# Issues on the dynamics of 1D quantum magnets

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#### issues

- novel magnetic mode of heat transport
- fractal Drude weight
- magnetothermal transport
- DTN a route to XXZ

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• TBA vs. low energy effective theories

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#### motivation

- thermal transport in 1D quantum magnets spin Seebeck effect
- dynamic heat transport
- transient grating spectroscopy
- spinon THz spectroscopy

### A novel mode of thermal transport<sup>1</sup>



$$J'/J~\sim~10^{-4}$$
  
 $J~\sim~2'400K$ 

 $\frac{Cu(C_4H_4N_2)(NO_3)_2}{J\sim 10K}$ 

 $\begin{array}{l} Cs_2 CuCl_4\\ S=3/2, \ J\sim 10K \end{array}$ 

<sup>1</sup>A. Revcolevschi, C. Hess, B. Büchner, A. Sologubenko, H.R. Ott, Y. Koike: □ ▷ < ♂ ▷ < ≥ ▷ < ≥ ▷ < ≥ ▷ < < ○ < < Rome 2019



#### magnetic thermal transport

- highly directional
- electrically insulating
- "metallic"  $J \sim \epsilon_F$
- "mechanical" switching

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<sup>2</sup>C. Hess Rome 2019

# flash method<sup>3</sup>



**Figure 2:** Left panel: Thermal image on the ab plane of  $La_5Ca_9Cu_{24}O_{41}$  showing very localized symmetric heating after a 40 ms heat pulse. Right panel: similar image on the ac plane showing a highly asymmetric streaked heating pattern due to the large magnon heat conductivity in the (diagonal) c-direction.



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#### integrable transport and Drude weights - a conjecture <sup>4</sup>



 $egin{array}{rcl} D &\sim & eta C_{jj} \ \sigma^{''} &= & \displaystyle rac{D}{\omega}|_{\omega 
ightarrow 0} \end{array}$  $\sigma'_{dc} \sim \beta$  $dt\langle j(t)j\rangle$ 

Image: A math



<sup>4</sup>W. Kohn 1964 Rome 2019

# Mazur inequality<sup>5</sup>

$$\begin{bmatrix} Q_n, H \end{bmatrix} = \mathbf{0}, \quad \langle Q_m Q_n \rangle = \delta_{mn}$$
$$\langle j(t) j \rangle_{t \to \infty} \sim C_{jj} \ge \sum_n \frac{\langle j Q_n \rangle^2}{\langle Q_n^2 \rangle}$$





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## S = 1/2 Heisenberg model

# $H = J \sum_{l=1}^{L} S_{l}^{x} S_{l+1}^{x} + S_{l}^{y} S_{l+1}^{y} + \Delta S_{l}^{z} S_{l+1}^{z} - h S_{l}^{z}$

- J > 0 antiferromagnet
- Δ < 1 easy-plane</li>
- Δ > 1 easy-axis
- $\Delta = cos(\pi/\nu)$

Bethe ansatz integrable model



•  $j_{S} = J \sum_{l} (S_{l}^{x} S_{l+1}^{y} - S_{l}^{y} S_{l+1}^{x})$ 



#### conservation laws <sup>6</sup>

$$Q_3 = j^E$$



<sup>6</sup>X.Z., F. Naef, P. Prelovšek 1997 *Rome 2019* 

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### Sr<sub>2</sub>CuO<sub>3</sub> from 2N to 4N





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# conservation laws 7

$$Q_3 = j_E$$

• 
$$\kappa(\omega) = D_{th}\delta(\omega)$$

• 
$$D_{th} = \beta^2 < j_E^2 >$$

•  $\kappa_{dc} = D_{th}\tau$ 

# spin Drude weight - $D_s$ • $D_s(T) \ge \frac{\beta}{2L} \frac{\langle j_S Q_3 \rangle^2}{\langle Q_3^2 \rangle}$ • $\beta \to 0$ • $D_s(T) \ge \frac{\beta}{2} \frac{8\Delta^2 m^2 (1/4 - m^2)}{1 + 8\Delta^2 (1/4 + m^2)}$ • $m = \langle S^z \rangle$

<sup>7</sup>X.Z., F. Naef, P. Prelovšek 1997 **Rome 2019** 

 $0 < \Delta < 1$ , m = 0, TBA <sup>8</sup>



$$egin{array}{rcl} D_0 &=& rac{\pi}{8}rac{\sin(\pi/
u)}{rac{\pi}{
u}(\pi-rac{\pi}{
u})} \ C_{jj} &=& 1-rac{\sin(2\pi/
u)}{2\pi/
u} \end{array}$$

<sup>8</sup>S. Fujimoto, N. Kawakami 1998, XZ 1999 Rome 2019

$$0 < \Delta < 1$$

$$D_s(T) = D_0 - cT^{2/(\nu-1)}$$

#### m=0

- alternative BA no strings<sup>9</sup>
- quasi-local conservation laws<sup>10</sup>
- numerical simulations ED, DMRG, "typicality" <sup>11</sup>
- Generalized Hydrodynamics (GHD) <sup>12</sup>
- Drude weights from GHD <sup>13</sup>

<sup>9</sup>A. Klümper

<sup>10</sup>T. Prosen, R. Pereira, J. Sirker, I. Affleck...

<sup>11</sup> F. Heidrich - Meisner, R. Steinigeweg...

<sup>12</sup>B. Doyon, M. Fagotti...

<sup>13</sup>J. Moore, C. Karrasch, E. Ilievski, J. De Nardis...

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#### $\beta \rightarrow 0$ fractal Drude weight

• 
$$\Delta = \cos(\frac{\pi l}{\nu})$$
$$D_{ql} = \frac{\sin^2(\frac{\pi l}{\nu})}{\sin^2(\frac{\pi}{\nu})}(1 - \frac{\nu}{2\pi}\sin(\frac{2\pi}{\nu}))$$





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#### $\omega < 1/L$ contribution ?



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# *D<sub>s</sub> scenario* transient gradient spectroscopy ?



#### magnetothermal transport<sup>14</sup>

$$j_Q = j_E - hj_S$$
 $\kappa_{th} = C_{QQ} - \beta C_{QS}^2 / C_{SS}$ 
 $C_{ij} = D_{ij} \tau_{ij}$ 
 $\kappa_{th} = (D_{QQ} - \beta D_{QS}^2 / D_{SS}) \tau$ 
 $MTC = \beta D_{QS}^2 / D_{SS}$ 

$$D_{QQ} = D_{EE} - 2\beta h D_{ES} + \beta h^2 D_{SS}$$

D<sub>EE</sub> = β<sup>2</sup> < j<sub>E</sub><sup>2</sup> >, D<sub>ES</sub> = β < j<sub>E</sub>j<sub>S</sub> > (QTM - Sakai, A. Klümper)

<sup>14</sup>K. Sakai - A. Klümper 2005, C. Psaroudaki, XZ 2015 Rome 2019

D<sub>SS</sub>





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 $D_{QQ} - MTC$ 





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 $\kappa_{\textit{th}}$ 





 $\kappa_{exp}^{15}$ 



Figure 4.3.13: Thermal conductivity measured parallel to the chains of  $Cu(C_4H_4N_2)(NO_3)_2$  as a function of magnetic field at several fixed temperatures. Figure taken from [196].

<sup>15</sup>T. Lorenz, A. Sologubenco Rome 2019



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# spin Seebeck coefficient- ${\it S}= abla h/ abla T$ <sup>16</sup>

$$S = rac{
abla h}{
abla T} = eta rac{D_{ES}}{D_{SS}} - eta h$$



# Effective s=1/2 model for S=1 easy - plane quasi-1D antiferromagnet or how to tune $\Delta^{17}$

NiCl<sub>2</sub>-SC(NH<sub>2</sub>)<sub>2</sub> (DTN) large D limit

$$egin{aligned} \mathcal{H} &= \sum_{n=1}^{N} [J(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) + D(S_n^z)^2 + HS_n^z] \ \mathcal{H}_{c_1} &= D - 2J + rac{J^2}{D} + rac{J^3}{2D^2}, \quad \mathcal{H}_{c_2} &= D + 4J \ \mathcal{H} &< \mathcal{H}_{c_1} \quad S^z = 0 \ \mathcal{H} &> \mathcal{H}_{c_2} \quad S^z = -N \end{aligned}$$



<sup>17</sup>S. Svyagin, C. Psaroudaki, N. Papanicolaou, G. Karadamoglou, J. Herbrych, XZ < (27) > < (27) > < (27) >



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#### Effective s=1/2 model

$$S_n^z = 0 o s_n^z = +1/2$$
  
 $S_n^z = -1 o s_n^z = -1/2$   
 $H_{eff} = \sum_n 2J(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y + \Delta s_n^z s_{n+1}^z) + hs_n^z$ 

where  $\Delta = 1/2$ , h = -J - D + H,  $h_c = \pm 2J(\Delta + 1)$ 



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#### magnetization





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#### specific heat





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#### 1D Heisenberg Hamiltonian

$$H = \sum_{i=1}^{N} J(S_{i}^{x}S_{i+1}^{x} + S_{i}^{y}S_{i+1}^{y} + \Delta S_{i}^{z}S_{i+1}^{z}) - hS_{i}^{z},$$

• 
$$\Delta = \cos \theta$$

• 
$$\theta = \pi/\nu$$

• 
$$(\theta = \frac{\pi}{\nu_1 + 1/(\nu_2 + 1/\nu_3 + ...)})$$

• excitations, strings of order  $n_j = j$ , parity  $\lambda_j$ ,  $j = 1, \nu$ 



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Thermodynamic Bethe Ansatz (TBA - C.N.Yang, C.P.Yang, 1969) M. Takahashi and M. Suzuki, 1972

$$\epsilon_j = \epsilon_j^{(0)} + h\mathbf{n}_j + T\sum_k \lambda_k T_{jk} \circ \ln(1 + e^{-\beta\epsilon_k}), \quad j = 1, ..., \nu$$

- $\epsilon_j$  thermal string energies
- x rapidity
- T<sub>jk</sub> phase shifts

• 
$$\boldsymbol{a} \circ \boldsymbol{b} = \int \boldsymbol{a}(\mathbf{x} - \mathbf{y}) \boldsymbol{b}(\mathbf{y}) d\mathbf{y}$$

• 
$$\boldsymbol{e}^{\beta\epsilon_j} = \rho_j^h / \rho_j$$

• 
$$n_k = \rho_k / (\rho_k + \rho_k^h).$$

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# dressed excitations <sup>18</sup>

$$\frac{\partial p_j}{\partial \mathbf{x}} = \frac{dp_j^{(0)}}{d\mathbf{x}} - \sum_k \lambda_k T_{jk} \circ n_k \frac{\partial p_k}{\partial \mathbf{y}}$$
$$E_j = \epsilon_j^{(0)} - \sum_k \lambda_k T_{jk} \circ n_k E_k$$
$$j_j^{\epsilon} = j_j^{\epsilon^{(0)}} - \sum_k \lambda_k T_{jk} \circ n_k j_k^{\epsilon}.$$

$$\mathcal{Q}_j = \mathcal{Q}_j^{(0)} - \sum_k \lambda_k T_{jk} \circ n_k \mathcal{Q}_k, \ \ \mathcal{Q}_j^{(0)} = \mathbf{n}_j, \ \ \ \mathcal{Q}_j = \partial \epsilon_j / \partial h$$

- h = 0,  $Q_j = 0$ ,  $j = 1, \nu 2$ ,  $Q_{\nu-1} = -Q_{\nu} = \nu/2$
- physically, uniform change of the S<sup>z</sup> component of the magnetization by ±1, e.g. in ESR experiments

<sup>18</sup>Doyon, Fagotti and collaborators *Rome 2019* 



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#### mean quantities

$$E = \sum_{j} \int dx \rho_{j} \epsilon_{j}^{(0)} = \sum_{j} \lambda_{j} \int \frac{dp_{j}^{(0)}}{2\pi} n_{j} E_{j}.$$
$$J_{E} = \sum_{j} \int dx \rho_{j} j_{j}^{\epsilon^{(0)}} = \sum_{j} \lambda_{j} \int \frac{dp_{j}^{(0)}}{2\pi} n_{j} j_{j}^{\epsilon}$$
$$v_{j} = \frac{\partial \epsilon_{j}}{\partial p_{j}}$$
$$J_{E} = \sum_{j} \lambda_{j} \int \frac{dp_{j}^{(0)}}{2\pi} n_{j} (v_{j} E_{j}).$$



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#### thermodynamics

$$f = -T \sum_{j} \lambda_{j} \int \frac{dp_{j}^{(0)}}{2\pi} \ln(1 + e^{-\beta\epsilon_{j}}).$$
$$c(T) = \frac{\partial\epsilon}{\partial T} = \beta^{2} \sum_{j} \int \frac{dp_{j}}{2\pi} n_{j}(1 - n_{j})E_{j}^{2}.$$
$$\chi(T) = \frac{\partial m}{\partial h}|_{h \to 0} = \beta \sum_{j} \int \frac{dp_{j}}{2\pi} n_{j}(1 - n_{j})Q_{j}^{2}.$$

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#### T ightarrow 0

$$T = 0$$
  

$$\epsilon_1 = -v \sin p_1, \quad 0 \le p_1 < \pi$$
  

$$\epsilon_j = 0, \quad j > 1$$
  

$$v = J \frac{p_i}{2} \frac{\sin \theta}{theta}$$

 $\begin{aligned} \epsilon_{1} &\simeq T \ln 3 - v \sin p_{1}, \quad 0 \leq p_{1} \leq \pi \\ \epsilon_{j} &\simeq T \ln(j^{2} - 1) + v |p_{j}|, \quad j = 2, ..., \nu - 2 \\ |p_{j}| &\leq p_{j}^{max}, \quad p_{j}^{max} = \frac{T}{v} \ln \left(\frac{(j + 1)^{2} - 1}{j^{2} - 1}\right) \\ \epsilon_{\nu - 1} &\simeq T \ln(\nu - 2) + v |p_{\nu - 1}| \\ |p_{\nu - 1}| &< p_{\nu - 1}^{max}, \quad p_{\nu - 1}^{max} = \frac{T}{v} \ln \left(\frac{\nu - 1}{\nu - 2}\right) \\ = -\epsilon_{\nu - 1} \end{aligned}$ Rome 2019



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$$T = 0$$
  
 $E_1 = \epsilon_1, E_j = 0, j > 1$ 

$$\begin{array}{ll} E_1 & \sim & -v|\sin p_1| \\ E_j & \sim & -T|\sin(\frac{\pi p_j}{p_j^{max}})|, \ j>1 \ |p_j| \leq p_j^{max} \end{array}$$

a note

$$f(p) = T \ln g - \epsilon_p$$
  
 $n_h = 1 - n = rac{g}{g + e^{eta \epsilon_p}}$ 







$$\epsilon_{spinon} = v |\sin p|, -\pi  $c_{spinon} \simeq \frac{\pi}{3} \frac{1}{\beta v}, (\pi/3 \simeq 1.047)$$$

$$c_{TBA}^{(1)} \simeq \beta^{2} 2 \int_{0}^{+\infty} \frac{dp_{1}}{2\pi} \frac{(vp_{1})^{2}}{4\cosh^{2}\frac{\beta(T\ln 3 - vp_{1})}{2}} \simeq 1.234 \frac{1}{\beta v}$$

$$c_{TBA}^{(j)} \sim \frac{1}{\beta v} \frac{1}{j^{3}}$$

$$\chi = \frac{1}{\pi v} K, \quad K = \frac{1}{2} \frac{1}{1 - 1/\nu}$$

## Drude weights - revisited<sup>19</sup>

• 
$$D_{th} = \frac{\beta^2}{2} \sum_j \lambda_j \int \frac{dp_j}{2\pi} n_j (1 - n_j) (v_j E_j)^2$$

• 
$$T \rightarrow 0$$
,  $v_j \rightarrow v$ ,  $D_{th} = \frac{v^2}{2}c$ 

• 
$$D_s = \frac{\beta}{2} \sum_j \lambda_j \int \frac{dp_j}{2\pi} n_j (1 - n_j) (v_j Q_j)^2$$

• 
$$T \rightarrow 0$$
,  $D_s = \frac{v^2}{2}\chi = \frac{1}{2\pi}vK$  (Shastry-Sutherland)

<sup>19</sup>Klümper, Sakai, XZ *Rome 2019* 



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- theory vs. experiment
- impurity scattering phonon scattering - microscopic theory
- TBA vs. low energy effective theories

