Neel transition in coupled spin-1/2 XXZ spin chains

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Outline

- Single XXZ chain and TLL
- coupled chains and Néel transition
- RPA approach

Phase diagram of the XXZ spin-1/2 chain

The XXZ spin chain Hamiltonian

$$H = J\sum_n \left[(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + \Delta S_n^z S_{n+1}^z\right]$$

From integrability:

- $\Delta < -1$: Ising Ferromagnet $\langle S_j^z\rangle = m_F$
- $\Delta > 1$: Ising Antiferromagnet $\langle S_j^z\rangle = (-1)^j m_{AF}$
- $|\Delta| < 1$ Tomonaga-Luttinger liquid

Tomonaga-Luttinger liquid (I)

Bosonized Hamiltonian

$$\begin{aligned} H &= \int \frac{dx}{2\pi}\left[uK(\nabla\theta)^2 + \frac{u}{K}(\partial_x\phi)^2\right], \\ [\phi(x), \nabla\theta] &= i\pi\delta(x-y). \end{aligned}$$

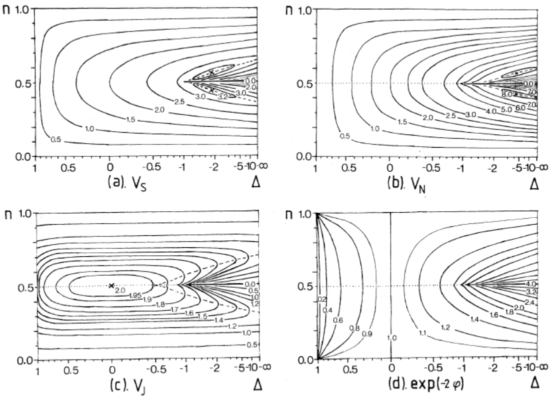
Zero magnetization

$$\begin{aligned} K &= \frac{1}{2 - \frac{2}{\pi}\arccos\Delta} \\ u &= \pi J \frac{\sqrt{1-\Delta^2}}{\arccos\Delta} \end{aligned}$$

isotropic case: $K = 1/2$

Tomonaga-Luttinger parameters for general magnetization

From F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).



$$K = e^{2\phi}, u = v_S, v_N = u/K, v_J = uK$$

Tomonaga-Luttinger liquid (II)

Bosonized spin operators

$$S^+(x) \sim \frac{e^{i\theta(x)}}{\pi a}\left[\cos(2\phi(x) - 2\pi m x) + e^{i\frac{\pi x}{a}}\right]$$

$$S^z(x) \sim m - \frac{\partial_x \phi}{\pi} + e^{i\frac{\pi x}{a}} \cos(2\phi(x) - 2\pi m x)$$

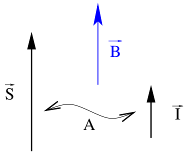
1. $z = 1$ quantum criticality in the ground state
2. correlation length u/T for $T > 0$.

Other Tomonaga-Luttinger liquid spin systems

Spin gap systems above C-IC transition

1. Two-leg ladders for $h > \Delta$: BPCB, DIMPY [Jeong et al. Phys. Rev. Lett. **117**, 106402 (2016)]
2. dimerized spin chains: Copper nitrate [Willenberg et al. Phys. Rev. B **91**, 060407 (2015)]
3. Haldane gap spin-1 chains: DTN [Mukhopadhyay et al. Phys. Rev. Lett. **109**, 177206 (2012)]

Nuclear Magnetic Resonance



Interaction Hamiltonian

$$H = H_0 + H_{\text{hyperfine}} + H_{\text{env.}} \quad H_0 = -\gamma_N B_z I_z$$

$$H_{\text{hyperfine}} = A\vec{S}\cdot\vec{I}$$

Phenomenological description

Bloch equations

$$
\begin{aligned}
\vec{\mu} &= \gamma_N \vec{I} \\
\frac{d\mu_z}{dt} &= \gamma_N (\vec{\mu} \times \vec{B})_z + \frac{\mu_{eq.} - \mu_z}{T_1} \\
\frac{d\mu_x}{dt} &= \gamma_N (\vec{\mu} \times \vec{B})_x - \frac{\mu_x}{T_{2L}} \\
\frac{d\mu_y}{dt} &= \gamma_N (\vec{\mu} \times \vec{B})_y - \frac{\mu_y}{T_{2L}}
\end{aligned}
$$

(Lorentzian) Relaxation rates

Longitudinal NMR relaxation rate

$$\frac{1}{T_1} = A^2 \int_{-\infty}^{+\infty} dt \cos(\omega_R t) \langle \{ S^+(t), S^-(0) \} \rangle$$

Transverse NMR relaxation rate

$$\begin{aligned} \frac{1}{T_{2L}} &= \frac{A^2}{2} \int_{-\infty}^{+\infty} dt \langle \{ S^+(t), S^-(0) \} \rangle \\ &\quad + A^2 \int_{-\infty}^{+\infty} dt \langle \{ S^z(t), S^z(0) \} \rangle \end{aligned}$$

Linear response formulation

By Fluctation-Dissipation theorem

$$\begin{aligned} \frac{1}{T_1} &= \frac{T}{\omega_R} \int \frac{dq}{2\pi} \mathrm{Im}\chi(q,\omega_R) \\ \chi(q,\omega) &= i \int dx dt e^{-i(qx-\omega t)} \theta(t) \langle [S^+(x,t), S^-(0,0)] \rangle \end{aligned}$$

NMR relaxation rates in the Luttinger liquid state

isotropic hyperfine interaction

$$
\begin{aligned}
\frac{1}{T_1} &= \frac{1}{T_1^{(q=0)}} + \frac{1}{T_1^{(q=\pi/a)}} \\
\frac{1}{T_1^{(q=\pi/a)}} &\sim \int dt \langle e^{i\theta(0,t)} e^{-i\theta(0,0)} \rangle \\
\frac{1}{T_1^{(q=0)}} &\sim \sum_{r=\pm 1} \int dt \langle e^{i\theta(0,t)+2r\phi(0,t)} e^{-i\theta(0,0)-2r\phi(0,0)} \rangle
\end{aligned}
$$

Staggered contribution

Correlation function

$$\langle e^{i\theta(0,t)} e^{-i\theta(0,0)} \rangle = \left(\frac{\pi T a}{u \sinh(\pi T t)} \right)^{\frac{1}{2K}}$$

Scaling result for $K > 1/2$

$$\frac{1}{T_1^{(q=\pi/a)}} \sim \frac{a}{u} \left(\frac{\pi T a}{u} \right)^{\frac{1}{2K}-1} \int_0^{+\infty} \frac{dw}{(\sinh w)^{\frac{1}{2K}}}$$

divergent as $T \to 0$

To Sum up . . .

Four Contributions

- $1/T_1 \sim T^{\frac{1}{2K}-1}$ from staggered S^+ fluctuations. (dominant)
- $1/T_1 \sim T^{2K+\frac{1}{2K}-1}$ from uniform S^+ fluctations
- $1/T_1 \sim T$ from uniform S^z fluctuations
- $1/T_1 \sim T^{2K-1}$ from staggered S^z fluctuations.

Crossover to high temperature

- Coira et al. `arXiv:1606.03985`
- Dupont et al. `arXiv:1606.09502`

The isotropic limit

taking $K \to 1/2$: simplistic

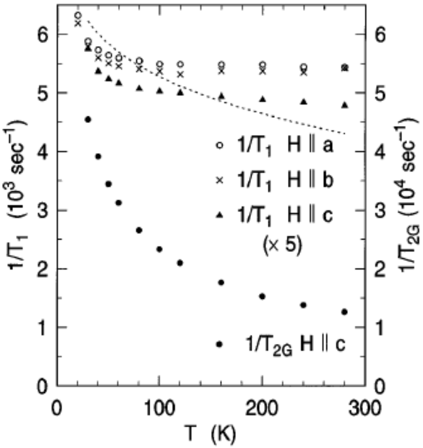
- $1/T_1 \sim T$ from uniform components
- $1/T_1 \sim T^0$ from staggered components

Logarithmic corrections from marginal operator

$$\frac{1}{T_1} \sim \sqrt{\ln \frac{T_0}{T} + \frac{1}{2} \ln \left(\ln \frac{T_0}{T} \right)} (1 + O(\ln(T_0/T))^{-1})$$

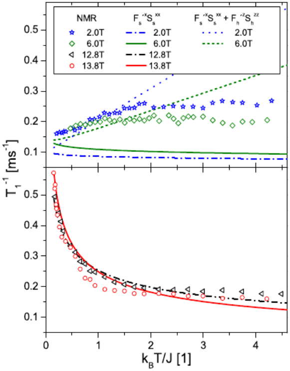
V. Barzykin J. Phys. Cond. Matt. **12**, 2053 (2000)

Experiments (I): isotropic case Sr_2CuO_3 ($T_N = 5K$)



From Takigawa et al. Phys. Rev. Lett. **76**, 4612 (1996).

Experiments (II): in field with CuPzN ($T_N = 0.1K$)



From Kühne et al. Phys. Rev. B **83**, 100407(R) (2011)

Array of coupled chains

Square array of chains

$$
\begin{aligned}
H &= J\sum_{n,j,k}(S^x_{n,j,k}S^x_{n+1,j,k} + S^y_{n,j,k}S^y_{n+1,j,k} + \Delta S^z_{n,j,k}S^z_{n+1,j,k}) \\
&\quad + J_\perp \sum_{n,j,k}(\vec{S}_{n,j,k}\cdot\vec{S}_{n,j+1,k} + \vec{S}_{n,j,k}\cdot\vec{S}_{n,j,k+1}) - \sum_{n,j,k} hS^z_{n,j,k}
\end{aligned}
$$

Néel transition

Mean Field theory

$4J_\perp \chi^{aa}(q = 0, \omega = 0, T_N) = 1$

1. $\langle S^z \rangle$ ordering $K < 1$
2. $\langle S^x \rangle$ ordering $K > 1/4$

Random Phase Approximation above the Néel temperature

Response in the RPA

$$\chi_{RPA}(\mathbf{q},\omega) = \frac{\chi_{1D}(q_z,\omega)}{1 - J(\mathbf{q}_\perp)\chi_{1D}(q_z,\omega)},$$

$\chi_{1D}(q_z,\omega)$: single chain response
$J(\mathbf{q}_\perp) = 2J_\perp(cos q_x + \cos q_y)$

expression of the NMR relaxation rate

Linear response expression of $1/T_1$

$$\frac{1}{T_1} = \lim_{\omega_R \to 0} \frac{T}{\omega_R} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \mathrm{Im}\chi(\mathbf{q}, \omega_R),$$

With RPA approximation

$$\left(\frac{1}{T_1}\right) = \left(\frac{1}{T_1}\right)_{q_z \simeq 0} + \left(\frac{1}{T_1}\right)_{q_z = \frac{\pi}{a}},$$

$$\left(\frac{1}{T_1}\right)_{q_z \simeq Q} = \lim_{\omega \to 0} \frac{T}{\omega} \int \frac{d^2\mathbf{q}_\perp}{(2\pi)^2} \int_{-\Lambda}^{\Lambda} \frac{dq_z}{2\pi} \mathrm{Im} \frac{\chi_{1D}(q_z + Q, \omega)}{1 - J(\mathbf{q}_\perp)\chi_{1D}(q_z + Q, \omega)}$$

Expression of relaxation rate

After integration of transverse modes

$$\left(\frac{1}{T_1}\right)_{q_z \simeq Q} = \int_{-\Lambda}^{\Lambda} \frac{dq_z}{\pi^2} \lim_{\omega \to 0} \frac{T}{\omega} \mathrm{Im}\chi_{1D}(q_z + Q, \omega) \times \frac{\mathrm{E}(16 J_\perp^2 \chi(q_z + Q, 0)^2)}{1 - 16 J_\perp^2 \chi(q_z + Q, 0)^2}$$

where E is a complete elliptic integral of the second kind.

Approximation for the uniform contribution

Neglect q_z in susceptibility

$$\left(\frac{1}{T_1}\right)_{q_z\simeq 0} \sim \frac{2}{\pi}\frac{\mathrm{E}(16J_\perp^2\chi_{1D}(0,0)^2)}{1-16J_\perp^2\chi_{1D}(0,0)^2}\left(\frac{1}{T_1}\right)_{q_z\simeq 0,1D},$$

$\Rightarrow$ only a weak change to the rate of the single chain.

The staggered contribution

Near the transiton

Divergence of RPA susceptibility at Néel transition
$\Rightarrow 1/T_1 \sim (T - T_N)^{-1/2}$
Giamarchi and Tsvelik Phys. Rev. B **59**, (1999)

Full expression of susceptibilities

$$\lim_{\omega \to 0} \frac{T}{\omega} \mathrm{Im}\chi^{zz}(k,\omega) = \frac{1}{4}\chi^{zz}(k + \frac{\pi}{a}, 0)\frac{\sin(\pi K)}{\sin^2 \frac{\pi K}{2} + \sinh^2\left(\frac{uk}{4T}\right)}$$

χ_{+-} : $K \to \frac{1}{4K}$.

Final expression: $1/T_1 = T^{1/(2K)-1}\varphi_K(T/T_N)$

$$\left(\frac{1}{T_1}\right)_{q_z\simeq\frac{\pi}{a},RPA} = \mathcal{C}\left(\frac{2\pi T}{u}\right)^{\frac{1}{2K}-1}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\xi}{\sin^2\left(\frac{\pi}{8K}\right)+\sinh^2(\pi\xi)}$$

$$\times\left|\frac{\Gamma\left(\frac{1}{8K}+i\xi\right)}{\Gamma\left(1-\frac{1}{8K}+i\xi\right)}\right|^2\frac{\mathrm{E}\left[\left(\frac{T_N}{T}\right)^{4-1/K}\left|\frac{\Gamma\left(1-\frac{1}{8K}\right)\Gamma\left(\frac{1}{8K}+i\xi\right)}{\Gamma\left(\frac{1}{8K}\right)\Gamma\left(1-\frac{1}{8K}+i\xi\right)}\right|^4\right]}{1-\left(\frac{T_N}{T}\right)^{4-1/K}\left|\frac{\Gamma\left(1-\frac{1}{8K}\right)\Gamma\left(\frac{1}{8K}+i\xi\right)}{\Gamma\left(\frac{1}{8K}\right)\Gamma\left(1-\frac{1}{8K}+i\xi\right)}\right|^4},$$

E is a complete elliptic integral of the second kind.

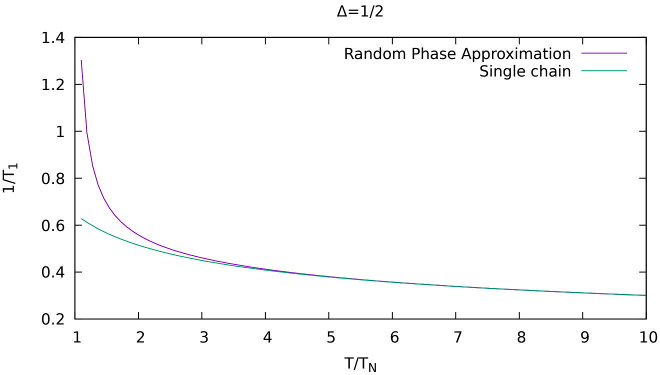
The vicinity of the Néel temperature

After expanding near $\xi = 0$

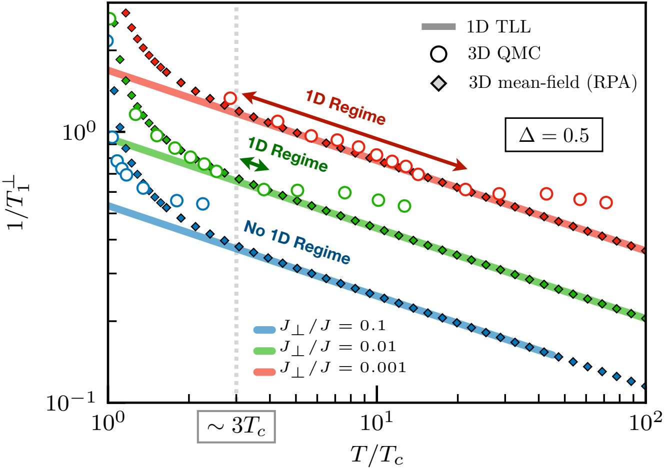
$$\frac{1}{T_1} \simeq \frac{a}{2a\Gamma^2(K)} \frac{\pi}{\sin^2(\pi K/2)\sqrt{\psi^{(1)}\left(\frac{K}{2}\right) - \psi^{(1)}\left(1-\frac{K}{2}\right)}} \times \left(\frac{2\pi T_N a}{u}\right)^{2K-1} \frac{1}{\sqrt{1-(T_N/T)^{2-2K}}},$$

$\rightarrow (T - T_N)^{-1/2}$ is recovered.

Comparing with the single chain



Comparing with QMC simulations



Dupont et al. Phys. Rev. B **98**, 094403 (2018).

Below T_N: self consistent Harmonic approximation

Variational method

$$H = \sum_n H_{TLL,n} - J \sum_{\substack{n \\ \alpha=y,z}} \cos(\theta_n - \theta_{n+e_\alpha})$$

$$H_{var.}(\lambda) = \sum_n H_{TLL,n} + \frac{\lambda}{2} \sum_{\substack{n \\ \alpha=y,z}} (\theta_n - \theta_{n+e_\alpha})^2$$

$$F_{var} = -T \ln \mathrm{tr}(e^{-\beta H_{var}}) + \langle H - H_{var} \rangle_{H_{var.}}$$

Low Temperature prediction

Goldstone mode contribution

$$\frac{1}{T_1^{\perp}} = \left[\frac{m^{\mathrm{AF}}(T)}{v_{\mathrm{sw}}^{b,c}}\right]^2 \frac{T}{4K},$$

Conclusions

Main findings

- Crossover from isolated chains to 3D behavior at $T = 3T_N$.
- Mean-field divergence of T_1 at $T = T_N$.
- Low temperature behavior $1/T_1 \sim T$.

Open questions

1. Isotropic case; Logarithmic corrections and low temperature Goldstone modes
2. Experiments indicate an intermediate temperature regime $0 \ll T \ll T_N$ where $1/T_1 \sim T^\alpha$ with $4 < \alpha < 5$.
3. Crossover to classical 3D XY model near T_N.
4. What about the two dimensional case ?