Dynamical Spin-structure Factor at small q for the XXZ $s = 1/2$ chain

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R.G. Pereira, JS, *et al.*, PRL **96**, 257202 (06)

JS PRB **73**, 224424 (06)

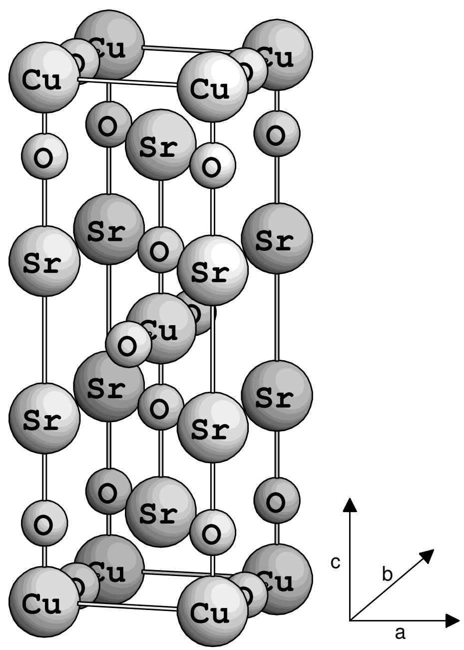
R.G. Pereira, JS, *et al.*, JSTAT P08022 (07)

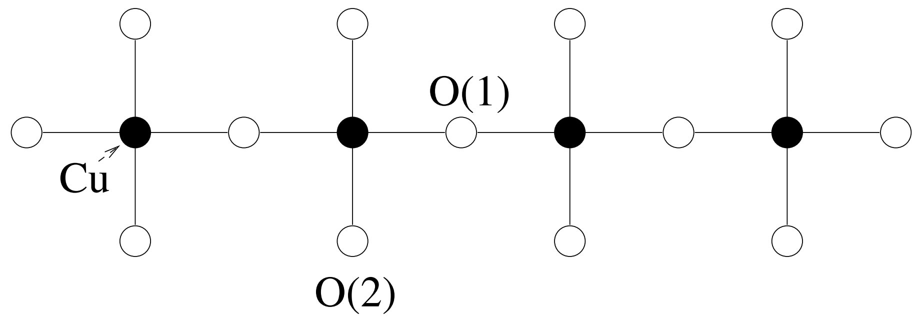
Topics

- The XXZ model
- The spin-structure factor at small q
- The spin-lattice relaxation rate

A realization of a spin chain: Sr_2CuO_3

- Sr_2CuO_3:





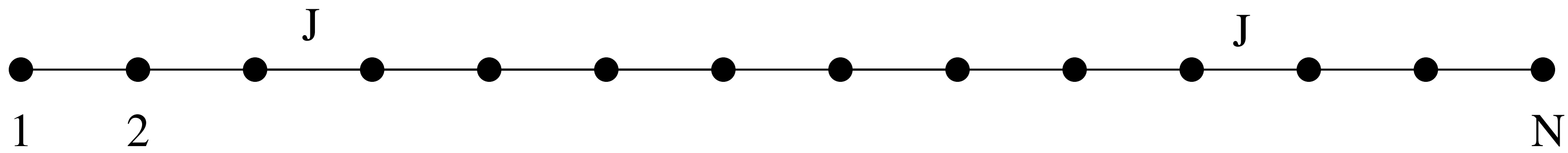
- neutron scattering $\rightarrow T_N \approx 5$ K
- $T_N/J_b \sim 10^{-3}$

- Antiferromagnet with strongly anisotropic couplings: ($S = 1/2$ spin of Cu ion)

Eff. Heisenberg model: $H = J_b \sum_i \boldsymbol{S}_i \boldsymbol{S}_{i+1} + J_a \sum_{<i,j>} \boldsymbol{S}_i \boldsymbol{S}_j + J_c \sum_{<i,j>} \boldsymbol{S}_i \boldsymbol{S}_j$

- $J_b \sim 2200$ K $\gg J_a \sim 0.002J \approx 5$ K $\gg J_c \sim 10^{-3}$ K

The XXZ-model: A theoretical model for 1D spin systems



Spin chain with N sites and $S = 1/2$ operators at each site interacting with

superexchange $J \longrightarrow$ Heisenberg model: $\quad H = J \sum_{j=1}^{N} \boldsymbol{S}_j \boldsymbol{S}_{j+1}$

Exchange anisotropy $\rightarrow$ XXZ-model:

$$H = J \sum_{j=1}^{N} \left[\frac{1}{2} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + \Delta S_j^z S_{j+1}^z \right] \quad ; \quad S_{\pm} = S^x \pm i S^y$$

Critical for $-1 \leq \Delta \leq 1$: Gapless excitations, no long range order, algebraically decaying correlation functions

Equivalent to interacting spinless fermions: (Jordan-Wigner)

$$H = J \sum_{j=1}^{N} \left[\frac{1}{2} \left(\psi_j^\dagger \psi_{j+1} + \psi_{j+1}^\dagger \psi_j \right) + \Delta \left(\psi_j^\dagger \psi_j - \frac{1}{2} \right) \left(\psi_{j+1}^\dagger \psi_{j+1} - \frac{1}{2} \right) \right]$$

$S^{zz}(q,w)$ at small q for the XXZ-model

$$H = J\sum_{j=1}^{N}\left[\frac{1}{2}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) + \Delta S_j^z S_{j+1}^z - hS_j^z\right]$$

- The longitudinal dynamical structure factor is defined by:

$$\begin{aligned} S^{zz}(q,\omega) &= \frac{1}{N}\sum_{j,j'=1}^{N} e^{-iq\left(j-j'\right)}\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\left\langle S_j^z(t)\, S_{j'}^z(0)\right\rangle \\ &= \frac{2\pi}{N}\sum_{\alpha}\underbrace{\left|\left\langle 0\left|S_q^z\right|\alpha\right\rangle\right|^2}_{\equiv\left|F(q,\omega)\right|^2}\delta\left(\omega - E_\alpha\right) \end{aligned}$$

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- $F(q,\omega)$ are called form factors; can be calculated for finite chains by BA (Biegel, Karbach *et al.* 02,03 ; Caux *et al.* 05)
- Calculation of $S^{zz}(q,w)$ by field theory methods and Bethe Ansatz (Pereira, JS *et al.*, PRL **96**, 257202 (06), JSTAT P08022 (2007))

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Motivation

$I)$ Spin-lattice relaxation rate studied by ^{17}O NMR in Sr_2CuO_3:

$$\frac{1}{T_1} \sim \int dq \cos^2(q/2) S^{zz}(q,\omega_N) \stackrel{?}{\sim} T + \frac{T^2}{\sqrt{\omega_N}} \quad ; \quad \omega_N \text{ resonance frequency}$$

Diffusive $q \sim 0$ mode ?

Thurber *et al.*, PRL **87**, 247202 (2001)

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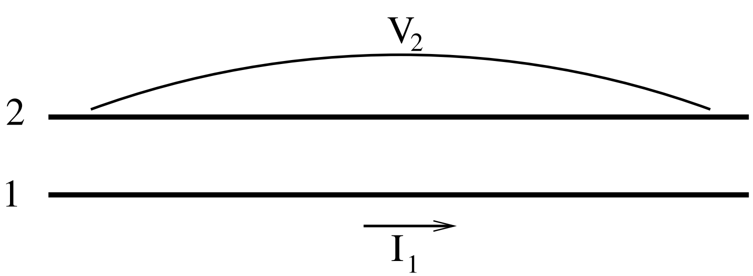
$II)$ Coulomb drag between quantum wires: (Fermion picture)



Drag resistivity: $r \sim -\lim_{I_1 \to 0} \frac{dV_2}{dI_1}$

$$r \sim \int dk\, dw\, k^2 U_{12}(k) \frac{\partial S_1(k,\omega)}{\partial \omega} S_2(-k,-\omega)$$

Overlap between structure factors important

Pustilnik *et al.*, PRL 91, 126805 (2003)

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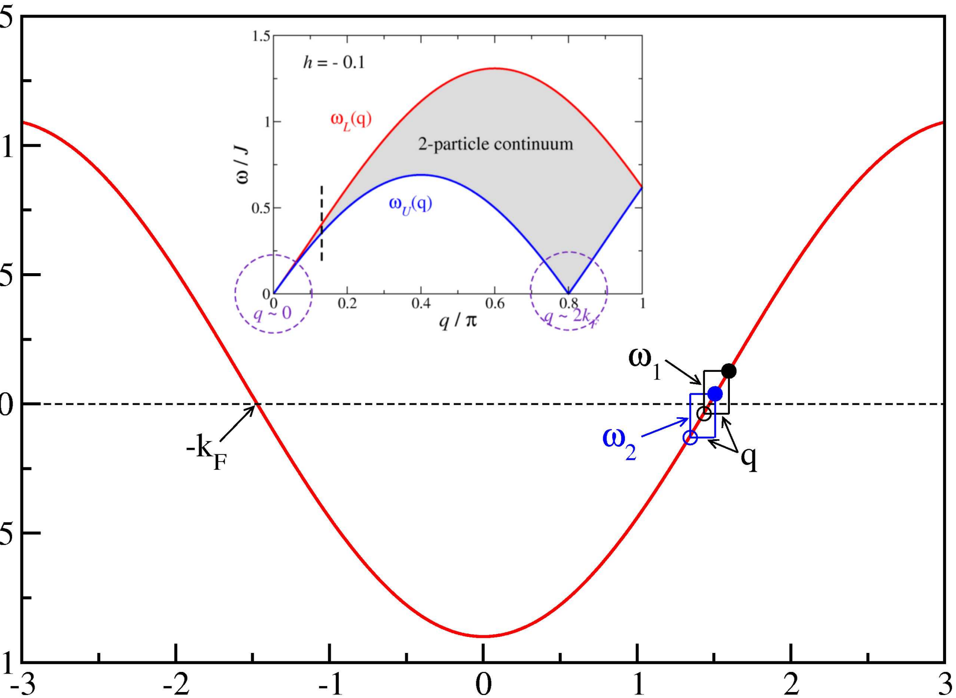
$S^{zz}(q,\omega)$ for $\Delta = 0$

$$H_0 = J\sum_{j=1}^{N}\left[\frac{1}{2}\left(\psi_j^\dagger\psi_{j+1} + \psi_{j+1}^\dagger\psi_j\right) - h\psi_j^\dagger\psi_j\right] = \sum_k (J\cos k - h)\psi_k^\dagger\psi_k$$



$$\langle 0|S_q^z|\alpha\rangle = \sum_p \langle 0|\psi_p^\dagger\psi_{p+q}|\alpha\rangle$$
$$= \theta(k_F - |p|)\theta(|p+q| - k_F)$$

$$\omega_L(q) = 2J\sin\tfrac{q}{2}\sin(k_F - \tfrac{q}{2})$$

$$\omega_U(q) = 2J\sin\tfrac{q}{2}\sin(k_F + \tfrac{q}{2})$$

$$\epsilon_{kR,L} \approx \pm v_F k + \frac{k^2}{2m} + \cdots$$

$$H_0 = \sum_k\left[\epsilon_{kR}\psi_{kR}^\dagger\psi_{kR} + \epsilon_{kL}\psi_{kL}^\dagger\psi_{kL}\right]$$

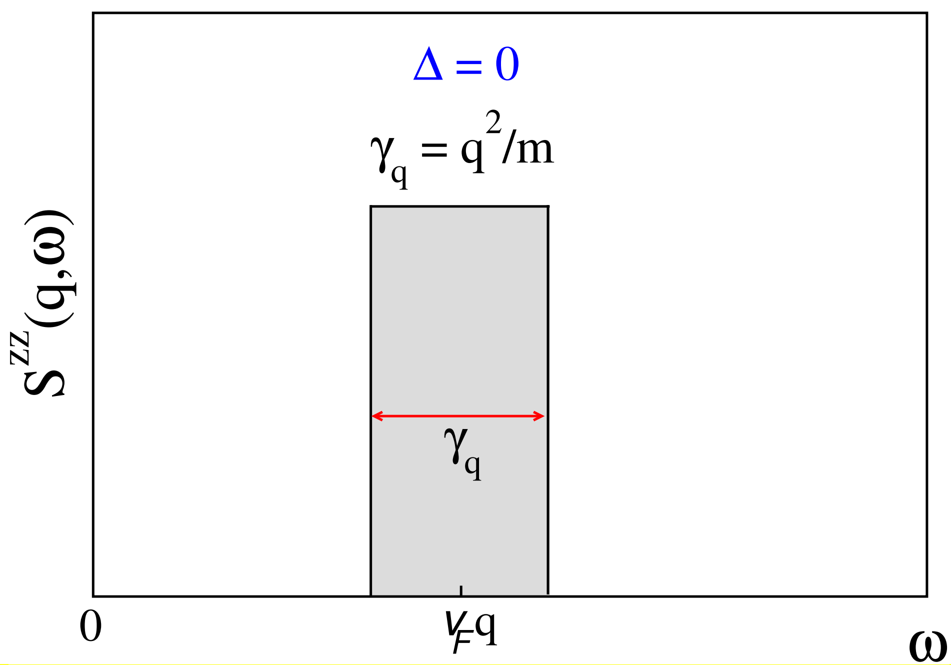
$S^{zz}(q,\omega)$ for $\Delta = 0$

- Linear approximation: $\epsilon_{kR,L} \approx \pm v_F k \rightarrow$ All particle hole excitations are degenerate

$$S^{zz}(q,\omega) = |q|\delta(\omega - v_F|q|)$$

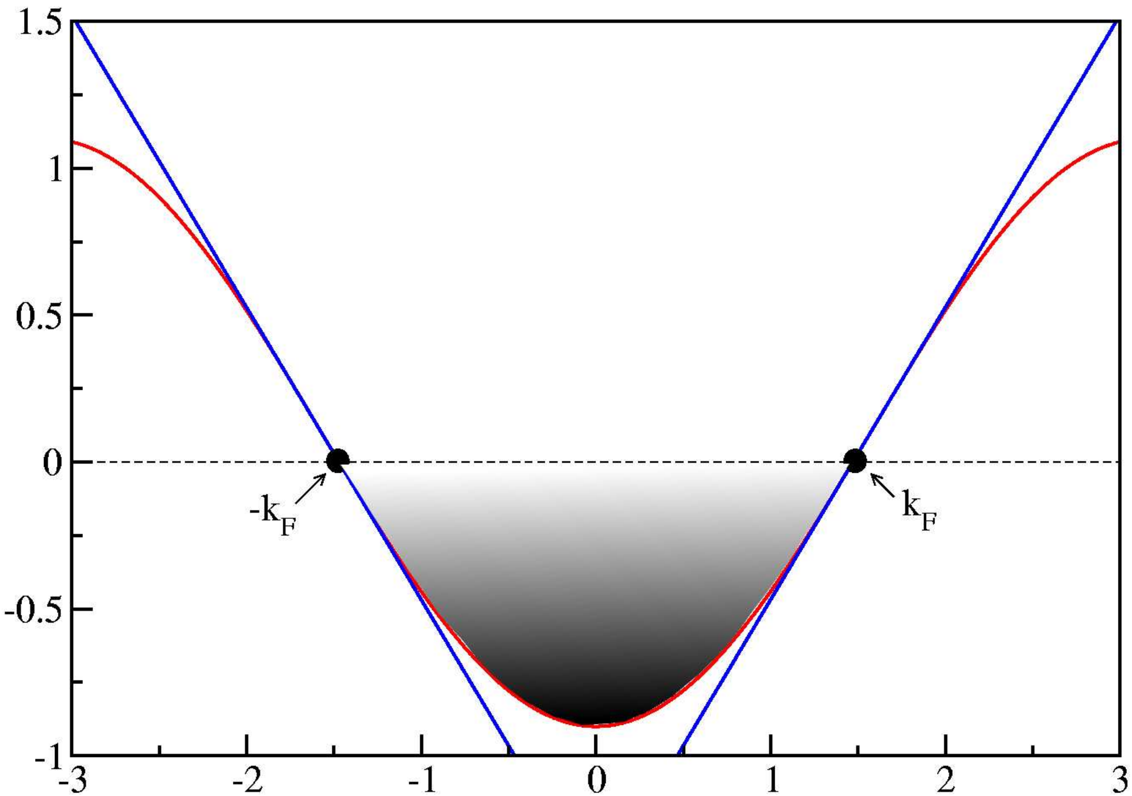
- $\epsilon_{kR,L} \approx \pm v_F k + \frac{k^2}{2m}$

$$S^{zz}(q,\omega) = \frac{m}{|q|}\theta\left(\frac{q^2}{2m} - |\omega - v_F|q||\right) \quad , \quad m = (J\cos k_F)^{-1}$$



Field theory: Luttinger liquid physics

Low energies $\rightarrow$ linearize dispersion around Fermi points + continuum limit



Bosonization:

$$H_{XXZ} \rightarrow H_{LL} + \text{irrel. operators}$$

$$H_{LL} = \sum_{q>0} vq \left(a_q^\dagger a_q + 1/2 \right)$$

$$q = 2\pi n/N, \; n = 1, 2, \cdots$$

Free Boson Model

- Collective modes, no Landau quasi-particles
- Correlation functions: Power laws with interaction-dependent exponents
- Corrections by perturbation theory in the irrelevant operators

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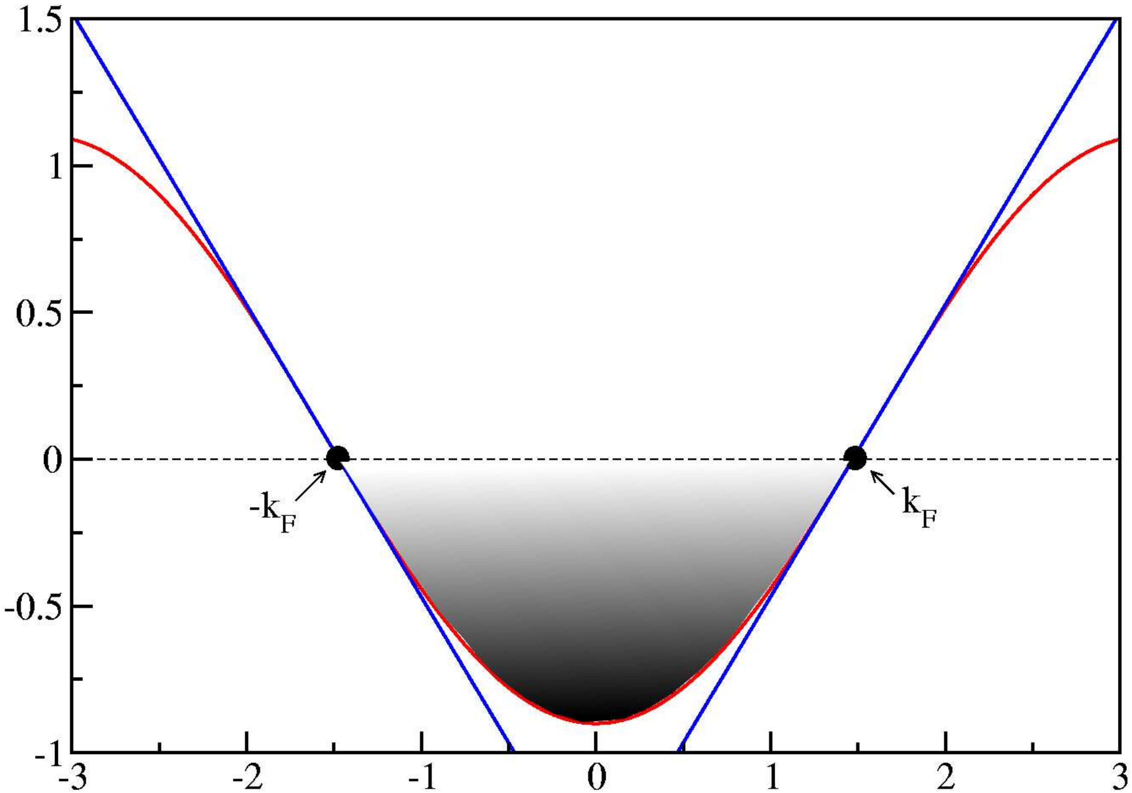
Luttinger liquid description

Linear dispersion:



Luttinger model:

$$H_{LL} = \sum_{q>0} vq \left(a_q^\dagger a_q + 1/2 \right)$$

Low-energy excitations exist only for $q \sim 0$ and $q \sim 2k_F$

Structure factor ($T = 0,\ q \sim 0$):

$$S^{zz}(q, \omega) = K\, |q|\, \delta(\omega - v\,|q|)$$

Boson with momentum $|q|$ always carries energy $\omega = v|q|$

$\rightarrow$ δ-function peak

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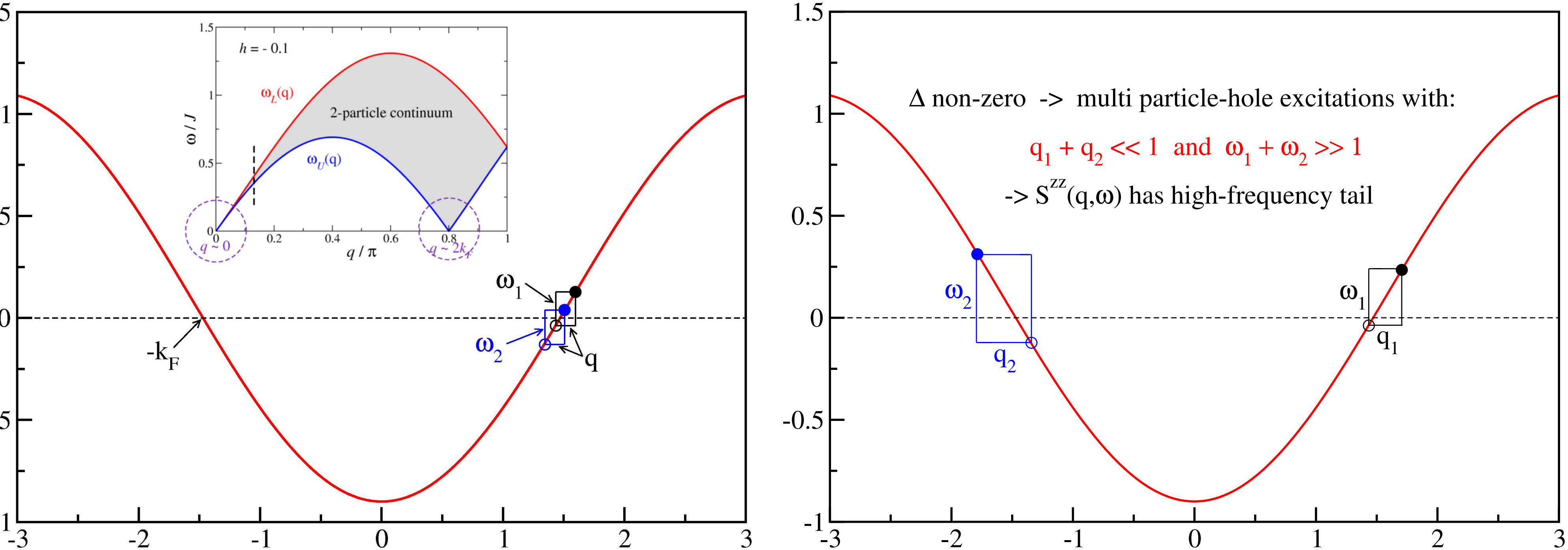
Beyond the Luttinger model



- Band curvature: $\epsilon_k = \pm vk + \frac{k^2}{2m}$

  Leads to a broadening of the δ-function peak

- Multi particle-hole excitations ($\Delta \neq 0$): Lead to a high-frequency tail

High-frequency tail

Perturbatively from the Luttinger model plus irrelevant operators: ($h \neq 0$)

$$\mathcal{H} = \frac{v}{2}\left[\Pi^2 + (\partial_x \phi)^2\right] + \eta_+ \left[(\partial_x \phi_L)^2 \, \partial_x \phi_R - (\partial_x \phi_R)^2 \, \partial_x \phi_L\right]$$

High-frequency tail

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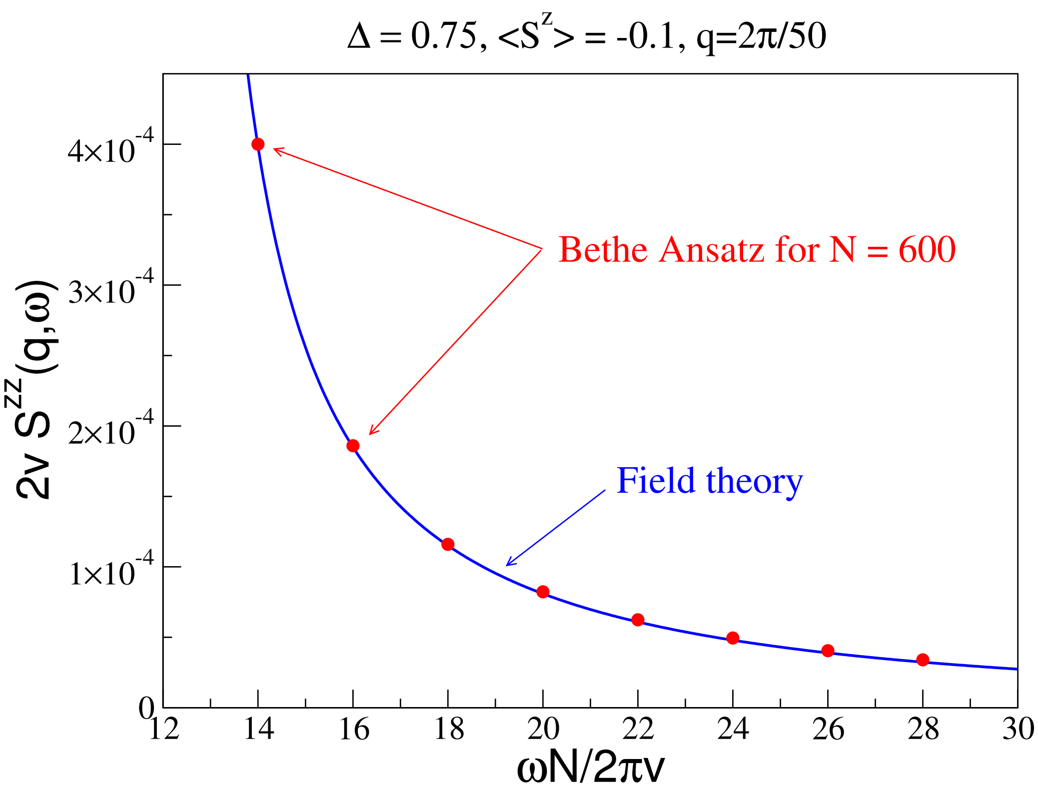

$$\delta S^{zz}_{\eta_+}(q,\omega) = \frac{K\eta_+^2 q^4}{v\pi} \frac{\theta(\omega - v|q|)}{\omega^2 - v^2 q^2}$$

valid for $\gamma_q \ll \omega - v|q| \ll J$

η_+ can be calculated from BA

Parameter-free result

(Pereira, JS *et al.* 06)

Linewidth

$$\mathcal{H} = \frac{v}{2}\left[\Pi^2 + (\partial_x \phi)^2\right] + \eta_+ \left[(\partial_x \phi_L)^2 \partial_x \phi_R - (\partial_x \phi_R)^2 \partial_x \phi_L\right]$$
$$+ \; \eta_- \left[(\partial_x \phi_L)^3 - (\partial_x \phi_R)^3\right]$$

In pert. theory η_--term produces terms increasingly singular at $\omega = vq$
$\rightarrow$ entire series has to be summed up

Linewidth

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Conjecture: If free fermion result is reproduced, then interacting case yields:

$$S(q,\omega) = \frac{K}{\eta_- q}\theta\left(\frac{\eta_- q^2}{2} - |w - vq|\right) \quad ; \quad \delta w = \eta_- q^2$$

$$\eta_- = \frac{v}{\sqrt{K}}\frac{\partial v}{\partial h} + \frac{v^2}{2K^{3/2}}\frac{\partial K}{\partial h} \quad ; \quad \eta_+ = \frac{3v^2}{2K^{3/2}}\frac{\partial K}{\partial h}$$

Exact results even for non-integrable models if $v(h)$, $K(h)$ can be determined

Agrees with boundaries of particle-hole excitation spectrum in Bethe Ansatz!

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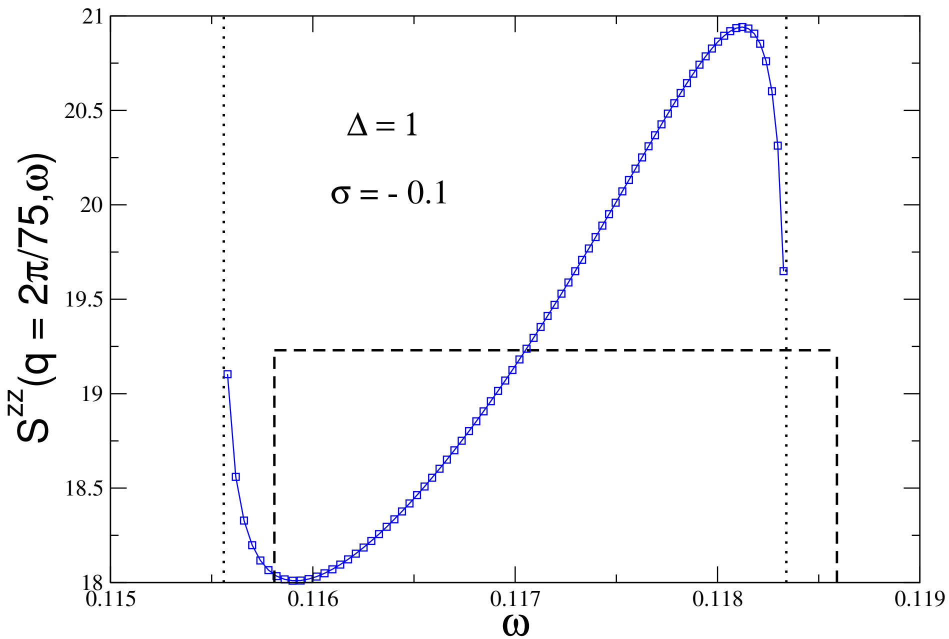
Lineshape and Edge Singularities

Lineshape obtained from factors calculated by Bethe Ansatz for $N = 6000$



- Maximum, minimum and power law edge singularities!
- Related to irrelevant operators of higher dimension
- $S^{zz}(q,\omega) \equiv \frac{q}{\delta\omega_q} f\left(q, \frac{\omega - vq}{\delta\omega_q}\right)$, $f(q,x)$ approaches flat distribution for $q \to 0$

- Lower edge: $S^{zz}(q,\omega) \sim [\omega - \omega_L(q)]^{-\mu}$ with $\mu = \mu(q,\Delta)$! (Pustilnik *et al.* (06))
- Edge singularities can be calculated exactly (Pereira *et al.* (07))

Spin-lattice relaxation rate in Sr_2CuO_3

- Nuclear spin relaxes due to hyperfine interaction: $H_{hf} = \sum_r A_r \boldsymbol{I}_0 \boldsymbol{S}_r$
- Relaxation rate: $\frac{1}{T_1} = \int \frac{dq}{2\pi} |A(q)|^2 S^{zz}(q, \omega_N)$
- Hyperfine form factor: $A(q) = \sum_r \mathrm{e}^{iqr} A_r$
- Directly measures structure factor

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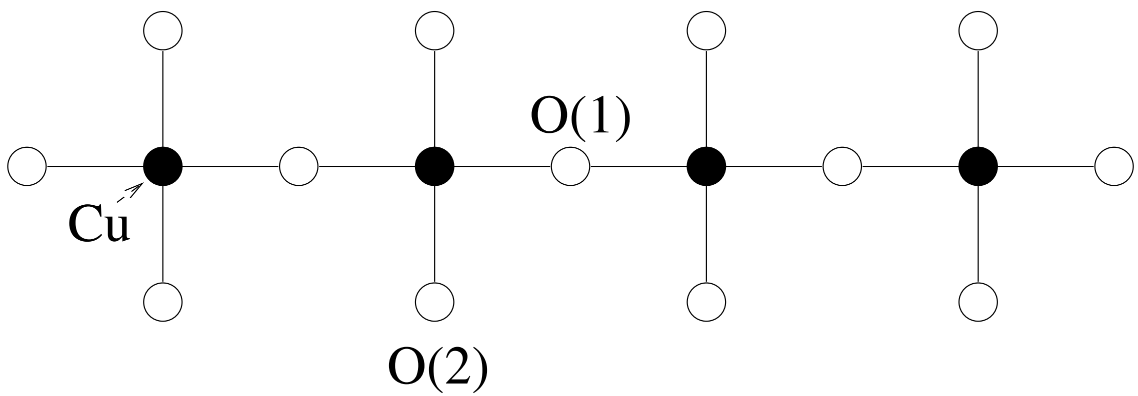

O(1): $A_r = A\delta(r \pm 1/2) \rightarrow A(q) = 2A\cos(q/2)$

Contributions from $q \sim \pi$ suppressed, mainly $q \sim 0$ important at low T!

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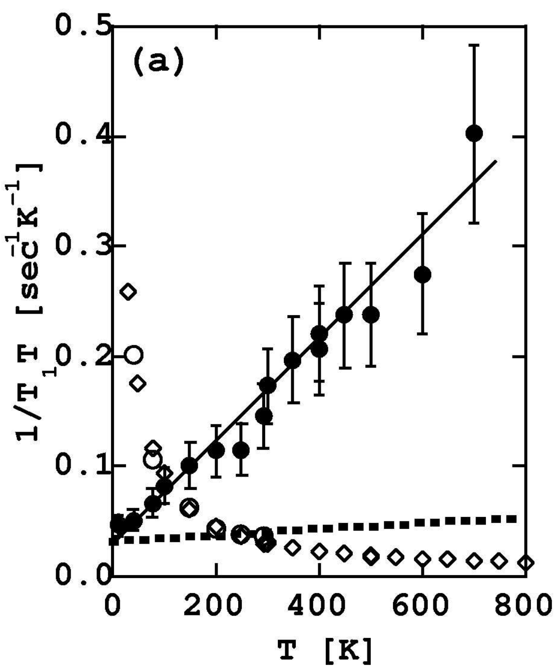
Spin-lattice relaxation rate in Sr_2CuO_3 (II)

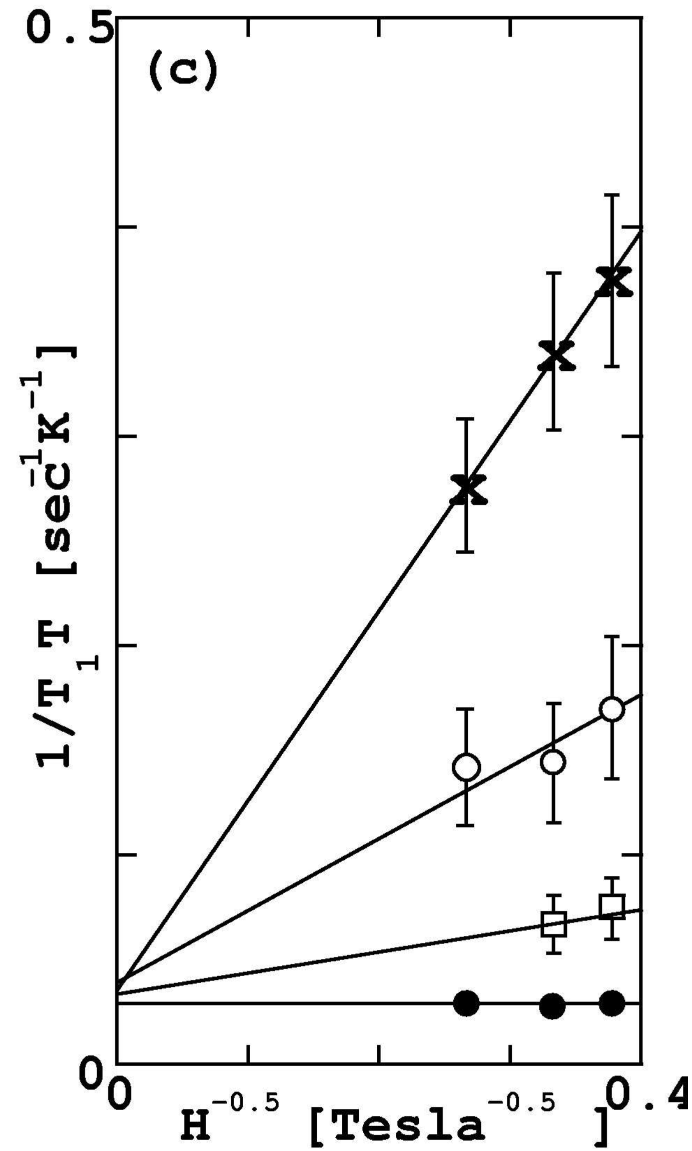
Experiment:

$$\frac{1}{T_1} \sim \int dq \cos^2\left(\frac{q}{2}\right) S^{zz}(q,\omega_N) \overset{?}{\sim} T + \frac{T^2}{\sqrt{\omega_N}}$$

Theory: $S^{zz}_u(q,\omega) \overset{T \gg \omega}{\approx} \frac{T|q|}{2\omega}\delta(w - v|q|)$

$$\frac{1}{T_1} \sim \frac{2T}{\pi^3 J^2} \cos^2\left(\frac{\omega}{\pi J}\right)$$





(Thurber *et al.* 01)

Spin-lattice relaxation rate in Sr_2CuO_3 (III)

$$\frac{1}{T_1} \sim \int dq \cos^2\left(\frac{q}{2}\right) S^{zz}(q,\omega_N)$$
$$\sim S_0^{zz}(\omega) + S_1^{zz}(\omega)$$

- Free fermions ($\Delta = 0$):

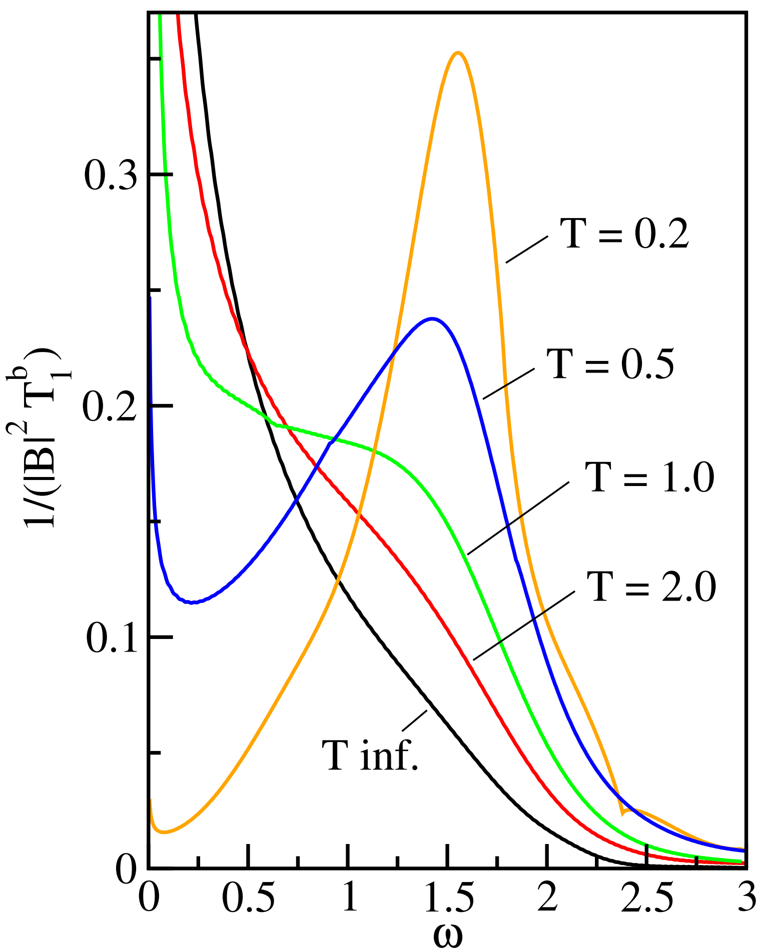
$$S_0^{zz}(\omega) \sim \underbrace{\frac{2}{\pi}T}_{\text{Fermi points}} + \underbrace{\frac{2}{\pi}e^{-J/T}(\text{const} - \ln\omega)}_{\text{top/bottom band}}$$

$$S_1^{zz}(\omega) \sim \underbrace{\frac{2}{\pi}T^3}_{\text{Fermi points}} + \underbrace{\frac{2}{\pi}e^{-J/T}(\text{const} - \ln\omega)}_{\text{top/bottom band}}$$

- TMRG: Diffusionlike contribution exists, but exponentially suppressed

$1/T_1 \sim \mathrm{e}^{-J/T}\omega^{-\alpha}$, $\alpha \sim 0.3$ for $\Delta = 1$

Spin-lattice relaxation rate (Δ=1)



(JS 06)

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Conclusions

- Calculation of the dynamical spin structure factor for the XXZ model at small q by a combination of bosonization and Bethe ansatz
  - Linewidth is proportional to q^2 for $h \neq 0$
  - Lineshape is non-Lorentzian: Maximum, minimum, power-law edge singularities
  - For $\Delta \neq 0$ there is a high-frequency tail

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  - For $\Delta \neq 0$ there is a high-frequency tail
- Experiments on Sr_2CuO_3 have suggested $1/T_1(q \sim 0) \sim T + T^2/\sqrt{w_N}$
  - Field theory gives $1/T_1(q \sim 0) \sim T$ plus non-singular terms in ω_N
  - Numerics shows that a singular contribution exists but exponentially suppressed $\sim \mathrm{e}^{-J/T}\omega^{-\alpha}$, $\alpha \approx 0.3$

Collaborations

- Ian Affleck (UBC, Vancouver, Canada)
- Michael Bortz (ANU, Canberra, Australia)
- Jean-Sebastian Caux (U Amsterdam, Netherlands)
- Sebastian Eggert (U Kaiserslautern, Germany)
- Satoshi Fujimoto (U Kyoto, Japan)
- Andreas Klümper (U Wuppertal, Germany)
- Nicolas Laflorencie (École Polytechnique, Lausanne, Switzerland)
- Jean Michel Maillet (École Normale Supérieure, Lyon, France)
- Rodrigo Pereira (UBC, Vancouver, Canada)
- Steve White (UC Irvine, USA)