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SMR. 767 - 15

**MINIWORKSHOP ON STRONG CORRELATIONS
AND QUANTUM CRITICAL PHENOMENA
(4 - 22 July 1994)**

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**A SYSTEMATIC UNDERSTANDING OF THE MAGNETIC AND TRANSPORT
PHENOMENA IN CUPRATES BASED ON THE t-J MODEL**

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

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A Systematic Understanding of the Magnetic and Transport Phenomena in Cuprates Based on the $t - J$ Model

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collaborator :

D.N. Sheng

- Introduction
- Framework: Flux-binding saddle-point state of the $t - J$ model
- Magnetic Properties
 - 1d: Exact results
 - 2d: Experimental results
 - commensurate vs. incommensurate magnetic fluctuations
 - “spin gap” behavior
 - NMR spin relaxation rate
 - pairing instability
- Charge Properties:
 - 1d: Luttinger liquid behaviors
 - 2d: Transport phenomena
 - linear-T resistivity
 - Hall effect; Hall angle phenomena; magneto-resistance
 - thermopower
- Conclusions

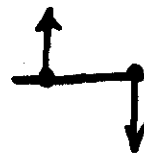
• Introduction

The t-J model $H_{t-J} = H_t + H_J$

hopping term $H_t = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}$



superexchange $H_J = J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4})$



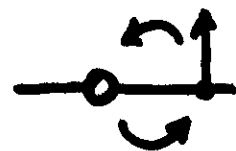
The Hilbert space is restricted by $\sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} \leq 1$

Slave-boson formulation

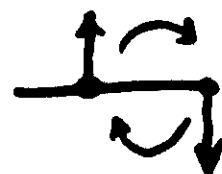
$$c_{i\sigma} = b_i^\dagger f_{i\sigma}$$

no double occupancy constraint $b_i^\dagger b_i + \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = 1$

$$H_t = -t \sum_{\langle ij \rangle \sigma} b_i^\dagger b_j f_{i\sigma}^\dagger f_{j\sigma} + \text{H.c.}$$



$$H_J = -\frac{J}{2} \sum_{\langle ij \rangle \sigma \sigma'} f_{i\sigma}^\dagger f_{j\sigma} f_{j\sigma'}^\dagger f_{i\sigma'}$$



The no double occupancy constraint is not
as crucial as in the original case

Mean-field decoupling

$$H_h^{MF} = -t \sum_{\langle ij \rangle \sigma} \chi_{ji}^{\sigma} h_i^{\dagger} h_j + \text{h.c.}$$

$$H_S^{MF} = -\frac{J}{2} \sum_{\langle ij \rangle \sigma \sigma'} \left(\chi_{ji}^{\sigma'} + \frac{t}{J} H_{ji} \right) f_{i\sigma}^{\dagger} f_{j\sigma} + \text{h.c.}$$

Mean-fields: $\chi_{ji}^{\sigma} = \langle f_{j\sigma}^{\dagger} f_{i\sigma} \rangle$, $H_{ji} = \langle h_j^{\dagger} h_i \rangle$

1. Uniform RVB state

$$\chi_{ji}^{\sigma} = \chi_0, \quad H_{ji} = H_0$$

phase fluctuation around the saddle-point:

Gauge field description

Ioffe & Larkin

Nagaoka & Lee

Kotliar

$\delta \rightarrow 0$, AF may underestimated

Wiegmann

...

$\delta = 0$, Variational energy 21% higher

NO AF long-range order

2. Flux-phase

$$\chi_{ji}^\sigma = \chi_0 e^{i\theta_{ij}} \quad (\delta=0, H_0=0)$$

Affleck & Marston

$$\phi_0 = \sum_{ij} \theta_{ij} = \pi$$



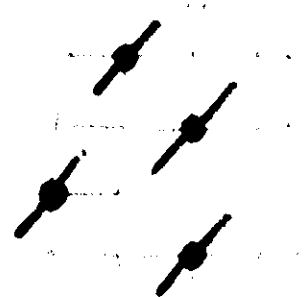
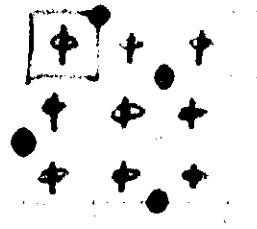
Variational energy by VMC: only 5% higher

AF long range order is still missing

3. Flux binding states

Exact diagonalization

(Canright, Girvin & Brass)
phys. Rev. Lett. 62 (1989)



... exactly by adding flux

Scheme one All spins, ...

no matter spins, are bound to the same flux quanta.

$$\sum_{ij} \theta_{ij} = \pi \sum_{\sigma} n_{\sigma}^f \quad \langle n_{\sigma}^f \rangle = \frac{1}{2} \quad \delta=0$$

Away from half-filling, $\sum_{ij} \langle \theta_{ij} \rangle = \pi (1-\delta) \rightarrow$ commensurate flux phase

$T=0$, Superfluid

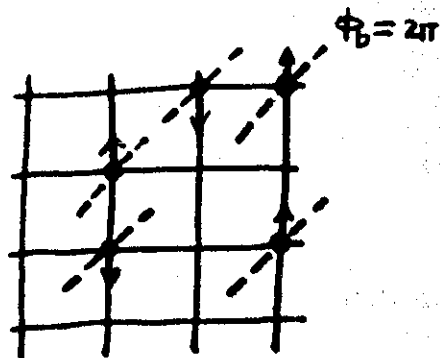
Z.Y. Wang, et al. Phys. Rev. B 49, 607 (1994)

$T > T_c$, anomalous transport properties

Z.Y. Wang et al.

Scheme two Spinons with different spins cannot see each other's flux tubes

$$\sum_a \theta_{ij}^\sigma = \underset{\substack{\uparrow \\ \Phi_b}}{2\pi} \sum_{l \in a} n_{lr}^f$$



each flux tube : 2π flux

Normal state is easily accessible in Scheme two

• Mathematical Framework

Identical transformation

$$H_J = -\frac{J}{2} \sum_{\langle ij \rangle \sigma \sigma'} \left(e^{i A_{ij}^\sigma} f_{i\sigma}^\dagger f_{j\sigma} \right) \left(e^{i A_{ji}^{\sigma'}} f_{j\sigma'}^\dagger f_{i\sigma'} \right)$$

$$A_{ij}^\sigma = \sigma \sum_{l \neq i,j} (\theta_i(l) - \theta_j(l)) \left[n_{l\sigma}^f + \frac{n_l^h}{2} - \delta_{\sigma,1} \right]$$

$\hookrightarrow \theta_i(l) = \text{Im} \ln(z_i - z_l)$

$$A_{ij}^\sigma \Leftrightarrow \theta_{ij}$$

Mean-field

$$\chi_0 = \langle e^{i A_{ij}^\sigma} f_{i\sigma}^\dagger f_{j\sigma} \rangle$$

Saddle-point Hamiltonian

$$H_{t-J}^{MF} = H_h + H_s$$

Spinon:

$$H_s = -J_s \sum_{\langle ij \rangle \sigma} e^{i A_{ij}^\sigma} f_{i\sigma}^\dagger f_{j\sigma} + H.c.$$

$$H_s = -J_s \sum_{\langle ij \rangle \sigma} \left(e^{i\sigma A_{ij}^h} \right) b_{i\sigma}^\dagger b_{j\sigma} + H.c.$$

$$A_{ij}^h = \frac{1}{2} \sum_{l \neq i,j} \text{Im} \ln \left(\frac{z_i - z_l}{z_j - z_l} \right) n_l^h$$

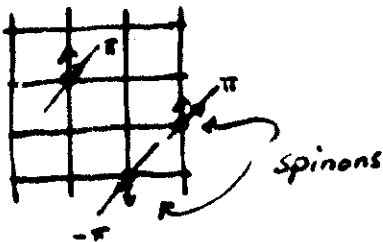
$$b_{i\sigma} = f_{i\sigma} e^{-i\sigma \sum_{l \neq i} \theta_i(l) (n_{l\sigma}^f - \delta_{\sigma,1})}$$

Jordan-Wigner transformation

Holon:

$$H_h = -t_h \sum_{\langle ij \rangle} \left(e^{i A_{ij}^b} \right) h_i^\dagger h_j + H.c.$$

$$A_{ij}^b = \frac{1}{2} \sum_{l \neq i,j} \text{Im} \ln \left(\frac{z_i - z_l}{z_j - z_l} \right) \left(\sum_{\sigma} \sigma n_{l\sigma}^b - 1 \right)$$



Half-filling: $A_{ij}^h = 0$ ($\delta = 0$)

$$S_i^+ = (-1)^i b_{i\uparrow}^+ b_{i\downarrow}$$

2d case: Bose condensation of $b_{i\sigma}$

$$\langle S_i^+ \rangle = (-1)^i \langle b_{i\uparrow}^+ \rangle \langle b_{i\downarrow} \rangle \neq 0$$

- AF LRO
- upper bound of GSE: 5% higher

1d case:

$$\langle S_i^+ S_j^- \rangle = (-1)^i \langle b_{i\uparrow}^+ b_{j\uparrow} \rangle \langle b_{i\downarrow} b_{j\downarrow}^+ \rangle$$

$$\propto \frac{\cos \frac{\pi}{2} (x_i - x_j)}{[(x_i - x_j)^2 - v_F^2]^{1/2}}$$

Luther & Peshel

(1975)

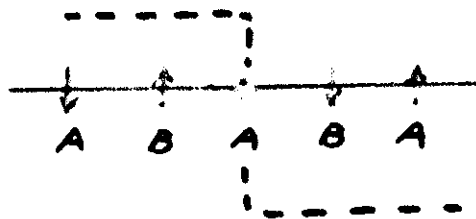
- Magnetic Properties Away From Half-Filling

- One-dimensional case

In bosonic representation

$$S_i^+ = (-1)^i b_{i\uparrow}^\dagger b_{i\downarrow} e^{i\pi \sum_{l<i} n_l^\uparrow}$$

Semiclassical picture:



Z. Y. Weng et al.

Phys. Rev. Lett.

67, 3318 (1991)

$$\begin{aligned} \langle S_i^+(t) S_j^-(0) \rangle &= (-1)^{i-j} \langle b_{i\uparrow}^\dagger(t) b_{j\uparrow}(0) \rangle \langle b_{j\downarrow}(t) b_{j\downarrow}^\dagger(0) \rangle \\ &\times \langle e^{i\pi \sum_{l<i} n_l^\uparrow(t)} e^{-i\pi \sum_{l<j} n_l^\uparrow(0)} \rangle \end{aligned}$$

$$\propto \frac{\cos(2k_f x)}{(x^2 - v_s^2 t^2)^{1/2} (x^2 - v_h^2 t^2)^{1/4}}$$

$$k_f = \frac{\pi}{2a} (1-\delta)$$

$$x = x_i - x_j$$

• Spin Dynamics in Two-dimension Doped Case

Saddle-point Hamiltonian

$$H_s = -J_s \sum_{\langle ij \rangle \sigma} \left(e^{i\sigma A_{ij}^h} \right) b_{i\sigma}^\dagger b_{j\sigma} + H.c.$$

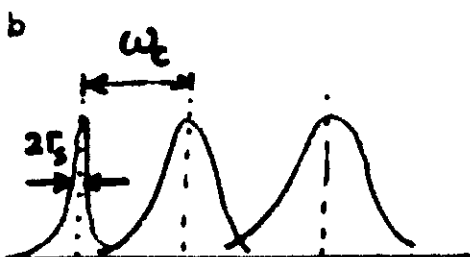
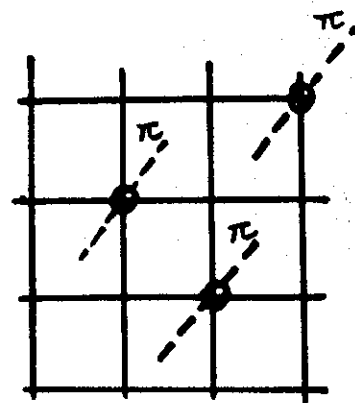
$$A_{ij}^h = \frac{1}{2} \sum_{l \neq i,j} \text{Im} \ln \left(\frac{z_i - z_l}{z_j - z_l} \right) n_l^h$$

$$n_l^h = \langle n_l^h \rangle + \delta n_l^h \Rightarrow A_{ij}^h = \bar{A}_{ij}^h + \delta A_{ij}^h$$

⚡ $\hookrightarrow$ fluctuating flux

$$B_h = \pi \delta$$

Levy & Laughlin
...



• Basic energy scales:

$$\omega_c = 2\pi J_s \delta \sim \delta J$$

• Basic length scale:

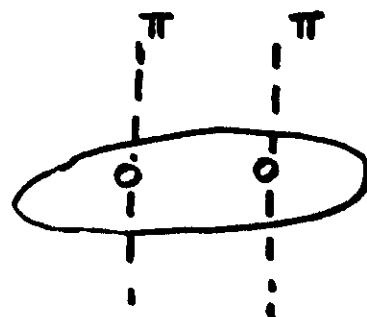
$\Gamma_s(n)$ — broadening

• Basic temperature scale:

$$l_c = 1/\sqrt{B_h} = a/\sqrt{\pi \delta} \quad \text{cyclotron length}$$

Bose condensation temperature T_c^*

Pairing instability at $T < T_c^*$:



Spin Susceptibility Function

$$\chi''(\mathbf{q}, \omega) = -\pi \sum_l K_{ll}(\mathbf{q}) \int \frac{d\omega'}{2\pi} \rho_b(l, \omega') \rho_b(l, \omega + \omega') [n(\omega + \omega') - n(\omega')] \\ - \pi \sum_{l \neq l'} K_{ll'}(\mathbf{q}) \int \frac{d\omega'}{2\pi} \rho_b(l, \omega') \rho_b(l', \omega + \omega') [n(\omega + \omega') - n(\omega')]$$

$$K_{ll'}(\mathbf{q}) = \frac{\delta}{16\pi} \int_0^\infty dy L_l(y) L_{l'}(y) e^{-y} J_0(\sqrt{2l_c^2 y} |\mathbf{q} - \mathbf{Q}|)$$

Small T , $\omega (< \omega_c)$

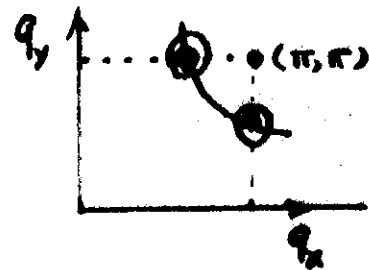
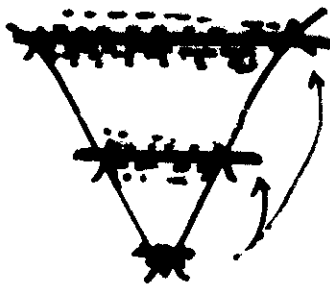


$$\chi''(\mathbf{q}, \omega) \propto K_{00}(\mathbf{q}) = \frac{\delta}{16} \exp\left(-\frac{|\mathbf{q} - \mathbf{Q}|^2}{2l_c^2}\right) \quad \vec{Q} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$$

Spin correlation length $l = \sqrt{2}l_c \propto a/\sqrt{\delta}$

Increase of T : width is not changed

Increase of ω : $K_{01}(\mathbf{q})$ involved $\rightarrow$ incommensurate structure

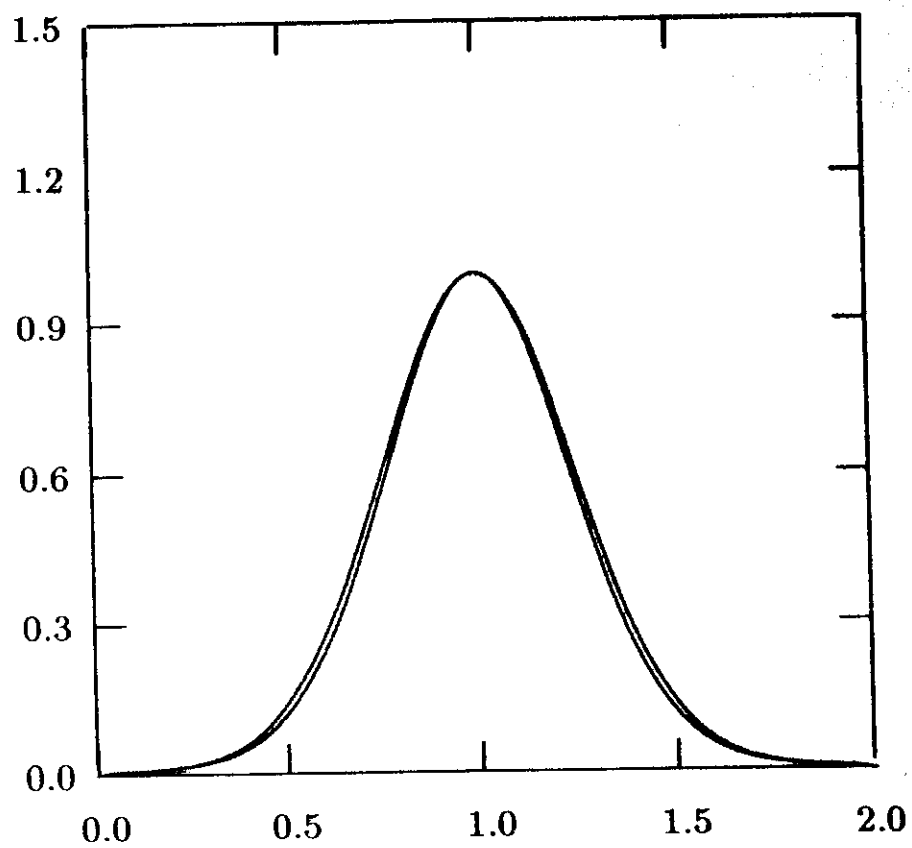


inter-Landau level transition



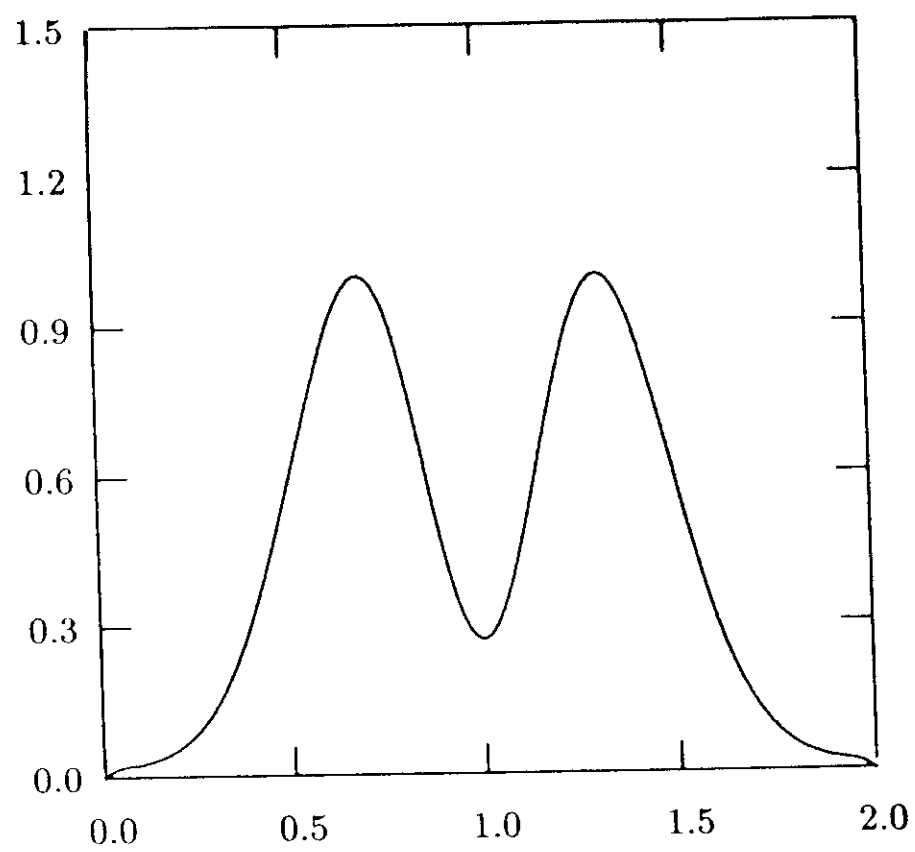
incommensurate peaks

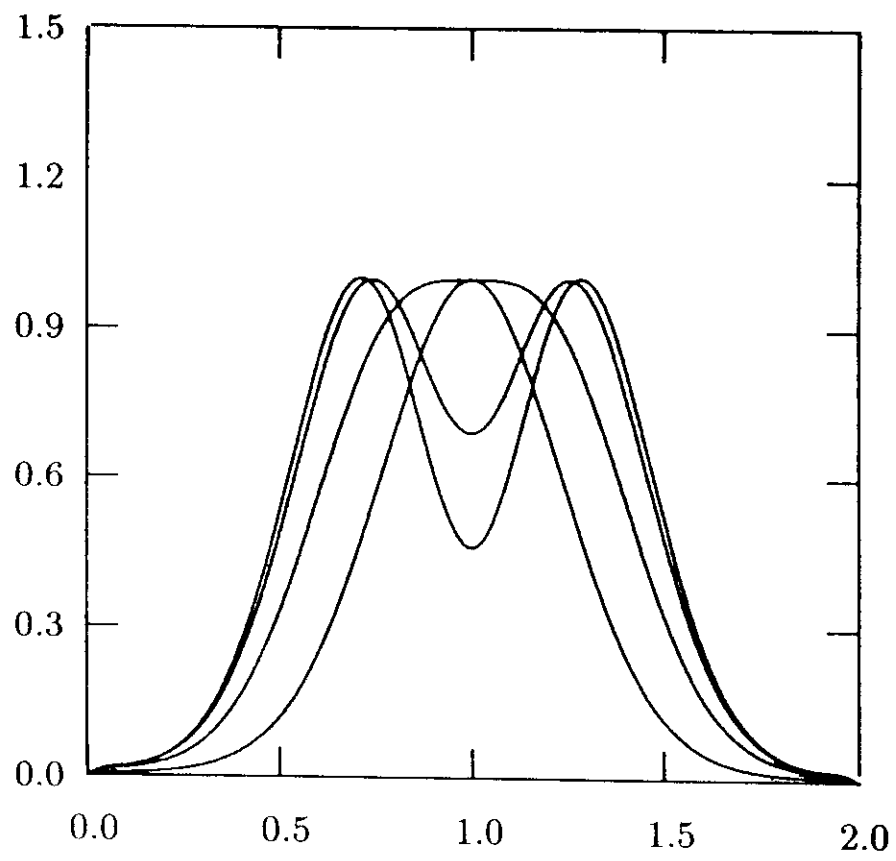
$\chi(q, \omega)$



$q, (\frac{\pi}{a})$

$(q_x = \frac{\pi}{a})$





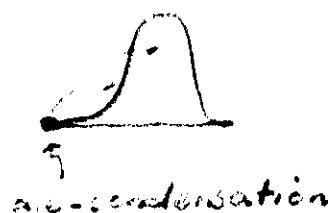
ω - dependence of the susceptibility function

$$\chi''(\mathbf{Q}, \omega) = -\frac{\delta}{16} \sum_l \int \frac{d\omega'}{2\pi} \rho_b(l, \omega') \rho_b(l, \omega + \omega') [n(\omega + \omega') - n(\omega')]$$

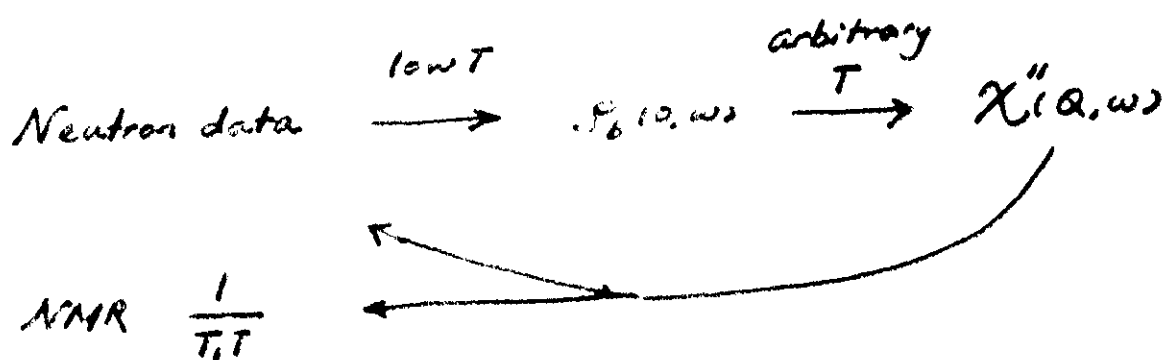
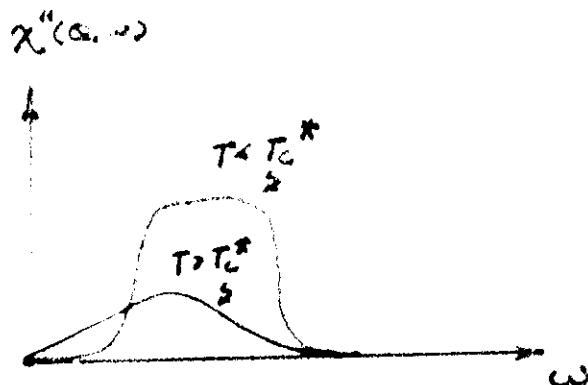


$$T > T_c^*, \chi''(\mathbf{Q}, \omega) \propto \frac{\omega}{T} \quad \left(\frac{\omega}{T} \ll 1 \right)$$

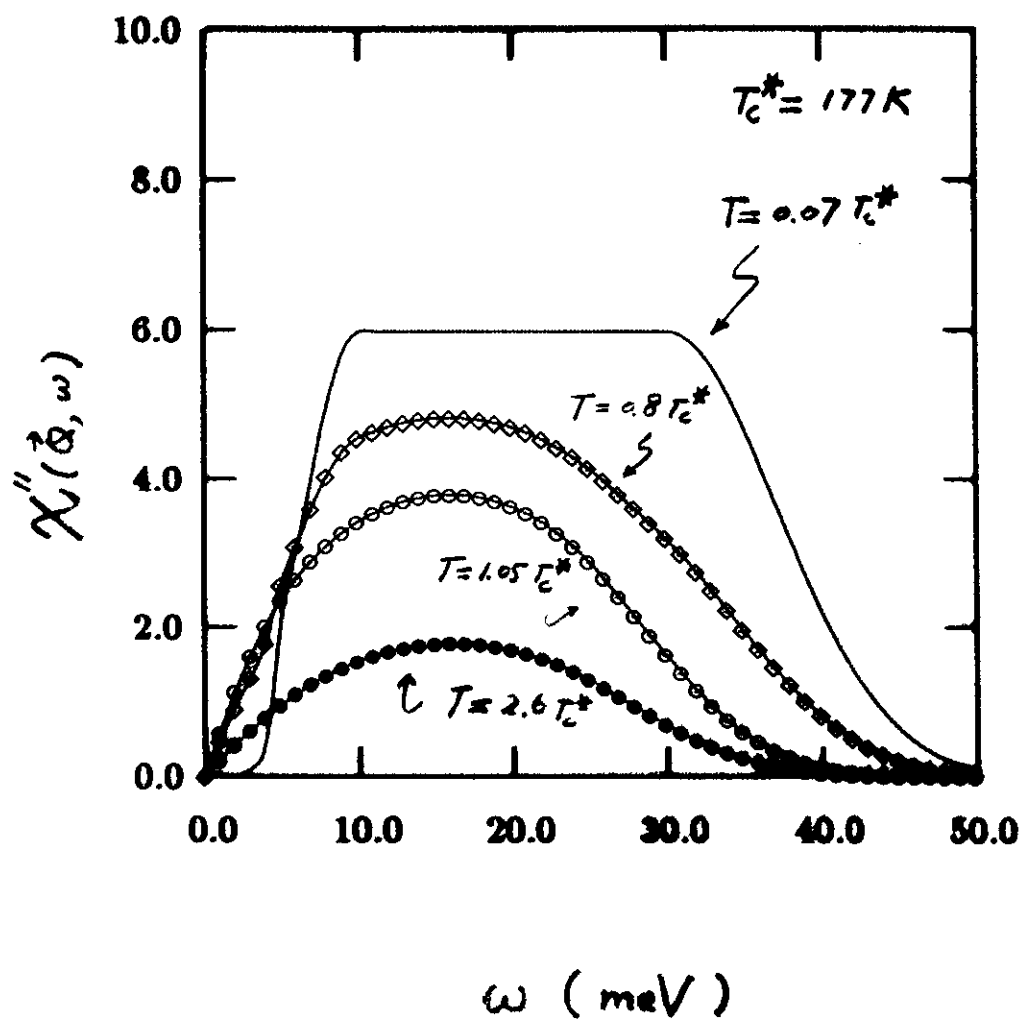
$$T = 0, \chi''(\mathbf{Q}, \omega) \propto \rho_b(0, \omega)$$



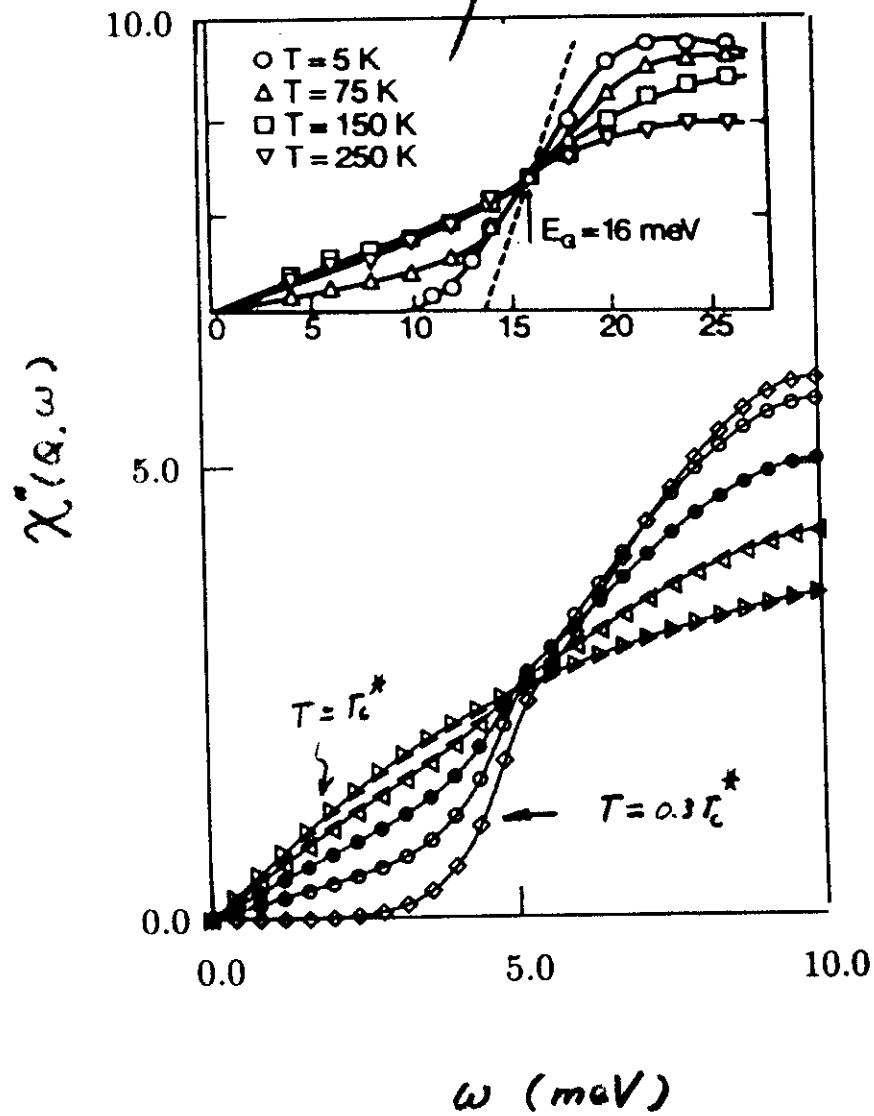
"Spring gap"
behavior

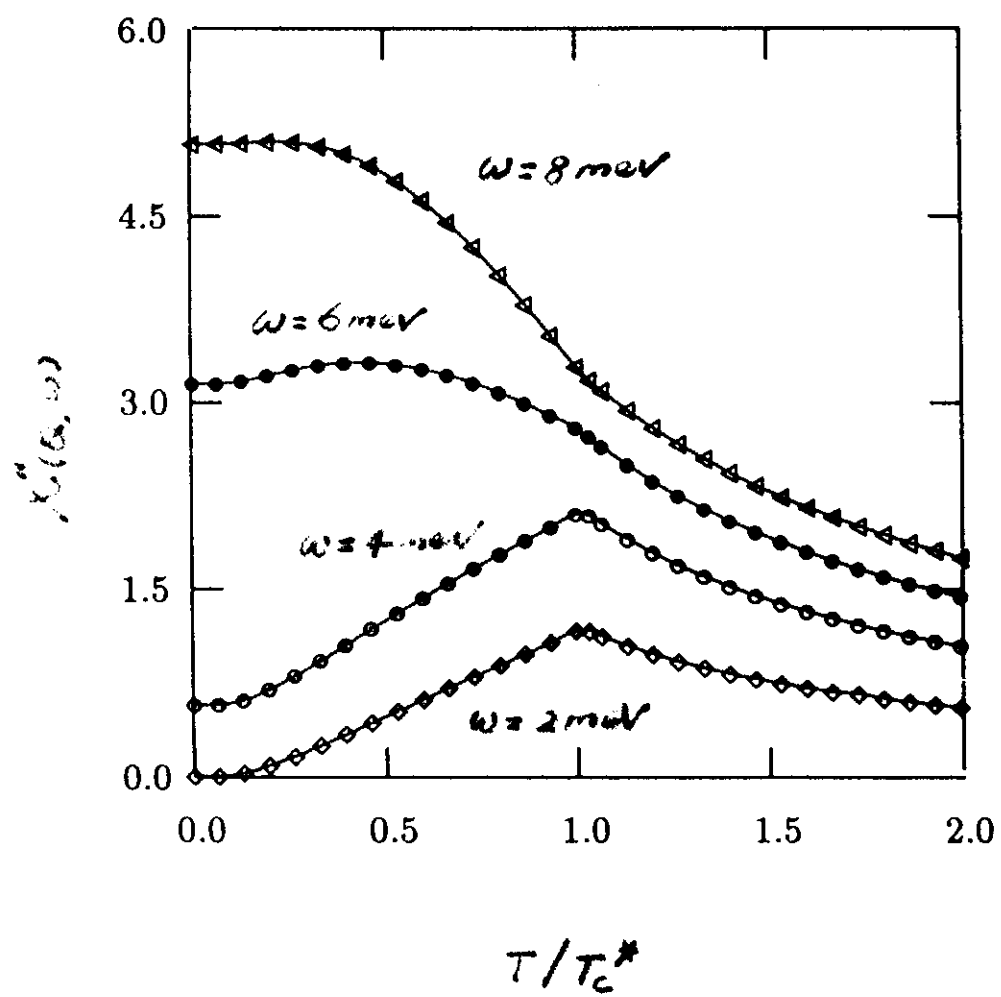


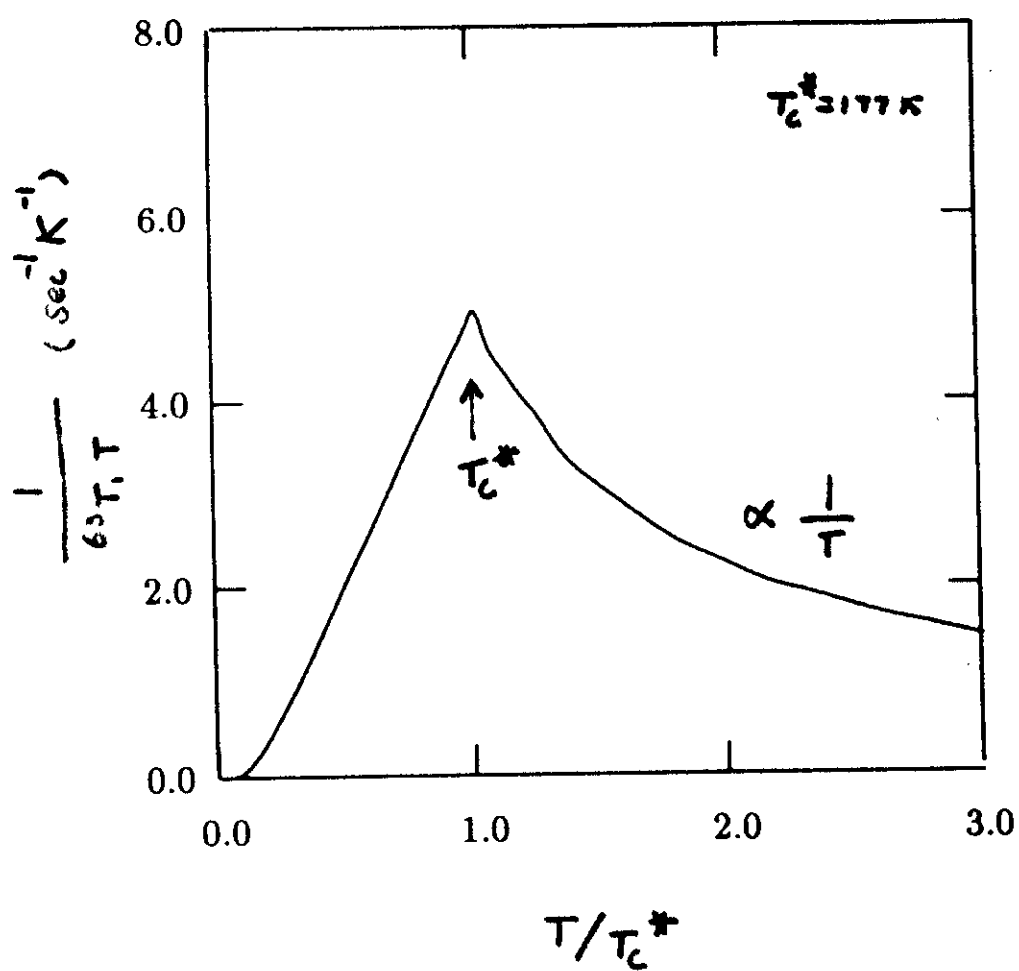
$\gamma\text{-Ba}_2\text{Cu}_3\text{O}_{6.6}$: Tranquada et al. Phys. Rev. B 46, 5561 (1992)



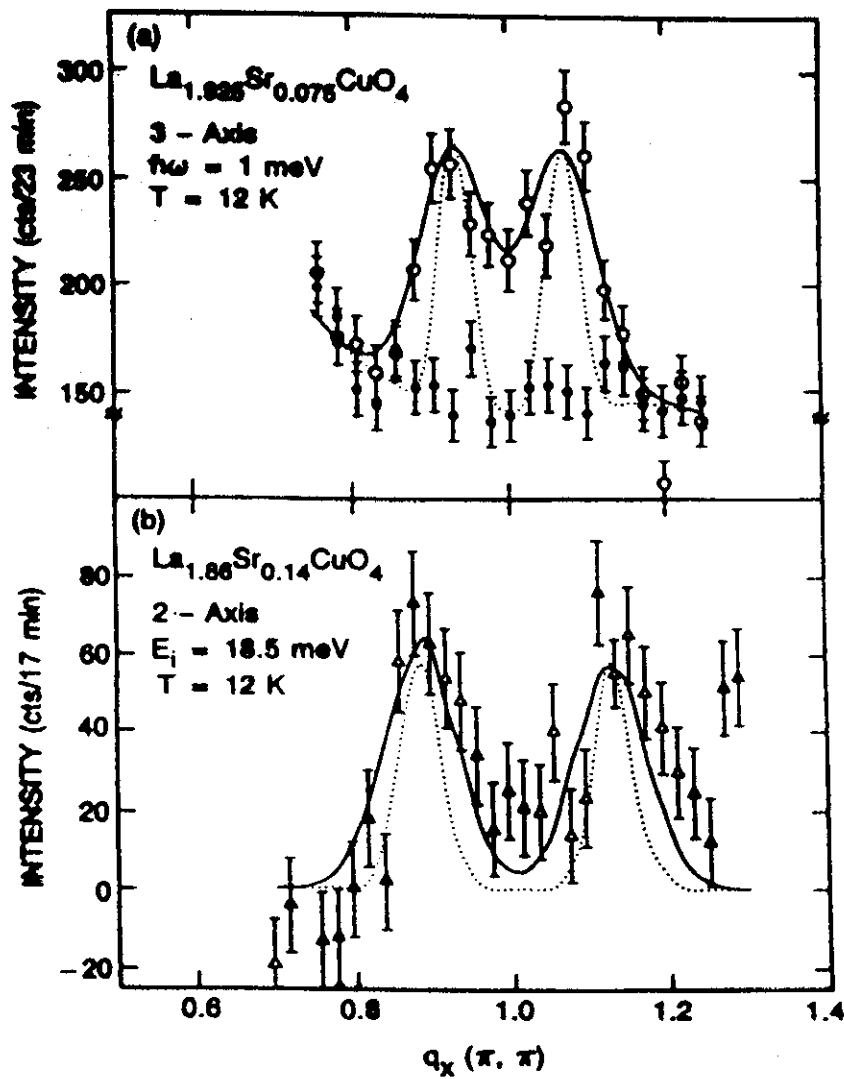
Rossat-Mignod et al. *Physica B* 185-189
86(1991)
 $\text{YBaCu}_3\text{O}_{8.69}$

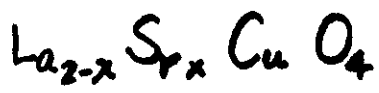




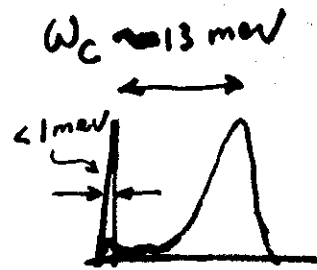


$$^{17}\text{T}_1^{-1} / ^{63}\text{T}_1^{-1} \approx \frac{1}{20}$$





A scenario for the spectral function



Consequences:

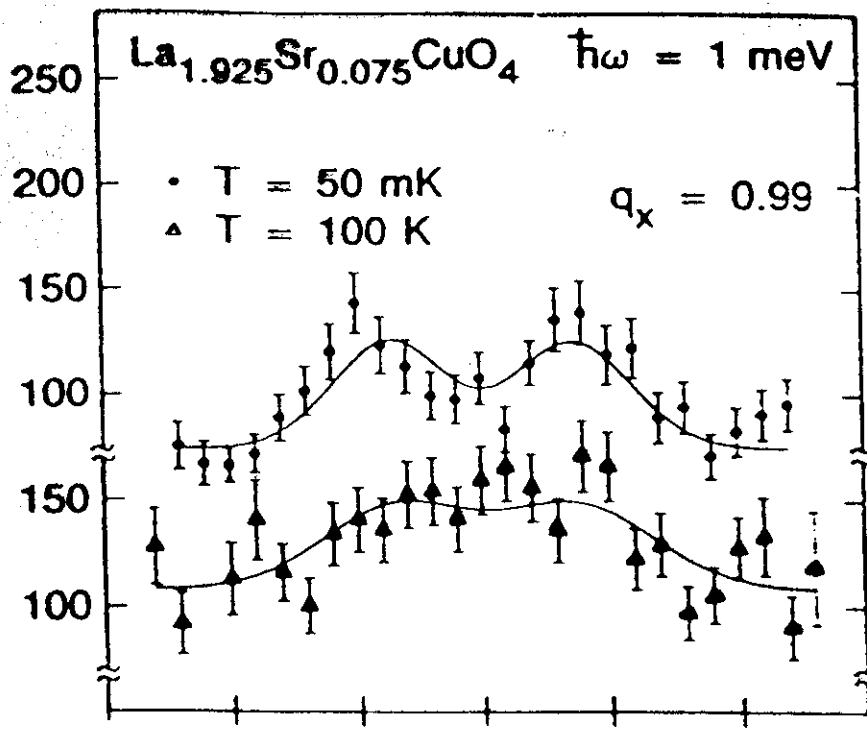
- NMR spin relaxation rate ($\omega \rightarrow 0$ case)

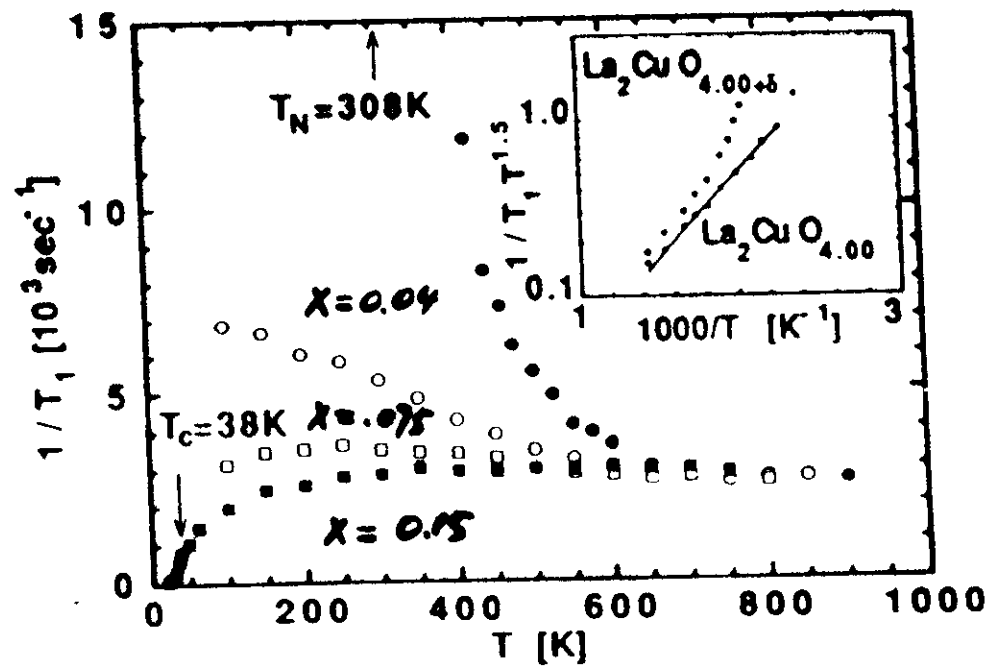
$$\left. \frac{1}{T_1 T} \right|_{^{63}\text{Cu}} \sim \frac{C}{T} \quad \text{persists to lower } T \quad (T > T_c^*)$$

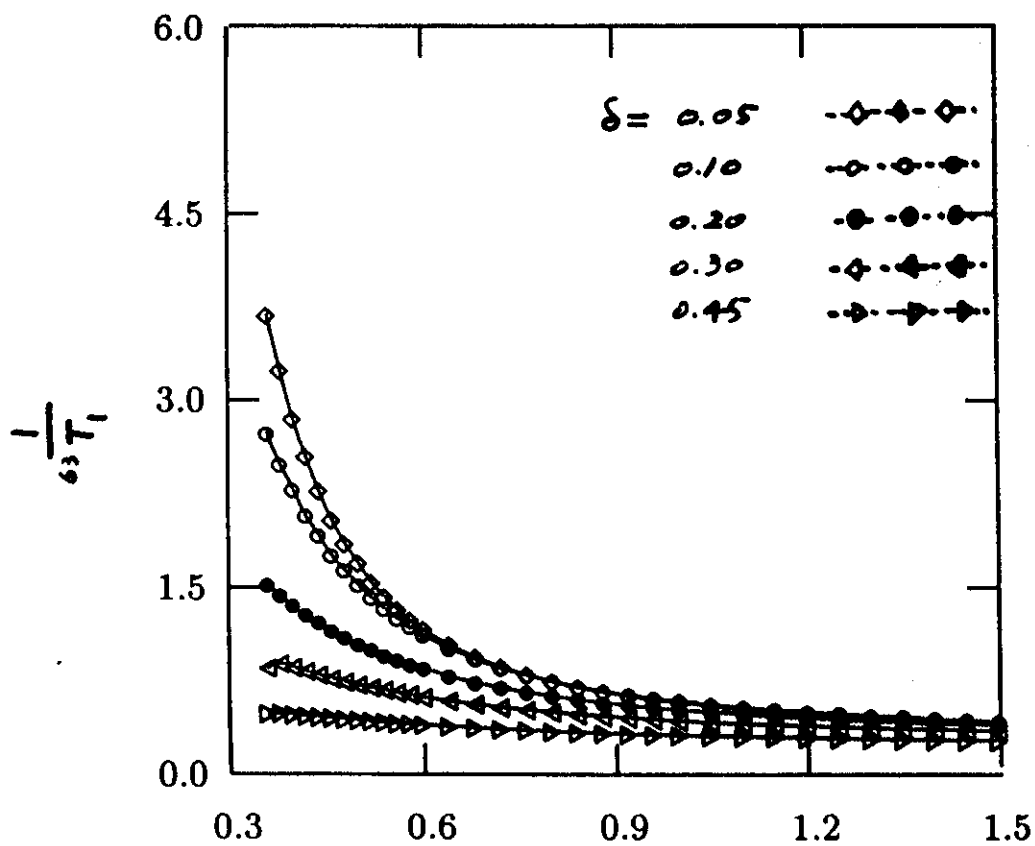
$$C = \frac{B^2 c_0(\delta)}{T_3} (1-\delta)^*$$

- High temperature $\chi''(q, \omega)$:

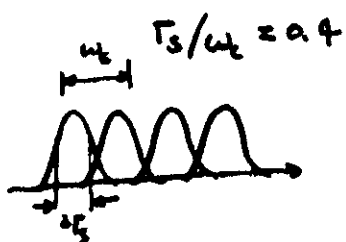
Incommensurate vs. commensurate







$$T(\omega_b) \rightarrow \frac{2\pi J}{s} \sim J$$



A Brief Summary of the Magnetic Properties

- Correct spin-spin correlation in 1d
- A consistent explanation of
 - “spin gap” behavior
 - commensurate & incommensurate structure
 - NMR spin relaxation rate
 - Others

- Open question:

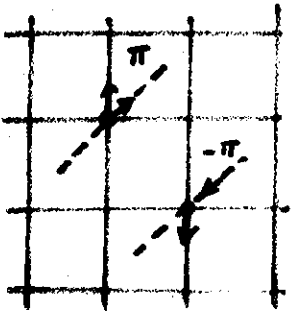
why spectral functions are different in

YBCO & LSCO compounds ?

• Charge Degree Of Freedom (2D)

Holon saddle-point Hamiltonian

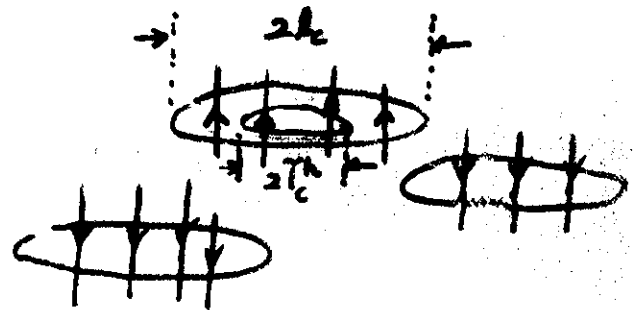
$$H_h = -t_h \sum_{\langle ij \rangle} e^{i\tilde{A}_{ij}^b} e^{-i\phi_{ij}^0} h_i^\dagger h_j + H.c.$$



$$\sum_{\square} \phi_{ij}^0 = \pi$$

$$\tilde{A}_{ij}^b = \frac{1}{2} \sum_{l \neq i,j} \text{Im} \ln \left(\frac{z_i - z_l}{z_j - z_l} \right) \sum_{\sigma} \sigma n_{l\sigma}^b$$

$$\langle \tilde{A}_{ij}^b \rangle = 0 \quad \text{random-flux?}$$

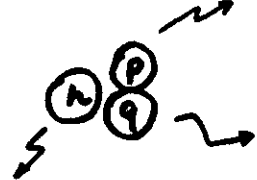


two length scales:

- length scale of the fluctuating flux $\sim l_c \propto \frac{a}{\sqrt{\epsilon}}$

- cyclotron length of holon under such a fluctuation flux $\tilde{l}_c^h \propto \frac{a}{\sqrt{1-\epsilon/2}}$

$$l_c > \tilde{l}_c^h$$

$\text{holon} =$


 external fields

 flux tubes carried by down spinors

Effective Lagrangian for the 2d Holon Degree of Freedom

$$\begin{aligned}
 L_h = & \int d^2 \mathbf{r} \{ h^+(\mathbf{r}) [\partial_\tau + a_0^{\text{ext}}] h(\mathbf{r}) + p^+(\mathbf{r}) \partial_\tau p(\mathbf{r}) + q^+(\mathbf{r}) \partial_\tau q(\mathbf{r}) \} \\
 & + \int d^2 \mathbf{r} \{ h^+ \frac{(-i\nabla - \mathbf{a}^{\text{ext}})^2}{2m_h} h + p^+ \frac{(-\nabla - \mathbf{A}^+)^2}{2m_p} p + q^+ \frac{(-\nabla - \mathbf{A}^-)^2}{2m_q} q \} \\
 & + \int d^2 \mathbf{r} \{ \lambda(\mathbf{r}) [p^+ p - h^+ h] + \beta(\mathbf{r}) [q^+ q - h^+ h] \}
 \end{aligned}$$

density constraint: $p^\dagger(\mathbf{r}) p(\mathbf{r}) = q^\dagger(\mathbf{r}) q(\mathbf{r}) = h^\dagger(\mathbf{r}) h(\mathbf{r})$ (scale $\sim \ell_c^{-1} = \frac{1}{\sqrt{B_z}}$)

$$\vec{A}^\pm = \pm \frac{B_z}{2} \vec{z} \times \vec{r}$$

$$B_z = \frac{\pi}{2a^2} (1-\delta)$$

Current constraint: $\mathbf{j}_h^L = \mathbf{j}_p^L = \mathbf{j}_q^L$

longitudinal gauge fluctuations of λ, β

→ Scattering mechanism

A Brief Summary

Normal state transport properties of the flux-binding phase:

- Resistivity

$$\rho \propto T$$

$$\rho = a \left(\frac{T}{T_h} \right) T + bT$$

$$\frac{\hbar}{\tau_s} \simeq \eta k_B T, \quad \eta \simeq 2.1$$

- Hall effect

$$\cot \theta = \frac{1}{\omega_H \tau_h} = \alpha T^2 + C$$

$$\cot \theta \approx \frac{f_{xx}}{f_{yx}}$$

$$R_H = \frac{1}{nec} \left(\frac{m_p + m_q}{m_H} \right) \frac{\tau_h}{\tau_s} \propto \frac{1}{T}$$

prediction $\frac{\Delta \rho}{\rho} \propto B^2 T^{-4}$

Observed!

Harris, Yan, Ong

U Anderson

(Princeton)

- Thermal power

$$S = \frac{k_B}{e} \ln \left(\frac{1 - 2\delta}{2\delta} \right) + f(T)$$