Diffusive transport in integrable lattice systems

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How to manipulate transport in simple, 1D quantum (classical) lattice systems?

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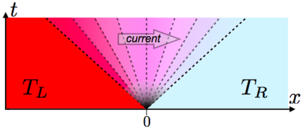
What is the mechanism for normal diffusion in integrable systems?

Three approaches to transport in Hamiltonian (conservative) systems:

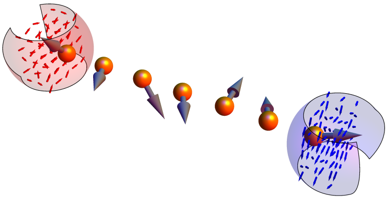
- Green-Kubo formulae and equilibrium dynamical correlation functions

$$\langle J(t)J(0)\rangle$$

- Inhomogeneous initial states in infinite systems



- Stochastic-boundary driven (finite) systems



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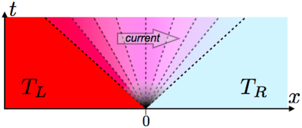

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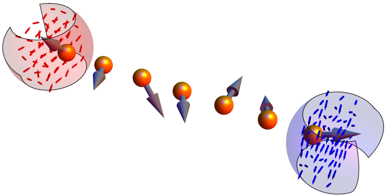

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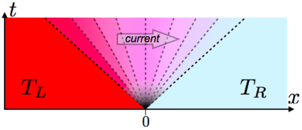

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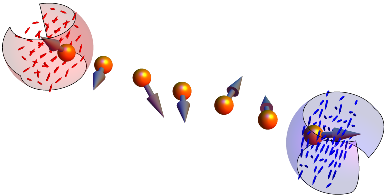

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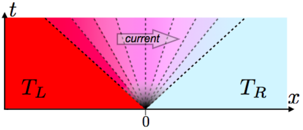

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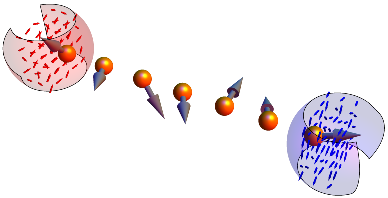

Green-Kubo formulae express the conductivities in terms of current a.c.f.

$$\kappa(\omega) = \lim_{t\to\infty} \lim_{n\to\infty} \frac{\beta}{n} \int_0^t \mathrm{d}t' e^{\mathrm{i}\omega t} \langle J(t'), J(0) \rangle_\beta$$

When d.c. conductivity diverges, one defines a Drude weight D

$$\kappa(\omega) = 2\pi D \delta(\omega) + \kappa_{\mathrm{reg}}(\omega)$$

which in linear response expresses as

$$D = \lim_{t\to\infty} \lim_{n\to\infty} \frac{\beta}{2tn} \int_0^t \mathrm{d}t' \langle J(t') J(0) \rangle_\beta .$$

Aren't integrable systems always ballistic?

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For integrable quantum systems, Zotos, Naef and Prelovšek (1997) suggested to use Mazur/Suzuki (1969/1971) bound:

$$D \geq \lim_{n\to\infty} \frac{\beta}{2n} \sum_m \frac{\langle J Q^{(m)}\rangle_\beta^2}{\langle [Q^{(m)}]^2\rangle_\beta}$$

with conserved $Q^{(m)}$ chosen mutually orthogonal $\langle Q^{(m)} Q^{(k)}\rangle_\beta = 0$ for $m \neq k$.

Mazur bound essentially follows from optimizing a trivial inequality

$$\left\langle \left(\int_0^t \mathrm{d}t' J(t) - \sum_m \alpha_m Q^{(m)} \right)^2 \right\rangle_\beta \geq 0$$

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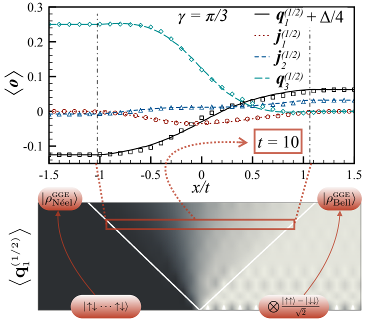
But what happens when all $Q^{(m)}$ are orthogonal to J, $\langle J Q^{(m)} \rangle_\beta = 0$?

Inhomogeneous initial states: Generalized hydrodynamics

Castro-Alvaredo, Doyon, Yoshimura, PRX **6**, 041065 (2016)
Bertini, Collura, De Nardis, Fagotti, PRL **117**, 207201 (2016)

Evolution of the initial state $\rho(t=0)=\rho_L\otimes\rho_R$



Generalized Euler equations for density of carriers of charge $Q^{(m)}$
(via *String-Charge Duality*, Ilievski et al JSTAT (2016) 063101)
along the *ballistic* rays $\zeta = x/t$:

$$\partial_t \rho_{\zeta,m}(\lambda) + \partial_x (v_{\zeta,m}(\lambda)\rho_{\zeta,m}(\lambda)) = 0.$$

Canonical model: XXZ spin 1/2 chain and $\mathbb{Z}_2$ symmetry

$$H = \frac{1}{4}\sum_{x=1}^{n-1}(2\sigma_x^+\sigma_{x+1}^- + 2\sigma_x^-\sigma_{x+1}^+ + \Delta\sigma_x^{\mathrm{z}}\sigma_{x+1}^{\mathrm{z}})$$

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$U_q(\mathfrak{sl}_2)$ Lax operator ($\Delta = \cos\eta$): $\mathbf{L}(\varphi, s) = \begin{pmatrix} \sin(\varphi + \eta\mathbf{S}_s^{\mathrm{z}}) & (\sin\eta)\mathbf{S}_s^- \\ (\sin\eta)\mathbf{S}_s^+ & \sin(\varphi - \eta\mathbf{S}_s^{\mathrm{z}}) \end{pmatrix}$

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Unitary (compact) representations ($s \in \frac{1}{2}\mathbb{Z}$) local $s = \frac{1}{2}$ and quasi-local charges

$$Q^{(\ell,s)} = \partial^{\ell-1}_\varphi \log \mathrm{tr}_{\mathrm{aux}}\mathbf{L}^{\otimes_x n}(\varphi, s)|_{\varphi=\frac{\eta}{2}}$$

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Nonunitary (noncompact) representations ($s \in \mathbb{C}$) quasi-local charges

$$Z(\varphi) = (\sin\varphi)^{-n}\partial_s \mathrm{tr}_{\mathrm{aux}} \mathbf{L}^{\otimes_x n}(\varphi, s)|_{s=0}, \quad \eta/\pi \in \mathbb{Q}$$

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Spin-reversal $S = \prod_x \sigma_x^{\mathrm{x}}$ and spin current $J = \mathrm{i}\sum_x(\sigma_x^+\sigma_{x+1}^- - \sigma_x^-\sigma_{x+1}^+)$:

$$[H, S] = 0, \qquad SJ = -JS,$$

$$[Q^{(\ell,s)}, S] = 0, \quad Z(\varphi)S = SZ(\pi - \varphi)^\dagger.$$

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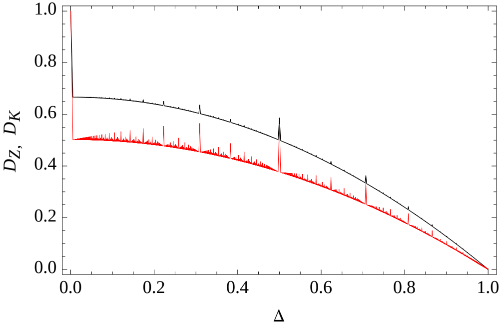
Important consequence: $\langle JQ^{(\ell,s)}\rangle_\beta = 0$, $\langle JZ(\varphi)\rangle_\beta \neq 0$.

High temperature Mazur bound on spin Drude weight using charges $\{Z(\varphi)\}$

$$\frac{D}{\beta} \geq D_Z := \frac{\sin^2(\pi l/m)}{\sin^2(\pi/m)}\left(1 - \frac{m}{2\pi}\sin\left(\frac{2\pi}{m}\right)\right), \quad \Delta = \cos\left(\frac{\pi l}{m}\right)$$



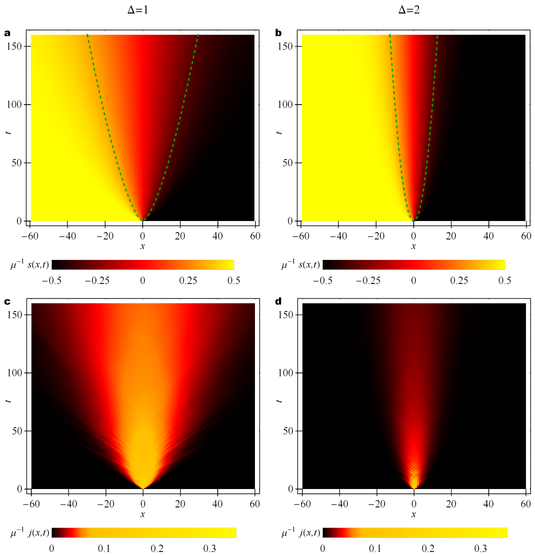
TP, PRL **106** (2011); TP and Ilievski, PRL **111** (2013)

And is argued to agree with exact expression obtained from Generalized Hydrodynamics (De Nardis and Ilievski, arXiv:1702.02930)

What about spin transport for $|\Delta| \geq 1$?

Quench from an inhomogeneous partly magnetized state

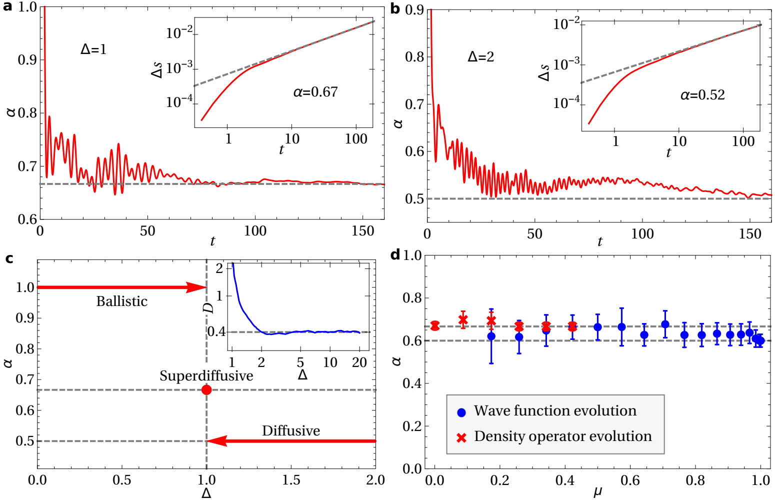
$$\rho(t=0) = (1+\mu\sigma^z)^{\otimes n/2} \otimes (1-\mu\sigma^z)^{\otimes n/2}$$



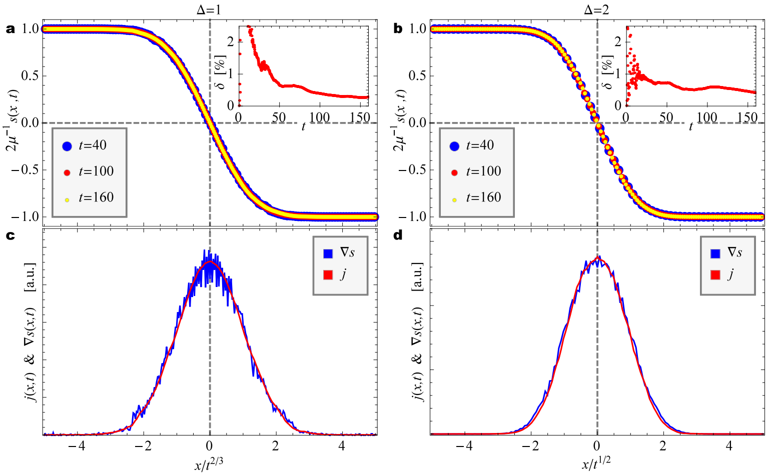
Ljubotina, Žnidarič and TP, arXiv:1702.04210; to appear in Nature Comm.

Scaling of the total transported magnetization

$$\Delta s(t) = \int_0^t j_{x=n/2}(t')\mathrm{d}t' \propto t^{\alpha}.$$



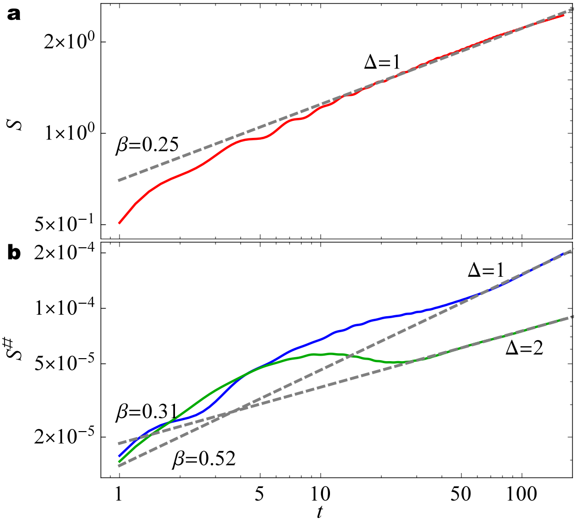
Scaling of magnetization profiles and diffusion equation



Curiously, for $\Delta = 1$ we have an effective diffusion in non-linearly scaled time

$$\partial_\tau s(x,t) = K\partial_x^2 s(x,t), \qquad \tau = t^{4/3}.$$

Why is this tDMRG simulation working for such long times?
Anomalously slow increase of bi-partitie entanglement entropies:



[Medenjak, Karrasch and TP, arXiv:1702.04677]
Finite-time T, finite-size n, fixed filling x, Drude weight and diffusion constant

$$\tilde{D}(x) = \frac{\beta}{4nT}\int_{-T}^{T} \mathrm{d}t \langle J_n(t), J\rangle_n^{\beta,x}, \quad \tilde{\mathcal{D}} = \frac{\beta}{4n\chi}\int_{-T}^{T} \mathrm{d}t \langle J_n(t), J\rangle_n^{\beta}$$

in terms of a projector P_n^m on a sector with fixed filling/magnetization m:

$$\langle A\rangle_n^{\beta,x} = \frac{\langle A P_n^{(x+1)n}\rangle_n^{\beta}}{\langle P_n^{(x+1)n}\rangle_n^{\beta}},$$

where χ is the static susceptibility.

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$$\tilde{D}(x) \propto x^2.$$

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Key idea:

- Write $\tilde{\mathcal{D}} = \frac{T}{\chi}\sum_x \langle P_n^{(x+1)n}\rangle_n^{\beta} \tilde{D}(x)$
- Scale the size as $n = vT$, where $v > v_{\mathrm{LR}}$ (Lieb-Robinson velocity), and consider large T asymptotics
- Expand Drude weight as $\tilde{D}(\beta) = D + \frac{1}{T}D_1 + \ldots$
- Throw away the term with D_1 which is strictly non-negative (D_1 agrees with the definition of the Diffusion constant in the presence of convective terms, see e.g. (Spohn, 1991)).

Lower bound on diffusion constant in terms of curvature of Drude weight

[Medenjak, Karrasch and TP, arXiv:1702.04677]

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In the limit $T \to \infty$, considering optimal $v = v_{\rm LR}$, the limits of $\tilde{D}(x)$ and $\tilde{\mathcal{D}}$ become the Drude weight and the diffusion constant, and we find:

$$\mathcal{D} \geq \frac{1}{8\beta\chi f v_{\rm LR}} \partial_x^2 D(x)\Big|_{x=0}, \qquad f = \lim_{n\to\infty} \frac{1}{4n} \partial_x^2 F_n(\beta, x)|_{x=0}$$

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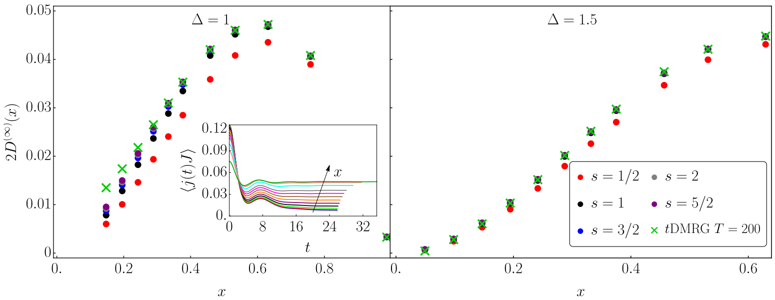
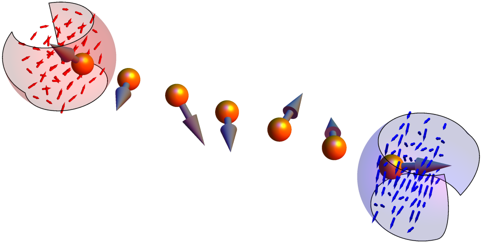
The bound is particularly simple at high temperature limit $\beta \to 0$:

$$\mathcal{D} \geq \frac{1}{4\chi v_{\rm LR}} \partial_x^2 D(x).$$

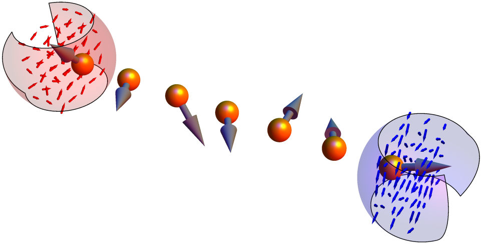




Canonical markovian master equation for the many-body density matrix:

The Lindblad (L-GKS) equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \hat{\mathcal{L}}\rho := -\mathrm{i}[H,\rho] + \sum_{\mu} \left(2L_\mu \rho L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho\} \right).$$



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- *Bulk*: Fully **coherent**, local interactions,e.g. $H = \sum_{x=1}^{n-1} h_{x,x+1}$.
- *Boundaries:* Fully **incoherent**, ultra-local dissipation, jump operators L_μ supported near boundaries $x = 1$ or $x = n$.

Nonequilbrium steady state (NESS)

Steady state Lindblad equation $\hat{\mathcal{L}}\rho_\infty = 0$:

$$\mathrm{i}[H, \rho_\infty] = \sum_\mu \left(2L_\mu \rho_\infty L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho_\infty\} \right)$$

The *XXZ* Hamiltonian:

$$H = \sum_{x=1}^{n-1} (2\sigma_x^+ \sigma_{x+1}^- + 2\sigma_x^- \sigma_{x+1}^+ + \Delta \sigma_x^{\mathrm{z}} \sigma_{x+1}^{\mathrm{z}})$$

and symmetric boundary (ultra local) Lindblad jump operators:

$$\begin{aligned} L_1^{\mathrm{L}} &= \sqrt{\frac{1}{2}(1-\mu)\varepsilon}\ \sigma_1^+, \quad L_1^{\mathrm{R}} = \sqrt{\frac{1}{2}(1+\mu)\varepsilon}\ \sigma_n^+, \\ L_2^{\mathrm{L}} &= \sqrt{\frac{1}{2}(1+\mu)\varepsilon}\ \sigma_1^-, \quad L_2^{\mathrm{R}} = \sqrt{\frac{1}{2}(1-\mu)\varepsilon}\ \sigma_n^-. \end{aligned}$$

Two key boundary parameters:

- ε System-bath coupling strength
- μ Non-equilibrium driving strength (bias)

TP, PRL**106**(2011); PRL**107**(2011); Karevski, Popkov, Schütz, PRL**111**(2013)

$$\rho_\infty = (\,\mathrm{tr}\, R)^{-1} R, \quad R = \Omega\Omega^\dagger$$

$$\Omega = \sum_{(s_1,\ldots,s_n)\in\{+,-,0\}^n} \langle 0|\mathbf{A}_{s_1}\mathbf{A}_{s_2}\cdots\mathbf{A}_{s_n}|0\rangle \sigma^{s_1}\otimes\sigma^{s_2}\cdots\otimes\sigma^{s_n} = \langle 0|\mathbf{L}(\varphi,s)^{\otimes_x n}|0\rangle$$

Cholesky decomposition of NESS and Matrix Product Ansatz (for $\mu = 1$)

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$$\mathbf{A}_0 = \sum_{k=0}^{\infty} a_k^0 |k\rangle\langle k|,$$

$$\mathbf{A}_+ = \sum_{k=0}^{\infty} a_k^+ |k\rangle\langle k+1|,$$

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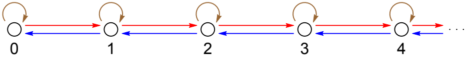

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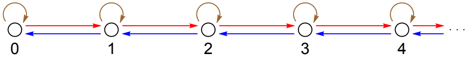

where (for symmetric driving):

$$\varphi = \frac{\pi}{2} \qquad \tan(\eta s) := \frac{\varepsilon}{2\mathrm{i}\sin\eta}$$

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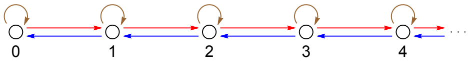

where (for symmetric driving):

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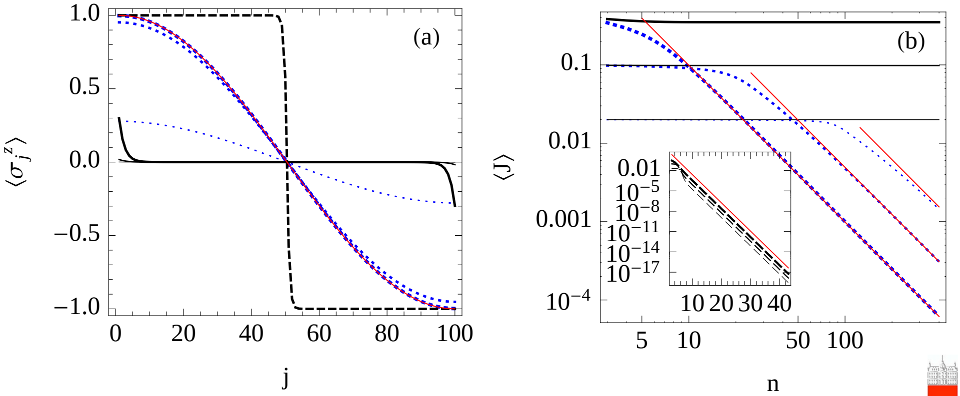
$\Omega(\varphi,s) = \langle 0|\mathbf{L}(\varphi,s)^{\otimes_x n}|0\rangle$ plays a role of a highest-weight transfer matrix corresponding to non-unitary representation of the Lax operator

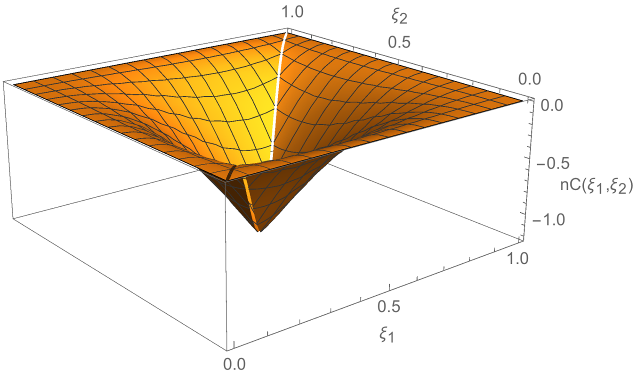
$$[\Omega(\varphi,s),\Omega(\varphi',s')] = 0, \quad \forall s,s',\varphi,\varphi'$$

- For $|\Delta| < 1$, $\langle J \rangle \sim n^0$ (ballistic)
- For $|\Delta| > 1$, $\langle J \rangle \sim \exp(-\mathrm{const}\, n)$ (insulating)
- For $|\Delta| = 1$, $\langle J \rangle \sim n^{-2}$ (anomalous)



$$C\left(\frac{x}{n}, \frac{y}{n}\right) = \langle \sigma^z_x \sigma^z_y \rangle - \langle \sigma^z_x \rangle \langle \sigma^z_y \rangle$$

for isotropic case $\Delta = 1$ (XXX)



$$C(\xi_1, \xi_2) = -\frac{\pi^2}{2n}\xi_1(1-\xi_2)\sin(\pi\xi_1)\sin(\pi\xi_2), \quad \text{for} \quad \xi_1 < \xi_2$$

How important is quantum mechanics for undertstanding quantum transport?

or

What about the ballistic-diffusive transitions in classical integrable lattices?

[TP and B. Žunkovič, PRL **111**, 040602 (2013)]

Locally interacting classical spin chain Hamiltonian

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

where for Lattice-Landau-Lifshitz model, the energy density reads

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

and $F(S) \equiv \sqrt{(\sinh^2(\rho R) - \sinh^2(\rho S))/(R^2 - S^2)}$.

Example: Classical "XXZ" model — Lattice-Landau-Lifshitz

[TP and B. Žunkovič, PRL **111**, 040602 (2013)]

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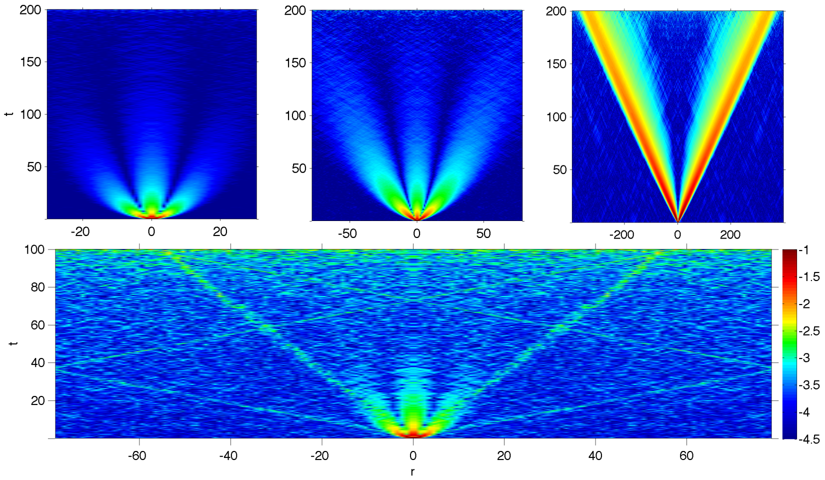
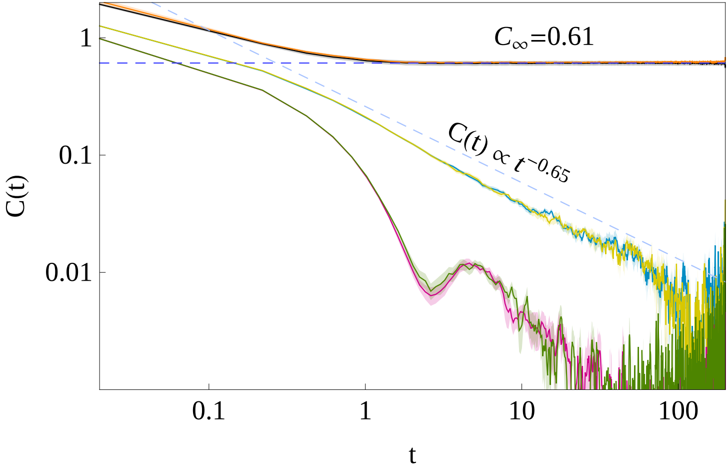
Writing **anisotropy parameter** $\delta = \rho^2$ we study three cases:

- $\delta > 0$, easy axis regime (Ising-like) **diffusive!!!**
- $\delta < 0$, easy plane regime (XY-like) **ballistic!!!**
- $\delta = 0$, isotropic regime (where $h(\vec{S}, \vec{S}') = \log\left(1 + \frac{\vec{S}\cdot\vec{S}'}{R^2}\right)$) **anomalous!!!**

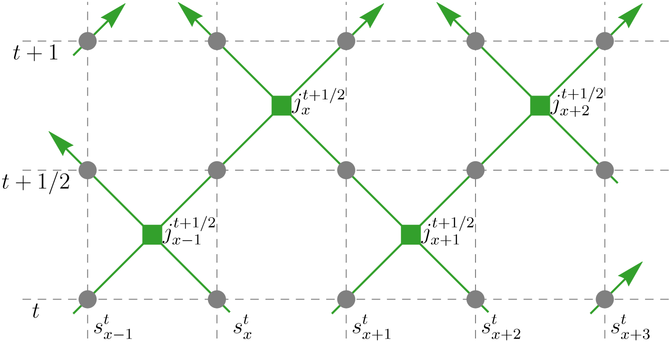


Spatio-temporal current-current c.f. shown in log-scale with color scale ranging from $10^{-4.5}$ to 10^{-1} indicated in the bottom-right. In the upper panels we show data averaged over ensembles of $N \approx 10^3$ initial conditions in easy-axis (left; $n = 5120$), isotropic (center; $n = 5120$) and easy-plane (right; $n = 2560$) regimes. Bottom: smaller $n = 160$, $N = 600$ where **scars of solitons** emerging from local thermal fluctuations are still clearly visible.



$C(t)$ 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).

[Medenjak, Klobas and TP, arXiv:1705.04636]



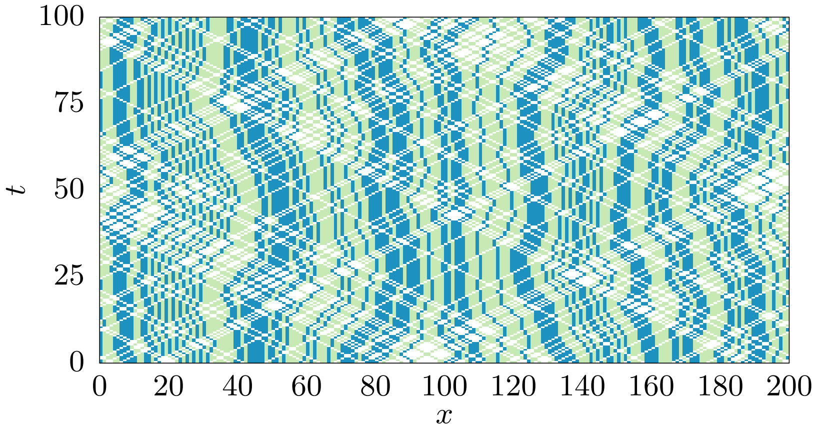
Local deterministic scattering rule (with three states $s \in \{\emptyset, +, -\}$):

$$\phi_{x,x+1} : (\emptyset, \emptyset) \leftrightarrow (\emptyset, \emptyset),\ (\emptyset, \alpha) \leftrightarrow (\alpha, \emptyset),\ (\alpha, \beta) \leftrightarrow (\alpha, \beta).$$

Global propagator $(s_{1,t+1}, s_{2,t+1}, \ldots, s_{n,t+1}) = \phi(s_{1,t}, s_{2,t}, \ldots, s_{n,t})$:

$$\phi = \phi^{\mathrm{o}} \circ \phi^{\mathrm{e}}, \quad \phi^{\mathrm{o}} = \phi_{1,2} \circ \cdots \circ \phi_{n-1,n}, \quad \phi^{\mathrm{e}} = \phi_{2,3} \circ \cdots \circ \phi_{n,1}.$$

An example of dynamics starting from a typical initial condition:



The model can be interpreted as a synchronized version of a hard-rod gas on $\mathbb{R}$ where diffusion has been established (Jepsen, JMP **6**, 405 (1965); Lebowitz, Percus, Sykes PR **171**, 224 (1968); **188**, 487 (1969))

Charge density:

$$q_x^t = s_x^t + s_{x+1}^t$$

Current density:

$$j_x^{t+1/2} = 2\,(-1)^x (s_x^{t+1/2} - s_{x+1}^{t+1/2})(s_x^{t+1/2} + s_{x+1}^{t+1/2})^2$$

Continuity equation:

$$q_x^{t+1} - q_x^t + \frac{1}{2}\left(j_{x+1}^{t+1/2} - j_{x-1}^{t+1/2}\right) = 0.$$

Define a commutative multilicative algebra of functions over micro-states $\underline{s} \in \{\emptyset, +, -1\}^n$ with a local basis

$$[\alpha]_x(\underline{s}) = \delta_{\alpha_{\boldsymbol{x}}, s_{\boldsymbol{x}}}, \quad \alpha \in \{\emptyset, +, -\},$$
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Dynamics, time-automorphism of algerba of observables:

$$a^t(\underline{s}) \equiv U^t a(\underline{s}) = a(\phi^t(\underline{s}))$$

where

$$U = U^{\mathrm{o}} U^{\mathrm{e}}, \; U^{\mathrm{o}} = \prod_{x=1}^{n/2} U_{2x-1,2x}, \; U^{\mathrm{e}} = \prod_{x=1}^{n/2} U_{2x,2x+1}.$$

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Model allows for a stochastic extension where charges $+$ and $-$ penetrate each other with probability λ

$$(\pm, \mp) \to (1-\lambda)(\pm, \mp) + \lambda(\mp, \pm).$$

Now, λ plays the role of spectral parameter.

Translationally invariant equilibrium state $p(\rho,\mu)$

Set $p(\pm) = \frac{1}{2}(\rho \pm \mu)$, $p(\emptyset) = 1 - \rho =: \bar{\rho}$ and define

$$\langle a \rangle_p = \sum_{\underline{s}} a(\underline{s}) \prod_x p(s_x).$$

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Useful local basis, orthonormal w.r.t. $pl(\rho, \mu = 0)$:

$$[0] = [\emptyset] + [+] + [-] \equiv 1, \quad [1] = [+] - [-], \quad [2] = \tfrac{\rho}{1-\rho}[\emptyset] - [+] - [-],$$

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Charge density and current density read

$$q_x = [10]_x + [01]_x, \quad j_x = 2(1-\rho)(-1)^x \left([10]_x - [01]_x + [12]_x - [21]_x \right).$$

Nice properties of U in basis 012 allow for explicit computation of $C(t) = \langle J U^t J \rangle_p$:

$$\frac{C(t)}{8\bar{\rho}} = \begin{cases} \mu^2 + \rho(2-\rho); & t = 0, \\ \frac{2\mu^2}{\rho} + 2\bar{\rho}^3 (1-2\rho)^{2t-2} \left(\rho - \frac{\mu^2}{\rho}\right); & t \geq 1. \end{cases}$$

Explicit evaluation of current-current correlations and Green-Kubo transport coefficients

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This yields the conductivity and the Diffusion constant for $\mu = 0$

$$\sigma = \frac{1}{2}C(0) + \sum_{t=1}^{\infty} C(t) = 4(1-\rho), \quad \mathcal{D} = \frac{\sigma}{\chi} = \frac{1}{\rho} - 1$$

where $\chi(\rho,\mu) = \langle q_x^2 \rangle_p = 4\rho - \mu^2$ is the static susceptibility.

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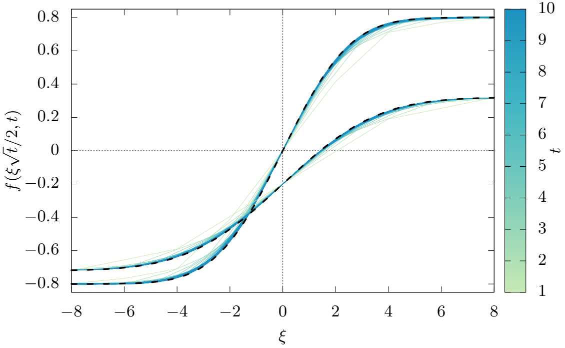
Note that this simple model saturates the curvature inequality (note $v_{\rm LR} = 2$)

$$\mathcal{D} = \frac{1}{4\chi v_{\rm LR}} \partial_\mu^2 D(\mu).$$

Using the nice algebra one can even completely solve the initial value problem for $\mu = \mu_{\rm L}$ for $x \leq n/2$ and $\mu = \mu_{\rm R}$ for $x > n/2$:

$$f(x,t) = \langle U^t q_{n/2+2x-1} \rangle_p,$$

$$\tilde{f}(\xi) = \lim_{t\to\infty} (\frac{1}{2}\xi\sqrt{t}, t) = (\mu_{\rm L} + \mu_{\rm R}) + (\mu_{rmR} - \mu_{\rm L}) {\rm erf}\left(\frac{\xi}{2\sqrt{\rho^{-1} - 1}}\right).$$



Conclusions

- No microscopic chaos needed for normal diffusion, extensive initial state randomness (entropy) suffices
- For systems with $\mathbb{Z}_2$ symmetries, such that the current is anti-symmetric, diffusion constant can be lower bounded by the curvature of the Drude-weight w.r.t. symmetry-breaking parameter (filling/magnetization). This could suggest perhaps to split the diffusion constant into a 'regular' (lower bound) and 'chaotic' (the rest) contributions.
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Conclusions

- No microscopic chaos needed for normal diffusion, extensive initial state randomness (entropy) suffices
- For systems with $\mathbb{Z}_2$ symmetries, such that the current is anti-symmetric, diffusion constant can be lower bounded by the curvature of the Drude-weight w.r.t. symmetry-breaking parameter (filling/magnetization). This could suggest perhaps to split the diffusion constant into a 'regular' (lower bound) and 'chaotic' (the rest) contributions.
- No clue on the mechanism for anomalous diffusion in isotropic Heisenberg model!?

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