New aspects of transport in spin chains

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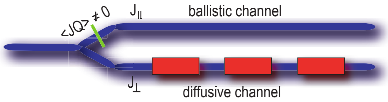
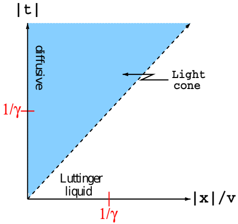
OPTIMAS

MATERIALS SCIENCE IN MAINZ

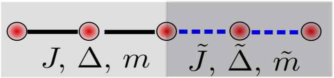
Outline

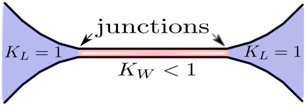
- Diffusive and ballistic spin transport in the anisotropic Heisenberg model





- Transport and scattering in inhomogeneous spin chains/quantum wires





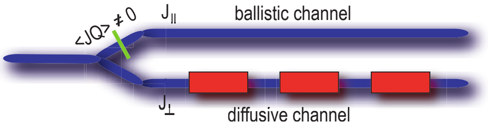
Collaborations

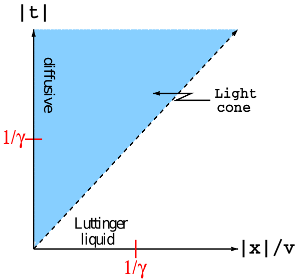
- Ian Affleck (UBC Vancouver)
- Sebastian Eggert (TU Kaiserslautern)
- Rodrigo Pereira (U Sao Paulo)
- Jan Ohst (TU Kaiserslautern)
- Nick Sedlmayr (TU Kaiserslautern)

- JS, R. G. Pereira, I. Affleck
  PRL **103**, 216602 (2009), PRB **83**, 035115 (2011)
- N. Sedlmayr, J. Ohst, JS, I. Affleck, S. Eggert
  arXiv: 1204.2565 (2012)

Spin transport

- Diffusive and ballistic spin transport in the anisotropic Heisenberg model



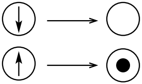


The anisotropic Heisenberg (XXZ) chain

- Spin-1/2 Heisenberg model with additional anisotropy Δ:

$$H = J\sum_j \left\{ \frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + \Delta S_j^z S_{j+1}^z \right\}$$

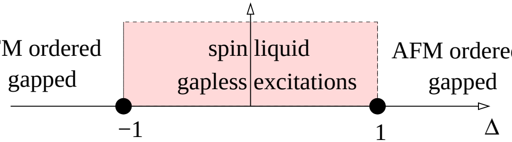
Jordan−Wigner transformation



- Equivalent to spinless fermion model:

$$H = J\sum_j \left\{ -\frac{1}{2}\left(c_j^\dagger c_{j+1} + c_j c_{j+1}^\dagger\right) + \Delta(n_j - 1/2)(n_{j+1} - 1/2) \right\}$$

Phase diagram:



The role of conservation laws in 1D quantum systems

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Is transport always ballistic? Thermalization in closed systems?

Current-current correlations and the Drude weight

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Drude weight measures part of the current which does not decay

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

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Ballistic versus diffusive based on current-current correlation:

Diffusive: $D(T>0)=0$

Ballistic: $D(T>0)\neq 0$

Phenomenological diffusion

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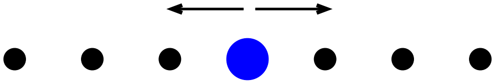

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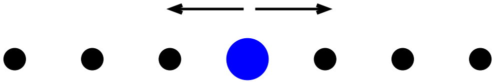

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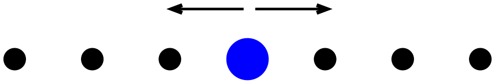

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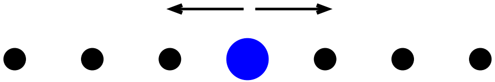

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Diffusion in the autocorrelation function of the conserved quantity does not exclude the possibility of ballistic transport $\leftrightarrow$ different correlation functions!

Drude weight in the anisotropic Heisenberg model

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

- Drude weight: $\sigma'(q=0,\omega) = 2\pi D\delta(\omega) + \sigma_{reg}(\omega)$
- Current operator: $\mathcal{J} = \frac{i}{2}\sum_l \left(S_l^+ S_{l+1}^- - S_{l+1}^+ S_l^-\right)$

The XXZ model is integrable, the energy current

$$\mathcal{J}_E = \sum_l j_l^E \quad \text{with} \quad j_l^E = -\mathrm{i}[h_{l-1,l}, h_{l,l+1}]$$

is conserved.

Finite magnetic field (broken particle-hole symmetry)

- $h \neq 0$: $\langle \mathcal{J}\mathcal{J}_E \rangle \neq 0$ then $\mathcal{J} = \mathcal{J}_\parallel + \mathcal{J}_\perp$, and $\mathcal{J}_\parallel = \frac{\langle \mathcal{J}\mathcal{J}_E \rangle}{\langle \mathcal{J}_E^2 \rangle}\mathcal{J}_E$ cannot decay

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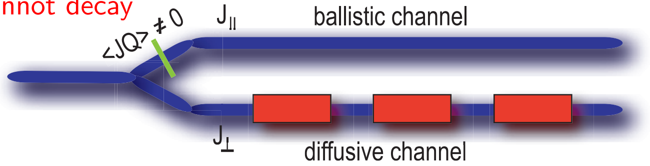

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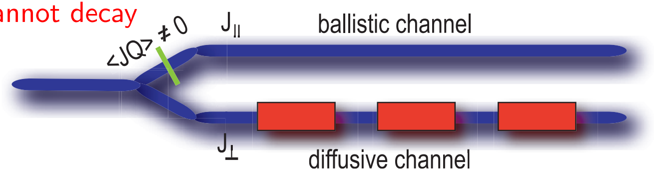
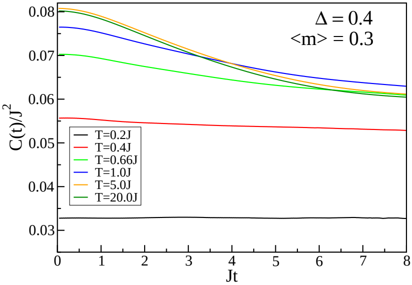


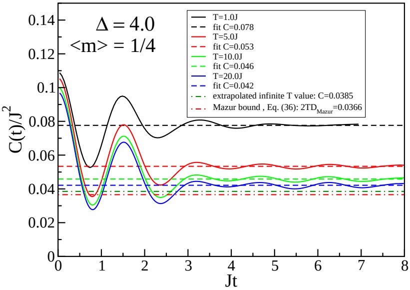
In general, ballistic and diffusive channels coexist

- Ballistic channel controls long-time asymptotics of the current-current correlation function
- Diffusive channel dominates long-time asymptotics of the low-energy, long-wavelength contribution of $\langle S^z_{l+x}(t) S^z_l(0) \rangle$

Transfer-matrix DMRG at finite magnetic field

- TMRG: Finite temperature, infinite system size
- Current CF: $C(t) = \lim_{L\to\infty} \langle \mathcal{J}(t)\mathcal{J}(0)\rangle / L$





If a local conservation law protects a substantial part of the current then $C(t)$ converges relatively fast towards the asymptotic value

Linear response and bosonization

- Bosonization of the XXZ model leads to:

$$H = H_0 + H_{\rm u} + H_{\rm bc}$$

$$H_0 = \frac{v}{2}\int dx\,\left[\Pi^2 + (\partial_x\phi)^2\right], \quad H_{\rm u} = \lambda\int dx\,\cos(\sqrt{8\pi K}\phi)$$

$$H_{\rm bc} = -2\pi v\lambda_+\int dx(\partial_x\phi_R)^2(\partial_x\phi_L)^2 - 2\pi v\lambda_-\int dx\,\left[(\partial_x\phi_R)^4 + (\partial_x\phi_L)^4\right]$$

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- In linear response we have to calculate the retarded spin-spin corr. fct. $\chi_{\rm ret}(q,\omega)$, related to the boson propagator:

$$\frac{\chi_{\rm ret}(q,\omega)}{Kq^2/2\pi} = \langle\phi\phi\rangle^{\rm ret}(q,\omega) = \frac{v}{\omega^2 - v^2q^2 - \Pi^{\rm ret}(q,\omega)}$$

related approach for Hubbard: [Giamarchi PRB **44**, 2905 (91)]

Linear response and bosonization (II)

- We have obtained a parameter-free result for $\Pi^{\mathrm{ret}}(q,\omega)$ in second order Umklapp, and first order in band curvature

$$\Pi^{\mathrm{ret}}(q,\omega) \approx -2i\gamma\omega - b\omega^2 + cv^2q^2$$

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  - Anisotropic case: $2\gamma \sim \lambda^2 T^{8K-3}$, $1/2 \leq K \leq 1$ for $0 \leq \Delta \leq 1$
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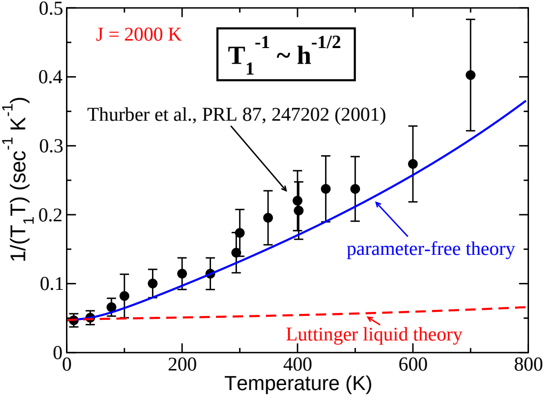
Spin-lattice relaxation: $\frac{1}{T_1 T} \sim \sqrt{\frac{\gamma(T)}{\omega_e}} \sim \sqrt{\frac{T/\ln^2(J/T)}{\omega_e}}$

^{17}O nuclear magnetic resonance for Sr_2CuO_3

$$\frac{1}{T_1} = \int \frac{dq}{2\pi} \underbrace{|A(q)|^2}_{\sim\cos(q/2)} S^{zz}(q,-\omega_e)\Big|_{h=0}$$

picks only $q \sim 0$ mode



Violations of the LL paradigm for time-like CF

- At $T = 0$ long-time asymptotics of $G(0,t) = \langle S_l^z(t) S_l^z(0) \rangle$ is dominated by high-energy excitations: (band curvature)

$$G(0,t) \sim \frac{e^{-ivt}}{t^\eta}, \quad \eta = K + 1/2$$

Pereira *et al* PRL **100**, 027206 (08)

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- At $T\gg h$ a low-energy term dominates: (Umklapp)

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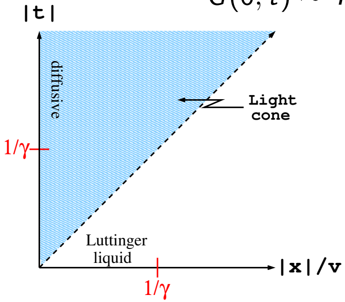

JS, Pereira, Affleck PRL **103**, 216602 (09)

JS, Pereira, Affleck PRB **83**, 035115 (11)

The conductivity and the memory matrix

- So far: purely diffusive response
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The conductivity and the memory matrix

- So far: purely diffusive response
- Conservation laws are not manifested in a lowest order self-energy approach
- Consider a single local conservation law $\langle JQ \rangle \neq 0$
- Can be implemented by a memory-matrix approach [Rosch, Andrei, PRL (00)], reduces to self-energy result if $\langle JQ \rangle \to 0$:

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

$$y \equiv \langle \mathcal{J} Q \rangle^2 / (\langle \mathcal{J}^2 \rangle \langle Q^2 \rangle - \langle \mathcal{J} Q \rangle^2) \sim (h/T)^2 \; (h \neq 0)$$

Sum rules: Weight shifts from diffusive into ballistic part

Relaxation rate: $\gamma \to (1+y)\gamma$

Drude weight in the half-filled case

$h = 0$: $\langle \mathcal{J} Q_n \rangle \equiv 0$ for all Q_n needed to construct the BA solution (particle-hole symmetry)

Zotos, Naef, Prelovsek, PRB **55**, 11029 (97)

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Numerical results and BA seemed to point to $D \neq 0$ but were partly contradictory:

- BA: Zotos PRL **82**, 1764 (99), Benz *et al* JPSJ **74**, 181 (05)
- ED: F. Heidrich-Meisner *et al*, PRB **68**, 134436 (03), J. Herbrych *et al*, PRB **84**, 155125 (11)
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Is there another local conservation law not obtained from the family of commuting transfer matrices (BA)?

A pseudo-local conservation law

- Construction of a pseudo-local conservation law $\mathcal{Q}$ for open boundary conditions: T. Prosen, PRL **106**, 217206 (11)

$$\mathcal{Q} = \sum_{d=1}^{L} \sum_{j} q_{d,j}, \quad ||q_d|| \sim \exp(-d)$$

$$[H, \mathcal{Q}] \sim -S_1^z + S_L^z$$

- The constructed quantity is odd under p-h transformations
- Overlap $\langle \mathcal{J} Q \rangle \sim L$ for $|\Delta| < 1$
- Exponential localization and conservation up to boundary terms are sufficient to give bound $D(T > 0, |\Delta| < 1) > 0$

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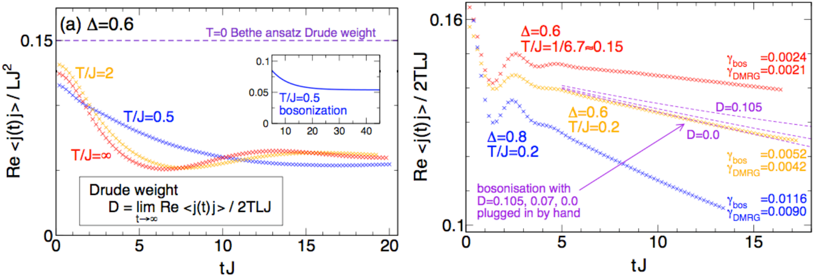
- Exponential localization and conservation up to boundary terms are sufficient to give bound $D(T > 0, |\Delta| < 1) > 0$

- Periodic boundary conditions?
- Connection to BA solution for open boundaries?

New numerical evidence for finite Drude weight

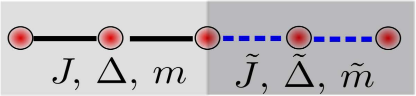


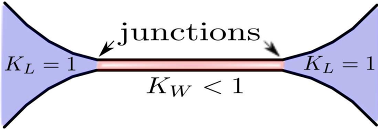
C. Karrasch *et al* arXiv: 1111.4508 (11)

- tDMRG extending my old calculation by factor 2 in time
- Solid evidence for $D > 0$ at large T
- relaxation rate γ at small T agrees well with bosonization

Inhomogeneous spin chains/quantum wires

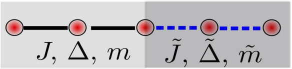
- Transport and scattering in inhomogeneous quantum wires/spin chains

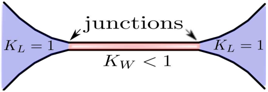




Is a perfect contact possible?

Hydrodynamic description





Effective action: $S_0 = \int_0^{1/T} \mathrm{d}\tau \int \mathrm{d}x \frac{v_x}{2K_x}\left[\frac{(\partial_\tau\phi)^2}{v_x^2} + (\partial_x\phi)^2\right]$

Maslov, Stone, PRB **52**, R5539 (95); Furusaki, Nagaosa, PRB **54**, R5239 (96)

- LL description with velocity v_x and LL parameter K_x

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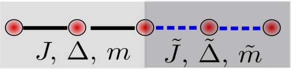

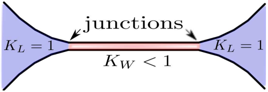

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Relevant backscattering operator: $e^{-i2k_F x}\psi_+^\dagger \psi_- \propto e^{-i2k_F x} e^{-i\sqrt{4\pi}\phi}$

Can no longer be neglected in the inhomogeneous case!

A single junction at $x = 0$

- Consider a single junction with $K_x = K_L\,(x<0)$, $K_x = K_R\,(x>0)$ and similarly for v_x
- We can calculate the full bosonic Green's fct:

$$
\begin{aligned}
\langle \phi(x,\tau)\phi(x',0)\rangle &= -\frac{\bar{K}}{\pi}\ln\left|\sinh\left[\pi T\left(\frac{|x|}{v_x}+\frac{|x'|}{v_{x'}}-i\tau\right)\right]\right| \\
&+ \frac{\mathcal{L}[x,x']K_x}{\pi}\ln\left|\frac{\sinh\left[\pi T\left(\frac{|x|}{v_x}+\frac{|x'|}{v_{x'}}-i\tau\right)\right]}{\sinh\left[\pi T\left(\frac{|x-x'|}{v_x}-i\tau\right)\right]}\right|,
\end{aligned}
$$

- $\mathcal{L}[x,x'] = 1$ if x and x' in same region, 0 otherwise
- Scaling exponent: $\bar{K} = 2/(1/K_L + 1/K_R)$

Backscattering at the junction

- Local perturbation: $H' \approx \lambda e^{-i\sqrt{4\pi}\phi_{x=0}} + h.c.$

Kane, Fisher, PRB **46**, 15233 (92)

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Furusaki, Nagaosa, PRB **54**, R5239 (96)

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Can we tune backscattering to zero?

Backscattering for a microscopic lattice model

- Spinless fermions, jump in t_x, U_x at $x = 0$:

$$H = \sum_x \left[-t_x(\psi_x^\dagger \psi_{x+1} + h.c.) + U_x(n_x - \tfrac{1}{2})(n_{x+1} - \tfrac{1}{2}) \right]$$

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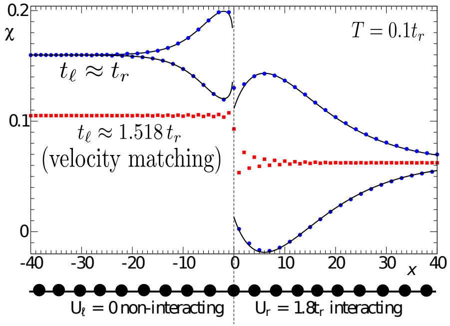
We have shown that this condition holds even for large interactions and jumps Sedlmayr, Ohst, JS, Affleck, Eggert, arXiv: 1204.2565 (12)

Strength of backscattering $\leftrightarrow$ Friedel oscillations

Density osc. at the junction: $\chi_x = \partial\langle n_x\rangle/\partial\mu = \chi_0 + (-1)^x\chi_{\mathrm{alt}}$



Friedel oscillations calculated analytically by bosonization (lines)

Relevant backscattering tuned to zero by matching the velocities

Conclusions

Spin transport in linear response

- *XXZ* model: ballistic and diffusive transport channels coexist
- Ballistic channel: Long-time behavior of current-current CF
- Diff. channel: Dominates $\langle S_r^z(t)S_0^z(0)\rangle$ for $vt \gg r$, $t \gg 1/\gamma$
- Violations of LL paradigm for time-like CF: band curvature (non-linear LL, $T=0$) and Umklapp scattering ($T>0$)

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Transport and scattering in inhomogeneous spin chains

- Generic junction: Relevant backscattering for $K_w < 1$
- Backscattering amplitude: $R \propto T^{\bar{K}-1}$, $\bar{K} = 2/(1/K_L + 1/K_w)$
- XXZ model: backscattering tuned to zero by velocity matching $\rightarrow$ unstable, perfectly conducting fixed point