Quantum traffic jam in far from equilibrium quantum systems

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Motivation and Outline

• Cooperative phenomena in low-dimensional quantum systems (ordering tendencies, collective quantum states)

• Unconventional transport properties (high thermal conductivity in quasi-1D magnetic compounds, ballistic spin transport in magnetic chains,...)

• Most theoretical studies in the linear response regime (Luttinger liquid,...)

• The far from equilibrium regime is very difficult both for analytic treatment and for numerical simulations

• New quantum phases and interesting physical phenomena might appear far from equilibrium

Long-range ordering into ferromagnetic domains and negative differential conductivity in anisotropic Heisenberg spin-$1/2$ chains - Hubbard model

Negative differential conductivity in far-from-equilibrium quantum spin chains,
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A model of open spin chain

XXZ Hamiltonian $\mathcal{H} = \sum_{k=1}^{N-1} \left[J_x(\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y) + \ J_z \sigma_k^z \sigma_{k+1}^z \right]$

Lindblad master equation $\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[\mathcal{H}, \rho] - \frac{1}{2} \sum_{m=1}^{4} \{L_m^\dagger L_m, \rho\} + \sum_{m=1}^{4} L_m \rho L_m^\dagger$

Coupling of both ends of the spin chain to magnetic baths

$$L_1 = \sqrt{\Gamma_L f_L}\, \sigma_1^+, \ \ L_2 = \sqrt{\Gamma_L (1 - f_L)}\, \sigma_1^-, \ \ L_3 = \sqrt{\Gamma_R f_R}\, \sigma_N^+, \ \ L_4 = \sqrt{\Gamma_R (1 - f_R)}\, \sigma_N^-$$

Γ_L, Γ_R system- left (right) bath coupling strength
f_L $(f_R) \in [0, 1]$ left (right) bath distribution function: $2f_{L,R} - 1$ bath's magnetization per spin

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Physical example: molecular spin wires with each boundary coupled to a magnetic impurity: the desired populations $\{f_{L,R}, 1 - f_{L,R}\}$ of up/down spins can be pumped by means of electromagnetic fields

Symmetric coupling and driving:
$\Gamma_L = \Gamma_R \equiv \Gamma$
$f_{L,R} = \frac{1}{2}(1 \mp f)$, so that $f \equiv f_R - f_L \in [0, 1]$

$f \ll 1$: linear response regime
$f = 1$: fully and oppositely polarized spin baths (ferromagnets)

Study the stationary, far-from-equilibrium, transport properties of this model

Charge and spin transport in strongly correlated one-dimensional quantum systems driven far from equilibrium,
Phys. Rev. B **80**, 035110 (2009)

Methods

Quantum trajectories:
up to $N \sim 20$ spins

Matrix product operator formalism:
up to $N \sim 100$ spins (small drivings) or $N \sim 40$ spins (far from equilibrium)

We study the stationary spin current $\langle j \rangle$ which can calculated (in the quantum trajectories approach) by looking at the left bath and summing up all up-down flips minus all down-up flips, and then dividing by the simulation time

Due to the conservation of the total magnetization in the XXZ Hamiltonian, this current is equal to the analogous quantity computed at the right bath and also to the expectation value $j_k = J_x(\sigma_k^x \sigma_{k+1}^y - \sigma_k^y \sigma_{k+1}^x)$ for any $k = 1, \ldots, N-1$

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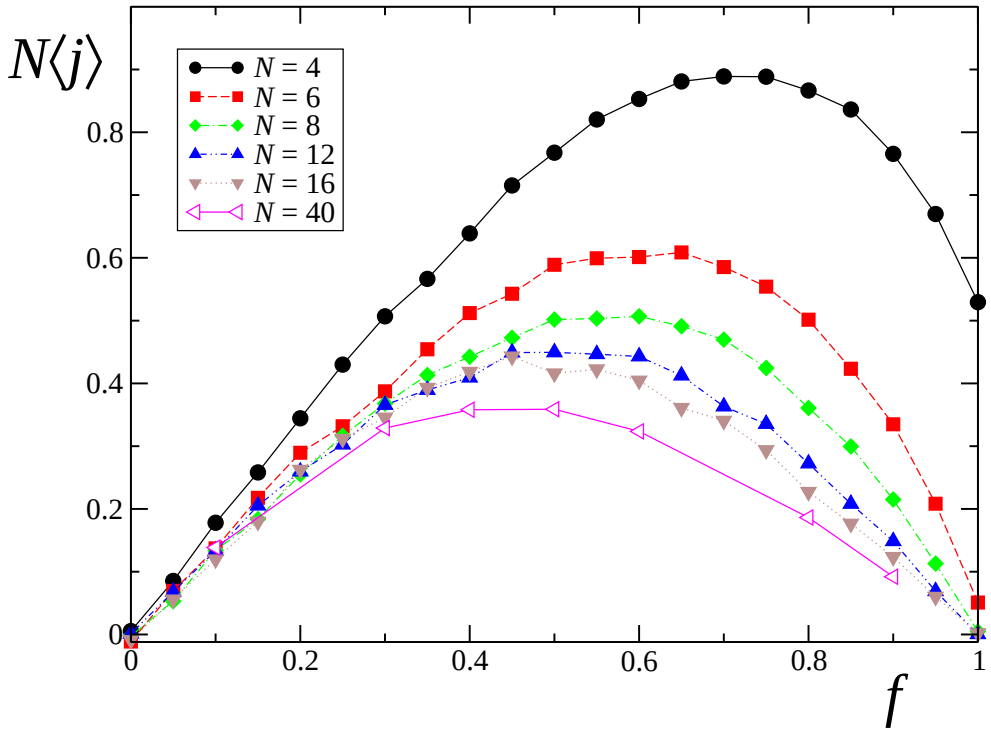
Negative differential conductivity



Set $\hbar = 1,\ J_x = 1$

Anisotropy $\Delta = J_z/J_x = 2$

Gapped regime $|\Delta| > 1$

Ohmic behavior in the linear response regime, for an integrable model [see Prelovsek and Zotos, e.g. PRB **70**, 205129 (2004)]

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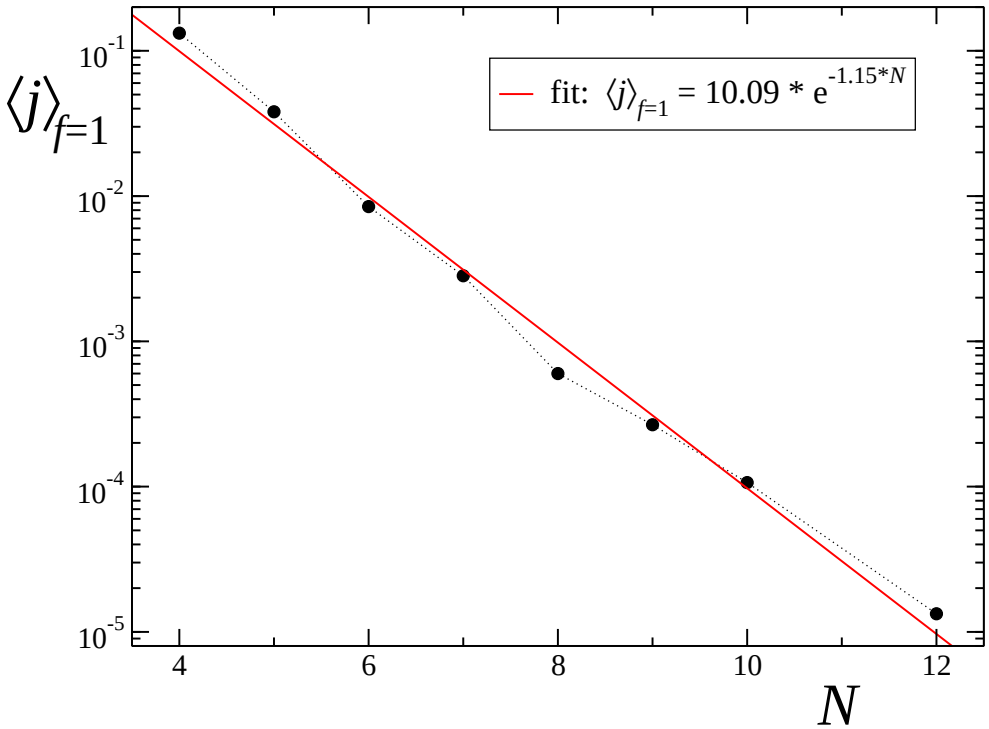
Behavior at maximum driving, $f = 1$



The current drops exponentially with the system size

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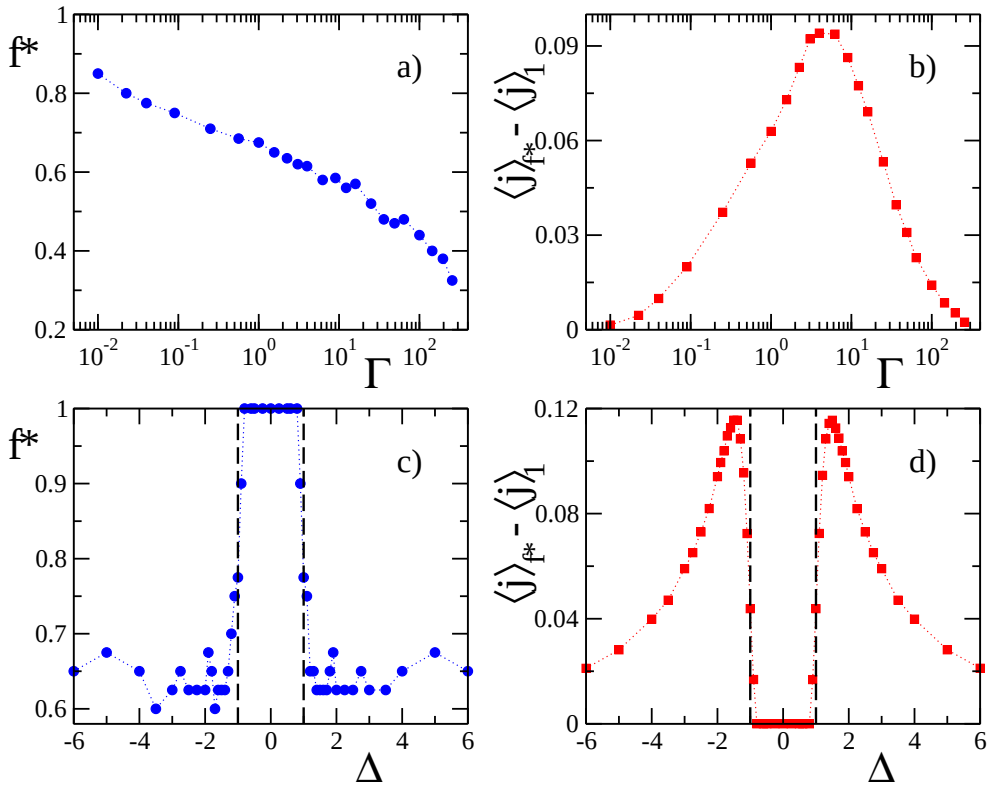
Find the "optimal working point"



The current reaches a maximum at a certain $f = f^\star$

Current small at small Γ: the "contact resistance" $1/\Gamma$ becomes large

Current small at large Γ: the system's dynamics is frozen by the strong coupling to reservoirs, quantum Zeno regime

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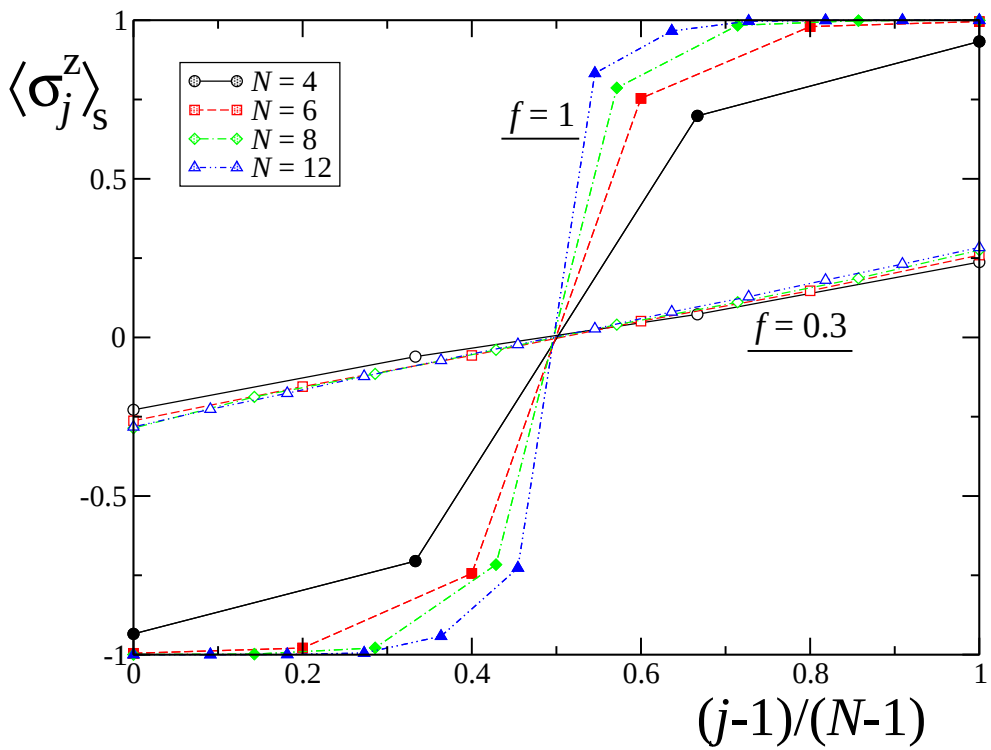
Long-range ordering: ferromagnetic domains at $f = 1$



Ferromagnetic domains are responsible for inhibiting spin flips, thus suppressing the spin current

No differences between a ferromagnetic $(J_z < 0)$ and an antiferromagnetic $(J_z > 0)$ spin coupling

Antiferromagnetic case: the baths pump energy into the system, while leading it to a stationary state with very low entropy

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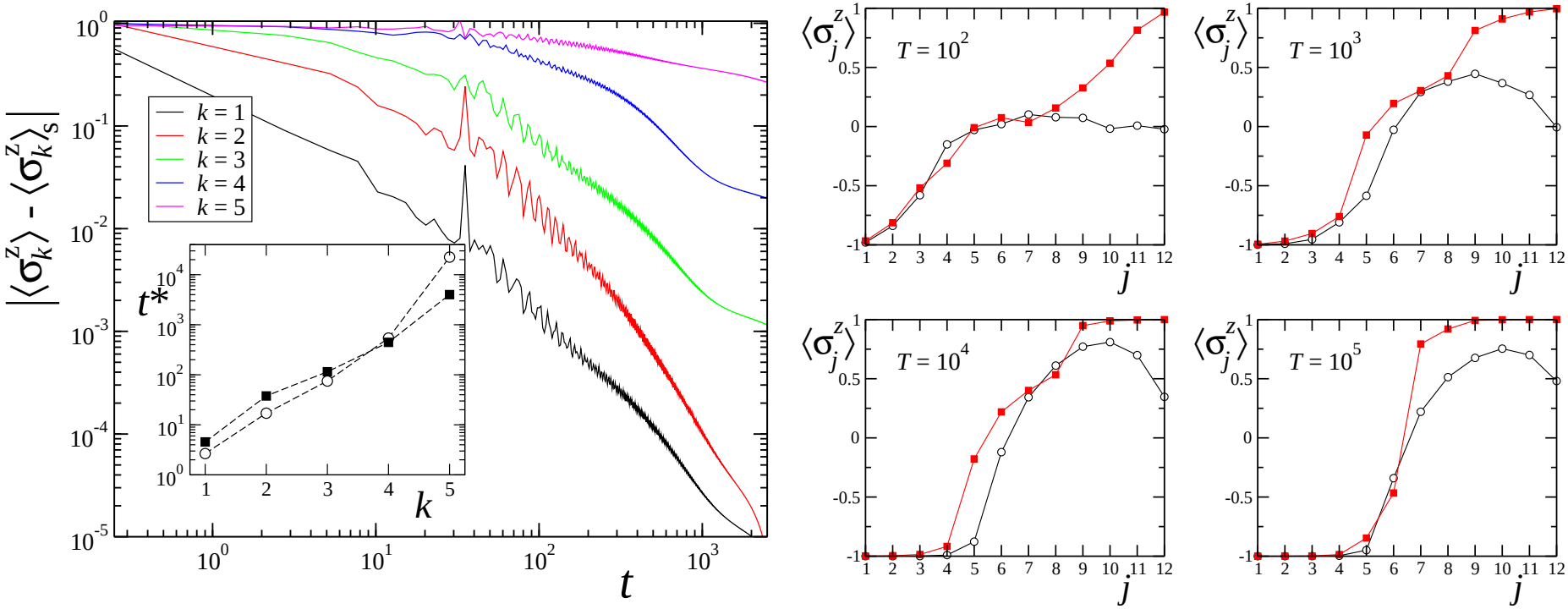
Exponentially slow approach to equilibrium, at $f = 1$



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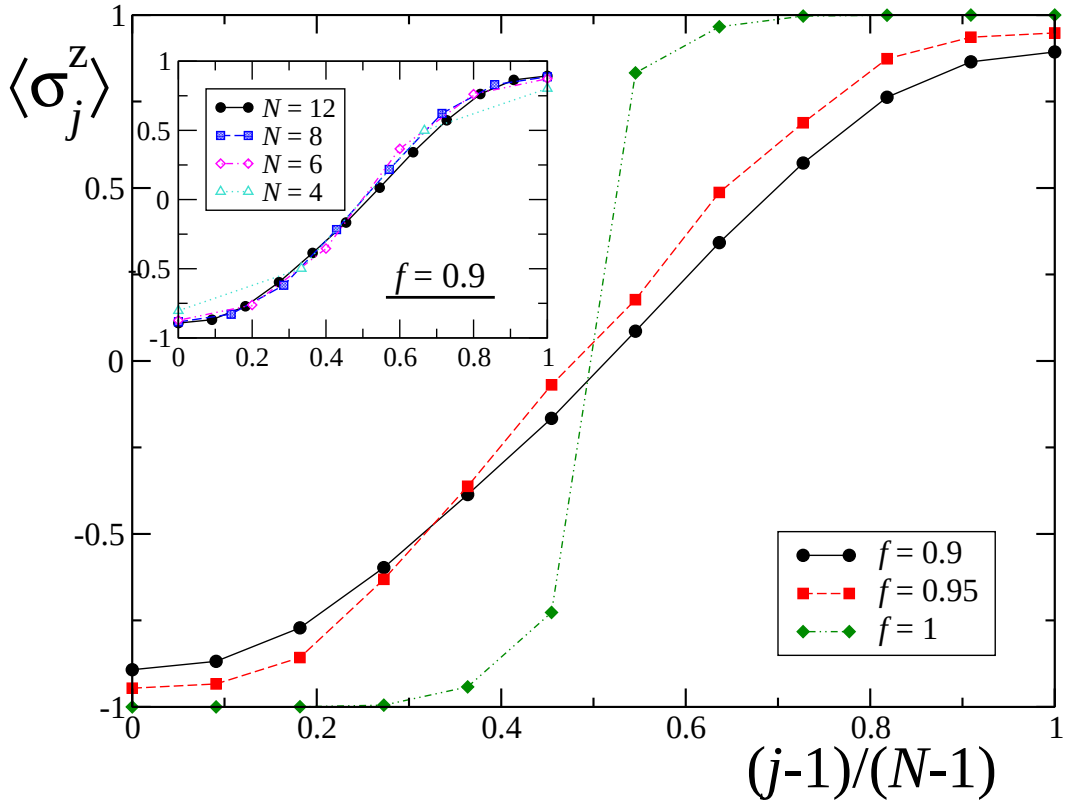
Spin blockade at $\mu < 1$



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One-magnon localization

One-magnon excitations: $\sum_{k=1}^{N} c_k|k\rangle$, $|k\rangle = \sigma_k^+|0\rangle$ (k-th spin flipped),
$|0\rangle \equiv |\downarrow\downarrow\cdots\downarrow\rangle$ ferromagnetic state

The autonomous XXZ chain has open boundary conditions: energy gap $2|J_z|$ between states $|1\rangle$ and $|N\rangle$ (spin-flip excitations at the boundaries) and states $|2\rangle$, $|3\rangle$,..., $|N-1\rangle$:

$$\langle 0|\mathcal{H}_s|0\rangle = (N-1)J_z,$$
$$\langle 1|\mathcal{H}_s|1\rangle = \langle N|\mathcal{H}_s|N\rangle = (N-3)J_z,$$
$$\langle 2|\mathcal{H}_s|2\rangle = ... = \langle N-1|\mathcal{H}_s|N-1\rangle = (N-5)J_z$$

Only nearest-neighbor spin-flipped states are coupled, with coupling strength $2|J_x|$:

$$\langle k|\mathcal{H}_s|k+1\rangle = 2J_x, \quad k = 1, ..., N-1$$

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In the one-magnon basis $\{|1\rangle, |2\rangle, ..., |N\rangle\}$

$$H = \begin{bmatrix} \alpha' & \beta & 0 & & & ... & & & 0 \\ \beta & \alpha & \beta & 0 & & ... & & & 0 \\ 0 & \beta & \alpha & \beta & 0 & ... & & & 0 \\ \vdots & & & & & & & & \vdots \\ \vdots & & & & & & & & \vdots \\ \vdots & & & & & & & & \vdots \\ 0 & & & & & ... & \beta & \alpha & \beta \\ 0 & & & & & ... & 0 & \beta & \alpha' \end{bmatrix},$$

$$\alpha' \equiv (N-3)J_z, \quad \alpha \equiv (N-5)J_z, \quad \beta \equiv 2J_x$$

This model is analytically solvable in the limit of large N: spin-flip excitations created at the borders of the chain remain exponentially localized when $|J_z|/|J_x| = |\Delta| > 1$, over a localization length $\ell \sim 1/\ln|\Delta|$

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One-magnon localization and the approach to equilibrium

SINGLE, FULLY POLARIZED RESERVOIR

The XXZ Hamiltonian conserves the overall magnetization and the only Lindblad operator, $L_2 \propto \sigma_1^-$, lowers magnetization; the equilibrium state is pure and ferromagnetic: $|\downarrow\downarrow\cdots\downarrow\rangle\langle\downarrow\downarrow\cdots\downarrow|$

Consider an intermediate state with the m leftmost spins down: The ferromagnetic domain enlarges when one-magnon excitations propagate, through $\sigma_j^x\sigma_{j+1}^x$ and $\sigma_j^y\sigma_{j+1}^y$ exchange couplings across the ferromagnetic domain to the left chain boundary

In the gapped phase ($|\Delta| > 1$) the one magnon propagation is exponentially localized: exponentially long time scales $\propto \exp(k/\ell) \sim \exp(k \ln|\Delta|)$ to polarize the k-th spin

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TWO, FULLY AND OPPOSITELY POLARIZED RESERVOIRS

Due to exponential one-magnon localization, essentially only the nearest bath is felt by the spins in the chain,

Exception: an interface region between the two ferromagnetic domains, whose length is of the order of the one-magnon localization length

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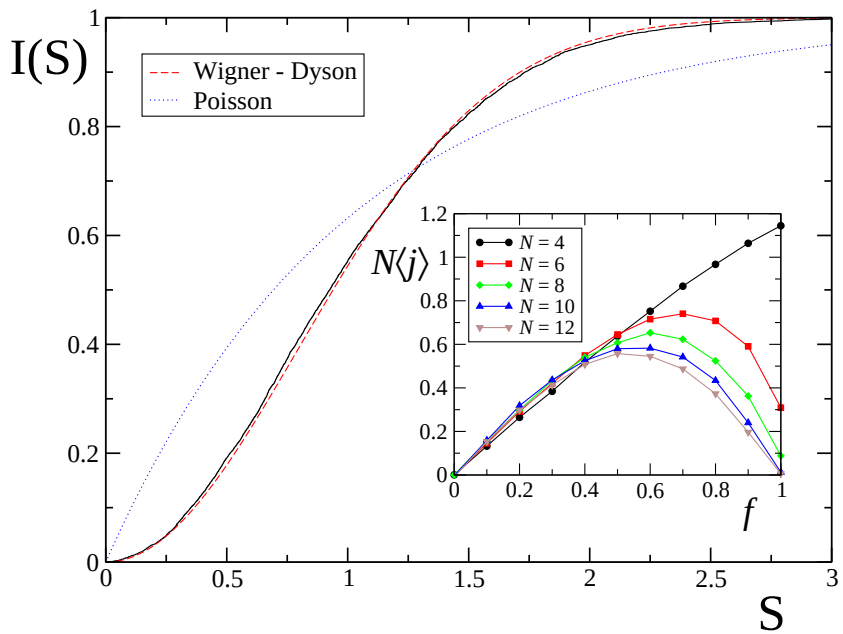
Non-integrable model: staggered magnetic field

$$\mathcal{H}_S = \sum_{j=1}^{N-1} \left[J_x(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + J_z \sigma_j^z \sigma_{j+1}^z \right] + B \sum_{j=1}^{N} (-1)^j \sigma_j^z$$



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Mapping into electronic transport model

Using the Jordan-Wigner transformation, mapping into the $t-V$ electronic model

$$\mathcal{H}_s = 2J_x \sum_{j=1}^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + 4J_z \sum_{j=1}^{N-1} n_j n_{j+1}$$

Lindblad operators $\longrightarrow$ operators injecting/extracting electrons at the lattice boundaries

Spin current $\longrightarrow$ charge current

$\frac{1}{2}(1 + \langle \sigma_k^z \rangle) \longrightarrow$ charge density at site k

Ferromagnetic domains at $f = 1 \longrightarrow$ phase separation in the fermionic model with all the electrons frozen in half of the lattice thus inhibiting charge transport, if $|V/t| > 2$, both for attractive and repulsive interactions

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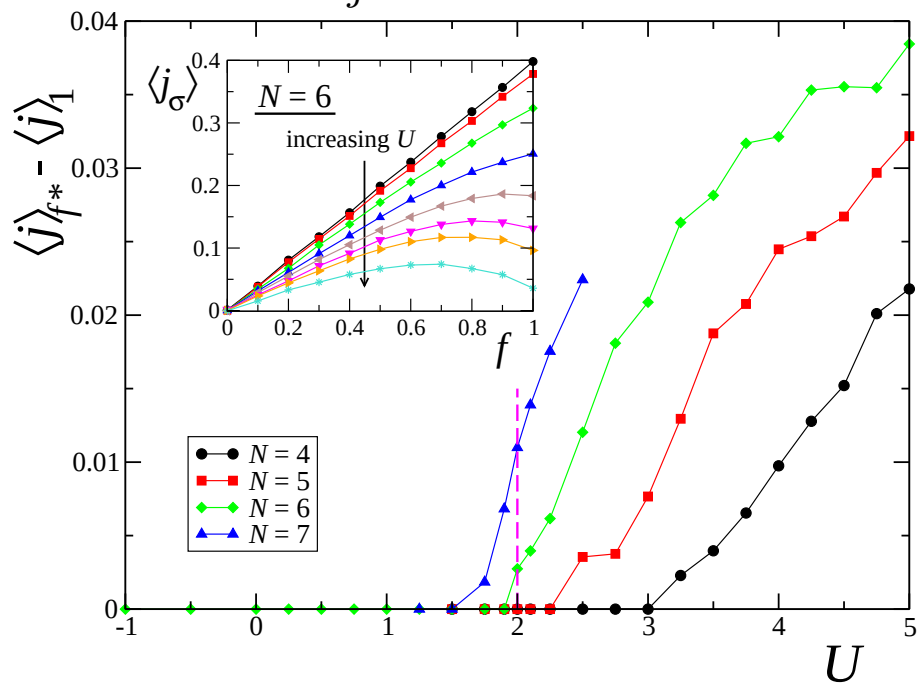
Negative differential conductivity in the Hubbard model

$$\mathcal{H}_s = -t \sum_{j,s} \left(c^\dagger_{j,s} c_{j+1,s} + \text{H.c.} \right) + U \sum_{j=1}^{N} n_{j,\uparrow} n_{j,\downarrow}$$

This model can be mapped into a spin ladder (two species of interacting spin-1/2 particles)



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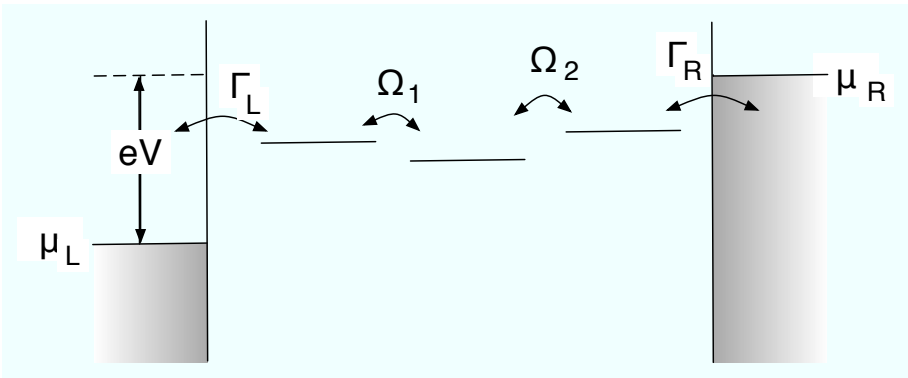
Derivation of the model



Tunneling Hamiltonian $\mathcal{H}_c = \sum_{k,s}(T_{Lk}c^\dagger_{Lk,s}c_{1,s} + T_{Rk}c^\dagger_{Rk,s}c_{N,s}) + \mathrm{H.c.}$

Leads modeled as ideal Fermi gases at (grand-canonical) equilibrium

Lindblad master equation obtained under the usual Born-Markov and rotating wave approximations

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Assume tunneling to leads much faster than the intrachain tunneling

Neglect the effects of Coulomb repulsion on the system-leads transition rates (wide-band limit)

$\Gamma_L \equiv 2\pi |T_L(E_1)|^2 g_L(E_1), \quad f_L \equiv f_L(E_1)$
$\Gamma_R \equiv 2\pi |T_R(E_N)|^2 g_R(E_N), \quad f_R \equiv f_R(E_N)$
E_1, E_N energy of the states involved for sites 1 and N
f_L (f_R) left (right) lead Fermi function
g_L (g_R) left (right) lead Fermi density of states
Neglect the charging energies: $E_c \ll k_B T$
Sequential tunneling approximation: $\Gamma_L, \Gamma_R \ll k_B T$

Far from equilibrium regime: large bias voltage $eV \gg k_B T$, $\mu_L \ll E_1, E_N \ll \mu_R$
In this limit, $f_L \to 0, f_R \to 1$: backward flow of electrons (against the applied bias) vanishes

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Conclusions and prospects

- New collective phase as an outcome of the interplay between coherent many-body quantum dynamics of the spin chain and incoherent spin pumping

- Negative differential conductivity potentially interesting for nanoscale devices such as current/heat diodes and transistors

- Integrable model: reduction of the complexity of the problem, thus addressing larger system sizes? Finite-size scaling? Analytical solution of the problem?

- How general is the described mechanism? Applicable to quantum transport in other spin/electronic systems? How does it depend on the specific bath model?

- Related topics: controllability of quantum systems, information flow through quantum channels