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IX TRIESTE WORKSHOP ON
OPEN PROBLEMS IN
STRONGLY CORRELATED SYSTEMS

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THE PHYSICS OF CHAINS AND LADDERS AS PROBED BY NMR

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These are preliminary lecture notes, intended only for distribution to participants.

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The physics of chains and ladders as probed by NMR

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1. Basic aspect of NMR

2. Understanding in S=1/2 Spin-Chains

3. Magnetism in Spin-Ladders

4. Spin Dynamics and Gap in Doped Spin-Ladders

5. Pressure Effect

Probing of spin fictuation from T_1 and neutron scattering experiments.

$\gamma\hbar I_z K H_o$

$$\mathcal{H} = -\gamma_n\hbar I_z \cdot H_o + A_{hf}\sum_l\{\underbrace{I_zS_l^z}_{\text{Knight shift}} + 1/2\overbrace{(I_+S(t)_l^- + I_-S(t)_l^+)}^{T_1}\} + H_e$$

the transition probability by the hyperfine interaction、W is given by

$\gamma_n\hbar(H_o+\Delta H)$

$$W(m \to m+1) = A^2\int_{\infty}^{\infty}\langle S_l(t)^+S_l(0)^-\rangle \exp(i\omega_o t)dt$$

$$W(m+1 \to m) = A^2\int_{\infty}^{\infty}\langle S_l(t)^-S_l(0)^+\rangle \exp(i\omega_o t)dt$$

$$\frac{1}{T_1} = W(m \to m+1) + W(m+1 \to m) = \frac{A^2}{2}\int_{\infty}^{\infty}\langle[S_l(t)^+S_l(0)^-]\rangle \exp(i\omega_o t)dt$$

Here、 $[AB] = (AB+BA)/2.$

$$\boxed{\frac{1}{T_1} = \frac{A^2}{2}\int_{\infty}^{\infty}\sum_q\langle[S_q(t)^+S_{-q}(0)^-]\rangle \exp(i\omega_o t)dt}$$

according to the fluctuation-dissipation theorem

$$\frac{1}{2}\int_{\infty}^{\infty}\sum_q\langle[S_q(t)^+S_{-q}(0)^-]\rangle \exp(i\omega t)dt = \frac{\hbar}{\pi}\frac{1}{1-\exp(-\hbar\omega/k_BT)}Im\chi\perp(q,\omega)$$

with $\omega_o \to 0$

$$\boxed{\frac{1}{T_1} = 2\gamma_n A^2 k_B T\sum_q\frac{Im\chi\perp(q,\omega_o)}{\omega_o}}$$

In comparison with the neutron scattering

$$\frac{d\sigma}{d\omega d\Omega} \sim \frac{1}{1-\exp(-\hbar\omega/k_BT)}Im\chi\perp(q,\omega)$$

For free electron model,

$$\chi_o(q, \omega + i\eta) = \sum_k \frac{f_k - f_{k+q}}{E_{k+q} - E_k - \hbar\omega + i\eta}$$

$q \to 0,\ \omega \to 0$

$$Im\chi_o(q,\omega) \sim \frac{\pi}{4} N(E_F) \frac{\hbar\omega}{q} \qquad \pi (f_k - f_{k+q}) \delta(E_{k+q} - E_k - \hbar\omega)$$

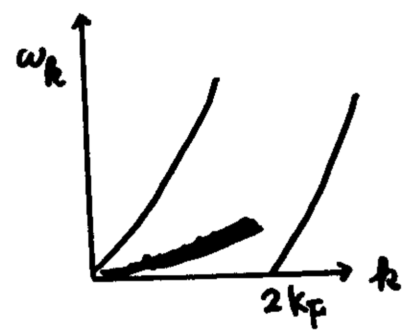
$$Re\chi_o(q,\omega) \sim \frac{\chi_{Pauli}}{2}(1 - q^2/12)$$

Paramagnetic Metal : $\sum_q Im\chi(q,\omega_o)/\omega_o \simeq$ **const.** $\longrightarrow T_1 T =$**const.**

Local moment system : $Im\chi(\omega_o)/\omega_o \simeq \frac{\chi_o(T)}{\Gamma} \sim 1/T \longrightarrow T_1 =$**const.**

Near the AF transition points or

for itinerant electron antiferromagnets



3D:

$$\frac{Im\chi(Q,\omega_O)}{\omega_O} \simeq \Gamma_Q(T)^{-\frac{1}{2}} \longrightarrow (T_1T)^{-1} \sim \frac{1}{\sqrt{\Gamma_Q(T)}}$$

2D:

$$\frac{Im\chi(Q,\omega_O)}{\omega_O} \simeq \Gamma_Q(T) \longrightarrow (T_1T)^{-1} \sim \frac{1}{\Gamma_Q(T)}$$

Nuclear Spin-Spin Relaxation Rate $\frac{1}{T_2}$

Indirect Nuclear Spin-Spin Interaction

$$\underline{H_{ij} = -I_i \hat{\Phi}(R_{ij}) I_j}$$

$$\hat{\Phi}(R_{ij}) = \int dr \int dr' A(R_i - r)\hat{\chi}(r - r')A(r' - R_j),$$

with $\hat{\chi}(r - r')$ being the susceptibility tensor of conduction electrons.

In case of $A(R_i - r) = A_s \delta(r_i - r_j)$,

$$\hat{\Phi}(R_{ij}) = \frac{1}{N}\sum_q A_s \hat{\chi}(q) A_s \exp(iq \cdot R_{ij}).$$

Spin Echo

Namely the spin-echo amplitude has the form of

$$M_\perp(2\tau) = M_\perp(0)\exp\left[-\frac{1}{2}\left(\frac{2\tau}{T_{2G}}\right)^2\right],$$

$$\begin{aligned}\left(\frac{1}{T_{2G}}\right)^2 &= \frac{1}{\hbar^2}\frac{3I(I+1)}{4}\sum_{i\neq j} \mid \Phi_{zz}(R_{ij}) \mid^2 \\ &= \underline{\frac{A_{zz}^4}{\hbar^2}\frac{3I(I+1)}{4}\left[\frac{1}{N}\sum_q \chi(q)^2 - \left(\frac{1}{N}\sum_q \chi(q)\right)^2\right]}\end{aligned}$$

For exmaple,

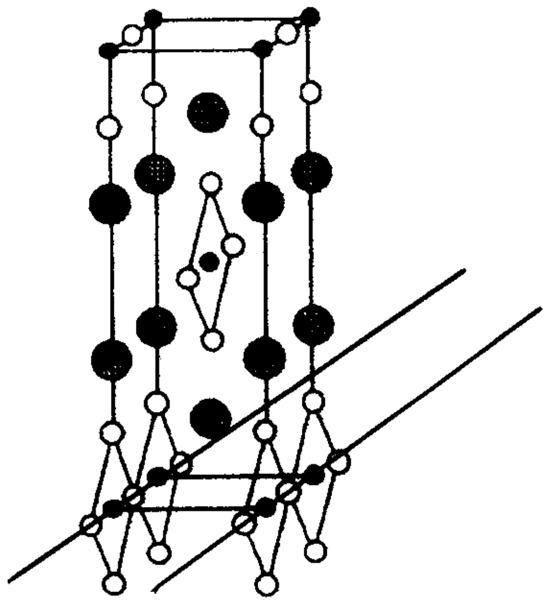
$$\chi(Q+q) = \frac{\chi(Q)}{1+q^2\xi^2},$$

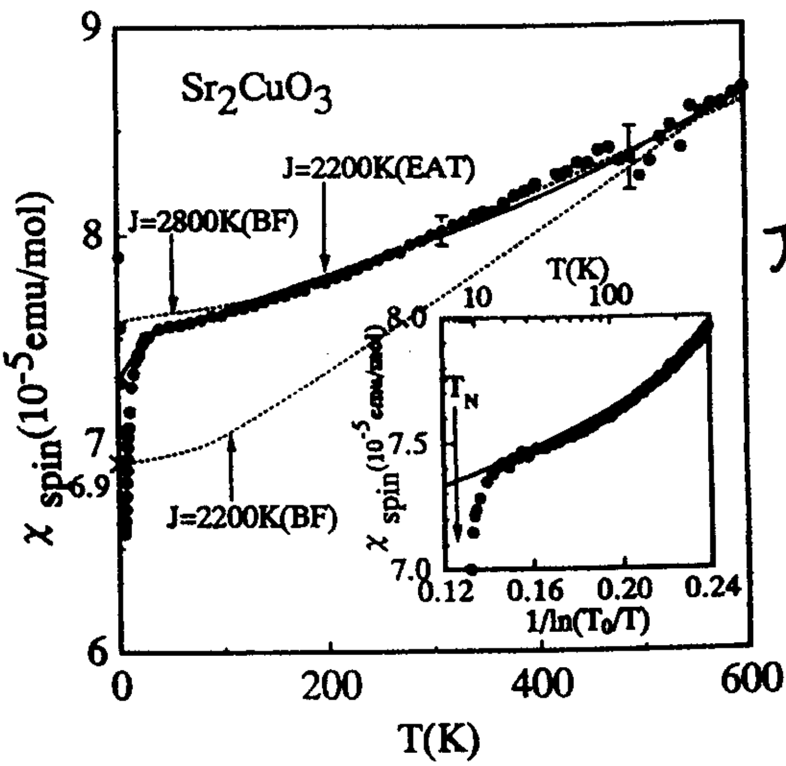
with the correlation length ξ.

$$\underline{\left(\frac{1}{T_2}\right)^2 \sim \int \{\frac{\chi(Q)}{1+q^2\xi^2}\}^2 dq \sim \frac{\chi(Q)^2}{\xi^3}.}$$

$S=1/2$ Antiferromagnetic Linear Chain System Sr_2CuO_3

Crystal Structure





$J_{\parallel} = 2200K$

Motoyama et al

Spin Dynamics in S=1/2 Antiferromagnetic Linear Chain System Sr_2CuO_3

Nuclear hyperfine Hamiltonian

$$H = \Sigma_{\alpha,i,j} A_{\alpha}^{ij} I_{i\alpha} S_{j\alpha} \qquad (\alpha = a, b, orc)$$

Nuclear spin-lattice rate, T_1

$$\frac{1}{T_1} = \frac{k_B T}{\hbar^2} \int \frac{dq}{2\pi} \left[A_x^2(q) + A_y^2(q)\right] \frac{Im\chi(q,\omega_n)}{\omega_n}$$

Nuclear spin-spin rate, T_{2G}

$$\left(\frac{1}{T_{2G}}\right)^2 = \frac{p}{8\hbar^2} \left[\int \frac{dq}{2\pi} A_z^4(q)\chi^2(q) - \left(\int \frac{dq}{2\pi} A_z^2(q)\chi(q)\right)^2\right]$$

Quatum-critical scaling (Schulz and Sachdev et al)

$$\chi(q,\omega) = \frac{1}{T}\tilde{\chi}\left(\frac{c(q-\pi)}{T}, \frac{\hbar\omega}{T}\right)$$

where $c = \pi J/2$.

$$\frac{1}{T_1} = \left[A_x^2(q) + A_y^2(q)\right] \frac{D}{\hbar J}$$

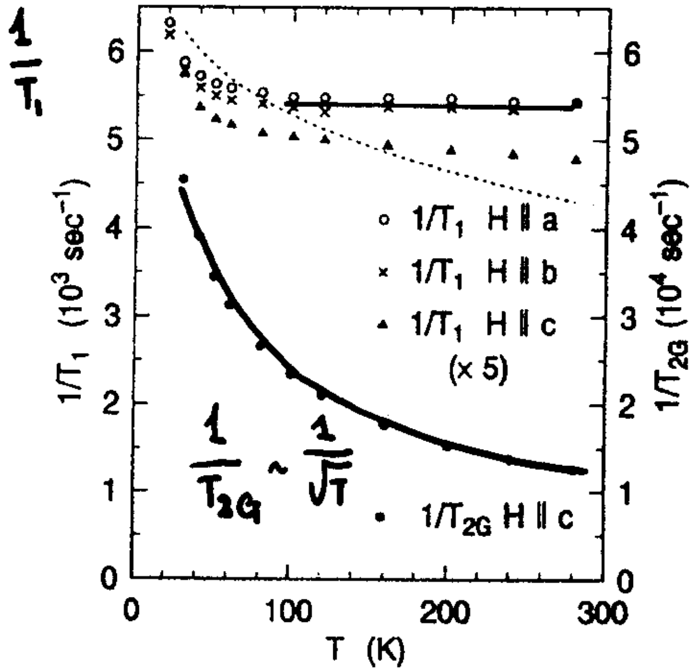
$$\frac{1}{T_{2G}} = \frac{A_z^2(\pi) D I}{4\hbar} \sqrt{\frac{p}{\pi k_B T J}} \propto \sqrt{\xi(T)}$$

Experimental Scaling

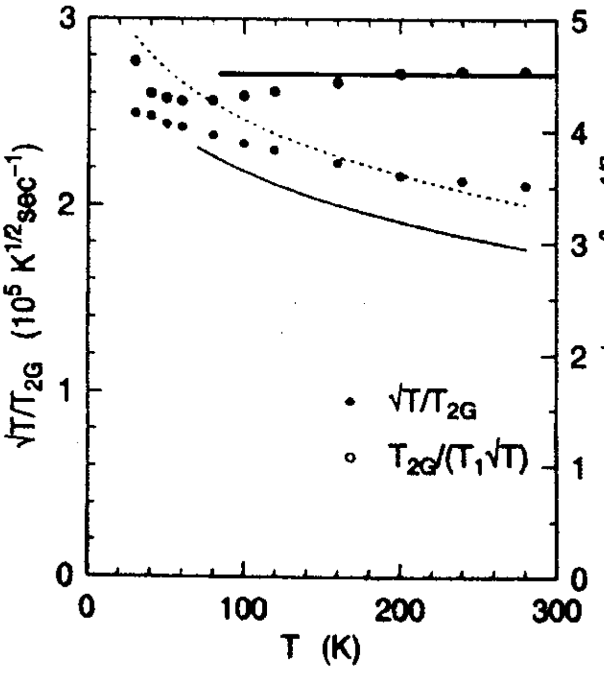
$$\frac{T_{2G}}{T_1\sqrt{T}} = \frac{A_x^2(\pi) + A_y^2(\pi)}{A_z^2(\pi)} \frac{4}{I} \sqrt{\frac{\pi k_B}{pJ}}$$

Comparison with experiment

Temperature dependence of $1/T_1$ and $1/T_{2G}$



Scaling with J=2200 K

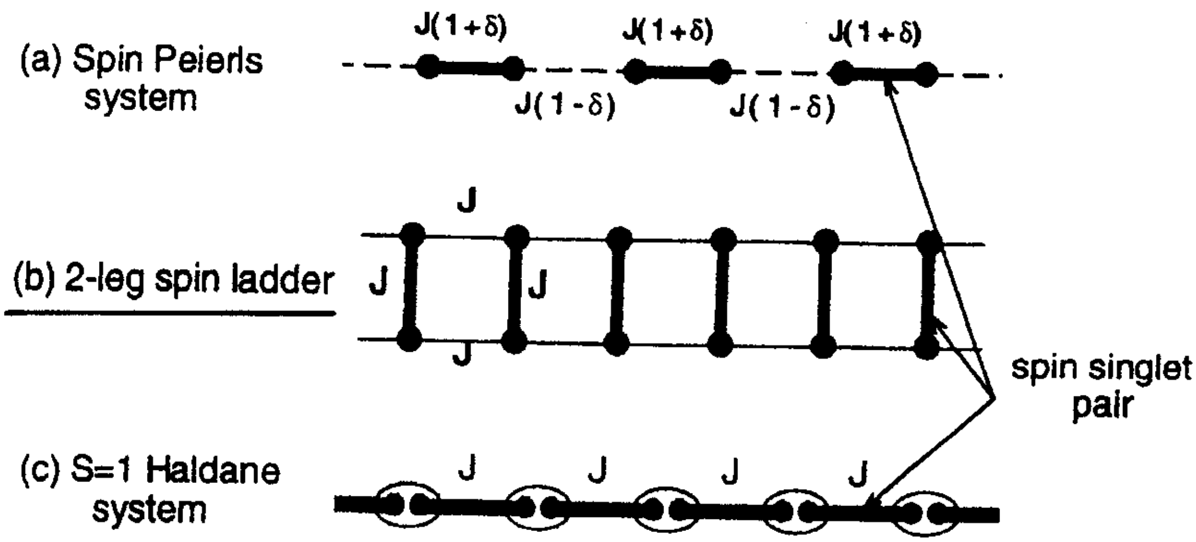


J = 2200K

$$\frac{T_{2G}}{T_1\sqrt{T}}$$

Takigawa et al

Spin Gap in Quatum Spin Systetm



Magnon Dispersion

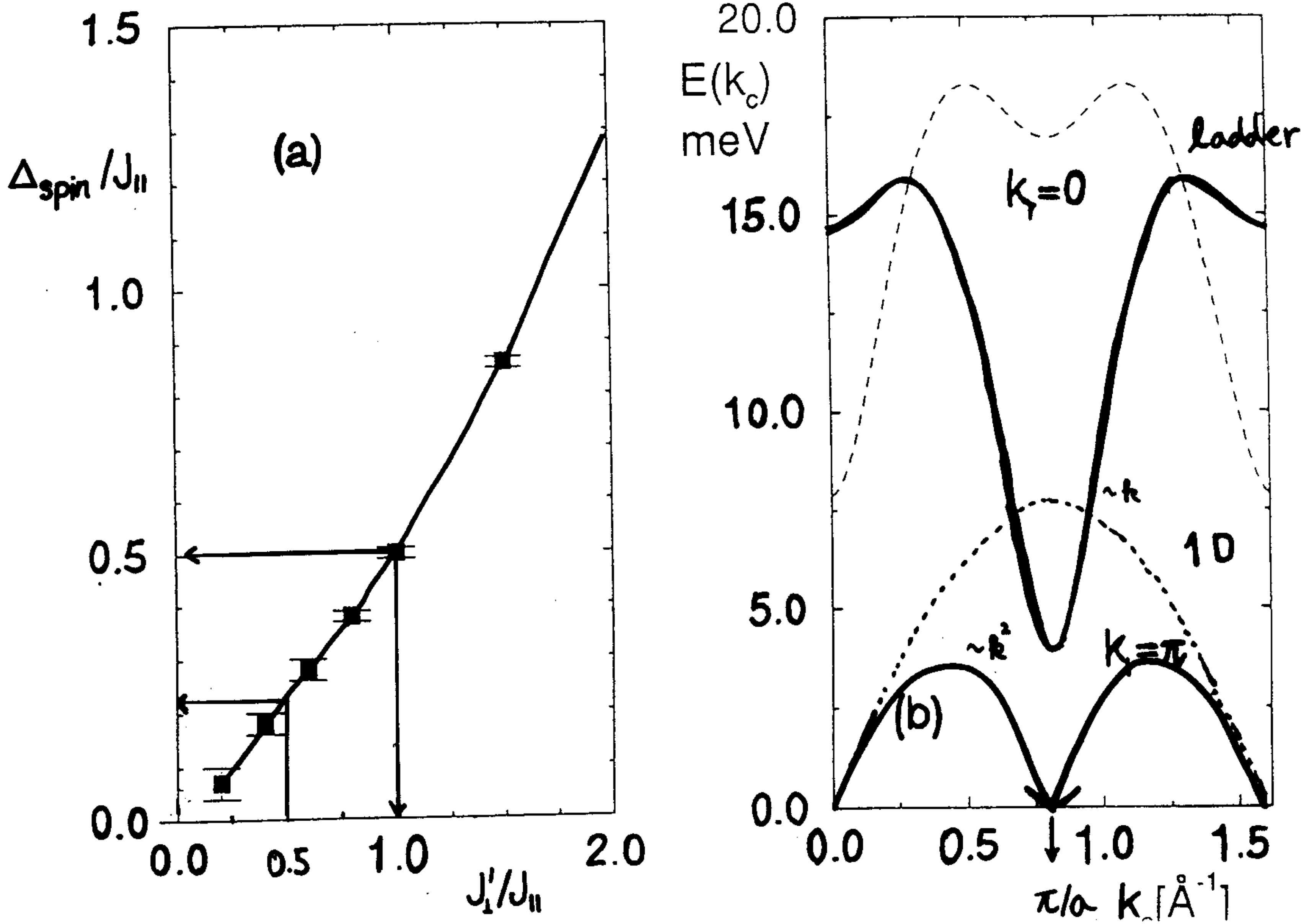
$$\varepsilon = \sqrt{c^2(k-\pi)^2 + \Delta^2}$$

Susceptibility

$$\chi_{spin} = \frac{2(g\mu_B)^2}{c\sqrt{2\pi}}\sqrt{(\Delta/T)}\exp\left(-\Delta/T\right)$$

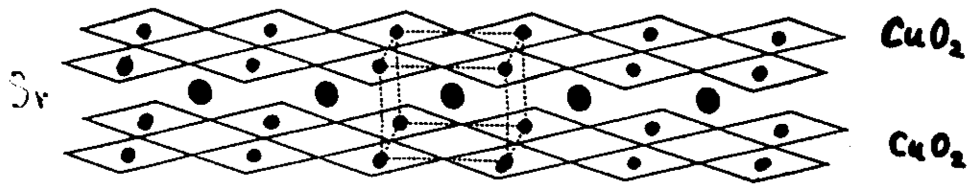
Nuclear Spin-Lattice Relaxation Rate, $1/T_1$

$$\begin{aligned}\frac{1}{T_1} &= \frac{A^2(0)}{2\hbar^2}\frac{2\Delta}{\pi c^2}K_0(\omega_n/2T)\exp\left(-\Delta/T\right) \\ &\simeq \frac{A^2(0)}{2\hbar^2}\frac{2\Delta}{\pi c^2}\left\{0.809 - \ln\left(g\mu_B H/T\right)\right\}\exp\left(-\Delta/T\right)\end{aligned}$$



Dagotto et al.

$Sr_{n-1}Cu_{n+1}O_{2n}$ Hiroi, Azuma, Takano

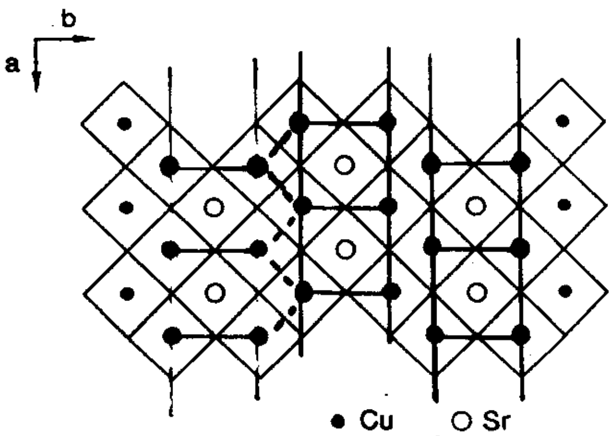


infinite layer $SrCuO_2$ (2D Heisenberg)

electron-doping hole-doping

$La_{1-x}Sr_xCuO_2$ $Sr_{1-x}CuO_2$: superconductivity

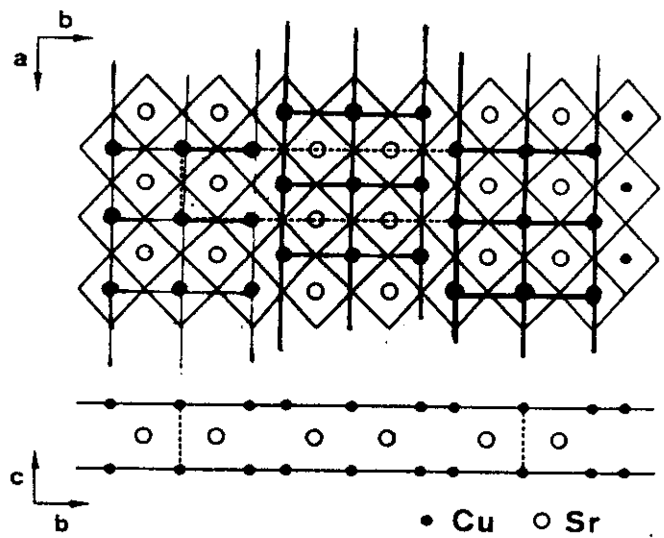
$n=3$ $n=5$



$\boxed{SrCu_2O_3}$

spin liquid

with spin gap



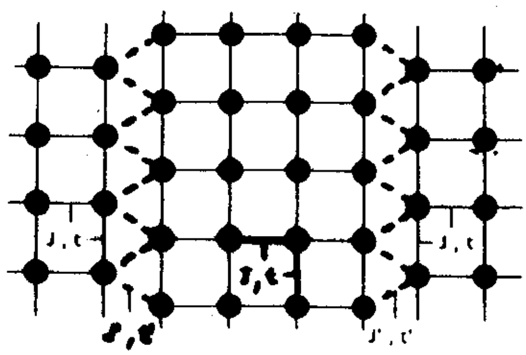
$\boxed{Sr_2Cu_3O_5}$

gapless spin liquid

$$\Delta = \frac{J}{2}$$

$$\sim J_\perp - \frac{J_{\parallel}}{2}$$

$$\frac{\xi}{a} \sim 3$$



$$\Delta \sim \frac{J}{4}$$

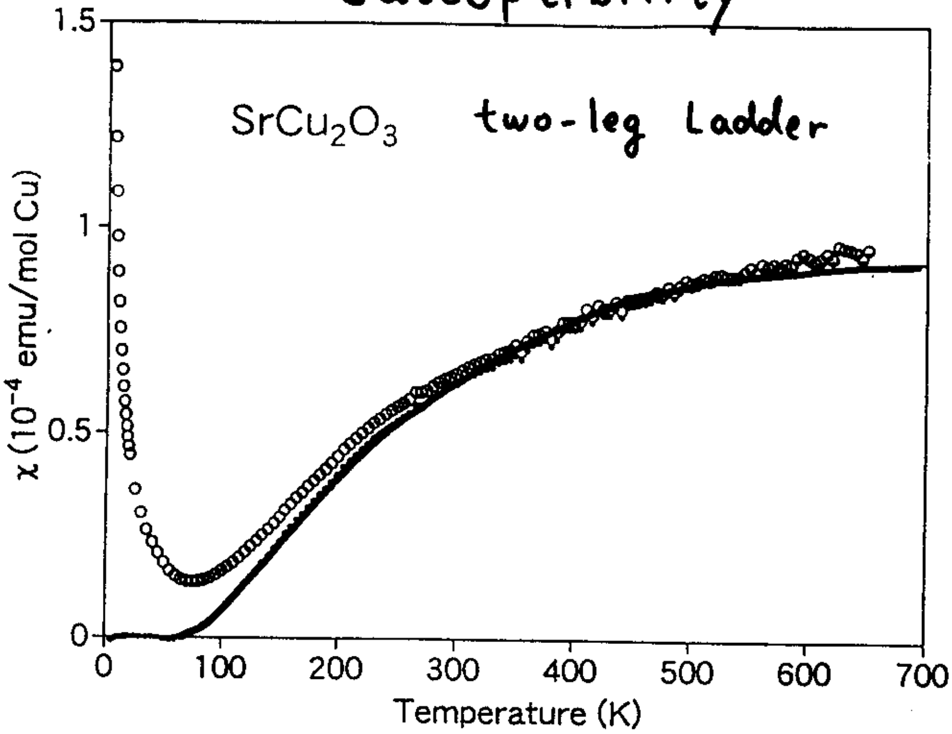
$$\frac{\xi}{a} \sim 5\sim6$$

Ladder t-J model

Imad, etal, Dagotto et al, White, Rice, et al.

帯磁率

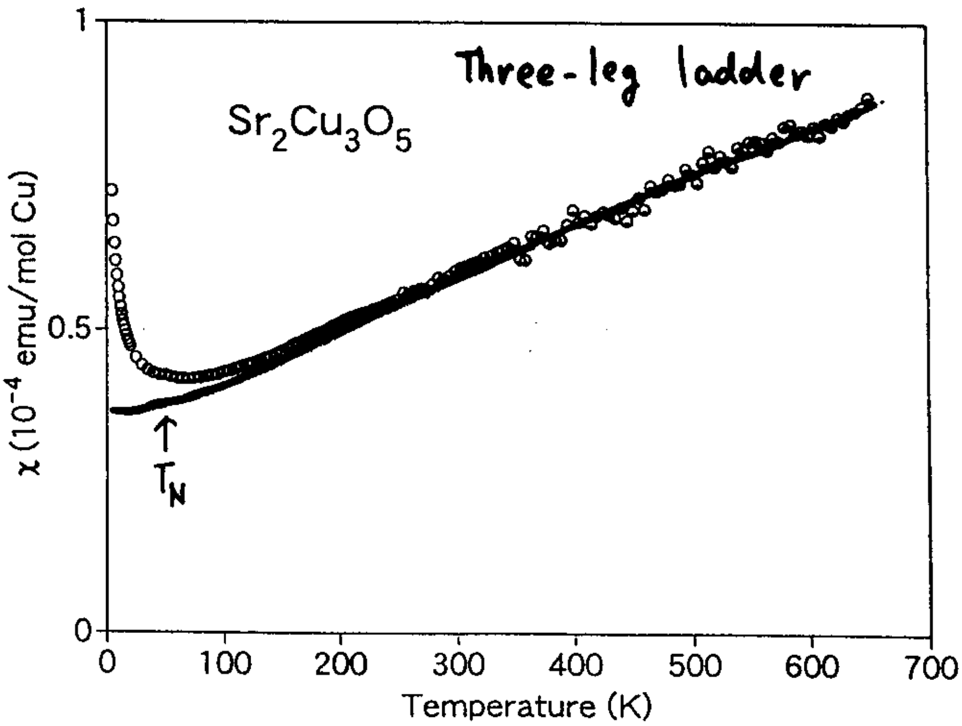
Susceptibility



$\Delta \simeq 420\,\mathrm{K}$

Spin-Gap behavior

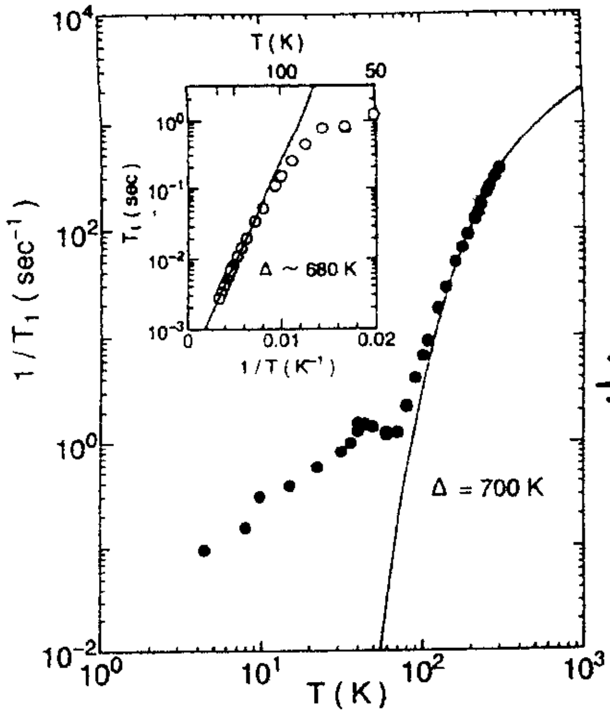
$$\chi(T) = \chi_s(T) + \frac{C}{T} \qquad \chi_s \propto \frac{1}{\sqrt{T}} \exp\left(-\frac{\Delta}{k_B T}\right)$$



Gapless

Azuma et al.

Nuclear Spin-Lattice Relaxation Rate, $1/T_1$



$$\frac{1}{T_1} \sim e^{-\frac{\Delta}{T}}\left(0.809 - \ln\frac{\omega_0}{T}\right)$$

Troyer et al

$$\Delta_{T_1} = 700K \;>\; \Delta_{K,\chi} = 420K$$

(1) massive Majonara fermion excitation with $m = \Delta_{K,\chi}$=440 K (Kishine and Fukuyama)

$$\Delta_{T_1} = \sqrt{3}\Delta_{K,\chi} \propto 700K$$

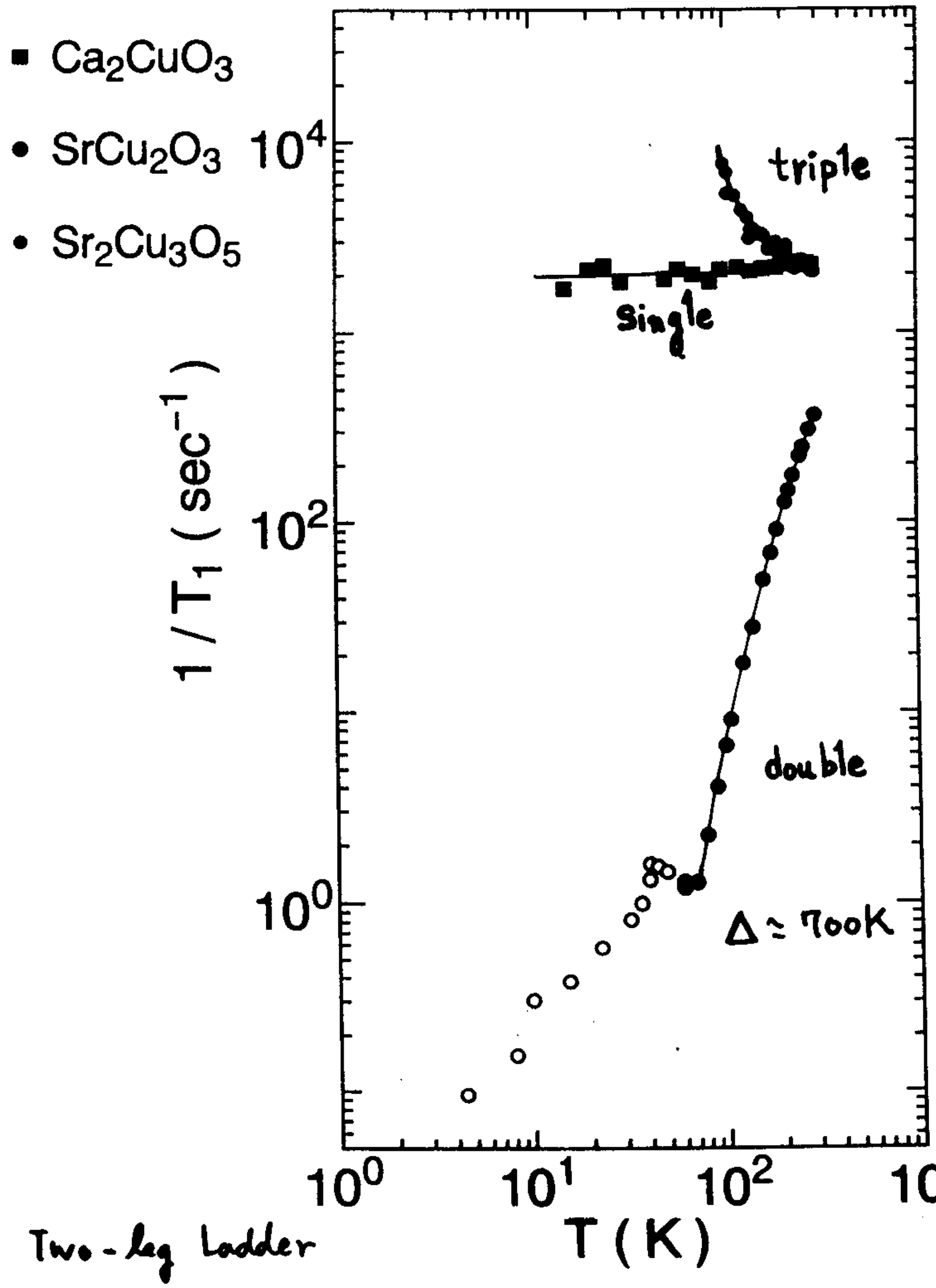
(2) 1D, gapped quantum $O(3)$ non-linear σ-model (Sachdev and Damle)

$$\frac{1}{T_1} \sim \frac{T\chi_s(T)}{\sqrt{2D_sH}} \sim \sqrt{3T/\pi H}\exp\left(-3\Delta/2T\right)$$

$$D_s = \frac{c^2\exp\left(\Delta/T\right)}{\Delta(1 + 2\cosh(H/T))}$$

$$\Delta_{T_1} = 1.5\Delta_{K,\chi} \propto 600K$$

Ishida et al



Sr_2CuO_3

Takigawa et al

Sachdev

Imada

Dagotto

Rice

$$\frac{1}{T_1} \approx \frac{1}{c^2} e^{-\frac{3\Delta}{2T}} \sqrt{\frac{3T}{\pi H}}$$

For Two-leg Ladder

$$\frac{1}{T_1} = \frac{3A_\perp^2(0)}{16a\pi^2} \exp(-\Delta/k_B T)\left[0.80908 - \ln(\omega_0/T)\right]$$

$$\frac{\Delta_{T_1}}{\Delta_\chi} = 1.5$$

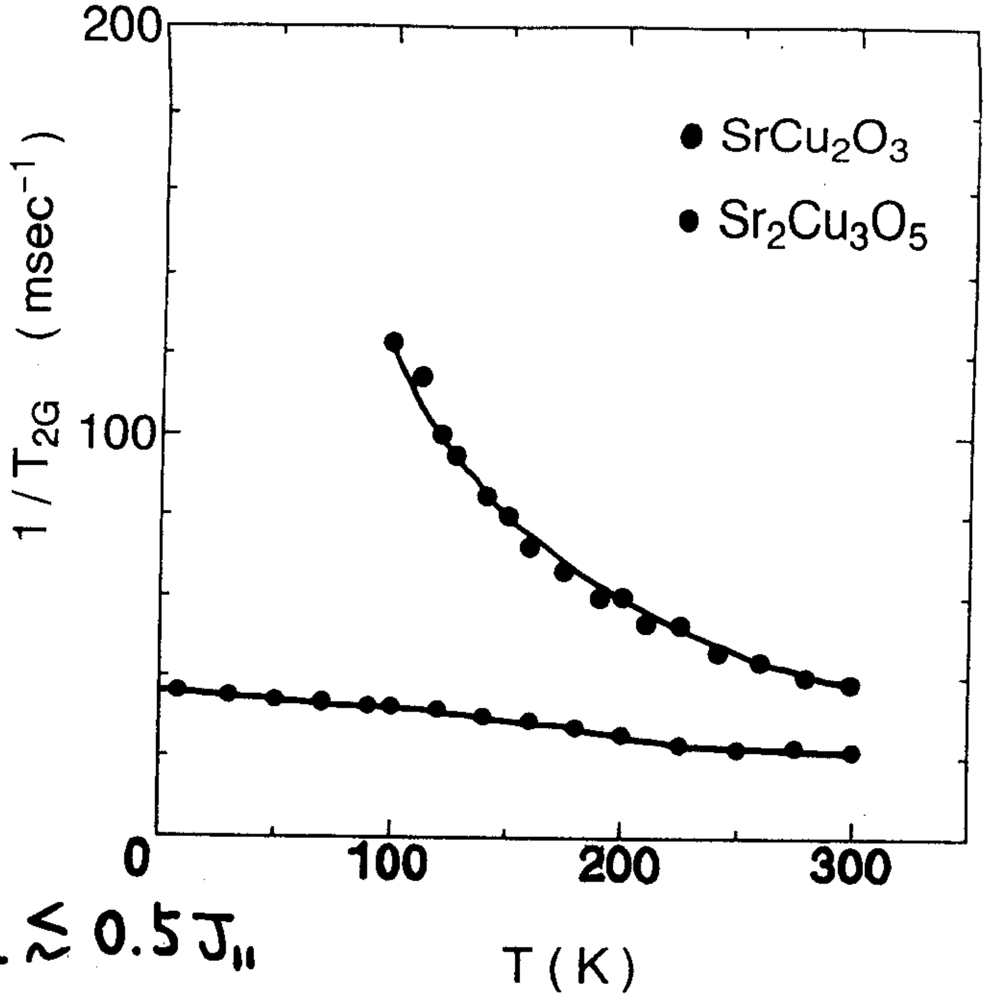
(Sachdev)

" $= 1.73$

(Kishine et al

ξ in $SrCu_2O_3$ ① $J_{\parallel} \sim 8$[illegible]K $\xi \sim 3.3a$

orrelation Length ② $J_{\parallel} \sim 2000K$ $\xi \sim 6 \sim 7a$



① Sandvik et al

② Johnston

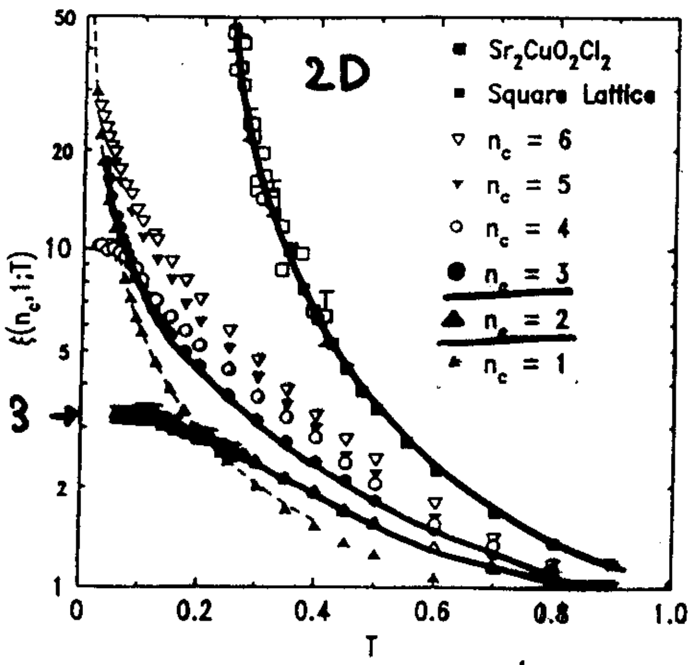
$\frac{1}{T_{2G}} \sim \sqrt{\xi}$

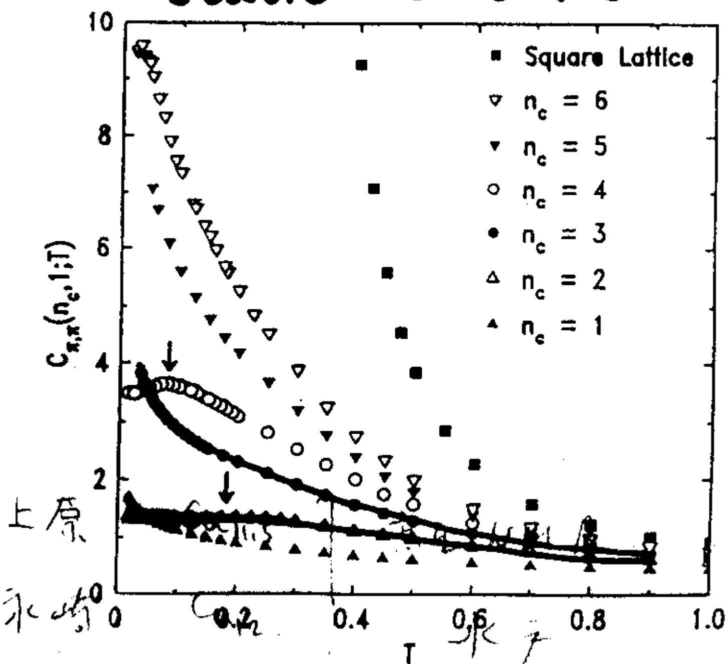
$J_{\perp} \lesssim 0.5 J_{\parallel}$

$\xi = \frac{\pi}{2}(J_{\parallel}/\Delta_{gap})$ $\Delta_{gap} \simeq 0.41 J_{\perp}$

ξ

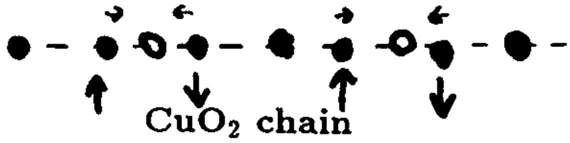
Static Structure

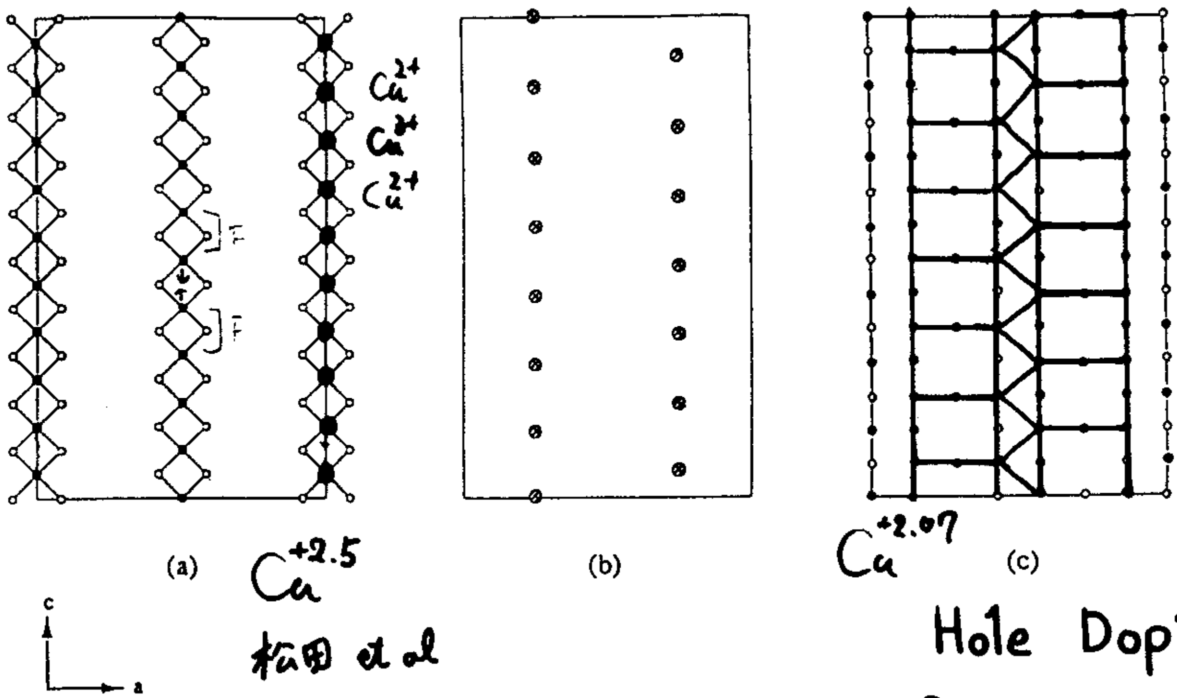




M. Greven et al.

$SrCu_2O_3$





(a) $Cu^{+2.5}$ (b) $Cu^{+2.07}$ (c)

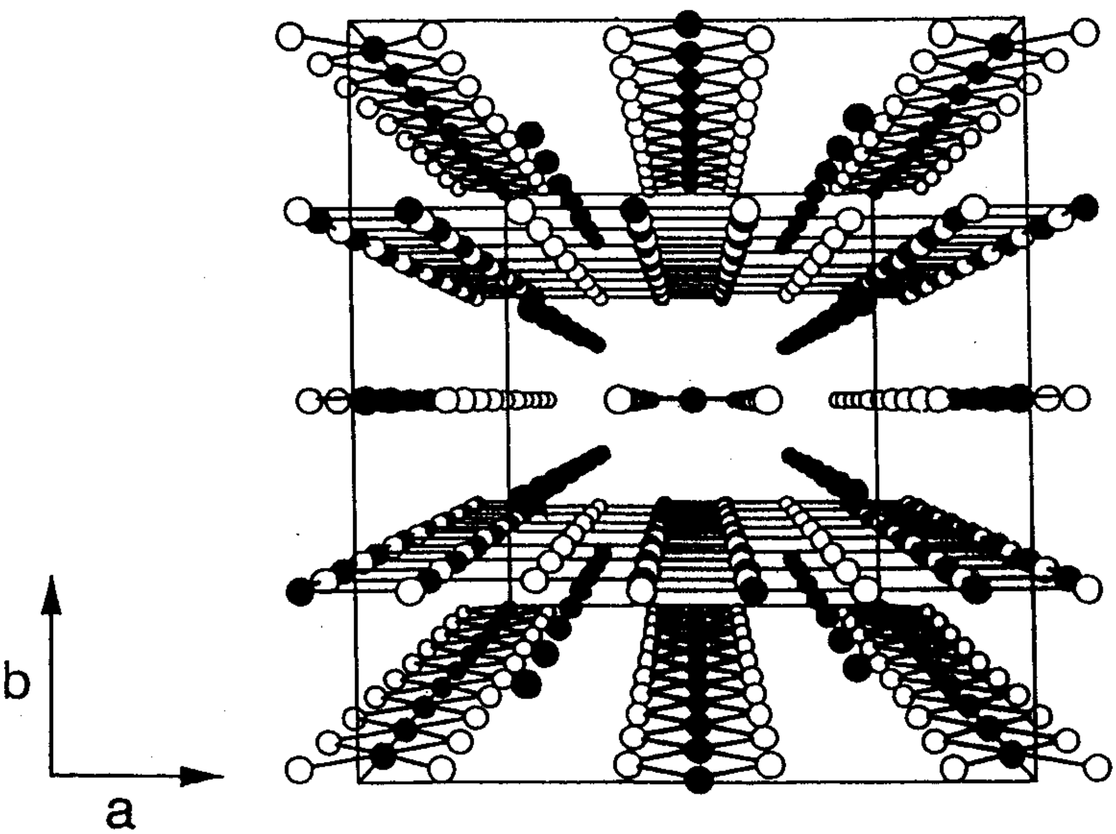
松田 et al

Hole Doping

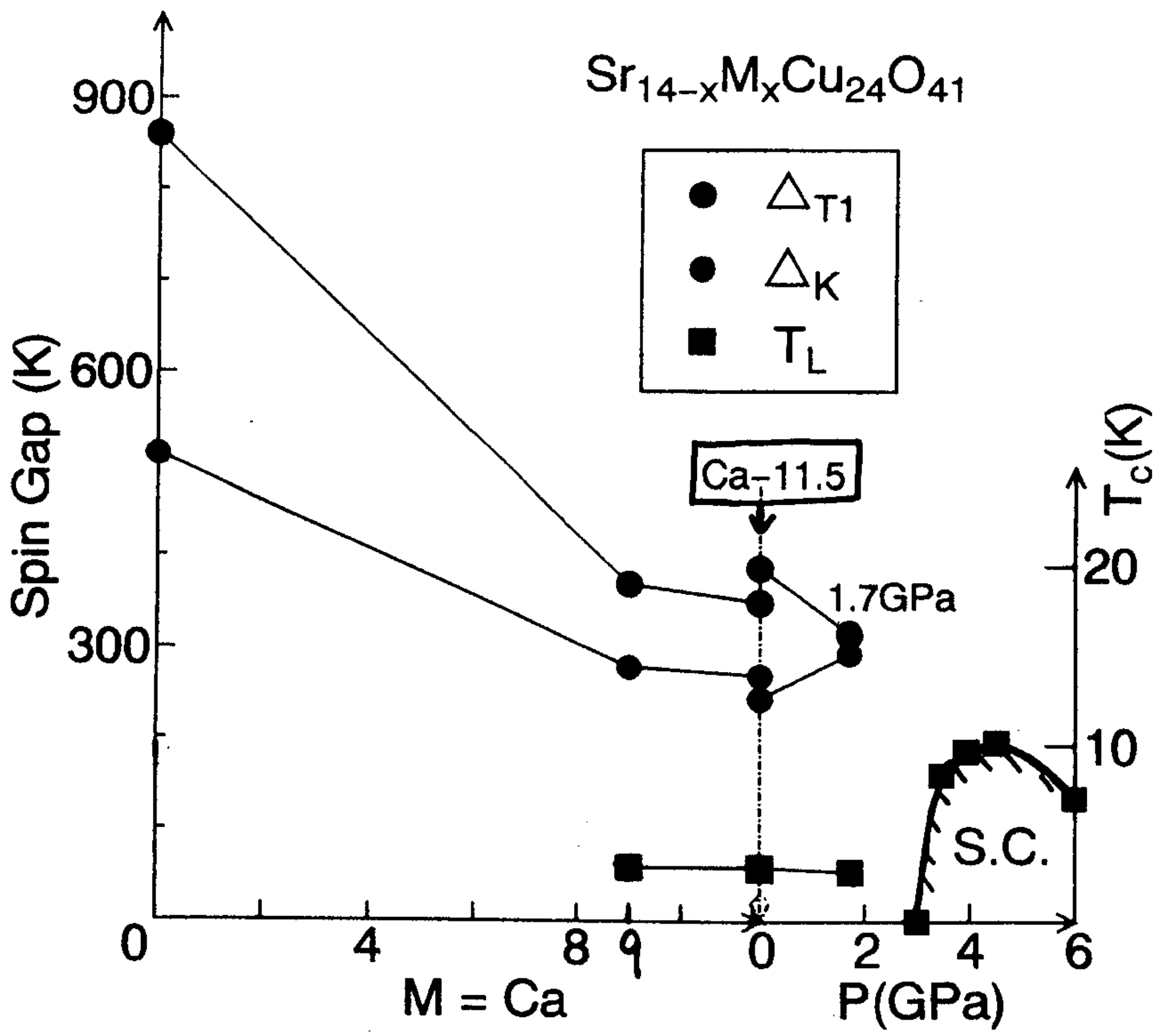
$Sr_{14} \rightarrow Cu^{+2.25}$

$Sr_{14.74} \rightarrow Cu^{+2.11}$

$\boxed{Sr_{14}Cu_{24}O_{41}}$

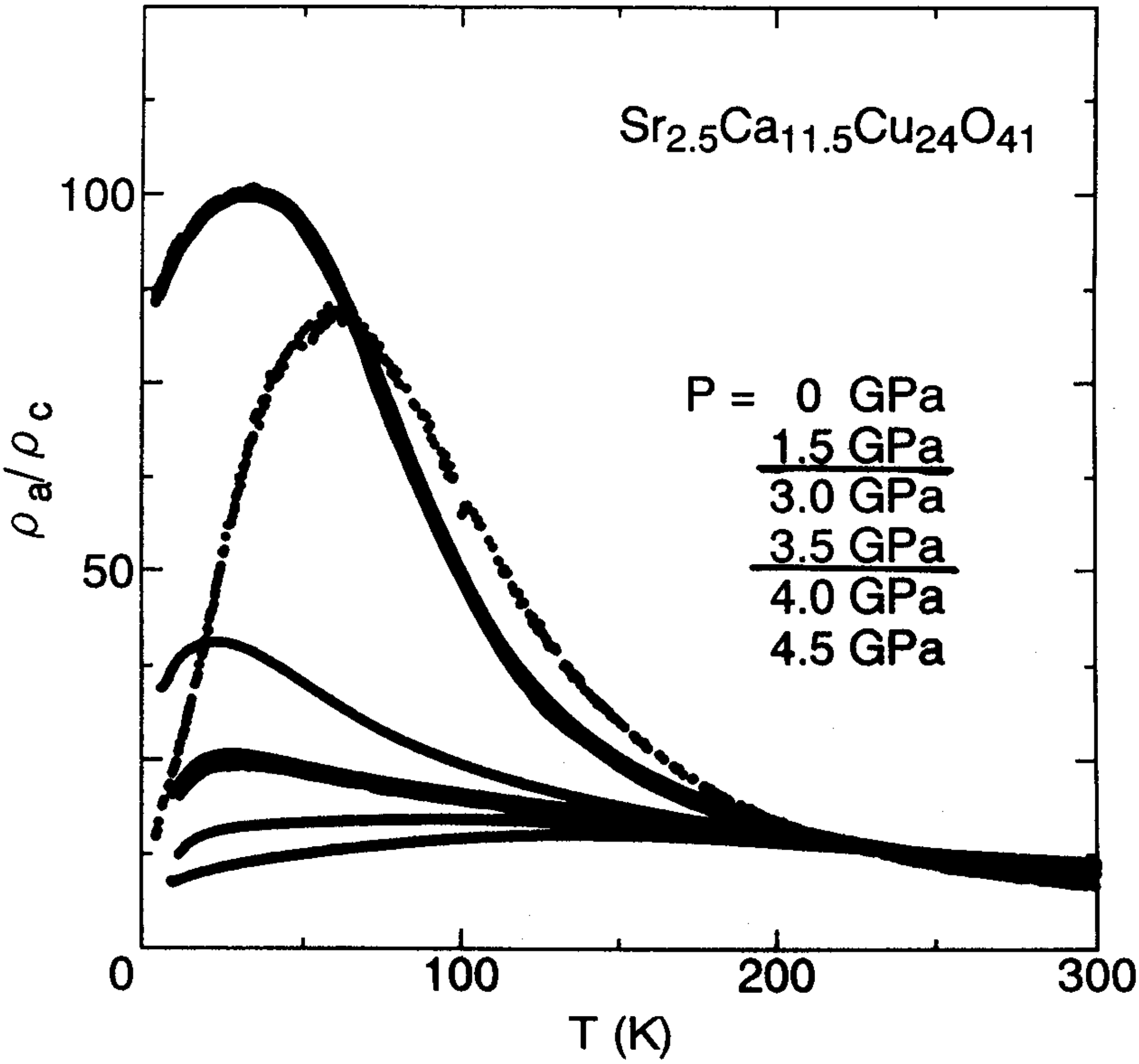


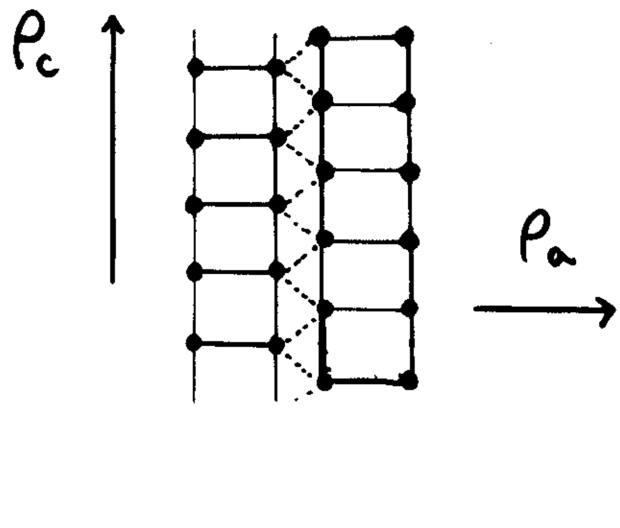
Spin Gap and Phase Diagram in $Sr_{14-x}Ca_xCu_{24}O_{41}$



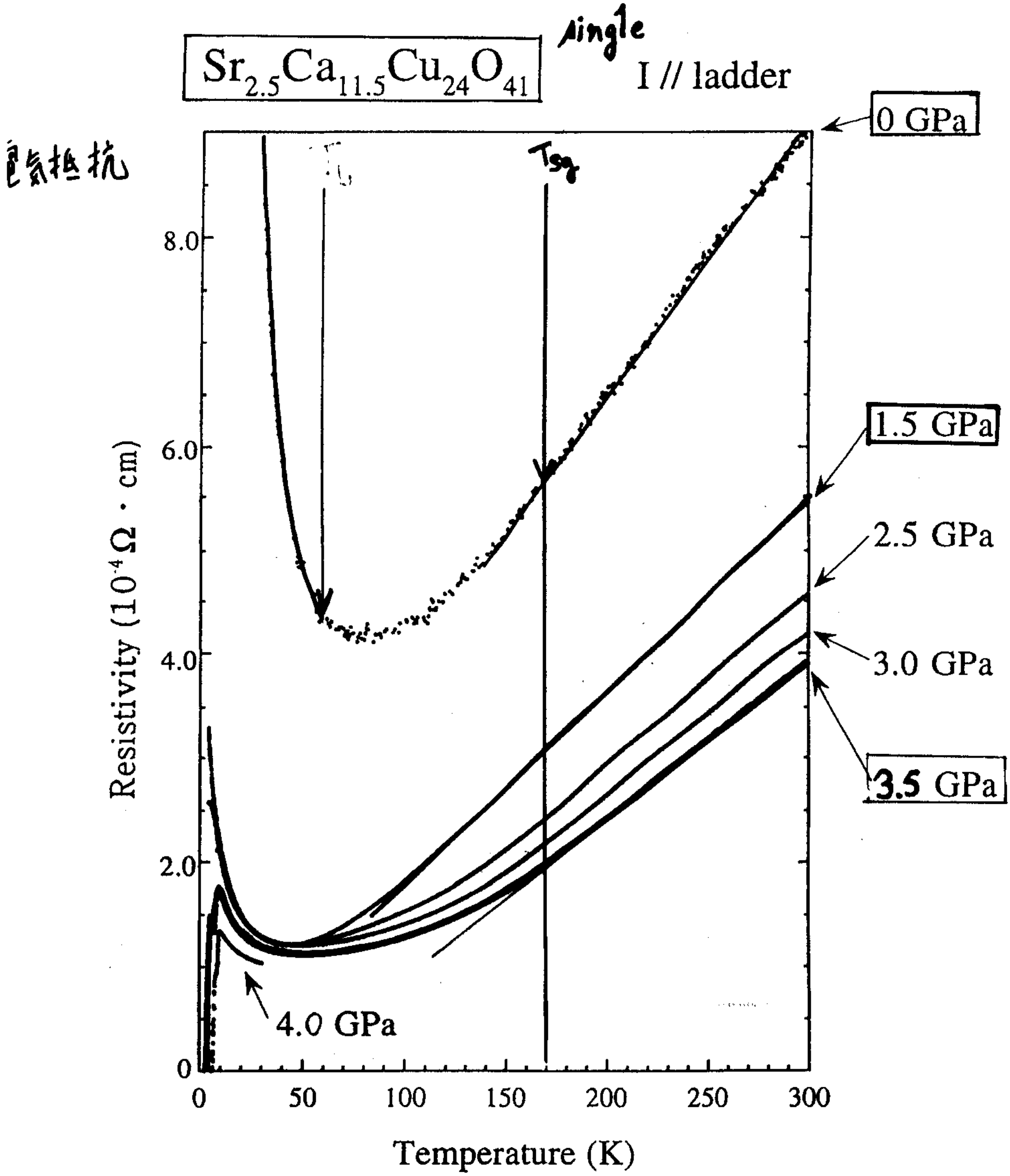
Anisotropy of Resistivity

電気抵抗の異方性 圧力変化





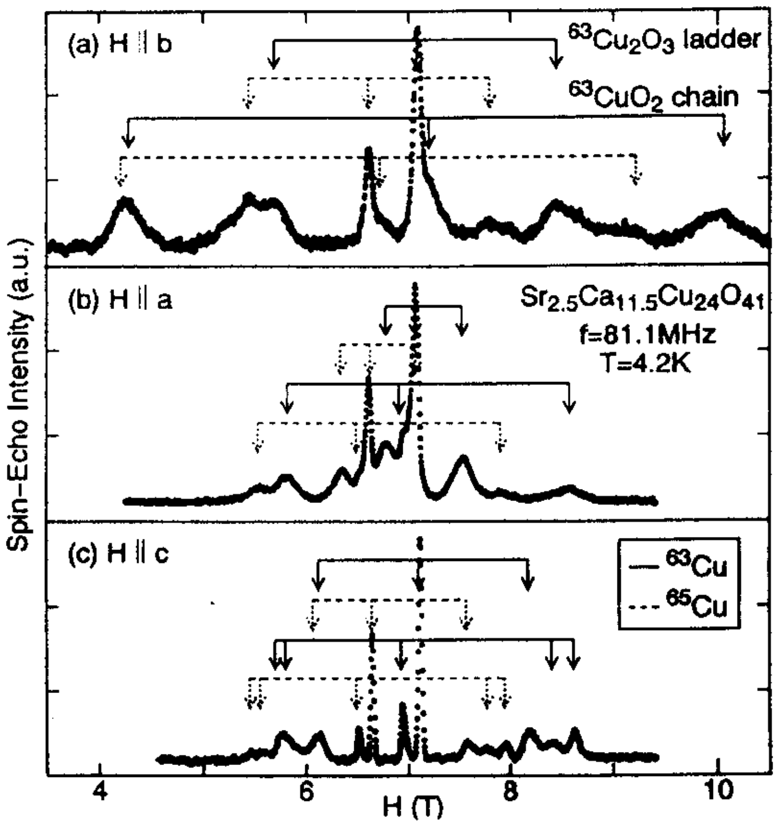
Pressure Dependence of Resistivity

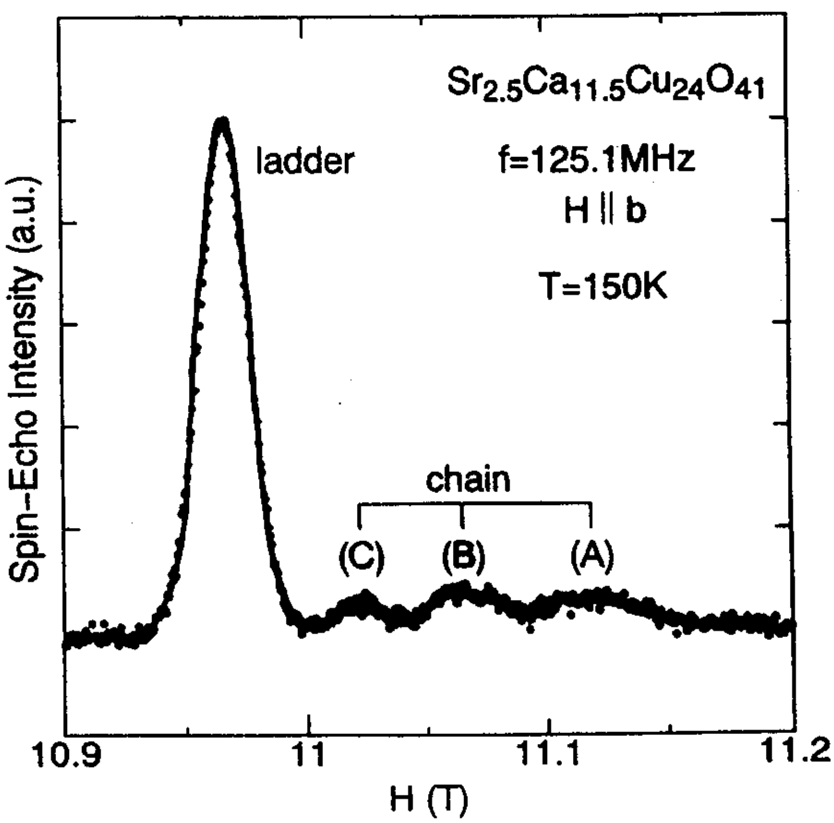


Uehara , Akimitsu

Takahashi Mori

NMR Spectra of Single Crystal $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$



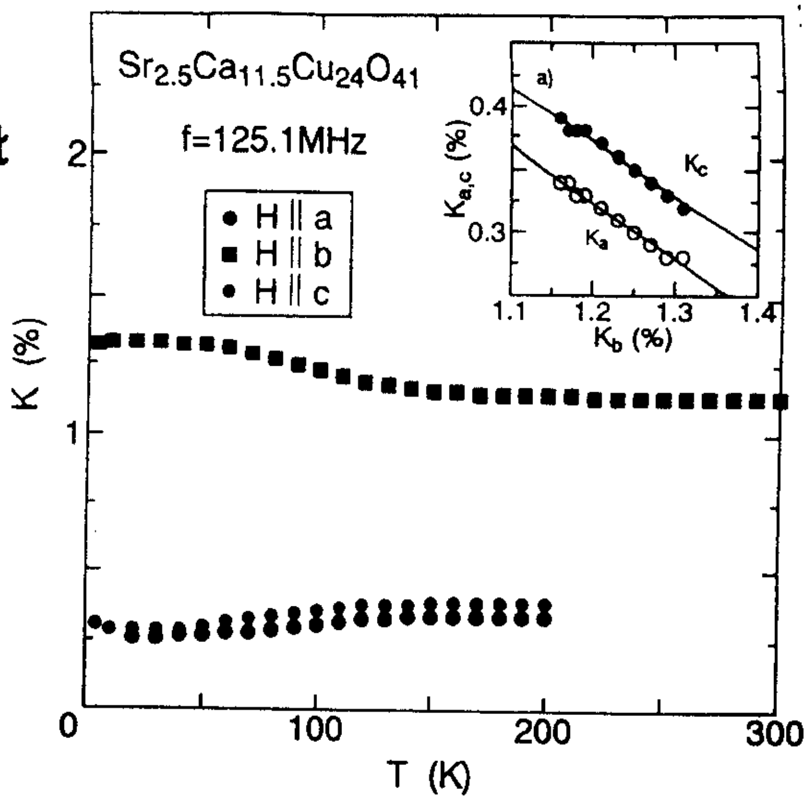


NMR shift of Cu_2O_3 ladder in $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$

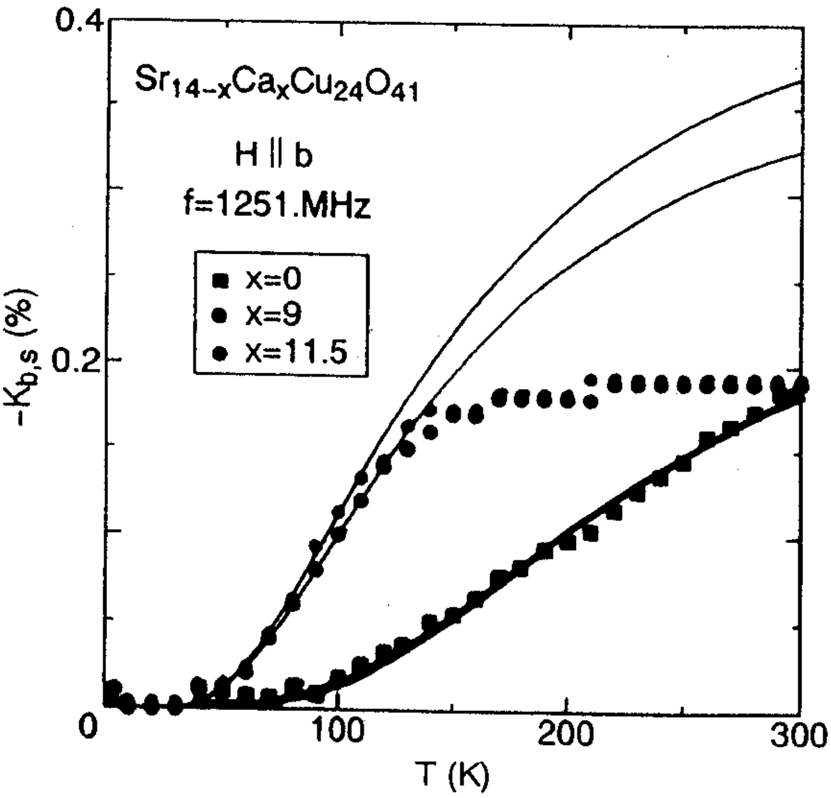
NMR shift

K_{obs}

$K_{obs} = K_s(T) + K_{orb}$



K_s



$\Delta \sim 510K$

$*$ 1D S=1/2 Heisenberg model (Sachdev *et al.*)

$\cdot \; T \ll J$

$$\left(\frac{1}{T_1}\right)_z = [A_x(\pi)^2 + A_y(\pi)^2]\frac{D}{\hbar J} \qquad = const.$$

exp.

$$\frac{1}{T_{2G}} = \frac{A_z(\pi)^2 DI}{4\hbar}\sqrt{\frac{p}{\pi k_B T J}} \qquad \propto \frac{1}{\sqrt{T}} \longrightarrow T_{2G}^2 \propto T$$

$$(\; I \simeq 8.4425, \; D \simeq 0.15, \; p = 0.69 \;)$$

$$\boxed{\left(\frac{T_{2G}}{T_1\sqrt{T}}\right)_z} = \frac{A_x(\pi)^2 + A_y(\pi)^2}{A_z(\pi)^2}\frac{4}{I}\sqrt{\frac{\pi k_B}{pJ}} \qquad \propto \frac{1}{\sqrt{J_\parallel}}$$

$$= 6.2 \times 10^{-3} K^{-1/2} \qquad \text{(for Ca11.5)}$$

$$= 4.4 \times 10^{-3} K^{-1/2} \qquad \text{(for } Sr_2CuO_3\text{)}$$

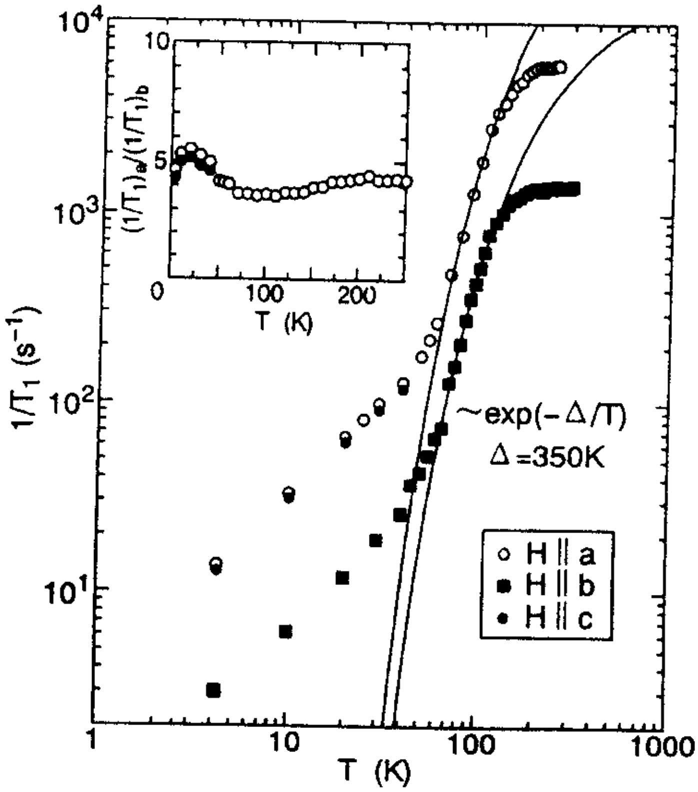
$$\begin{aligned}
\frac{A_x(\pi)^2 + A_y(\pi)^2}{A_z(\pi)^2} &= \frac{2(1/T_1)_z}{(1/T_1)_x + (1/T_1)_y - (1/T_1)_z} \\
&\simeq \frac{2(1/T_1)_\parallel}{2(1/T_1)_\perp - (1/T_1)_\parallel} \\
&= \frac{2}{2R_{q\sim\pi} - 1} \\
&= 0.263 \qquad \text{(for Ca11.5)} \\
&= 0.203 \qquad \text{(for } \underline{Sr_2CuO_3\text{)} \longrightarrow J_\parallel \simeq 2200K}
\end{aligned}$$

$\longrightarrow$ $\underline{J_\parallel \simeq 1700 \text{ K for Ca11.5}}$

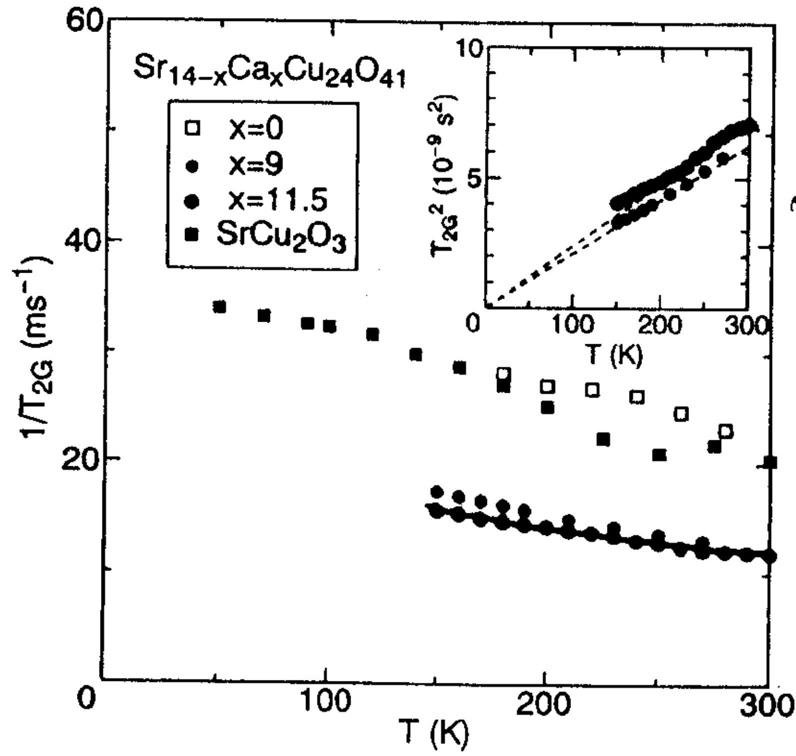
Takigawa et al

Spin Dynamics and Correlation in Hole-Doped $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$

$\frac{1}{T_1}$



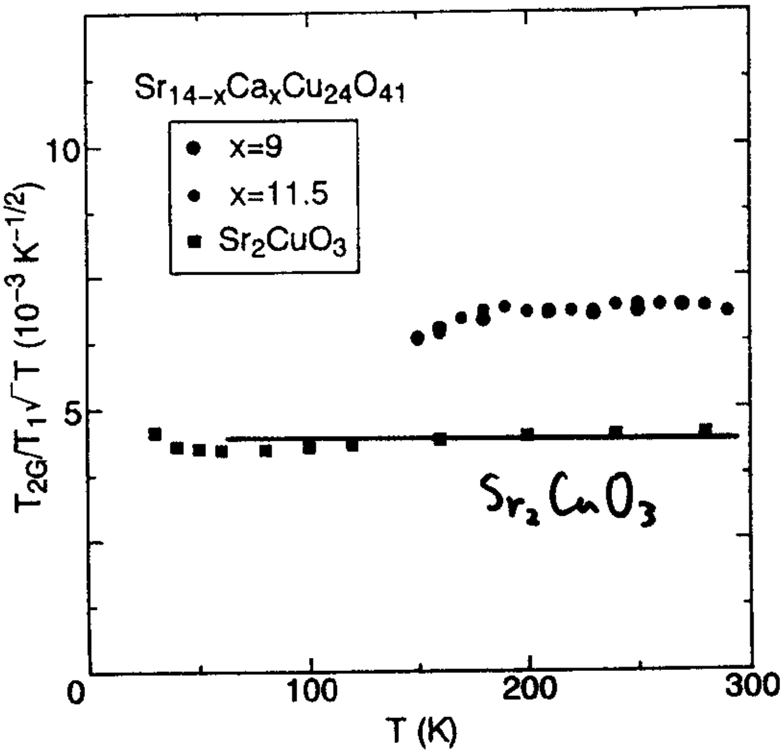
$\frac{1}{T_{2G}}$



$\sim \frac{1}{\xi(T)}$

1D like Spin Dynamics in Hole-Doped $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$

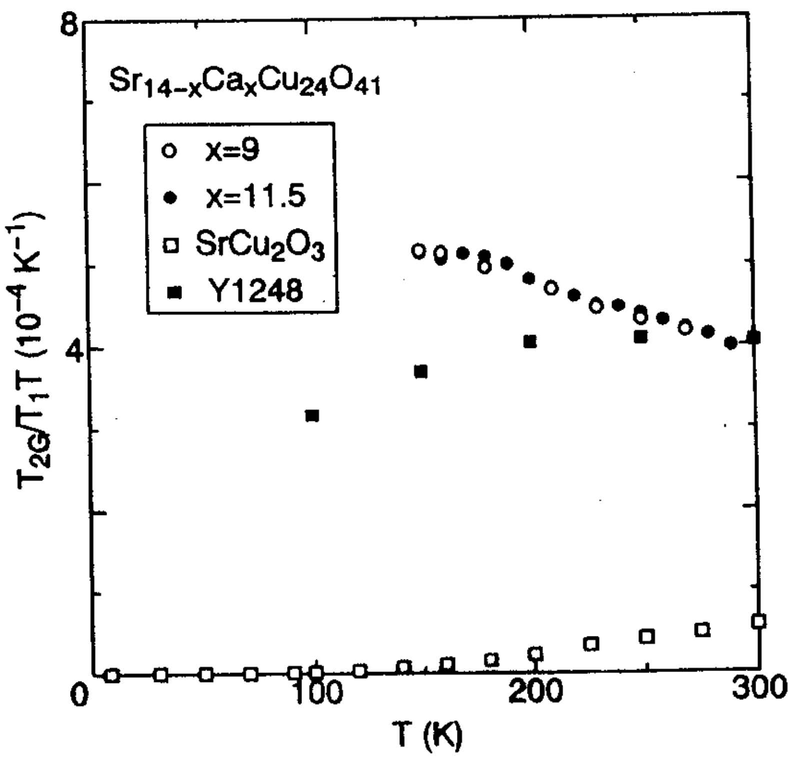
$\frac{T_{2G}}{T_1\sqrt{T}}$



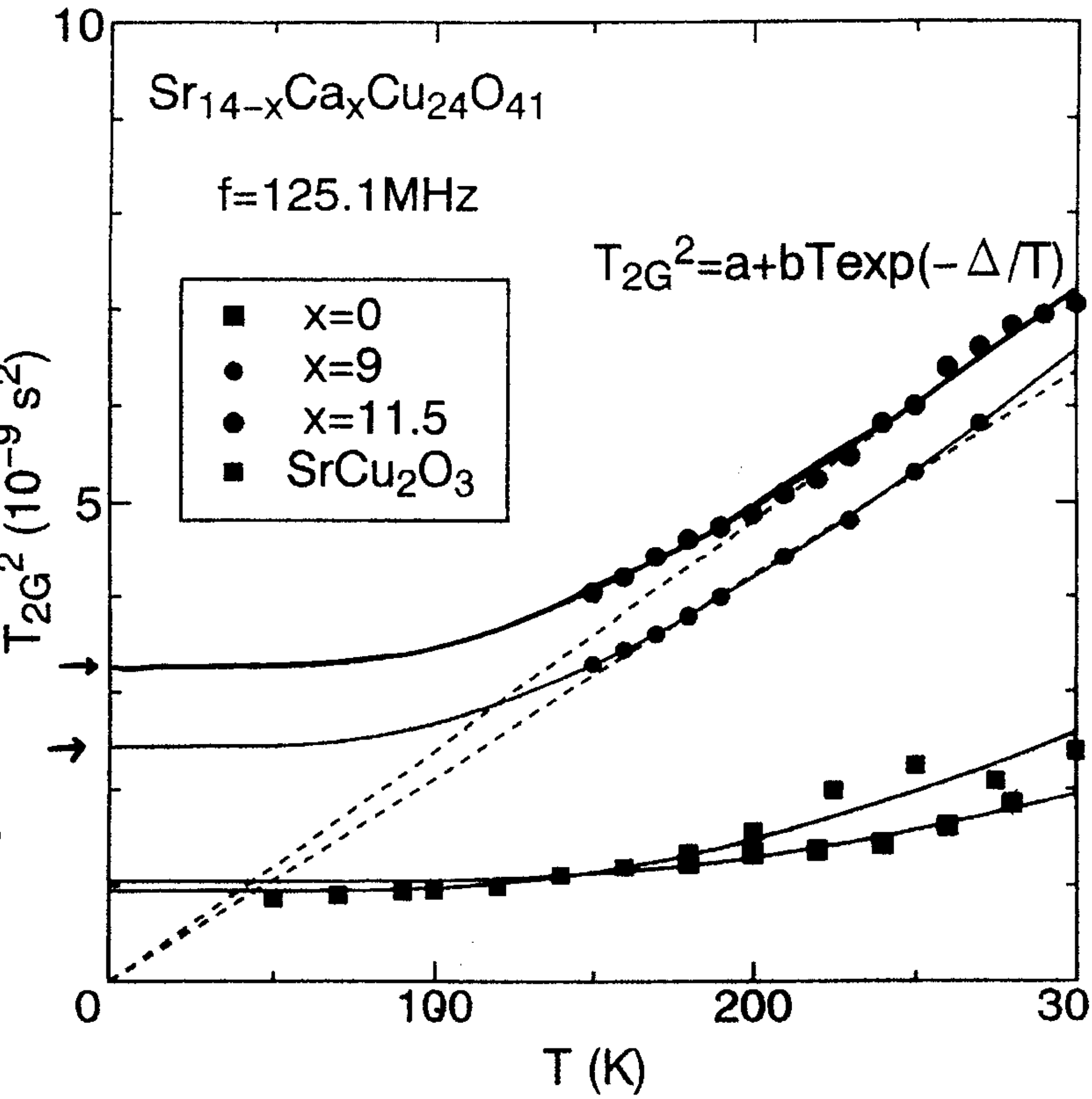
$J_\parallel = 1700K$

$J_\parallel = 2200K$

$\frac{T_{2G}}{T_1 T}$



Temperature Dependence of $\xi(T)$



$a \sim \frac{1}{\xi_0}$

Correlation Length $\xi(T)$ in Spin-Ladders

$$\frac{1}{\xi(T)_{ladder}} = \frac{1}{\xi_0} + \frac{1}{\xi_{1D}(T)} \exp\left(-\Delta/T\right)$$

$$\frac{1}{\xi_0} = \frac{\Delta}{c_{1D}} \qquad c_{1D} = \pi/2J_{\parallel}$$

$$\frac{1}{\xi_{1D}(T)} = T[2 - b^{-1}(1 - 0.486 b^{-1}\ln(b))]$$

$Sr_{14}Cu_{24}O_{41}$ (Δ_K=510 K, $J_{\parallel}$ ~1700 K)

$$\xi_0 \sim 5.2 \quad \text{with} \quad J_{\perp}/J_{\parallel} \sim 0.7$$

Hole-Doped Ca11.5 (Δ_K=270 K, $J_{\parallel}$ ~1700 K)

$$\xi_0 \sim 10 \quad \text{with} \quad J_{\perp}/J_{\parallel} \sim 0.4$$

Scaling between $\xi(T)$ and Gaussian Spin-Echo Decay Rate, $1/T_{2G}(T)$ (Sandvik et al)

$$T_{2G}^2(T) = \alpha + \frac{\beta}{\xi(T)}$$

$$T_{2G}^2(T) = a + bT\exp\left(-\Delta/T\right)$$

Correlation Length ξ_h in Hole-Doped Spin-Ladders

$$\frac{1}{\xi_h(T)} = \frac{1}{\xi_h(0)} + \frac{1}{\xi_{ladder}(T)}$$

Hole-Doped Ca11.5 (Δ_K=270 K, $J_\parallel$ ~1700 K)

$$\xi_o \sim 10 \quad \text{with} \quad J_\perp/J_\parallel \sim 0.4$$

$$T^2_{2\mathrm{G}}(T=0) \sim \frac{1}{\xi_h(0)} + \frac{1}{\xi_o(0)}$$

doped 1D
Imada et al

$$\frac{T^2_{2\mathrm{G}}(hole)}{T^2_{2\mathrm{G}}(ladder)} = \frac{\xi_h^{-1}(0) + \xi_o^{-1}(0)}{\xi_o^{-1}(0)}$$

$$\frac{T^2_{2\mathrm{G}}(\mathrm{Ca11.5})}{T^2_{2\mathrm{G}}(\mathrm{Sr14})} = \frac{\xi_o^{-1}(\mathrm{Ca11.5})}{\xi_o^{-1}(\mathrm{Sr14})} = 5.2/10$$

Ca9

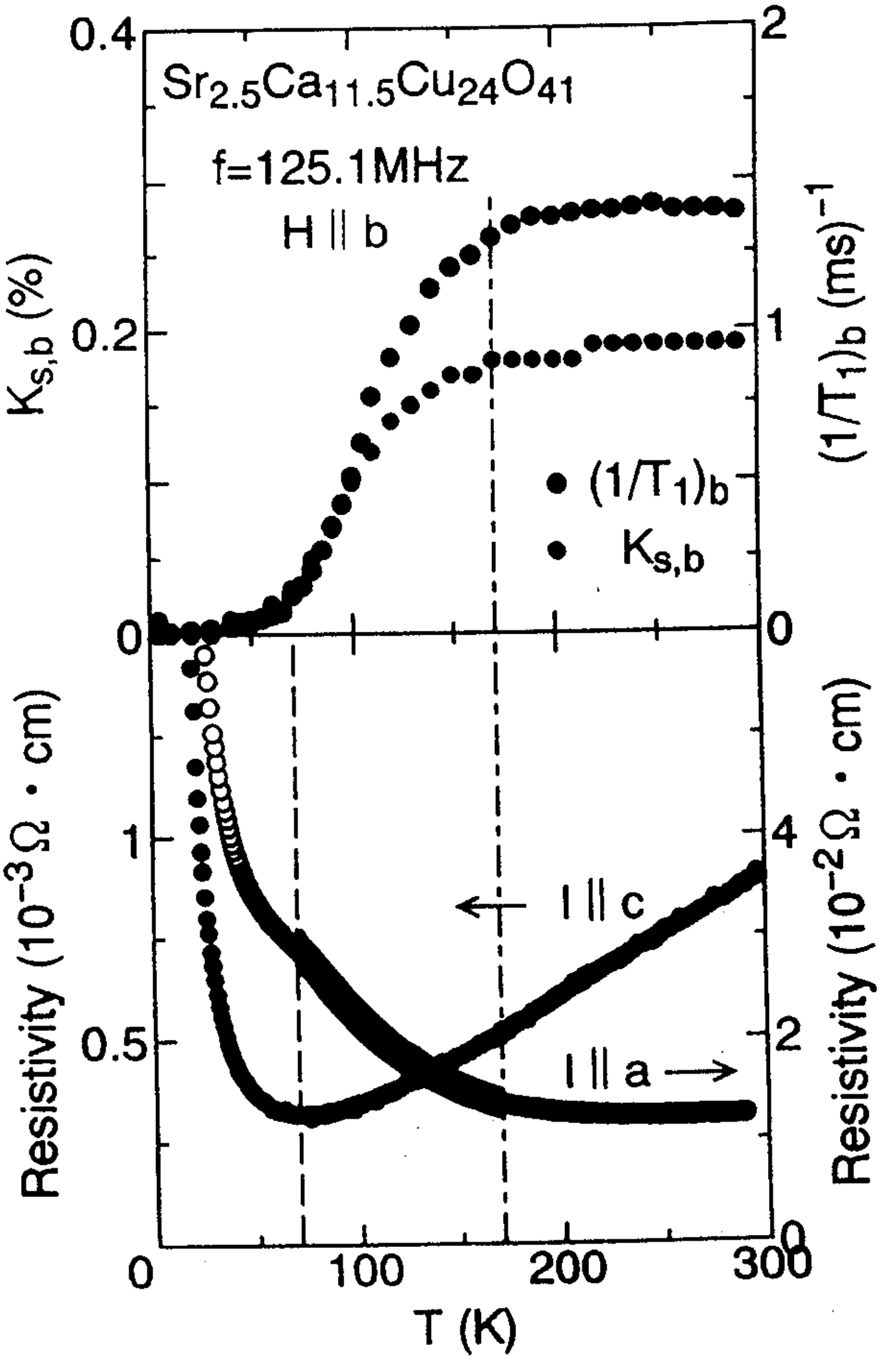
$\xi_h \sim 2.6$ **Hole Content : $x \sim 0.19$**

Ca11.5

$\xi_h \sim 1.9$ **Hole Content : $x \sim 0.25$**

Optical Conductivity $x = 0.2$ Osafune et al

Spin Gap and Transport Property
– A Class of Luther-Emery Liquid –



Pairs are formed below ~150K, But confined in each ladder

increase of anisotropy in Resistivity