $\rho(0)$ in Eq. (6), of course. Nevertheless, due to its concrete form, this initial state represents an ensemble average w.r.t. to typicality[45–47] or, more precisely, the dynamical typicality of quantum expectation values.[48] Thus, the overwhelming majority of all possible initial states with the same $d_\mu(0)$ as $\rho(0)$ is also expected to approximately yield the $d_\mu(t)$ corresponding to $\rho(0)$, if the dimension of the relevant Hilbert space is sufficiently large, see especially Ref. 48. The latter largeness is certainly fulfilled for all practical purposes. Or, in other words, the concrete curves for $d_\mu(t)$ and thus for $W^2(t)$ only slightly "fluctuate" around the curve of the ensemble average. In fact, for the single-particle quantum system in Refs. 25, 26, 29, and 49 it has been demonstrated that Eqs. (12)–(14) correctly describe the dynamics for all pure initial states $|\psi(0)\rangle$ which are not created explicitly in order to violate these equations, see Ref. 25 and 49.

Eventually, let us relate the nonperturbative result for the diffusion constant $\mathcal{D}(t)$ to the standard result of linear-response theory for the dc conductivity σ_{dc}.[38,39] In the limit of high temperatures this conductivity may be written as

$$\sigma_{\mathrm{dc}} = \frac{\beta}{N} \int_0^\infty dt' C(t'), \tag{15}$$

where β is the inverse temperature. The comparison of Eq. (15) with Eq. (13) yields

$$\mathcal{D}(t \to \infty) = \frac{\sigma_{\mathrm{dc}}}{\beta\epsilon^2}, \tag{16}$$

i.e., it leads to an Einstein relation. It is well known that the integral in Eq. (15) will diverge, whenever $C(\omega)$, the Fourier transform of $C(t)$, has a finite contribution at $\omega = 0$, see Ref. 7, for example. As routinely done, we may hence define a Drude weight D, e.g.,

$$D \equiv \lim_{t\to\infty} \frac{\mathcal{D}(t)}{t} = \frac{C(\omega = 0)}{N\epsilon^2}. \tag{17}$$

B. Finite time and length scales

If the total current is strictly preserved, i.e., $[\hat{H}, \hat{J}] = 0$, the diffusion constant $\mathcal{D}(t)$ is completely governed by the Drude weight D, i.e., $\mathcal{D}(t) = Dt$ for all t. Consequently, transport is

purely ballistic at each time, respectively, length scale. Even if the total current does not represent a strictly conserved quantity, a nonzero Drude weight directly implies that the diffusion constant $\mathcal{D}(t)$ is still approximately given by the straight line Dt in the limit $t\to\infty$. However, at some finite time or length scale the diffusion constant $\mathcal{D}(t)$ may nevertheless appear to be almost constant, i.e., $\mathcal{D}(t)\approx\mathcal{D}$, as expected for diffusive behavior. Such a behavior requires that the Drude weight D is not relevantly large (on the corresponding scale), the finiteness of D by itself is not crucial in this context. In fact, it is well known that the classification of transport types for a given quantum system generally is a concept which crucially depends on the considered time or length scale, see Refs. 25, 26, and 29, for example.

The above line of reasoning becomes also relevant in those situations where some model parameter λ induces a transition from a finite toward a zero Drude weight D, e.g., where D vanishes above some critical value of λ, say λ_C. Then at this critical value λ_C a sharp transition from ballistic toward nonballistic transport is to be expected at the infinite time scale. However, such a transition does not necessarily appear at some finite time, respectively, length scale. Even if there was a transition, a sharp one would require at the critical value λ_C a sudden jump of the Drude weight D from a finite and relevantly large number (on the corresponding scale) to zero.

We hence do not concentrate merely on Drude weights and their finiteness, although those are also discussed, of course. Instead of that we focus on the diffusion constant $\mathcal{D}(t)$, as defined in Eq. (13), at finite times and for finite systems as well. According to Eq. (13), we can evaluate the underlying current-autocorrelation function directly in the time domain, i.e., $C(t)$, instead of the frequency domain, i.e., $C(\omega)$. This way we are not concerned with the problems which may arise due to the fact that $C(\omega)$ is a highly nonsmooth function for a finite system. We particularly exploit that the $\mathcal{D}(t)$ curve does not change at sufficiently short-time scales any more, when the size of a system becomes large enough. Thus, at those short-time scales, interesting signatures of the infinitely large system may already be extractable for a system with an accessible size. In the following Secs. III–V this concept will be demonstrated in full detail.

III. ISING CHAIN WITHIN A TILTED FIELD

In the present section we will study a first example of a translationally invariant spin system. This system is an Ising chain which is exposed to a, say, tilted magnetic field $\mathbf{B}$. Concretely, its Hamiltonian reads ($\hbar=1$),[13,21,22]

$$\hat{H}=\sum_{\mu=1}^{N}\hat{h}_{\mu},$$

$$\hat{h}_{\mu}=\frac{J}{4}\hat{\sigma}_{\mu}^{z}\hat{\sigma}_{\mu+1}^{z}+\frac{B_z}{4}(\hat{\sigma}_{\mu}^{z}+\hat{\sigma}_{\mu+1}^{z})+\frac{B_x}{4}(\hat{\sigma}_{\mu}^{x}+\hat{\sigma}_{\mu+1}^{x}), \quad (18)$$

where B_z and B_x denote the z component, respectively, x component of the total vector $\mathbf{B}=(B_x,0,B_z)$. Here, one might think of some magnetic field which originally was in line with the z direction and has been rotated about the y axis with the angle $\alpha=\arctan(B_x/B_z)$.

In Hamiltonian (18) the operators $\hat{\sigma}_{\mu}^{i}(i=x,y,z)$ are the standard Pauli matrices (corresponding to site μ); J denotes the coupling strength; and N represents the total number of sites. Throughout this work we use periodic boundary conditions, i.e., $N+1\equiv 1$.

Due to the presence of the tilted magnetic field, the only trivial symmetries are translational invariance and mirror symmetry[21] such that the whole Hilbert space is decomposable into $2N$ decoupled subspaces with similar dimensions. For the present model the component of the total spin $\hat{\mathbf{S}}=1/2\Sigma_{\mu=1}^{N}\hat{\sigma}_{\mu}$ in $\mathbf{B}$ direction (and any other direction) is nonpreserved. Therefore magnetization (or spin) is not a suitable transport quantity here.

However, this model is appropriate to investigate the transport of energy, i.e., it allows to study the density dynamics of the local quantities $\hat{h}_{\mu}$, see Eq. (18). Note that these quantities contain contributions from both the Ising interaction and the Zeeman energy. The respective energy current $\hat{J}^{E}$ is given by[13,21,22]

$$\hat{J}^{E}=\sum_{\mu=1}^{N}\hat{j}_{\mu}^{E},$$

$$\hat{j}_{\mu}^{E}=\imath[\hat{h}_{\mu},\hat{h}_{\mu+1}]=-\frac{B_x J}{8}(\hat{\sigma}_{\mu}^{z}-\hat{\sigma}_{\mu+2}^{z})\hat{\sigma}_{\mu+1}^{y} \quad (19)$$

and the factor ϵ^2, as defined in Eq. (7), reads

$$\epsilon^2=\frac{1}{16}(J^2+2B_z^2+2B_x^2). \quad (20)$$

If the component B_z is identical to zero ($\alpha=90°$), the energy current, Eq. (19), is strictly preserved. Furthermore, Hamiltonian (18) is well known to be integrable. But it can become quantum chaotic for $B_z\neq 0$, e.g., for the special set of parameters $J=-8$, $B_z=4$, $B_x=6.75(\alpha\approx 59°)$.[13,21,22] Recently, for exactly this parameter set, a strong evidence for diffusive behavior has been found from nonequilibrium bath scenarios.[13,21,22]

Figure 1 (top) shows the diffusion constant $\mathcal{D}(t)$, as given by Eq. (13), for the above set of parameters. We observe that $\mathcal{D}(t)$ increases within the correlation time of the underlying current-autocorrelation function but, already on this time scale, essentially the Drude weight governs the overall shape of the curve, at least for small lengths $N\approx 8$. But when N is increased, the Drude weight D rapidly becomes smaller, i.e., D decreases faster than a power law, see Fig. 2 (squares). In particular, there is no need to assume a finite and relevant value for D in the thermodynamic limit $N\to\infty$. Already for $N\approx 16$ the Drude weight D is such small that the tendency of the diffusion constant $\mathcal{D}(t)$ to gradually develop toward a horizontal line becomes visible. Nevertheless, only from those lengths which are available from numerically exact diagonalization a definite conclusion may still be vague, particularly conclusions about the time after which $\mathcal{D}(t)$ possibly remains constant and about the constant value $\mathcal{D}$, too.

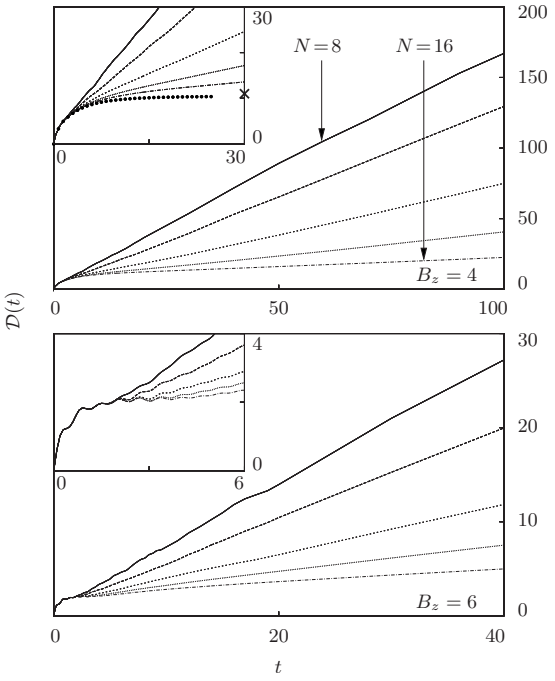

FIG. 1. The diffusion constant $\mathcal{D}(t)$, as given by Eq. (13), for energy transport in the Ising chain within a tilted field in the high-temperature limit ($T=\infty$). Insets zoom in $\mathcal{D}(t)$ at short t. Parameters: $J=-8$, $B_x=6.75$, $B_z=4$ (top) as well as $B_z=6$ (bottom). All curves are evaluated numerically (exact diagonalization) for chain lengths $N=8,10,\ldots,16$ (arrows). The circles (top inset) represent additional data for $N=24$, extracted from Ref. 21 and computed by the use of approximative numerical integrators. The cross (top inset) indicates the conductivity $\mathcal{D}_{\text{bath}}=11$ from Ref. 13 (Ref. 50), as obtained from a nonequilibrium bath scenario for the same set of parameters.

Fortunately, additional data is available in literature: In Ref. 21 the current-autocorrelation function has been evaluated also by the use of an approximative numerical integrator. Based on this data the time evolution of the diffusion constant $\mathcal{D}(t)$ can be extracted[51] for the length $N=24$, see Fig. 1 (top inset). And in fact, for times which are larger than $t\approx 10$ we observe that $\mathcal{D}(t)$ takes on a constant value $\mathcal{D}\approx 10.5$. The latter value further is in excellent agreement with the conductivities $\mathcal{D}_{\text{bath}}\approx 10.3$ from Ref. 21 and $\mathcal{D}_{\text{bath}}=11$ from Ref. 13 (Ref. 50), as obtained therein for the same set of parameters from nonequilibrium bath scenarios. (In these works $\mathcal{D}_{\text{bath}}$ is denoted by κ.)

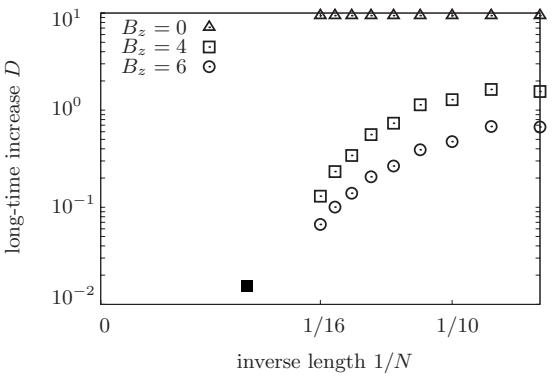

FIG. 2. The long-time increase D of the diffusion constant $\mathcal{D}(t)$, the Drude weight, for energy transport in the Ising chain within a tilted field at high temperatures ($T=\infty$). Parameters: $J=-8$ and $B_x=6.75$. All open symbols are evaluated numerically (by the use of exact diagonalization) for chain lengths $N\leq 16$ and for z components $B_z\leq 6$. The filled square is extracted from Ref. 21 and represents an upper bound for $N=24$.

When the z component is decreased from $B_z\approx 4$ down to 0, diffusive behavior eventually breaks down toward ballistic transport, because the current becomes strictly preserved for $B_z=0$. Unfortunately, it is hardly possible to give a critical value for this transition, simply due to the limited system sizes which are accessible by the use of exact diagonalization. However, such a value may be very unsharp for a continuous transition, i.e., if the Drude weight changes smoothly and does not jump suddenly from zero (or a finite, irrelevantly small number) to a finite, relevantly large number, cf. Sec. II.

Contrary, when the z component is increased from $B_z\approx 4$, the indications of diffusive behavior become much more pronounced for the accessible system sizes, cf. Fig. 1 (bottom). Respective diffusion constants may therefore be suggested for this parameter regime.

IV. ANISOTROPIC HEISENBERG CHAIN

In this section we will investigate transport in the anisotropic Heisenberg chain (or XXZ model) as another and certainly more interesting example of a translationally invariant spin system. It is described by a Hamiltonian of the form ($\hbar=1$),[6,7,13,16]

$$\hat{H}=\sum_{\mu=1}^{N}\hat{h}_\mu,$$

$$\hat{h}_\mu=\frac{J}{4}(\hat{\sigma}_\mu^x\hat{\sigma}_{\mu+1}^x+\hat{\sigma}_\mu^y\hat{\sigma}_{\mu+1}^y+\Delta\hat{\sigma}_\mu^z\hat{\sigma}_{\mu+1}^z) \tag{21}$$

with the anisotropy parameter Δ. Independent from the concrete choice of Δ, Hamiltonian (21) is integrable in terms of the Bethe Ansatz, see Ref. 1, for example.

In the presence of an external (uniform) magnetic field B one may add to Hamiltonian (21) a Zeeman term of the form $\hat{H}_B=B\hat{S}^z$. However, because the following investigation (at infinite temperature) will not depend on the concrete choice of B, we set $B=0$ for simplicity.

As well known, Hamiltonian (21) is invariant under rotations about the z axis, i.e., it commutates with $\hat{S}^z$. As a consequence $\hat{H}$ can be diagonalized within decoupled subspaces with dimensions N over $M+N/2$, where M is the quantum number w.r.t. $\hat{S}^z$. Moreover, due to the translational invariance as well as the mirror symmetry of Eq. (21), the problem can be reduced further by a factor $2N$.

Since $\hat{S}^z$ represents a strictly conserved quantity, this model allows to investigate the density dynamics of the local quantities $\hat{\sigma}_\mu/2$, i.e., magnetization transport (or spin trans-

port). The respective magnetization current $\hat{j}^S$ is given by[6,7,13,16]

$$\hat{j}^S = \sum_{\mu=1}^{N} \hat{j}^S_\mu,$$

$$\hat{j}^S_\mu = \imath\left[\frac{1}{2}\hat{\sigma}^z_\mu, \hat{h}_\mu\right] = \frac{J}{4}(\hat{\sigma}^x_\mu\hat{\sigma}^y_{\mu+1} - \hat{\sigma}^y_\mu\hat{\sigma}^x_{\mu+1}) \tag{22}$$

and the factor ϵ^2, as defined in Eq. (7), takes on the fixed value 1/4.

Similarly, an energy current can be also introduced via the relation $\hat{j}^E_\mu = \imath[\hat{h}_\mu, \hat{h}_{\mu+1}]$. But, since its commutator with Hamiltonian (21) vanishes exactly, this current is strictly conserved such that energy transport is purely ballistic at each time scale and length scale (and for all finite temperatures, see Ref. 19).

Except for the special case of $\Delta=0$ (XY model) the magnetization current is nonpreserved. On that account it could be, in principle, possible to find diffusive behavior for nonzero anisotropies. Nevertheless, in the literature there is strong evidence that such a behavior is restricted to the regime $\Delta>1$ only,[1,2,4–8,11,13,14,16] most promising appear those Δ which are close to 1.5.[13,14,16] Those expectations are also due to results on the Drude weight D,[1,4,8] e.g., Bethe Ansatz approaches suggest that D is finite for the regime $\Delta<1$ and zero for the regime $\Delta>1$.[1,8] Still controversial is the special case of $\Delta=1$, where D may be already zero[1] or not.[8]

For completeness, we also show numerical results for the Drude weight in Fig. 5, although respective data can be found already in Ref. 4, also obtained by the use of exact diagonalization and additionally extrapolated to $N\to\infty$. This data can be transferred directly to the present investigation, if the concrete values for the Drude weight are multiplied by a factor $1/(\epsilon^2\pi)=4/\pi$. Further results on Drude weights from exact diagonalization can be found in, e.g., Refs. 2, 5, and 6.

A. Anisotropies $\Delta<1$

Figure 3 shows the diffusion constant $\mathcal{D}(t)$, as defined in Eq. (13), for the anisotropy parameter $\Delta=0.5$. For $N=8$ the Drude weight D determines the overall shape of the $\mathcal{D}(t)$ curve, i.e., on all time scales $\mathcal{D}(t)$ is very close to the straight line Dt. There is only an insignificant deviation from this line at short-time scales below the correlation time of the underlying current-autocorrelation function, see Fig. 3 (inset). For $N=20$, i.e., when the length of the chain is more than doubled, the $\mathcal{D}(t)$ curve remains practically the same. On that account it appears to be justified to assume a similar curve in the thermodynamic limit $N\to\infty$. This assumption is consistent with the extrapolation of the Drude weight in Ref. 4, see Fig. 5 (squares), too. We may therefore suggest purely ballistic behavior for the case $\Delta=0.5$.

Note that Sirker *et al.* have recently presented results in Ref. 12 which point toward a coexistence of diffusive and ballistic dynamics, where the ballistic distribution is small due to a small Drude weight. Even though we reproduce that the Drude weight is large for $N\leq 20$ and does not depend significantly on N, we cannot exclude the possibility that the Drude weight eventually becomes small for $N\gg 20$, of course.

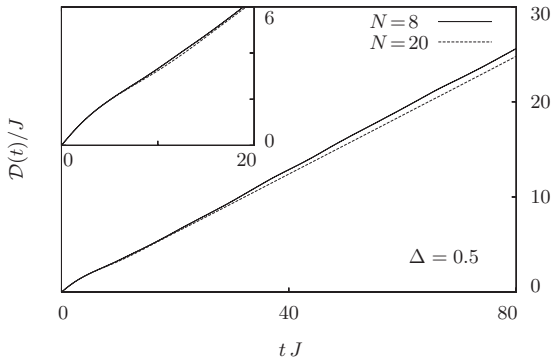

FIG. 3. The diffusion constant $\mathcal{D}(t)$, as given by Eq. (13), for magnetization transport (spin transport) in the anisotropic Heisenberg chain (XXZ model) in the high-temperature limit ($T=\infty$). Insets zoom in $\mathcal{D}(t)$ at short t. The curves are evaluated numerically (by the use of exact diagonalization) for the anisotropy parameter $\Delta=0.5$ and for chain lengths $N=8$ and 20.

B. Anisotropies $\Delta>1$

In Fig. 4 (middle) we display the diffusion constant $\mathcal{D}(t)$ for the anisotropy $\Delta=1.5$. We observe that $\mathcal{D}(t)$ increases at short-time scales, i.e., within the correlation time of the underlying current-autocorrelation function $C(t)$, and then remains approximately constant for an interval at intermediate time scales, i.e., a "plateau" is formed at those times. Finally, a renewed increase takes place on long-time scales which is completely governed by the Drude weight or by the zero-frequency distribution of $C(\omega)$. Note that the plateau cannot be seen, if zero- and finite-frequency parts are treated separately from each other. It is a feature which arises from a combination of both contributions.

The above plateau remarkably is already visible for $N=8$. Moreover, its "height" does not change with N, while its "width" seems to increase gradually, see Fig. 4 (middle inset). The latter increase particularly appears to be plausible because the Drude weight is commonly expected to vanish in the thermodynamic limit $N\to\infty$, as already outlined above. We hence make the educated guess that the plateau of $\mathcal{D}(t)$ will be continued to, say, arbitrary long times, when only N becomes sufficiently large, e.g., $N\to\infty$. Then the height $\mathcal{D}/J\approx 0.60$ directly determines the concrete value of the diffusion constant, of course. And indeed, the latter value for $\mathcal{D}$ also is in excellent agreement with the conductivity $\mathcal{D}_{\text{bath}}/J=0.58$ in Ref. 13 (Ref. 50), as found therein from a nonequilibrium bath scenario. Although a respective figure is not shown for $\Delta=1.6$, such an agreement is additionally obtained with the results in Ref. 16, namely, $\mathcal{D}/J\approx 0.55$ and $\mathcal{D}_{\text{bath}}/J=0.585\pm 0.020$. (In these works $\mathcal{D}_{\text{bath}}$ is denoted by κ.) Those quantitative agreements support the correctness of our guess and the emergence of diffusive transport appears to be verified for those Δ which are close to 1.5.

Independent from the above arguments regarding the long-time extrapolation for $N\to\infty$, we should mention that for $N=20$ the $\mathcal{D}(t)$ curves have already converged for those

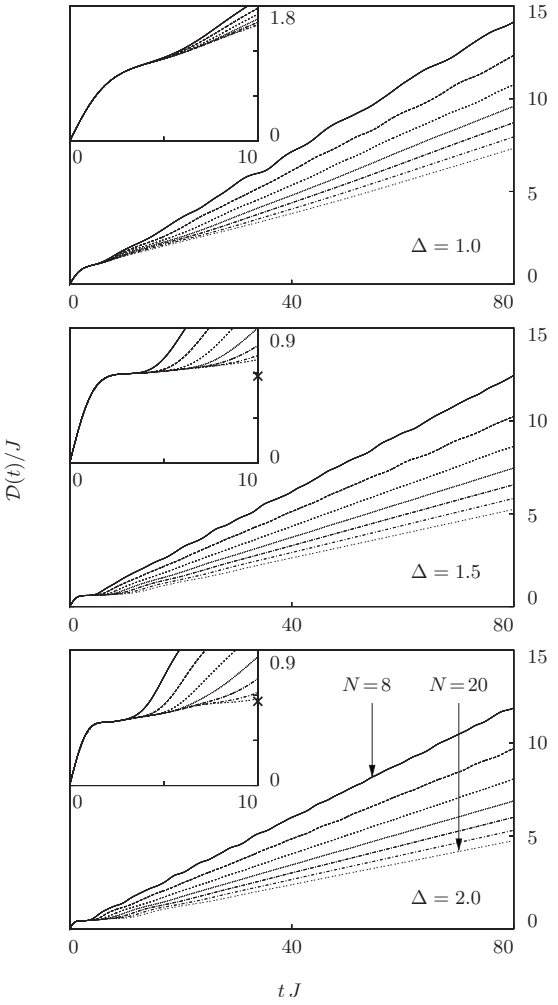

FIG. 4. The diffusion constant $\mathcal{D}(t)$, as given by Eq. (13), for magnetization transport (spin transport) in the anisotropic Heisenberg chain (XXZ model) in the high-temperature limit ($T=\infty$). Insets zoom in $\mathcal{D}(t)$ at short t. The curves are evaluated numerically (by the use of exact diagonalization) for chain lengths $N=8,10,\ldots,20$ (arrows) and for anisotropy parameters $\Delta=1.0$ (top), 1.5 (middle), as well as 2.0 (bottom). One cross (middle inset) indicates the conductivity $\mathcal{D}_{\mathrm{bath}}/J=0.58$ in Ref. 13 (Ref. 50), as found therein from a nonequilibrium bath scenario. Another cross (bottom inset) represents the value $\sigma_{\mathrm{dc}}/(\beta\epsilon^2 J)=0.56$ with the dc conductivity $\sigma_{\mathrm{dc}}/(\beta J)=0.14$ according to Ref. 15.

times which are shorter than $t\approx 8/J$, see Fig. 4 (middle inset). Due to Eq. (12), this time corresponds to a length scale W on the order of about three sites. Thus, at least for $W\leq 3$ the dynamics should be known.

For larger anisotropy parameters Δ we find a similar situation: again there is a clearly developing plateau at intermediate time scales, see Fig. 4 (bottom) for the case $\Delta=2.0$. For the accessible system sizes, however, the final plateau height $\mathcal{D}$ does not seem to be reached yet, i.e., $\mathcal{D}$ cannot be read off with the same accuracy, as done before for $\Delta\approx 1.5$. For comparison we hence indicate in Fig. 4 (bottom inset) the quantity $\sigma_{\mathrm{dc}}/(\beta\epsilon^2 J)=0.56$ with the dc conductivity $\sigma_{\mathrm{dc}}/(\beta J)=0.14$ according to Ref. 15, obtained therein from an analysis on the basis of the standard Green-Kubo formula. The good agreement with this result is noticeable.

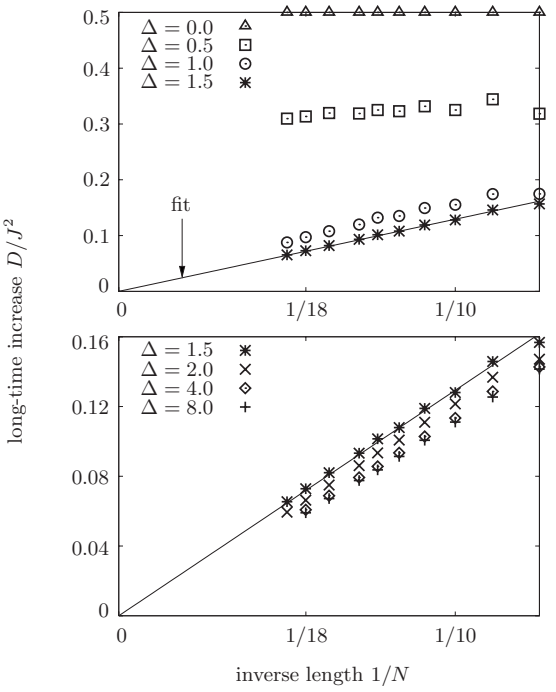

FIG. 5. The long-time increase D of the diffusion constant $\mathcal{D}(t)$, the Drude weight, for magnetization transport (spin transport) in the anisotropic Heisenberg chain (XXZ model) at high temperatures ($T=\infty$). The symbols are evaluated numerically (by the use of exact diagonalization) for chain lengths $N\leq 20$ and for anisotropy parameters $\Delta\leq 8$. The line indicates a fit for the special case of $\Delta=1.5$.

C. Anisotropy $\Delta=1$

As already mentioned above, it is still controversial, whether or not the Drude weight is finite in the limit $N\to\infty$, when Δ becomes exactly 1.0. However, let us for the moment assume that the Drude weight is indeed finite in that limit. Then at the infinite time scale the diffusion constant $\mathcal{D}(t)$ is completely governed by this nonzero Drude weight and increases linearly. At finite time scales, however, $\mathcal{D}(t)$ may still appear to be almost constant and feature a plateau like the one for the case $\Delta=1.5$. In principle, such a plateau can be very wide, if only its height is large in comparison with the Drude weight D such that the finiteness of D is by itself not crucial in this context, cf. Sec. II.

We hence show in Fig. 4 (top) the diffusion constant $\mathcal{D}(t)$ for the special case $\Delta=1$. The initial short-time increase directly passes into the final long-time increase, i.e., in between a horizontal line is not observable for the accessible system sizes. Nevertheless, we cannot exclude the possibility that a plateau with a height on the order of $\mathcal{D}/J\approx 1.0$ will eventually develop, when the system size is further increased, cf. Fig. 4 (top inset). We may thus compare this value for $\mathcal{D}$ with the extrapolated Drude weight $D/J^2\approx 0.025$ in Ref. 4 (Ref. 52), for example. (The latter extrapolated D is about 1/4 of the long-time slope for $N=20$, cf. Figs. 4 and 5.) By the use of the rough estimation $D|t_2-t_1|/\mathcal{D}\ll 1$ we directly obtain that an interval with $\mathcal{D}(t)\approx\mathcal{D}$ cannot be wider than some time scale $|t_2-t_1|\ll 40/J$, respectively, length scale $|W_2-W_1|\ll 9$. Thus, if the above extrapolation for the Drude weight was indeed

correct, diffusion would be restricted to very few sites only. Contrary, if the Drude weight was zero (or a finite, irrelevantly small number), diffusion could occur for a possible arbitrary number of sites, of course.

V. HEISENBERG CHAIN WITHIN AN ALTERNATING FIELD

In this section we are going to concentrate exclusively on the pure Heisenberg chain, i.e., $\Delta=1$, and investigate another modification of Hamiltonian (21) which may lead to diffusive transport. Such a modification certainly is the incorporation of disorder, i.e., coupling constants or field strengths which vary randomly from one site to another.[9,10,23,53,54] But the investigation of disorder is numerically rather challenging and conceptually more subtle due to the localization phenomenon, even for a noninteracting single-particle system.[29,55] Instead we will consider another scenario without disorder, where the Heisenberg chain is exposed to a strictly alternating field. This scenario is concretely described by Hamiltonian (21) and an additional Zeeman term of the form[13,16]

$$\hat{H}_B = \sum_{\mu=1}^{N} \frac{B+(-1)^{\mu}\delta B}{2}\hat{\sigma}_{\mu}^{z}, \tag{23}$$

where δB is the deviation from the mean B. As already done before, we may set $B=0$ for simplicity.

The presence of the Zeeman term, Eq. (23), does not affect the commutation of $\hat{H}$ and $\hat{S}^z$, i.e., the Hamiltonian can be diagonalized within decoupled M subspaces, too. As long as N is even, there also is translational invariance (w.r.t two sites) such that the problem can be reduced further by a factor $N/2$. (There is no mirror symmetry for even N.)

Since $\hat{S}^z$ still represents a strictly conserved quantity, the present model allows to investigate the transport of magnetization w.r.t. the field parameter δB. Note that the respective current $\hat{J}^S$ and factor ϵ^2 are identical to those in Sec. IV. When δB is increased from zero and becomes comparative with the coupling strength J, the model undergoes a transition to quantum chaos,[13] i.e., one may assume that the latter transition already is a first pointer toward the onset of diffusion. Even though it is entirely independent from those assumptions, we start our investigation with $\delta B/J=0.5$.

For $\delta B/J=0.5$ the curve for the diffusion constant $\mathcal{D}(t)$ has changed from Fig. 4 (top) into Fig. 6 (top). In particular, the initial short-time increase does not directly pass into the final long-time increase any more. Instead there is an oscillation in between such that, at the first view, the situation appears to be much more complicated than a simple horizontal line. However, for $N=18$ the $\mathcal{D}(t)$ curve has already converged until the end of this oscillation, see Fig. 6 (top inset). Exactly at this position the curve seems to gradually develop a plateau with a height on the order of $\mathcal{D}\approx 0.42J$. The plateau becomes visible since the Drude weight rapidly decreases with N, i.e., it is about one order of magnitude smaller for $N=18$ than for $N=8$, cf. Fig. 7 (circles). Note that the Drude weight does not fulfill a simple $1/N$ dependence

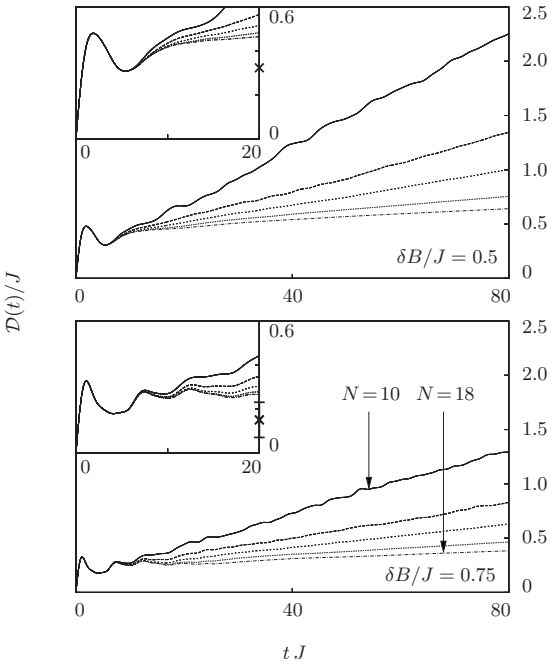

FIG. 6. The diffusion constant $\mathcal{D}(t)$, as given by Eq. (13), for magnetization transport (spin transport) in the Heisenberg chain within an alternating field in the high-temperature limit ($T=\infty$). Insets zoom in $\mathcal{D}(t)$ at short t. The curves are evaluated numerically (by the use of exact diagonalization) for chain lengths $N=10,12,\ldots,18$ (arrows) and for field strengths $\delta B/J=0.5$ (top) as well as 0.75 (bottom). The crosses (insets) indicate the conductivities $\mathcal{D}_{\mathrm{bath}}/J=0.323\pm0.010$ and 0.15 ± 0.08 in Ref. 16, as obtained from a nonequilibrium bath scenario.

and decays faster than a power law. Thus, there is no need to suppose a finite and relevant Drude weight in the limit $N\to\infty$.

Remarkably, the above suggested $\mathcal{D}$ for $\delta B/J=0.5$ agrees well with the conductivity $\mathcal{D}_{\mathrm{bath}}/\lambda=0.323\pm0.010$ from Ref. 16, as found therein from a nonequilibrium bath scenario. The deviation from this conductivity is on the order of 30% solely. However, the small deviation may be explained as

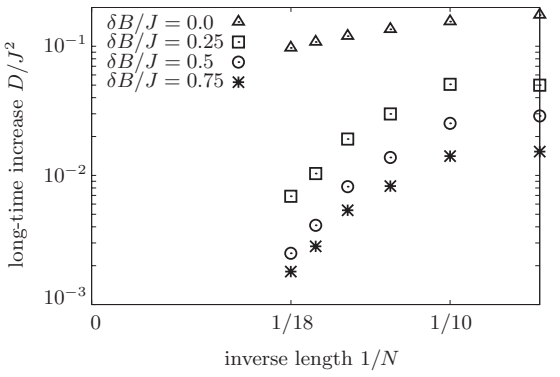

FIG. 7. The long-time increase D of the diffusion constant $\mathcal{D}(t)$, the Drude weight, for magnetization transport (spin transport) in the Heisenberg chain within an alternating field at high temperatures ($T=\infty$). The symbols are evaluated numerically (by the use of exact diagonalization) for chain lengths $N\leq 18$ and for field strengths $\delta B/J\leq 0.75$.

follows: in Ref. 16 the conductivity is evaluated by the use of the Lindblad equation, i.e., it is extracted from the steady state of a finite chain which is at both ends weakly coupled to baths at different temperatures. This weak bath coupling is essential for the validity of the Lindblad approach. But, for a finite chain, a too weak bath coupling may also yield a value $\mathcal{D}_{\mathrm{bath}}$ which is lower than the correct value, say, $\mathcal{D}$, see Ref. 31. Since in Ref. 16 the independence of the conductivity from the bath-coupling strength is not analyzed in detail, we suppose that the above deviation results from a slightly too weak coupling of chain and reservoirs.

For larger field parameters δB suggestions are less reliable, since the initial oscillations of the $\mathcal{D}(t)$ curves become much more pronounced, as already visible in Fig. 6 (bottom). Even though there are oscillations, $\mathcal{D}(t)$ still remains strictly positive, i.e., those oscillations probably are no pointer toward insulating behavior.

Note that definite conclusions cannot be made for the parameter regime $\delta B/J<0.5$, since the curves for $\mathcal{D}(t)$ continuously change from Fig. 4 (top) into Fig. 6 (top), i.e., one basically is concerned with the problem that the Drude weight governs the overall shape of the curve, at least for accessible system sizes.

VI. SUMMARY AND CONCLUSION

In the present paper we have investigated transport in several translationally invariant spin-$\frac{1}{2}$ chains in the special limit of high temperatures. We have concretely considered spin transport in the anisotropic Heisenberg chain, in the pure Heisenberg chain within an alternating field, and energy transport in an Ising chain which is exposed to a tilted field.

To this end we have first reviewed on a recently derived connection between the evolution of the variance of some "typical" inhomogeneous nonequilibrium density and the current-autocorrelation function at finite times.[34] In the limit of infinitely long times this connection was shown to yield a generalized Einstein relation which relates the diffusion constant (in the absence of any external force) to the dc conductivity (as the linear-response coefficient in the presence of an external force, i.e., as evaluated from the standard Green-Kubo formula[38,39]). However, we have additionally demonstrated that the great advantage of the above connection is given by its direct applicability at finite times and for finite systems, e.g., at short times interesting signatures of an infinitely large system may be extractable for a system with an accessible size.

By means of numerically exact diagonalization we have indeed observed strong indications for diffusive behavior in the considered spin chains for a range of model parameters. Moreover, the suggested diffusion constants have been found to be in quantitative agreement with recent results on diffusion coefficients which were obtained for the same spin chains from numerically involved investigations of nonequilibrium bath scenarios in Refs. 13, 16, 21, and 22.

Amongst all those and our findings at high temperatures the emergence of diffusive transport of magnetization appears to be verified in the anisotropic Heisenberg chain with the anisotropy parameter $\Delta=1.5$,[13,16] despite the integrability of the model. It is known that the onset of quantum chaos is not a sufficient condition for diffusion[9,10] but the latter result suggests also that nonintegrability is not necessary at all.

Unfortunately, it is still an open question whether spin transport in the pure Heisenberg chain is diffusive or ballistic. Simply by the use of numerically exact diagonalization we were not able to reach those system sizes which are required for any definite conclusion on that question.

Therefore the next step certainly is the application of approximate methods in order to obtain the current-autocorrelation function at finite times, either numerical ones, e.g., Suzuki-Trotter decompositions,[56,57] or analytical ones, e.g., projection operator techniques[29,32,58,59] or moment methods.[17,18] Approximative methods will also be in indispensable, when the investigation is extended from one-dimensional spin chains to, e.g., more-dimensional spin lattices.

Apart from the above methodic details, a physically interesting question is the dependence of transport on temperature, of course. Since the connection between the evolution of the variance and the current-autocorrelation function is not restricted to infinite temperature, further investigations may be done in this direction, too. However, we expect that for low temperatures the convergence of the diffusion constant at finite times is much slower, when the system size is increased. Thus, for low temperatures conclusions on the basis of a finite system may be less reliable.

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[50] There systematically is a factor 2 between the diffusion constants in the present work and the conductivities in Ref. 13 for both examples in Secs. III and IV. We suppose that this factor 2 has been missed in the definition of the currents in Ref. 13.
[51] In Ref. 21 the current-autocorrelation function $C(t)$ has been normalized to 1, i.e., $C(0) \equiv 1$. In order to extract the exact value for the diffusion constant $\mathcal{D}(t)$, one has to know that $C(0) = N2^N B_x^2 J^2/32$. One has to incorporate additionally that in Ref. 21 the time axis is stretched by a factor 2.
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