Macroscopic Diffusive Transport in a Microscopically Integrable Hamiltonian System

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We demonstrate that a completely integrable classical mechanical model, namely the lattice Landau-Lifshitz classical spin chain, supports diffusive spin transport with a finite diffusion constant in the easy-axis regime, while in the easy-plane regime, it displays ballistic transport in the absence of any known relevant local or quasilocal constant of motion in the symmetry sector of the spin current. This surprising finding should open the way towards analytical computation of diffusion constants for integrable interacting systems and hints on the existence of new quasilocal classical conservation laws beyond the standard soliton theory.

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Introduction.—Derivation of irreversible macroscopic transport (e.g., Fourier's, Ohm's, or Fick's) laws from reversible, deterministic, microscopic equations of motion is one of the central questions of statistical physics which remains largely unsolved even today. It has been believed [1–6] that chaotic dynamics in classical systems, or more generally strong nonintegrability in either quantum or classical systems, are necessary conditions for diffusive transport. Recently, few examples of spin diffusion at high temperature in completely integrable but strongly interacting quantum spin or particle chains have appeared [7–11], suggesting that complete integrability might not exclude the possibility of macroscopically diffusive dynamics. It has remained unclear, however, whether quantum nature of the corresponding many-body dynamics supporting macroscopic entanglement is a necessary condition. Here, we show that even quantum correlations are not necessary. By performing extensive numerical simulations in a family of integrable classical spin chains with local interactions—the lattice Landau-Lifshitz model [12]—we show that spin transport at finite temperature is diffusive in the easy-axis regime, while it becomes ballistic in the easy-plane regime and anomalous at the isotropic point. This opens up the possibility for analytic computations of diffusion constants in interacting many-body systems. In the context of spin transport, our results have potential applications to nanomagnetism and the theory of data storage devices where the soliton based transport of magnetization plays a crucial role [13].

Liouville integrability [14] is the central concept in the analytic theory of classical mechanics. A Hamiltonian, i.e., conservative system in classical mechanics, is integrable if it possesses the same number of independent conserved quantities as the number of degrees of freedom, call it n. In other words, its motion can be reduced to quasiperiodic winding around n-dimensional torus embedded in $2n$-dimensional phase space [14]. Thus, integrable dynamics is regular and manifestly free of sensitive dependence on initial conditions. Nevertheless, integrable systems, though being sparse in nature, represent one of the key topics in mathematical physics as they gave birth to the celebrated soliton theory [12] explaining a variety of observable phenomena, ranging, to name just a few, from localized light in nonlinear optics, waves on shallow water, and tsunami waves, to elementary particles and localized excitations in condensed matter at low temperatures.

The solitons, indestructible localized packages of energy which propagate through the system and scatter from each other like elastic hard balls, have been believed to be the reason why integrable extended systems behave as ideal ballistic conductors of heat, particles, electric charge, magnetization, etc. [1,2]. Being particularly interested in the one-dimensional lattice systems, where n particles are arranged along a line or a ring such that only nearest neighbors can interact representing the simplest model of crystalline solids, one finds that the existence of nontrivial conservation laws (besides the transported quantity, e.g., energy, particle number, electric charge, magnetization) generically implies the ballistic (nondiffusive) transport [15]. This statement, which builds on an old idea of Mazur [16] but has only recently been formally proven [17], essentially states the following. Whenever there exists a quantity I which is conserved in time $I(t) \equiv I$ and independent of the transported quantity itself, such that $\langle IJ \rangle \neq 0$, where $J(t) = \sum_{x=1}^{n} j(x, t)$ is the current with $j(x, t)$ being the current density at time t and at site x in the lattice, and $\langle \cdots \rangle$ denotes the thermodynamic average (for fixed, specified values of temperature, electrochemical potential, magnetization, etc.), then the transport is ballistic and the corresponding Kubo conductivity κ diverges. Conductivity is related to a diffusion constant D, via the generalized Einstein relation $\kappa = D/T$ where T

is the absolute temperature, and the latter can be within Green-Kubo linear response theory expressed

$$D = \lim_{\tau\to\infty}\lim_{n\to\infty}\sum_{r=1}^{n}\int_0^{\tau} C(r,t)dt, \qquad (1)$$

in terms of the integrated spatiotemporal current-current correlation function $C(r,t) = \langle j(x,0)j(x+r,t)\rangle$. Lattice site x is arbitrary for translationally invariant systems which exhaust major examples of integrable systems. Note that in statistical mechanics the thermodynamic limit of size $n\to\infty$ has to be taken always before the time $\tau\to\infty$ limit. It is clear that the above expression for the diffusion constant can be given in terms of time correlations only, namely $D = \lim_{t\to\infty} D(t)$, introducing a time-dependent diffusion constant as

$$D(\tau) = \int_0^{\tau} C(t)dt, \qquad (2)$$

where we can write the total current time autocorrelation as $C(t) = \frac{1}{n}\langle J(0)J(t)\rangle$. The existence of solitons and nontrivial conserved quantities in integrable systems implies nonvanishing tails of the time correlations [15,17] $C_\infty = C(t\to\infty) \neq 0$, in turn implying linear divergence of the time-dependent diffusion constant $D \to C_\infty t \to \infty$ which is a signature of ballistic transport. To date, all studies of transport in classical integrable particle chains have persistently showed ballistic transport (see e.g., Ref. [18] and references therein). On the other hand, for diffusive transport ($D < \infty$), we have evidence that not even microscopic chaos [6] is necessary, but a weaker property of dynamical mixing [19] is sufficient [18,20,21]. Furthermore, some recent numerical studies of quantum spin $1/2$ chains with anisotropic Heisenberg interaction (*XXZ* chains) indicated [8,9,22,23] that the high temperature spin transport is diffusive in the easy-axis regime, despite the fact that the *XXZ* chains are quantum integrable by the algebraic Bethe ansatz which is the quantum version of the soliton theory. These results have been further corroborated with evidence of particle and spin diffusion in another Bethe ansatz integrable model, namely the one-dimensional Hubbard model [11]. Nevertheless, as the completeness of Bethe ansatz solutions has not been proven in these models and as quantum dynamics supports a high degree of complexity as opposed to classical dynamics due to exponentially large (in n) Hilbert space dimension and possibility of macroscopic entanglement [24], it has remained unclear whether the key to the observed diffusion really lies in the integrability structures of the Heisenberg and Hubbard models.

Model and methods.—However, in this Letter we show a convincing numerical evidence for spin diffusion at high temperature in a fully classical completely integrable model. We consider a lattice Landau-Lifshitz (LLL) model [12] for a chain or a ring of n classical spins described by angular-momentum vectors $\vec{S}_x$, $x = 1,\ldots,n$

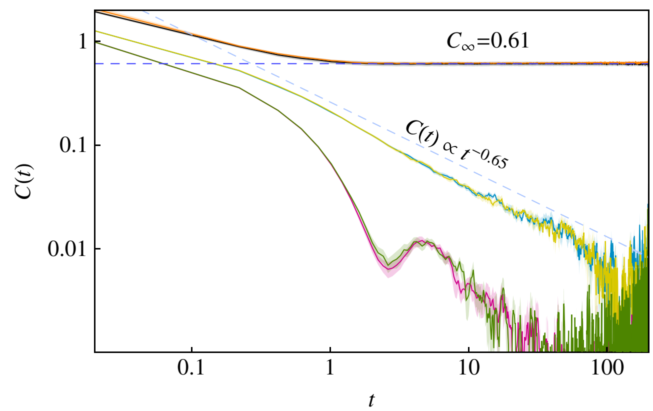

FIG. 1 (color online). Current autocorrelation function $C(t)$ in log-log scale for easy-plane regime (top curves, orange: $n = 160$, black: $n = 2560$), isotropic regime (middle curves, yellow: $n = 2560$, blue: $n = 5120$), and easy-axis regime (bottom curves, violet: $n = 2560$, green: $n = 5120$). Shaded regions denote the estimated statistical error for ensemble averages over $N \approx 10^3$ initial conditions. Dashed lines denote asymptotic behavior for large time in the easy-plane regime (dark blue) and isotropic regime (light blue).

of equal fixed length $|\vec{S}_x| \equiv R$ and the Hamiltonian function of the form

$$H = \sum_{x=1}^{n} h(\vec{S}_x, \vec{S}_{x+1}), \qquad (3)$$

where the nearest-neighbor spin interaction density $h(\vec{S}, \vec{S}')$ is given by

$$\begin{aligned} h(\vec{S},\vec{S}') = \log|&\cosh(\rho S_3)\cosh(\rho S_3') \\ &+ \coth^2(\rho R)\sinh(\rho S_3)\sinh(\rho S_3') \\ &+ \sinh^{-2}(\rho R) F(S_3)F(S_3')(S_1 S_1' + S_2 S_2')|, \end{aligned} \qquad (4)$$

and $F(S) \equiv \sqrt{[\sinh^2(\rho R) - \sinh^2(\rho S)]/(R^2 - S^2)}$ (as defined by Faddeev and Takhtajan, Ref. [12], Chapter III.5). ρ is the model's parameter, which can be real or purely imaginary. So we shall reparametrize it with an alternative real parameter $\delta = \rho^2$, which may—in analogy with the closely related *XXZ* spin chain [25]—be called an anisotropy parameter. The cases with $\delta > 0$ correspond to easy-axis spin-spin interaction, those with $\delta < 0$ to easy-plane interaction, whereas $\delta = 0$ designates the case of isotropic interaction.

As the third component M_3 of the total magnetization $\vec{M} = \sum_{x=1}^{n} \vec{S}_x$ is a constant of motion, one finds that the equation of motion for local magnetization $dS_{x,3}/dt = j_x - j_{x-1}$ has a form of a local continuity equation from which we read out the expression for the spin current density $j_x = j(\vec{S}_x, \vec{S}_{x+1})$ in the LLL model, namely

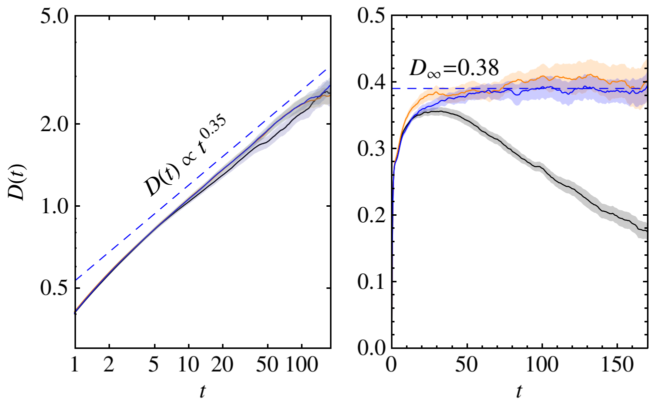

FIG. 2 (color online). Time dependent diffusion constant $D(t)$ in isotropic regime (left) and easy-axis regime (right) comparing different system sizes $n = 640$ (black), $n = 2560$ (orange), and $n = 5120$ (blue). The shaded region denotes estimated statistical error and the dashed lines show estimated asymptotic behavior.

$$j(\vec{S}, \vec{S}') = \sinh^{-2}(\rho R)(S_2 S_1' - S_1 S_2') \times F(S_3)F(S_3')\exp[-h(\vec{S}, \vec{S}')]. \quad (5)$$

The Hamiltonian and the current density in the easy-plane regime $\delta < 0$ can be obtained from (4) and (5) by analytic continuation, i.e., by replacing $\cosh(\rho \cdots)$ by $\cos(s \cdots)$ and $\sinh(\rho \cdots)$ by $\sin(s \cdots)$ where $s = \sqrt{-\delta}$. In the isotropic case $\delta = 0$, one performs the limit $\rho \to 0$ in (4) and (5) and obtains explicitly

$$h(\vec{S}, \vec{S}') = \log\left(1 + \frac{\vec{S} \cdot \vec{S}'}{R^2}\right), \qquad j(\vec{S}, \vec{S}') = \frac{S_2 S_1' - S_1 S_2'}{R^2 + \vec{S} \cdot \vec{S}'}. \quad (6)$$

Time development of each spin is given by solving Hamilton's equations $d\vec{S}_x/dt = \frac{\partial H}{\partial \vec{S}_x} \times \vec{S}_x$, where $\times$ denotes the cross product. These equations of motion for $\vec{S}_x(t)$ are then solved using a variable step integrator of MATLAB with required relative accuracy of better than 10^{-6} for all trajectories (see [26] for more details). Besides checking the accuracy of trivial conservation laws, such as H and M_3, we have also checked that numerically determined Lyapunov exponents [14] vanish asymptotically in all three regimes ($\delta >, =, < 0$) as required for a completely integrable system.

We chose N initial conditions generated by the Metropolis algorithm [27] yielding a thermal Gibbs ensemble with given temperature T and vanishing $M_3 = 0$ component (along the symmetry axis of the spin-spin interaction) of the magnetization. We note that ensembles with nonvanishing or nonfixed M_3 would not yield the

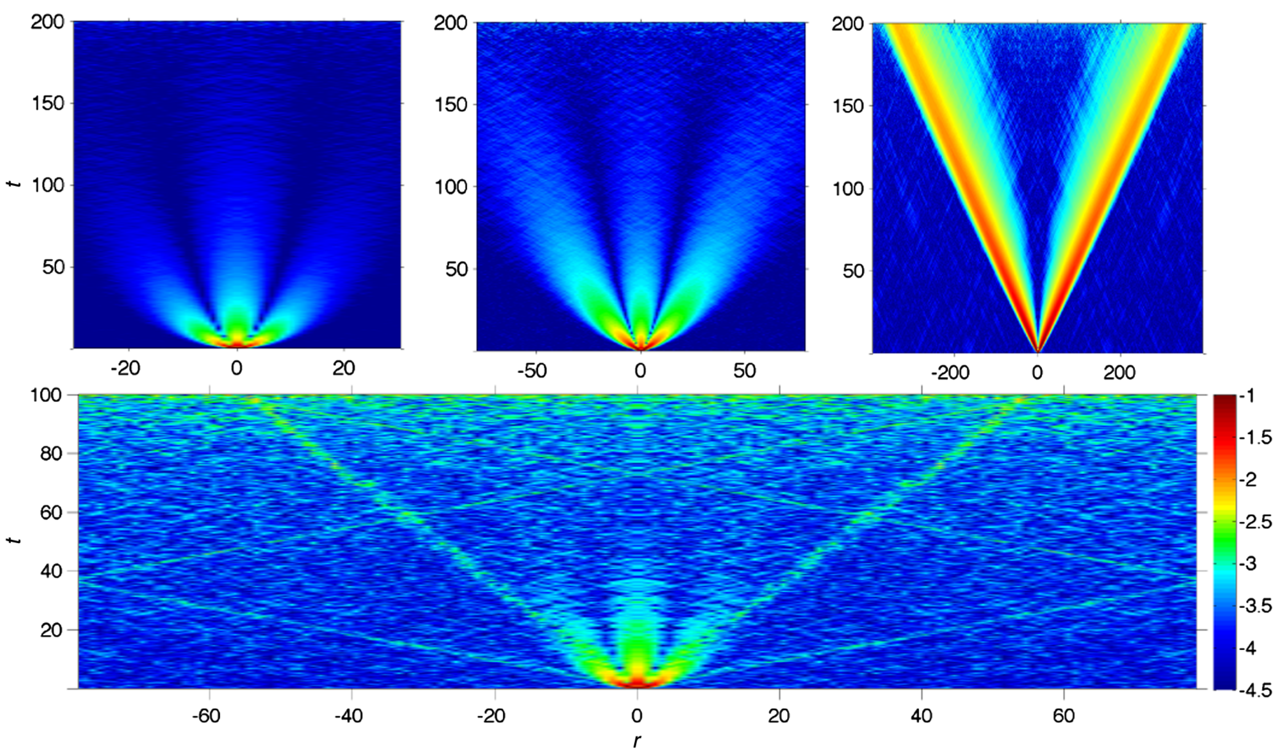

FIG. 3 (color online). Modulus of spatiotemporal spin current autocorrelation function $|C(r, t)|$ shown in log scale with color scale ranging from $10^{-4.5}$ to 10^{-1} indicated in the bottom right. In the upper panels we show data averaged over ensembles of $N \approx 10^3$ initial conditions in easy-axis (left; $n = 5120$), isotropic (center; $n = 5120$), and easy-plane (right; $n = 2560$) regimes. The bottom plot shows the easy-axis regime again with a smaller system or ensemble size $n = 160$, $N = 600$ where scars of solitons emerging from local thermal fluctuations are still clearly visible.

correct Kubo formula [4] for the spin-diffusion constant in the absence of an external magnetic field. The LLL model is invariant under a canonical transformation

$$\mathcal{R}\colon (S_{x,1}, S_{x,2}, S_{x,3}) \to (S_{x,1}, -S_{x,2}, -S_{x,3}), \qquad (7)$$

i.e., a π rotation around the first Cartesian axis, namely $\mathcal{R}H = H$. As the LLL r matrix [12] is invariant under $\mathcal{R}$, so are also all the derived local conserved quantities $\mathcal{R}I_k = I_k$. However, the spin current is odd under the symmetry transformation, $\mathcal{R}J = -J$, so all (ballistic) terms in the Mazur bound [15] have to vanish, $\langle I_k J\rangle = \langle \mathcal{R}I_k \mathcal{R}J\rangle = -\langle I_k J\rangle$, allowing for the possibility of non-ballistic transport.

Results.—Solving Hamilton's equations numerically we compute the spatiotemporal current-current autocorrelation function $C(r, t)$, as well as the temporal autocorrelation $C(t)$ and obtain the time-dependent spin diffusion constant $D(t)$ (2). We chose several different chain sizes n (up to $n = 5120$) and ensemble size N large enough (typically $N \sim 10^3$) so that finite size effects, and the statistical error scaling as $\sim 1/\sqrt{nN}$, appear negligible. Representative values of the anisotropy parameters are chosen as $\delta = 1$ (easy-axis regime), $\delta = -1$ (easy-plane regime), and $\delta = 0$ (isotropic regime) while fixing $R = 1$. In all cases, the temperature of the initial Gibbs ensemble is $T = 4$. In Fig. 1, we plot spin current autocorrelation $C(t)$ in all three regimes and find a finite saturation value $C_\infty \neq 0$ implying ballistic transport in the easy-plane regime, whereas, in the isotropic and easy-axis regimes the tails of the current autocorrelation function are vanishing. To elaborate on the tails of the current autocorrelation function, we plot in Fig. 2 the time dependent diffusion constant $D(t)$, which in the isotropic regime shows power law behavior $D(t) \propto t^\alpha$ with $\alpha \approx 0.35$, and in the easy-axis regime saturates at a finite value $D(\infty) \approx 0.38$, providing a firm evidence of anomalous spin transport in the isotropic regime and diffusive spin transport in the easy-axis regime. These results can be even better illustrated by portraying spatiotemporal correlations $C(r, t)$ in Fig. 3. In the easy-plane regime, we find a clear causality-cone structure with nondecaying tails whereas in the easy-axis case, the cone is curved inwards and the tails are strongly damped in time resulting in suppression of all ballistic contributions for long times. In the bottom panel of Fig. 3, we present data for much a smaller ensemble of initial conditions and smaller system size showing "scars," i.e., ballistic solitons which may emerge in initial conditions with localized large thermal fluctuations and which can travel much faster than the correlation velocity, but contributions of which (due to the existence of $\mathcal{R}$ symmetry) vanish in the limit of the infinitely large ensemble $N \to \infty$. Therefore, one would recognize the fact that we are dealing with a completely integrable system (in particular in the easy axis regime) only by looking at a finite N data.

Conclusion.—The surprising possibility of having a regime with normal, diffusive transport in a completely integrable classical system (as found in the easy-axis regime of the LLL model), which is associated with the existence of parity-type symmetry of the classical r matrix whose operation changes the sign of the corresponding transporting current, opens up the immediate question regarding whether the classical r matrix theory [12] can be updated to allow for analytical calculations of diffusive transport coefficients. Equally interesting is the problem of explaining the ballistic regime in such a situation (say in the easy-plane regime of the LLL model), since the Mazur bound identically vanishes. As the LLL model can be considered as a classical limit of the XXZ spin chain (see also [25]), we conjecture the existence of a classical analog of the construction of quasilocal conserved quantities with negative parity [29] going beyond the standard soliton theory [12].

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[26] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.111.040602 for details and tests of numerical integration scheme and Metropolis sampling, in particular time-invariance of equilibrium distributions.
[27] The ensemble of initial conditions is sampled via a standard Metropolis algorithm [28], where the new configuration in each Metropolis step is generated by choosing two random spins and changing their values randomly in the ϕ-z plane (ϕ denotes the angle of a spin-vector in the xy plane and z is its component along the z-axis) according to a uniform probability with a constraint preserving the total magnetization (assuring $M_3 = 0$), namely $dP \propto d\phi_1 d\phi_2 dz_1 dz_2 \delta[z_1 + z_2 - (z_1' + z_2')]$, where $z_{1,2}'$ denote the spin components before the change. The acceptance probability of the step is given by the Gibbs factor $\exp[(E' - E)/T]$, where E' and E denote the values of H, Eqs. (3), (4), and (6), of the configurations before and after the step, respectively, and T is the temperature. (see also [26]).
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