Transport in quantum spin chains (notes Boulder '23, Marko Žnidarič)

1.) Introduction

[arXiv:2003.03334 Bertini et al.]

transport of conserved quantity

Example:

- $\underline{H_{XXZ} = \sum_x \sigma_x^x \sigma_{x+1}^x + \sigma_x^y \sigma_{x+1}^y + \Delta \sigma_x^z \sigma_{x+1}^z = \sum_x h_{x,x+1}}$ Heisenberg XXZ model
- $H_{XYZ} = \sum_x \frac{1+\gamma}{2} \sigma_x^x \sigma_{x+1}^x + \frac{1-\gamma}{2} \sigma_x^y \sigma_{x+1}^y + \Delta \sigma_x^z \sigma_{x+1}^z$ XYZ model

- magnetization $Z = \sum_x \sigma_x^z$

$[Z, H_{XXZ}] = 0$ transport of spin in XXZ ok ✓

$[Z, H_{XYZ}] \neq 0$ "spin created locally" ✗

Conserved quantity → continuity equation $\frac{\partial \rho}{\partial t} + \mathrm{div}\, \vec{j} = 0$

defines the current $\frac{\partial \rho_x}{\partial t} + (j_x - j_{x-1}) = 0$

Example: for H_{XXZ} spin current is

$$\frac{d\sigma_x^z}{dt} = -i[\sigma_x^z, H_{XXZ}] = j_{x-1} - j_x, \quad \text{with}$$

$$\underline{j_x \equiv i[\sigma_x^z, h_{x,x+1}] = 2(\sigma_x^x \sigma_{x+1}^y - \sigma_x^y \sigma_{x+1}^x)}$$

For XXZ we can study transport of spin, or energy. (Ex. 1.: energy current XXZ)

fermionic language: particle = spin (Ex. 2.: Jordan-Wigner)

Comment: energy ≠ heat transport !

- spin and energy have microscopic definition, heat does not
  (no "heat operator")
  not state function

- def. of heat always requires excursion into thermodynamics

$$dE = đQ + đW \quad \Rightarrow \quad j_E = j_Q + \mu j_N \quad \text{or}$$

$$\underbrace{j_Q = j_E - \mu j_N}$$

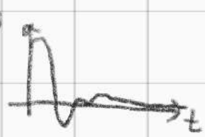
microsc. j_E and j_N
thermodynamic μ

{requires splitting j_E into "stochastic" part - heat, and "deterministic" work}

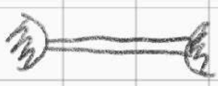
- Using $j_E = i[h, h] = \hat{j}_Q$ as "heat" current $\hat{j}_Q$ is WRONG
  (violates the II. law, see Ex. 3.: heat vs. energy)

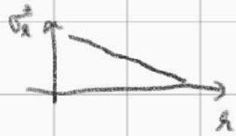
2.) Theory

(a) Linear response

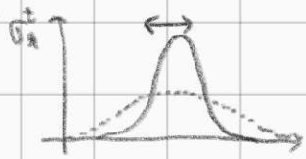


(b) explicit driving - NESS





(c) unitary evolution of inhomogeneous states



(a) Linear response

[Pottier: Noneq. Stat. Phys.]

transport coefficient (eg. diffusion constant) = integral of current autocorrel.)

remember general L.-R.: $H = H_0 - a(t)\, A$

$$\langle B(t) \rangle = \int_{-\infty}^{\infty} \chi_{BA}(t-\tau)\, a(\tau)\, d\tau$$

response function of B to pert. A

$$\chi_{BA}(t) = \frac{i}{\hbar}\,\Theta(t)\,\langle [\,B^{(\infty)}(t), A\,]\rangle_{eq.} =$$ commutator

$$= \Theta(t)\,\beta \cdot \underbrace{\frac{1}{\beta}\int_0^\beta \langle \dot{A}(-i\hbar\lambda)\,B(t)\rangle_{eq.}\,d\lambda}_{\text{Kubo correlation function}}$$

in Fourier space : $\underbrace{\langle B(\omega)\rangle = \chi_{BA}(\omega)\,a(\omega)}$

generalized susceptibility

Example : (electric / spin) particle conductivity

$$H = H_0 - e\,E(t)\,x$$

$a(t) = e\,E(t)$, $A = x$

$B = j$ particle current

$j = e\dot{A} = e\,v$

by definition $\underbrace{j(\omega) = \sigma(\omega)\,E(\omega)}$

conductivity

$$\text{L.-R.} \Rightarrow \quad \sigma(\omega) = e\,\chi_{jx} = \int_0^\infty e^{i\omega t}dt \int_0^\beta \langle j(-i\hbar\lambda)\,j(t)\rangle_{eq.}\,d\lambda$$

we use Kubo
corr. to have $\dot{A} \sim j$

For spin chains exactly the same : $J = \sum_x j_x$ extensive current

$$\underbrace{\sigma(\omega) = \beta \lim_{t\to\infty}\lim_{L\to\infty} \frac{1}{\beta}\int_0^\beta d\lambda \int_0^t e^{i\omega\tau}\,\frac{\langle J(0)\,J(\tau + i\hbar\lambda)\rangle_{eq}}{L}\,d\tau}$$

$\sigma(\omega) \equiv \sigma'(\omega) + i\,\sigma''(\omega)$

$$\langle * \rangle_{eq} = \mathrm{tr}\left(* \,\frac{e^{-\beta H_0}}{Z_0}\right)$$

* correct thermodynamic limit : $\lim_{t\to\infty}\lim_{L\to\infty}$, ie., first $L \to \infty$!
* central object $\frac{\sigma(\omega)}{\beta}$
* classical ($\hbar \to 0$) or high-T ($\beta \to 0$) limit : $\sigma(\omega) = \beta \int_0^\infty e^{i\omega t}\,\frac{\langle J(0) J(t)\rangle}{L}\,dt$

* Kubo correlation function can be expressed in terms of classical, commutator,... correlation functions, e.g.,

$$\sigma'(\omega) = \frac{1-e^{-\beta\omega}}{\omega}\int_0^\infty \frac{\mathrm{Re}\left[e^{i\omega t}\langle J(0)J(t)\rangle\right]}{L}\,dt$$

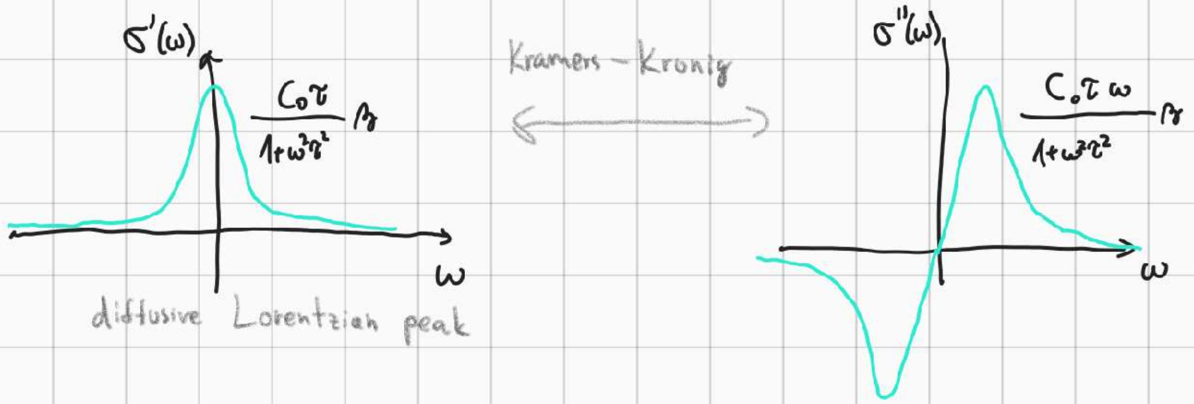
Behavior of $\sigma(\omega)$

let's take classical current autocorrelation function $C(t) = \frac{1}{L}\langle J(0)J(t)\rangle = C_0 e^{-t/\tau}$

$\equiv$ classical Drude model [Ashcroft & Mermin Ch. 1.] (classical particle damped by force $F \propto v$)

$$\Rightarrow \quad \sigma(\omega) = \frac{C_0\tau}{1-i\omega\tau}\beta$$

{see Ex. 4. for connection with Langevin eq. and C_0}



for $\tau \to \infty$ (no dissipation) peak at $\omega = 0$ goes into a δ-function

$$\sigma'(\omega) \xrightarrow{\tau\to\infty} 2\pi \underbrace{D}_{\text{Drude weight}}\,\delta(\omega) \quad , \quad D = \frac{C_0}{2}\beta$$

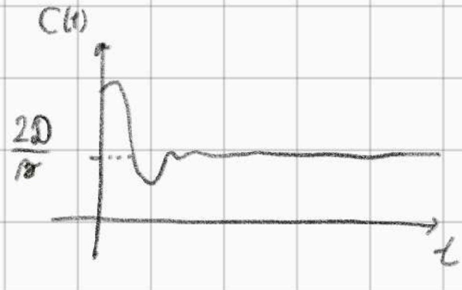
(Ex. 4.: derivation)

In general split:

$$\underbrace{\sigma'(\omega) = 2\pi D\,\delta(\omega) + \sigma_{reg}(\omega)}$$

* D: Drude weight

$\frac{D}{\beta} = \frac{1}{2}$ plateau signals ballistic transport



* $\frac{\sigma_{reg}(\omega)}{\beta} \sim \omega^{\alpha}$ for $\omega \ll 1$ $\left(\text{implies } C(t) \propto \frac{1}{t^{\alpha+1}} \right)$

+ $\alpha = 0$: diffusion
+ $\alpha > 0$: subdiffusion
+ $\alpha < 0$: superdiffusion

* diffusion constant

+ $\sigma'(\omega=0)$ relates current j and perturbation in H that induces σ^z, i.e.,

$H = H_0 - \sum \sigma^z_r h_r \Rightarrow$ gradient of magnetic field

$$j = -\sigma'(\omega) \nabla h$$

+ diffusion constant defined in terms of "Fick's" law

$$j = -D \nabla \sigma^z$$

$$\boxed{D = \frac{\sigma(0)}{\chi}} \quad , \quad \chi = \frac{\partial \sigma^z}{\partial h} = \frac{\beta}{L}\left[\langle Z^2\rangle - \langle Z\rangle^2\right]$$

"static spin susceptibility"

$Z = \sum_r \sigma^z_r$

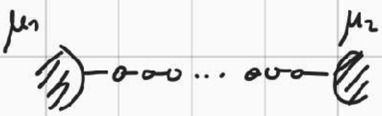
(Ex.5.: derive χ)

at $\beta \to 0$ one has $\chi = \beta$ and $D = \frac{\sigma(\omega)}{\beta}$

(Ex.6.: def. of D in d-dimensions)

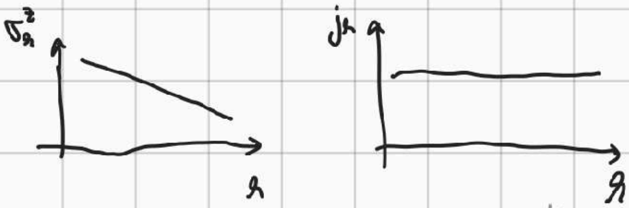
(b) nonequilibrium steady state – NESS

like "experiment" – couple to a "bath"



$\rho(t) \rightarrow \rho_\infty$ NESS

$$j = \mathrm{tr}(\rho_\infty j_r)$$

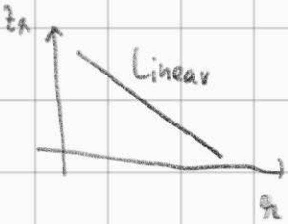


diffusion

conservation $j_r = j$

in NESS

* transport type : scaling of NESS j with L at fixed $\Delta\mu$

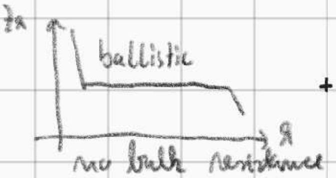


+ diffusion : $j = -D\,\frac{z_L - z_1}{L}$, ie, $j \sim \frac{1}{L}$ (the same D as in L.R. arXiv: 1806.11050, Dz PRB'19)

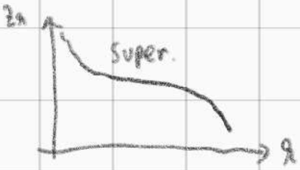
diffusion is a prefactor

in general transport $\underbrace{j \sim \frac{1}{L^{\gamma}}}$, scaling exponent γ

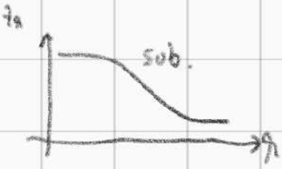
$\left\{ \text{finite-size } D \sim L^{1-\gamma} \right\}$



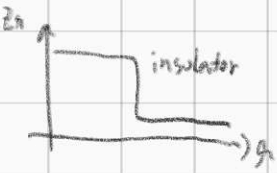
+ ballistic : $\gamma = 0$



+ superdiffusion : $0 < \gamma < 1$



+ subdiffusion : $\gamma > 1$



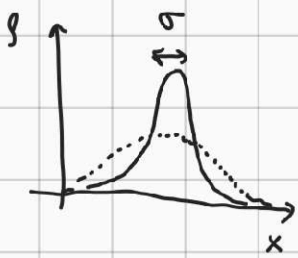
+ insulator : $\gamma \to \infty$

* how to drive?

for generic systems does not matter in the TDL (selfthermalization)

+ thermodynamic parameters like $\mu, T, \dots$, must be measured in the system (not some bath parameters; boundary jumps / contact resistance)

(c) unitary evolution



$\underbrace{\langle \sigma^2 \rangle \simeq t^{2\beta}}$ $\left(\Rightarrow \text{finite-time } D \sim t^{2\beta - 1} \right)$

scaling exponent β :

+ $\beta = \frac{1}{2}$: diffusion
+ $\beta = 1$: ballistic
+ $\frac{1}{2} < \beta < 1$: superdiffusion
+ $\beta < \frac{1}{2}$: subdiffusion

* Exponents:
+ $\sigma'(\omega) \sim \omega^{\alpha}$ (LR)
+ $j \sim \frac{1}{L^{\gamma}}$ (NESS)
+ $\sigma \sim t^{\beta}$ (spreading)

assuming single-parameter scaling they are related.

+ $\sigma \sim t^{\beta} \Rightarrow t \sim L^{1/\beta} \Rightarrow j = L \cdot \frac{1}{t} = \frac{1}{L^{1/\beta - 1}}$

$$\Downarrow$$

$$\underbrace{\beta = \frac{1}{\gamma+1}} \qquad \left(\gamma = \frac{1}{\beta} - 1\right)$$

+ $\sigma' \sim \omega^{\alpha} \Rightarrow C(t) \sim \frac{1}{t^{\alpha+1}} \Rightarrow D(t) = \int_0^t C(\tau) d\tau \sim \frac{1}{t^{\alpha}} \sim t^{2\beta - 1}$

$$\Downarrow$$

$$\underbrace{\alpha = \frac{\gamma - 1}{\gamma + 1}} \qquad (\alpha = 1 - 2\beta)$$

often one uses dynamical scaling exponent $z = \frac{1}{\beta} = 1 + \gamma$.

* Linear response depend on current-current correlation function $C(t) = C_{JJ}(t)$.

important also density-density correlation function C_{zz}. (Scattering exper.)

Are the two related? yes

(Ex. 7.: Use cont. eq. to connect C_{zz} and C_{JJ})

$$\underbrace{\langle \ddot{z}(x,t) z(0,0) \rangle = \langle j''(x,t) j(0,0) \rangle}$$

(dots: time-deriv, prime: space deriv. / using cont. space index x)

from which one gets

$$\underbrace{\ddot{\Sigma}_2(t) = 2\, C_{JJ}(t)}, \qquad \Sigma_2(t) \equiv \int x^2 \langle z(x,t) z(0,0) \rangle dx$$

{could be used to get relation between α and β}

3.) Methods

how do we calculate objects from 2) Theory?

Hard, because the many-body limit $L \to \infty$ is needed!

Few methods mentioned:
+ exact diagonalization and L.R.
+ Lindblad master eq. and NESS
+ generalized hydrodynamics (GHD)

+ exact diagonalization (easy, but has serious limitations)

- limited to small L (in some classical systems we know that large L is needed ($\gtrsim 10^3$) to reach TDL; in transport size can be everything)

- as soon as one works with eigenenergies E_n and eigenstates $|n\rangle$ one is immediately in the wrong TDL of first $t\to\infty$ (to resolve eigenstates) and only then $L\to\infty$.
  Generic issue with ED, not particular to transport.

Example of such failure:

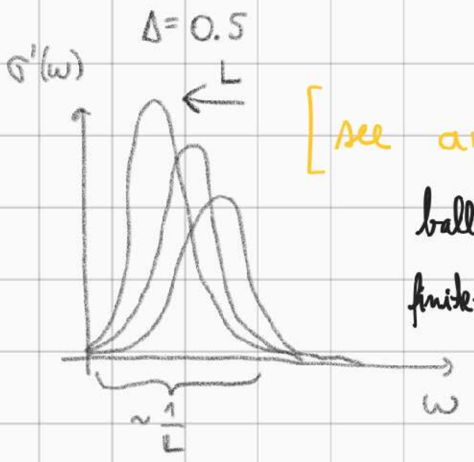
Drude weight (ballistic) is $\frac{1}{2}$ of the plateau in $C(t), \infty$

$$\frac{D}{\beta} = \frac{1}{2}\,\frac{1}{L}\sum_{E_n=E_{n'}} p_n |\langle n|J|n'\rangle|^2$$

given by diagonal matrix elements of $J=\sum_n j_n$ (in absence of degeneracies)

these can be zero due to e.g. symmetries. One should also take into account close-to-diagonal, i.e., not take $t\to\infty$ first.

+ For instance, in the XXZ with OBC (but not PBC) all diagonal are zero ?! despite ballistic transport



[see arXiv: 1810.03640 Brenes et al. (PRB 98, 235128 '18)]

ballistic transport (Drude weight) is shifted to finite $\omega \sim \frac{1}{L}$

finite-L $C(t)$ does not have a plateau, just finite-time plateau

+ on a similar note (from the same paper), XXZ with a single impurity stays ballistic (single "scattering" among L sites). $\sigma'(\omega)$ behaves similar as above. "Favorite" quantum chaos criterion – level spacing distribution is "chaotic". system is not chaotic! (eigenstates in a many-body system are not observable)

+ Lindblad master equation and NESS

(sometimes works for large systems)

[Alicki & Lendi: Quantum Dynamical Semigroups and Application

Breuer & Petruccione: The Theory of Open Q. Systems]

$$\underbrace{\frac{d\rho}{dt} = \underbrace{i[\rho,H]}_{\text{unitary}} + \sum_j{}' \underbrace{[L_j\rho, L_j^\dagger] + [L_j, \rho L_j^\dagger]}_{\substack{2L_j\rho L_j^\dagger - L_j^\dagger L_j\rho - \rho L_j^\dagger L_j \\ \text{dissipation}}} \equiv \mathcal{L}\rho}$$

Lindblad (Gorini-Kossakowski-Sudarshan) equation [history arXiv: 1710.05993 Chruscinski & Pascazio]

* the most general evolution of $\rho(t)$:
  + linear and preserves positivity $\rho(0) \geq 0 \xrightarrow{t} \rho(t) \geq 0$

    (implies positive map Λ, $\rho(t) = \Lambda(t)\rho(0)$)
  + completely positive: $\mathbb{1} \otimes \Lambda(t)$ also positive
  + dynamical semigroup: $\Lambda(t)\Lambda(t') = \Lambda(t+t')$

* formal solution $\rho(t) = e^{\mathcal{L}t}\rho(0)$, but $\mathcal{L}$ complicated (for spin $\frac{1}{2}$ $4^L \times 4^L$)

* of special interest is fixed point

  $\underbrace{\mathcal{L}\rho_\infty = \rho_\infty}$ steady state

* derivation: + $H_{sys} + H_{bath} + V$ weak coupling, Markovian, fast environment, secular

  ie., complicated with nonlocal L_j

  + noisy $H(t)$, eg., $H(t) = \xi(t)\sigma^z$ with white noise $\xi(t)$

    results in Lindblad average dynamics with $L = \sqrt{\gamma}\sigma_z$

    $\gamma \propto \langle \xi^2(t) \rangle$

  + continuous measurement, repeated interaction, ...

* just postulate: in TDL for generic systems (self thermalize)

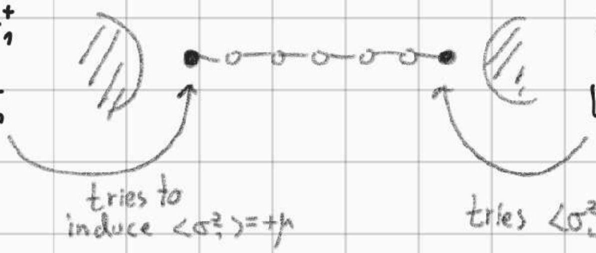
(Ex. 8.: simple Lindblad eq.)

Spin driving:

common choice for spin transport

$L_1 = \sqrt{\Gamma(1+\mu)}\,\sigma_1^+$

$L_2 = \sqrt{\Gamma(1-\mu)}\,\sigma_1^-$



$L_3 = \sqrt{\Gamma(1-\mu)}\,\sigma_L^+$

$L_4 = \sqrt{\Gamma(1+\mu)}\,\sigma_L^-$

* for $\mu = 0$ the SS is $\rho_\infty = \mathbb{1}\frac{1}{2^L}$ infinite-T equilibrium
* nonzero μ: "artificial" driving at infinite T and finite $\beta\mu$. ρ_∞ is NESS with nontrivial $\langle\sigma_k^z\rangle$ and $\langle j_k\rangle$

How to find ρ_∞?

* exact solution (rare!)

  + XX chain with any μ: ballistic
    MPO form of ρ_∞ with $\chi = 4$ [arXiv:1006.5368, MZ JPA '10]

  + XXZ with $\mu = 1$ (maximal driving): ballistic ($\Delta<1$), subdiffusive ($\Delta=1$), insulating ($\Delta>1$)
    nongeneric physics
    [arXiv:1106.2978, Prosen PRL '11]

  + $\mathcal{L}$ is quadratic: diagonalization of $L\times L$ matrix
    [arXiv:0801.1257, Prosen NJP '08]

  + H quadratic and L_j Hermitian, eg., XX chain with dephasing $L_j = \sqrt{\gamma}\,\sigma_j^z$:
    ballistic ($\gamma = 0$) $\rightarrow$ diffusive [arXiv:1005.1271, MZ JSTAT '10]
    hierarchy of correlations

* numerics :

$$\rho(t) = \sum_{\vec{s}}' c_{\vec{s}} \sigma^{\vec{s}} \quad , \quad \vec{s} \in \{x,y,z,\mathbb{1}\}^{\otimes L}$$

$$c_{\vec{s}} = \langle L | M_1^{(s_1)} M_2^{(s_2)} \cdots M_L^{(s_L)} | R \rangle$$ matrix product operator ansatz (MPO)

↖ bond size χ

+ time evolve by $e^{\mathcal{L} t}$, splitting into small steps Δt (Trotter-Suzuki)

+ use local L_j so that $\mathcal{L}$ is a sum of local terms

$e^{\mathcal{L}_{\ell,\ell+1} \Delta t}$ transforms $M_\ell^{(s_\ell)} M_{\ell+1}^{(s_{\ell+1})}$ into $\Theta_{s_\ell' i, s_{\ell+1}' j} \xrightarrow{\text{SVD}} M_\ell^{(s_\ell')} M_{\ell+1}^{(s_{\ell+1}')}$

cost $\mathcal{O}((d\chi)^3)$ TEBD

d = basis dimension, is 4 for spin $\frac{1}{2}$

[arXiv: 2104.14350, Landi, Poletti, Schaller RMP '22 boundary-driven Lindblad]

evolve until NESS $\rho_\infty = \rho(t \to \infty)$ is reached (inverse gap of $\mathcal{L}$, but not always)

efficiency depends on χ – "entanglement" of $\rho(t)$

$$\rho(t) = \sum_\alpha \lambda_\alpha A_\alpha \otimes B_\alpha$$ Schmidt decomposition

χ = # of nonzero λ_α (for exact MPO)

Example: + $\rho = \mathbb{1} = \mathbb{1} \otimes \mathbb{1}$ requires $\chi = 1$

separable/product operator

(infinite-T ρ_∞ is easy)

⇓

often TEBD works well at high-T (even $L \sim 10^3$ in couple weeks CPU)

+ $\rho = \mathbb{1} + \alpha\, \sigma_1^z \otimes \sigma_2^z \Rightarrow \chi = 2$

+ generalized hydrodynamics

[arXiv: 1912.08496, Doyon SciPost '20]

for integrable systems – extensive number of local conserved quantities

[arXiv: 1012.3587, Caux & Mossel JSTAT '11] like "free (quasi) particles" with nontrivial momenta, and only 2-body scatterings that cause phase shifts (velocity depends on density)

conservation laws for conserved densities ϱ_m: $\dot{\varrho}_m + \mathrm{div}\, \vec{j}_m = 0$

$\vec{j}_m = \varrho_m \vec{v}_m$

to treat conserved ϱ_m use thermodynamic Bethe ansatz

* can evolve inhomogeneous initial states (e.g. a domain wall) in the scaling limit (local relaxation, $\varrho \sim e^{-\sum_m \lambda_m \varrho_m}$)
(generalized) Gibbs state

.... and extract transport parameters, like $\mathcal{D}$ and D.

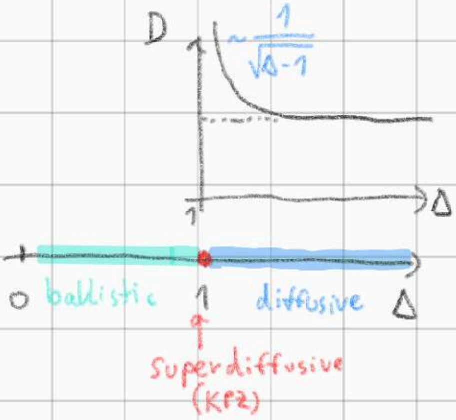
4.) Results for XXZ

* energy current conserved, $[J_E, H] = 0 \Rightarrow$ ballistic

* spin transport

  + in sector with $Z \neq 0$ $\langle J J_E \rangle \neq 0 \Rightarrow$ ballistic spin

  + interesting regime for $Z = 0$ (half-filling)



• for $\Delta < 1$: $\mathcal{D} \neq 0$ known for long time

fractal $\mathcal{D}(\Delta)$ due to quasi-local ϱ_m
[arXiv: 1103.1350 Prosen; 1306.4498 Prosen & Ilievski]

• $\Delta = 1$: superdiffusive $(z = \frac{3}{2})$
[arXiv: 1103.4094 ...]

• $\Delta > 1$: debatable, but solved by GHD

[arXiv: 1812.00767 De Nardis, Bernard, Doyon; 1812.02701 Gopalakrishnan, Vasseur]

* breaking integrability

+ strong breaking into chaos → diffusion
+ weak breaking more subtle: (no quantum KAM thm.)
  - single impurity → remains ballistic [1810.03640 Brenes et al.]
  - finite density of impurities → diffusion with $D(\rho) \sim \frac{1}{\rho^{2-z}}$ [2006.09793 MZ]

beware: at small ε → long times (size) needed

transport well defined only for $t \to \infty$ (finite window / arbitrary fitting ≠ transport)

5.) Open questions

* numerical methods ("entanglement barrier")

  benchmark D at $\Delta = 1.5$

* Lindblad and integrable systems

* quantum KAM

* disorder in XXZ : subdiffusion → MBL ?

  large scales (classical Heisenberg: arXiv 2304.05423 Scardicchio et al.)

* integrable : • is XXZ $\Delta > 1$ really diffusive?

  • can answer depend on the quantity? (higher correlations, fluctuations, ...)

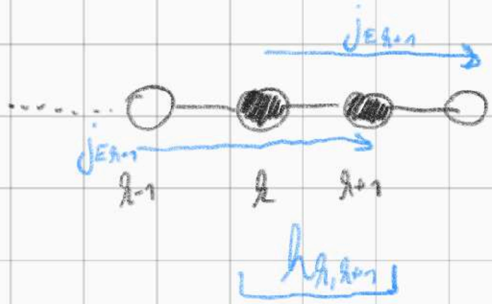
  numerical indication not all is diffusive, e.g.,

  + 1405.5541 MZ in XXZ
  + 2109.13088 Krajnik et al. in classical
  + 2306.09333 Google AI in Floquet XXX

Exercises – Lecture notes on "Transport...." (Boulder '23 M. Žnidarič)

Exercise 1. energy current for the XXZ model

$$j_{E\ell} = i\left[h_{\ell-1,\ell},\, h_{\ell,\ell+1}\right] = 2\left\{ yzx - xzy + \Delta(xy-yx)z + \Delta z(xy-yx) \right\}_{\ell-1,\ell,\ell+1}$$



Q.: what are symmetries connected to spin/energy transport?

Exercise 2. Jordan–Wigner transform.: Paulis $\leftrightarrow$ fermions

W.-J.: $Z_\ell = \sigma_1^z \sigma_2^z \cdots \sigma_\ell^z$, spinless fermions:

$$c_j = Z_{j-1}\sigma_j^-, \quad c_j^+ = Z_{j-1}\sigma_j^+$$

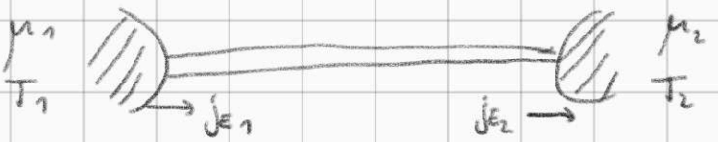
show
$$H_{XXZ} = \sum_\ell 2\left(c_\ell c_{\ell+1}^+ + c_{\ell+1} c_\ell^+\right) + \Delta \sum_\ell (2n_\ell - 1)(2n_{\ell+1} - 1)$$

t-V model

spin transport = magnetization = particle-charge transport

Exercise 3. heat vs. energy

* use incorrect $j_Q = j_E$ and show that one can have SS with nonzero currents and zero entropy production (violating the 2nd Law of TD)



in SS: $j_{E_1} = j_{E_2}$

entropy current : $j_{S_1} = \frac{j_{Q_1}}{T_1}$ and $j_{S_2} = \frac{j_{Q_2}}{T_2}$

if $j_Q = \tilde{j}_Q$ and one takes $T_1 = T_2$ (but non-equal $\mu_1 \neq \mu_2$)

$\Downarrow$

{ A: transversal area, $\frac{dS_{int}}{dt}$: entropy generated in the system }

$$\frac{1}{A}\frac{dS_{int}}{dt} = \frac{j_{Q_2}}{T_2} - \frac{j_{Q_1}}{T_1} = \frac{j^E}{T_1} - \frac{j^E}{T_1} = 0 \qquad (\rightarrow\leftarrow)$$

* use correct $j_Q = j_E - \mu j_N$ and show that in this case entropy production is always positive (II. law).

(see eg. Pottier's book)
$$\begin{pmatrix} j^N \\ j^E \end{pmatrix} = \begin{pmatrix} L_{NN}, & L_{NE} \\ L_{EN}, & L_{EE} \end{pmatrix} \begin{pmatrix} \nabla(-\frac{\mu}{T}) \\ \nabla(\frac{1}{T}) \end{pmatrix}, \quad \underline{L} \geq 0 \text{ positive semi-definite}$$

for $T_1 = T_2$: $\underbrace{j^N = -L_{NN}\frac{\nabla\mu}{T}, \; j^E = -L_{EN}\frac{\nabla\mu}{T}}$

$$j_Q = (-L_{EN} + \mu L_{NN})\frac{\nabla\mu}{T}$$

and $$\frac{1}{A}\frac{dS_{int}}{dt} = \frac{L_{NN}}{T^2}(\mu_2 - \mu_1)^2 \geq 0 \quad \checkmark$$

Exercise 4.: exponential $C(t)$

+ calculate Fourier transformation of $C(t) = C_0 e^{-t/\tau}$.
+ use Plemelj-Sohotski formula $\frac{1}{\omega \mp i\varepsilon} = \mathcal{P}\left(\frac{1}{\omega}\right) \pm i\pi\delta(\omega)$ and show that in the limit $\tau \to \infty$ one has

Drude weight $$\mathcal{D} = \frac{C_0\beta}{2}, \quad \text{with def. } \sigma'(\omega) = 2\pi\mathcal{D}\,\delta(\omega)$$

+ Langevin equation and Drude model:

$\langle v v(t)\rangle = \frac{D}{\gamma}e^{-\gamma|t|}$, ie, $\langle v^2\rangle = \frac{D}{\gamma} = \frac{kT}{m}$ (Einstein relation) ; $J = ev \Rightarrow C_0 = e^2\frac{D}{\gamma} = e^2\frac{kT}{m}$

we get $\underline{\sigma(\omega=0) = C_0\tau\beta = \frac{e^2\tau}{m}}$ this is standard Drude ($\sigma = \frac{ne^2\tau}{m}$, using $n=1$ for lattice)

<u>Note</u>: $\sigma(0)$ is not explicitly proportional to β. This is because $C_0 \propto T \xrightarrow{T\to\infty} \infty$

Different than in spin chains, where C_0 will not grow with T (bounded op. j_s), and $\Rightarrow \sigma \sim \beta$

Exercise 5.: use partition function $\mathcal{Z} = \mathrm{tr}\left(e^{-\beta(H_0 - \sum \sigma_i^z h)}\right)$ and

show that $\frac{\partial \sigma^z}{\partial h} = \frac{\beta}{L}\left(\langle Z^2\rangle - \langle Z\rangle^2\right)$, where $\sigma^z = \langle \sigma_i^z \rangle =$

$= \frac{1}{\mathcal{Z}}\, \mathrm{tr}\left(Z\, e^{-\beta(H_0 - Zh)}\right)$

Exercise 6.: diffusion in d-dim.

what we call diffusion constant is a matter of definition.

Fick's law $\underbrace{\vec{j} = -D\nabla\rho}$ D: diffusion const.

together with cont. eq. $\rho_t + \mathrm{div}\,\vec{j} = 0$ gives

diffusion equation $\underbrace{\rho_t = D\,\nabla^2\rho}$

+ Green's function in 1-d and infinite space is

$$G(x, x_0, t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-(x-x_0)^2/4Dt},$$

meaning that $\langle x^2\rangle = 2Dt$ for diffusion

+ in d-dimensions one has $G = \frac{1}{(4\pi D t)^{d/2}}\, e^{-(\vec{r}-\vec{r}_0)^2/4Dt}$

and therefore $\langle(\vec{r}-\vec{r}_0)^2\rangle = 2dDt$

diff. constant is therefore $\underbrace{D = \lim_{t\to\infty} \frac{\langle r^2(t)\rangle}{2dt}}$

Exercise 7.: relation between $C_{zz}(x,t)$ and $C_{JJ}(x,t)$.

denote local current $j(x,t)$, $J(t)=\int dx\, j(x,t)$, and local magnetization by $z(x,t)$

$$C_{zz}(x,t) = \langle z(x,t)\, z(0,0)\rangle$$
$$C_{JJ}(x,t) = \langle j(x,t)\, j(0,0)\rangle$$
, where $\langle * \rangle = \mathrm{tr}(\rho *)$

* use $\underline{\text{cont. eq.}}$: $\dot{z}(x,t) + j'(x,t) = 0$,

and $\underline{\text{stationarity in time of eq. correlations}}$: $\langle A(t) B(0)\rangle = \langle A(0) B(-t)\rangle$

$$\Downarrow$$

$$\langle \dot{A}(t) B(0)\rangle = -\langle A(t) \dot{B}(0)\rangle$$

and $\underline{\text{stationarity in space}}$: $\langle a(x) b(0)\rangle = \langle a(0) b(-x)\rangle$

$$\Downarrow$$

$$\langle a'(x) b(0)\rangle = -\langle a(x) b'(0)\rangle$$

to show that $\underbrace{\langle \ddot{z}(x,t) z(0,0)\rangle = \langle j''(x,t) j(0,0)\rangle}$

* use the above to show that the 2^{nd} moment of C_{zz} obeys

$$\underbrace{\ddot{\Sigma}_2(t) = 2\, C_{JJ}(t)}, \quad C_{JJ}(t) = \frac{1}{L}\langle J(t) J(0)\rangle$$

(hint: twice per-partes)

* alternative relation :

cont. equation in Fourier space gives

$$z(q,\omega) = \frac{q}{\omega}\, j(q,\omega)$$
, where eg. $z(x,t) = \int z(q,\omega)\, e^{iqx - i\omega t}\, dq\, d\omega$

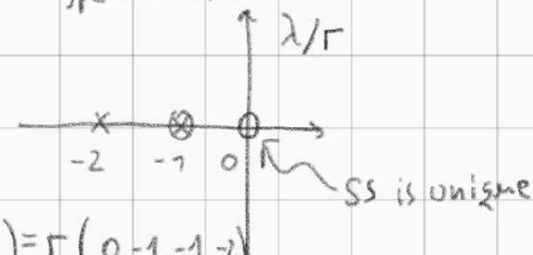
assuming stationarity Wiener-Khinchin thm. gives $C_{zz}(q,\omega) = \frac{q^2}{\omega^2} C_{JJ}(q,\omega)$

Exercise 8.: single-spin dissipation

Take $H=0$ and $L=\sqrt{\Gamma}\,\sigma^-$, and initial state $|\psi(0)\rangle = |\uparrow = +1\rangle$ and calculate $\rho(t)$.

we have $\rho(0) = \frac{1}{2}(\mathbb{1}+\sigma^z)$, $\mathcal{L} = \Gamma \begin{pmatrix} -1 & & & \emptyset \\ & -1 & & \\ \emptyset & & -2 & -2 \\ & & & 0 \end{pmatrix}$ in basis $(\sigma^x, \sigma^y, \sigma^z, \mathbb{1})$

spectrum of $\mathcal{L}$



$\sigma(\mathcal{L}) = \Gamma(0,-1,-1,-2)$

$\Downarrow$

$$e^{\mathcal{L}t} = \begin{pmatrix} a & & & \emptyset \\ & a & & \\ \emptyset & & a^2 & a^2-1 \\ & & & 1 \end{pmatrix}, \quad a = e^{-\Gamma t}$$

$\Downarrow$

$$\rho(t) = \rho_\infty + e^{-2\Gamma t}\sigma^z \quad , \quad \rho_\infty = \frac{1}{2}(\mathbb{1}-\sigma^z) = |\downarrow\rangle\langle\downarrow|$$

Bloch sphere $\rho(t) = \frac{1}{2}(\mathbb{1} + \vec{r}\cdot\vec{\sigma})$