Diffusion and Ballistic Transport in One-Dimensional Quantum Systems

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It has been conjectured that transport in integrable one-dimensional systems is necessarily ballistic. The large diffusive response seen experimentally in nearly ideal realizations of the $S = 1/2$ 1D Heisenberg model is therefore puzzling and has not been explained so far. Here, we show that, contrary to common belief, diffusion is universally present in interacting 1D systems subject to a periodic lattice potential. We present a parameter-free formula for the spin-lattice relaxation rate which is in excellent agreement with experiment. Furthermore, we calculate the current decay directly in the thermodynamic limit using a time-dependent density matrix renormalization group algorithm and show that an anomalously large time scale exists even at high temperatures.

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For a generic system of interacting particles at sufficiently high temperatures, transport is expected to be scattering limited. In d spatial dimensions, the signature of diffusive motion is the characteristic long-time decay of the autocorrelation function $\langle n_{\mathbf{r}}(t) n_{\mathbf{r}}(0)\rangle \sim t^{-d/2}$. Here, $n_{\mathbf{r}}$ represents the density of a globally conserved quantity $\sum_{\mathbf{r}} n_{\mathbf{r}}$. In very clean systems, however, transport can be a subtle issue because constants of motion may slow down the current decay or even prevent currents from decaying completely. An important role in our understanding of strongly correlated electrons is played by *integrable* quantum models. Since these models possess an infinite number of *local* conserved quantities, one might expect ideal (*ballistic*) transport to be the rule rather than the exception [1]. Whether or not diffusive behavior is possible at all in such systems is indeed an intensely studied [1–13] but still open question. Experimentally, the question if spin diffusion holds in Heisenberg chains has been investigated for decades [14–17].

In the thermodynamic limit, ballistic transport can be defined from the condition that the current-current correlation function $\langle \mathcal{J}(t)\mathcal{J}(0)\rangle$, where $\mathcal{J}$ is the spatial integral of the current density operator and the brackets denote thermal average, does not decay to zero at large times. This happens, for example, in a free electron gas, where $\mathcal{J}$ is proportional to the momentum operator and therefore conserved in a translationally invariant system [13]. The dc conductivity is then infinite. Next, we consider the case where the current operator itself is not conserved but a conserved quantity Q exists which has finite overlap with $\mathcal{J}$. We can then write $\mathcal{J} = \mathcal{J}_{\parallel} + \mathcal{J}_{\perp}$, with $\mathcal{J}_{\parallel} = (\langle \mathcal{J}Q\rangle/\langle Q^2\rangle)Q$ being the part which cannot decay [9], leading to parallel diffusive and ballistic channels as indicated in Fig. 1. This idea can be generalized to a set of orthogonal conserved quantities Q_n, $\langle Q_n Q_m\rangle = \langle Q_n^2\rangle \delta_{n,m}$, and leads to Mazur's inequality [6,18]

$$D = \frac{1}{2LT}\lim_{t\to\infty}\langle \mathcal{J}(t)\mathcal{J}(0)\rangle \geq \frac{1}{2LT}\sum_n \frac{\langle \mathcal{J}Q_n\rangle^2}{\langle Q_n^2\rangle}. \quad (1)$$

Here, L is the system size and T the temperature. The *Drude weight* D measures the weight of the delta-function peak in the real part of the optical conductivity at zero frequency, $\sigma'(\omega) = 2\pi D\delta(\omega) + \sigma_{\mathrm{reg}}(\omega)$. In principle, both D and $\sigma_{\mathrm{reg}}(\omega = 0)$ can be nonzero [2]. Weak breaking of the conservation laws renders the conductivity finite, but in this case the projection of the current onto the longest lived Q_n sets a lower bound for the conductivity [9].

It is important to note that the right-hand side of Eq. (1) can vanish even if integrability allows us to construct an infinite set of conserved quantities. In the following, we consider the integrable model of *spinless* fermions (*XXZ* model)

$$H = J\sum_{l=1}^{N}\left[-\frac{1}{2}(c_l^{\dagger}c_{l+1} + \mathrm{H.c.}) + \Delta\left(n_l - \frac{1}{2}\right)\left(n_{l+1} - \frac{1}{2}\right)\right]. \quad (2)$$

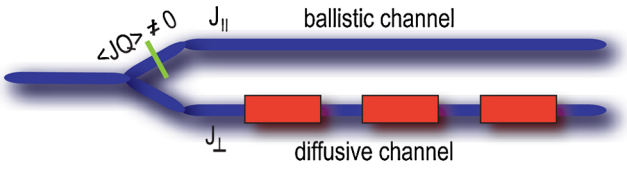

FIG. 1 (color online). In a diffusive channel, the conductivity is limited by the dominant of the various scattering processes pictured as a serial arrangement of resistors. If part of the current is, however, protected by a conservation law, a parallel ballistic channel for charge transport is opened.

Here N is the number of sites, J the hopping amplitude, c_l annihilates a fermion at site l, and Δ is the interaction strength. This model is equivalent to the anisotropic spin-1/2 chain and is exactly solvable by Bethe ansatz (BA) [19]. At half filling, $\langle n_l \rangle = 1/2$, the excitation spectrum is gapless for $|\Delta| \leq 1$ and gapped for $|\Delta| > 1$. The current operator is $\mathcal{J} = \sum_l j_l$, with $j_l = -iJ(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l)/2$ as follows from a discretized continuity equation.

At zero temperature, the Drude weight can be calculated by BA [20] and is found to be finite in the gapless and zero in the gapped regime. Mazur's inequality can be used to show that $D(T) \neq 0$ away from half filling at arbitrary temperatures [6]. Remarkably, at half filling the Mazur bound for the Drude weight obtained from *all local* conserved quantities vanishes identically due to particle-hole symmetry. Since this is only a lower bound, it does not imply that D itself vanishes. However, one can argue [21] that in the gapped regime D should remain zero at finite temperatures. The main open question is whether the Drude weight is finite at finite temperatures in the half filled gapless case. Since Eq. (1) is actually an equality if all conserved quantities are included [22], a nonzero D at half filling requires the existence of a *nonlocal* conserved quantity which has finite overlap with the current operator [9]. $D(T > 0) \neq 0$ at half filling has been found in two independent BA calculations [4,10]. However, these results disagree and they both violate exact relations for $D(T)$ at high temperatures [10]. Further evidence for $D(T > 0) \neq 0$ stems from exact diagonalization (ED) [7–9] and quantum Monte Carlo (QMC) calculations [5,23]. We will discuss these numerical works in relation to our own results at the end of this Letter.

Evidence for diffusion in the spin-spin autocorrelation function at high temperatures has been sought via ED [11], QMC [24], and density matrix renormalization group (DMRG) methods [12,25]. The results at infinite temperature seemed consistent with an algebraic decay $\langle S_l^z(t) S_l^z(0) \rangle \sim t^{-\alpha}$ with exponent α close to 1/2 as expected for $d = 1$. At low temperatures, the diffusive contribution was practically undetectable [12]. Meanwhile, nuclear magnetic resonance (NMR) [16] and muon spin relaxation [17] experiments even found evidence for *low-temperature diffusive behavior* in two completely different $S = 1/2$ Heisenberg chain compounds, but have so far remained unexplained.

In the NMR experiment on the spin chain compound Sr_2CuO_3, spin diffusion is observed as a characteristic magnetic field dependence of the spin-lattice relaxation rate, $1/T_1 \sim 1/\sqrt{h}$ [16]. Here, only excitations with momentum $q \sim 0$, relevant for the studied transport properties, contribute. Clearly, Sr_2CuO_3 is not exactly an integrable system. However, the behavior is expected to be different depending on whether the diffusion constant is determined by intrinsic umklapp scattering within the integrable model or by integrability-breaking perturbations. The spin excitations propagating in a given channel only contribute to the diffusive response at frequencies which are small compared to the relaxation rate in that channel. If the Drude weight of the XXZ model is large in the regime $h \ll T \ll J$, then we expect a large fraction of the excitations in Sr_2CuO_3 to propagate in a quasiballistic channel with a very small relaxation rate. The diffusive response should therefore be suppressed compared to the case where the integrable model has a dominant diffusive channel.

We now calculate $1/T_1$ by a standard field theory approach based on the Luttinger model [19] assuming that there is no unknown nonlocal conservation law that has a finite overlap with $\mathcal{J}$. For $T \gg \omega_e$ and $\Delta = 1$ we have

$$\frac{1}{T_1} \approx -\frac{2T}{\omega_e} \int \frac{dq}{2\pi} |A(q)|^2 \chi''_{\mathrm{ret}}(q, \omega_e). \tag{3}$$

Here $\chi''_{\mathrm{ret}}(q, \omega)$ is the imaginary part of the *longitudinal* retarded spin-spin correlation function $\chi_{\mathrm{ret}}(q, \omega)$ and $\omega_e = \mu_B h$. $1/T_1$ is determined by the *transverse* spin Green's function at the *nuclear* resonance frequency, $\omega_N \approx 0$. By including the Zeeman term in the time evolution of the transverse spin operator but ignoring its negligible effects on the Boltzmann weights and using the resulting $SU(2)$ symmetry we express $1/T_1$ in terms of the *longitudinal* Green's function at the *electron* resonance frequency ω_e in (3). For the in-chain oxygen site in Sr_2CuO_3, we have $A(q) = A\cos(q/2)$ with $|A|^2 = k_B(g\gamma_N\hbar)^2[(2C^b)^2 + (2C^c)^2]/(2\hbar\pi^3 k_B^2 J^2)$ where k_B is the Boltzmann constant, $C^{b,c}$ are the dimensionless components of the hyperfine coupling tensor, $g\gamma_N\hbar = 4.74 \times 10^{-9}$ eV, and J is the exchange coupling measured in kelvin. To obtain the curve shown in Fig. 2, we used $J = 2000$ K and $2C^b = 105$, and $2C^c = 54$ [16]. For small momentum q we find

$$\chi_{\mathrm{ret}}(q, \omega) = \frac{vKq^2}{2\pi} \frac{1}{\omega^2 - v^2 q^2 - \Pi_{\mathrm{ret}}(q, \omega)}. \tag{4}$$

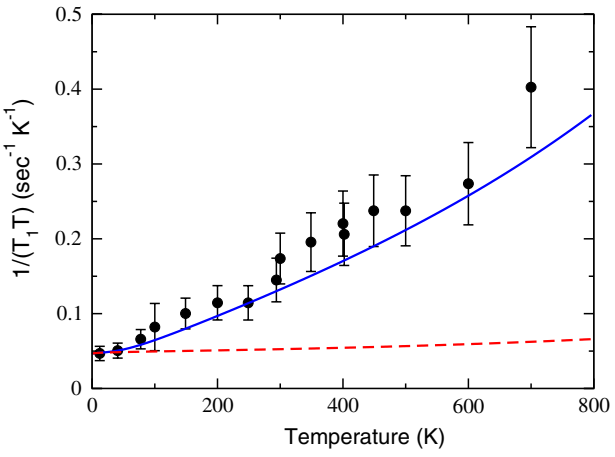

FIG. 2 (color online). Experimental data for $1/T_1$ of the spin chain compound Sr_2CuO_3 at $h = 9$ T taken from Ref. [16] (dots) compared to our theory (blue solid line). Without diffusion, $\gamma = 0$, $1/(T_1T)$ would be almost constant (red dashed line).

Here K is the Luttinger parameter and v the spin velocity. For the pure Luttinger model, $\Pi_{\rm ret}(q,\omega) \equiv 0$, leading to $1/T_1 \sim T$ in the limit $T \to 0$ [26]. In second order in the umklapp scattering and first order in band curvature the self-energy has the form

$$\Pi_{\rm ret}(q,\omega) \approx -2i\gamma\omega - b\omega^2 + cv^2q^2. \tag{5}$$

For the experimentally relevant isotropic case ($\Delta = 1$), $K \approx 1 + g/2$ and $v = J\pi/2$. For the decay rate $\gamma(T)$ and the parameters b and c we find in this case

$$2\gamma = \pi g^2 T, \qquad c = \frac{g^2}{4} - \frac{3g^3}{32} - \frac{\sqrt{3}}{\pi}T^2,$$
$$\underbrace{b = \frac{g^2}{4} - \frac{g^3}{32}\left(3 - \frac{8\pi^2}{3}\right)}_{b_2} + \underbrace{\frac{\sqrt{3}}{\pi}T^2}_{b_1}. \tag{6}$$

Following Lukyanov [27], the running coupling constant $g(T)$ is determined by the equation

$$\frac{1}{g} + \frac{\ln g}{2} = \ln\left[\sqrt{\frac{\pi}{2}}\frac{e^{1/4+\tilde{\gamma}}}{T}\right], \tag{7}$$

where $\tilde{\gamma}$ is the Euler constant. Similarly, the parameters γ, b, and c can be determined for the anisotropic case $0 < \Delta < 1$ (see Ref. [28]). Importantly, we always find a finite decay rate implying spin diffusion in the sense that $\langle n_l(t)n_l(0)\rangle \sim T\sqrt{\gamma/t}$ at large times. At high temperatures such that $\gamma \gg h$ but still $T \ll J$, we find $1/T_1 \sim T\sqrt{\gamma/h}$ with $\gamma \sim T/\ln^2(J/T)$ for the isotropic Heisenberg model. A comparison of the essentially parameter-free calculated temperature dependence with experiment is shown in Fig. 2. The good agreement indicates that a large diffusive response is present in the integrable Heisenberg model near half filling. Furthermore, this result shows that umklapp scattering is a "dangerously irrelevant" perturbation of the Luttinger model [26], completely changing the behavior of $1/T_1$ in the regime $h \ll T$ from a constant to a square-root divergence $1/\sqrt{h}$, as seen in experiment.

Our field theory calculation assumed $D(T > 0) = 0$. The optical conductivity $\sigma(q,\omega) = i\omega\chi_{\rm ret}(q,\omega)/q^2$ can be obtained from Eq. (4) and we find that

$$\sigma'(\omega) = \frac{vK}{2\pi}\frac{2\gamma}{[(1+b)\omega]^2 + (2\gamma)^2} \tag{8}$$

is a Lorentzian with width set by γ. If conservation laws protecting the Drude weight are present, they can be naturally incorporated using the memory matrix formalism [2]. For a single conservation law $[Q, H] = 0$, this formalism yields

$$\sigma'(\omega) = \frac{Kv}{2\pi(1+y)}\left[\pi y(1-b_1)\delta(\omega) + \frac{2\gamma'}{[(1+b_1+b_2')\omega]^2 + (2\gamma')^2}\right], \tag{9}$$

where the parameter $y \equiv \langle \mathcal{J}Q\rangle^2/(\langle \mathcal{J}^2\rangle\langle Q^2\rangle - \langle \mathcal{J}Q\rangle^2)$ measures the overlap of $\mathcal{J}$ with the conserved quantity, and $\gamma' = (1+y)\gamma$ and $b_2' = (1+y)b_2$. Here b_1 and b_2 in the isotropic case are the parameters defined in Eq. (6). Note that for $y = 0$, Eq. (9) reduces to the optical conductivity (8) obtained in the self-energy approach. According to Eq. (9), $\sigma'(\omega)$ has a ballistic and a regular (diffusive) part, with the weight in each part being controlled by y. Away from half filling (finite magnetic field in the spin chain), a lower bound for y is provided by the overlap with the conserved energy current operator $Q = \mathcal{J}_E$ [1]. In this case, $y \sim (h/T)^2$. In the half filled case a possible unknown nonlocal conservation law would mean that spectral weight is shifted from the Lorentzian into a ballistic part that does not contribute to the temperature dependence of $1/(T_1T)$ (see dashed line in Fig. 2). That the experimental points in Fig. 2 are actually mostly *above* the theoretical prediction suggests that D is rather small near half filling.

In order to clarify the contradiction with previous studies that supported a large Drude weight at half filling [7,8], we used a DMRG algorithm [12,25] to calculate the current-current correlation $C(t) \equiv \langle \mathcal{J}(t)\mathcal{J}\rangle/L$ directly in the ther-

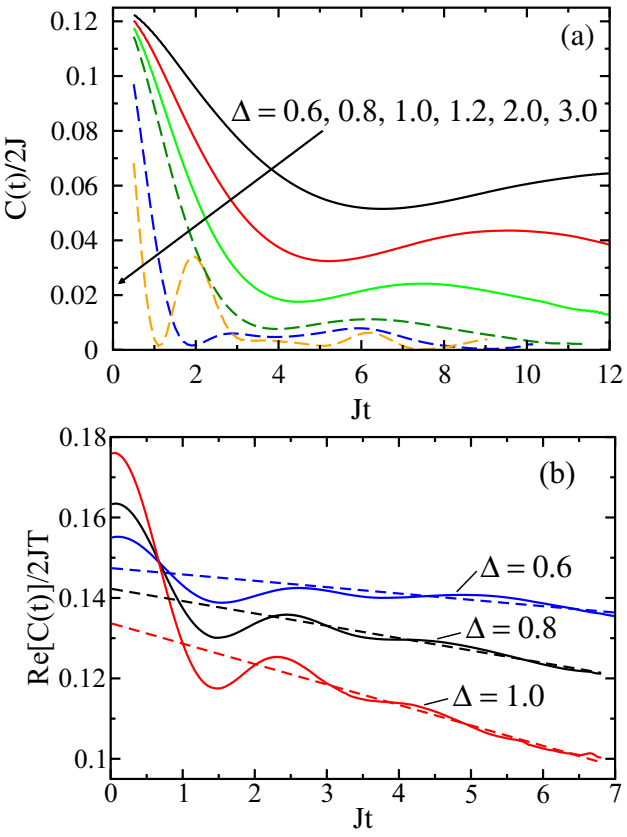

FIG. 3 (color online). (a) $C(t) = \langle \mathcal{J}(t)\mathcal{J}(0)\rangle/L$ at $T = \infty$ for various Δ as indicated on the plot. The solid (dashed) lines correspond to Δ in the critical (gapped) regime, respectively. (b) $\mathrm{Re}[C(t)]/2JT$ at $T = 0.2J$ for $\Delta = 0.6$, $\Delta = 0.8$, and $\Delta = 1.0$ (solid lines). The dashed lines are linear fits $\mathrm{Re}[C(t)]/2JT = A - BJt$ for $Jt \in [3.5, 7]$.

TABLE I. Parameters obtained by fitting $\mathrm{Re}[C(t)]/T$ in Fig. 3(b) to $\mathrm{Re}[C(t)]/T = A - Bt$. According to Eq. (11), we expect $A = vK/\pi(1+b)$ and $B/A = 2\gamma$ with parameters γ and b as given in Eq. (6) for $\Delta = 1$ and in Ref. [28] for the anisotropic case, respectively.

Δ	A	$vK/4\pi(1+b)$	$B/2A$	γ
0.6	0.147	0.147	0.0054	0.0052
0.8	0.142	0.140	0.0109	0.0116
1	0.134	0.135	0.0190	0.0297

modynamic limit. According to Eq. (1), this correlation function asymptotically yields D. Remarkably, the results in Fig. 3(a) show that $C(t)$ is nonmonotonic and does not converge to an asymptotic value for times up to $Jt = 11$ even for infinite temperature. This is true within the critical as well as the gapped regime. Note that the time scales reached in our DMRG calculations are about a factor of 2 larger than what can be achieved by ED where only times $vt < N/2$ are accessible. We conclude that a large time scale persists at $T = \infty$ posing a serious challenge for ED studies.

While previous QMC results [5] are unable to resolve the small decay rate, $\gamma \ll T$, very recent ones [29] seem to strongly support our expression for $\gamma(T)$ in Eq. (6). Further evidence that $\gamma(T)$ is nonzero for $T \ll J$ is provided by Fig. 3(b) showing $\mathrm{Re}[C(t)]/2JT$ at $T = 0.2J$. The result in Eq. (9) predicts for the decay of the current-current correlation function for $t \gg (2\pi T)^{-1}$ and neglecting the small imaginary part (suppressed by a factor γ/T):

$$C(t) \sim \frac{vKT}{2\pi(1+y)}\left(y(1-b_1) + \frac{e^{-2\gamma' t}}{1+b_1+b_2'}\right). \quad (10)$$

At intermediate times $(2\pi T)^{-1} \ll t \ll 1/\gamma'$ we obtain a linear decay independent of y if $b_1, b_2' \ll 1$

$$C(t) \approx KvT(1-2\gamma t)/[2\pi(1+b)]. \quad (11)$$

A linear fit in this regime yields values which are consistent with our theory (see Table I). We also note that the values of $C(t)/2JT$ for $Jt \approx 6$ are already smaller than the Drude weight found in [10] by BA.

To summarize, we have shown that in integrable 1D systems diffusion can coexist with ballistic transport, in the sense illustrated in Fig. 1. This is the scenario for the XXZ model away from half filling. For the half filled case, however, we have argued that the large diffusive response measured experimentally in spin chains and seen in our numerical calculations suggests that, contrary to common belief, the low-temperature Drude weight is either zero or surprisingly small for Δ near 1.

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