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INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY

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EXPERIMENTAL WORKSHOP ON
HIGH TEMPERATURE SUPERCONDUCTORS AND RELATED MATERIALS
(BASIC ACTIVITIES)

(11 February - 1 March 1991)

" HTS Materials and Neutron Scattering "

presented by:

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

HTS materials and Neutron Scattering

Second lecture:

- Magnetic excitations (ILL, BNL, ..)
- Phonon anomalies (Paris - Karlsruhe)

Materials: $La_{2-x}Sr_xCuO_4$

$YBa_2Cu_3O_{6+\delta}$

T5, T6, T9

Magnetic fluctuations of quasi 2 dimensional Quantum-Anti-Ferro-Magnets - "QAFM".

Experimental: $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+\delta}$

Theory : Spin 1/2 Heisenberg Model

$$H = \sum J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Discuss: Correlation function, susceptibility χ

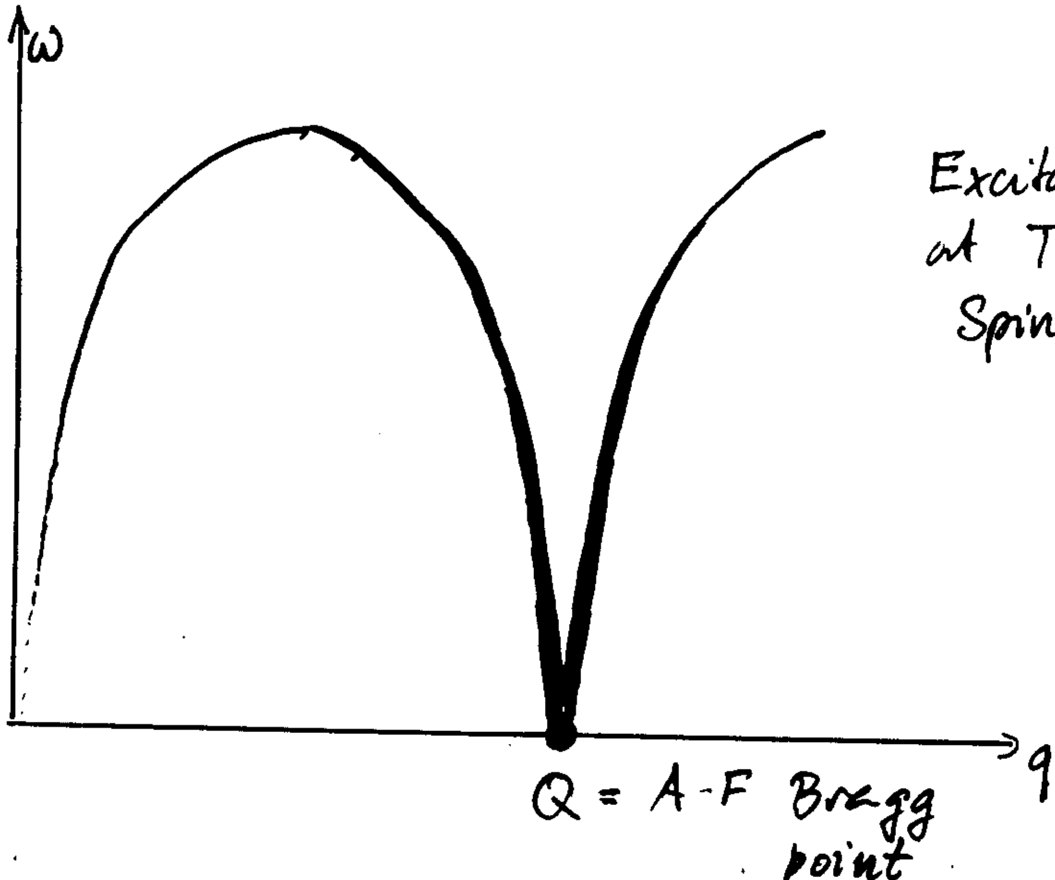
$$\mathcal{S}(\vec{q},\omega) = \int dt\, e^{i\omega t} \sum_{ij} e^{i\vec{q}(\vec{R}_i-\vec{R}_j)} \langle \vec{S}_i \cdot \vec{S}_j(t) \rangle$$

$$\mathcal{S}(\vec{q},\omega) = \frac{1}{1-e^{-\hbar\omega/kT}} \operatorname{Im} \chi(\vec{q},\omega) \quad ; \quad \omega \neq 0.$$

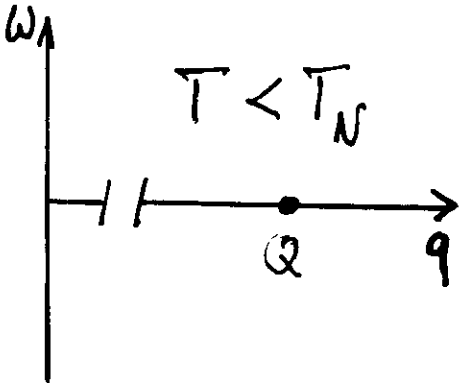
Sum rule: $\frac{1}{N}\sum_q \int d\omega\, \mathcal{S}(\vec{q},\omega) = \langle \vec{S}_i^2 \rangle = S(S+1)$

if stable moments exist.

Heisenberg model, $T=0$; $\langle \vec{S}_i \rangle = D e^{i Q \cdot R_i} \cdot \vec{e}_z$



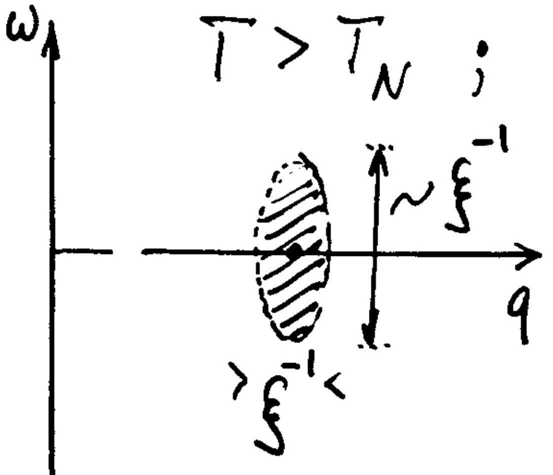
Excitation spectrum at $T=0$: Spin waves



Bragg-peak at $q = Q$

Bragg-intensity makroskopic

$I_B \sim \mathcal{O}(N)$

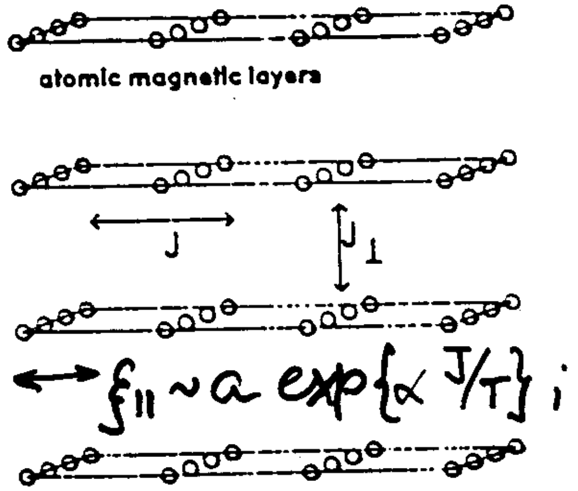


$T > T_N$; $\frac{k_B T}{J} \ll 1$: Braggintensity is smeared out over region of width

$\sim \xi^{-1}$ in q

$\sim \sqrt{TJ} \cdot \xi^{-1}$ in ω

ξ = correlation length



$$\xi_{\parallel} \sim a \exp\{\alpha\, J/T\};$$

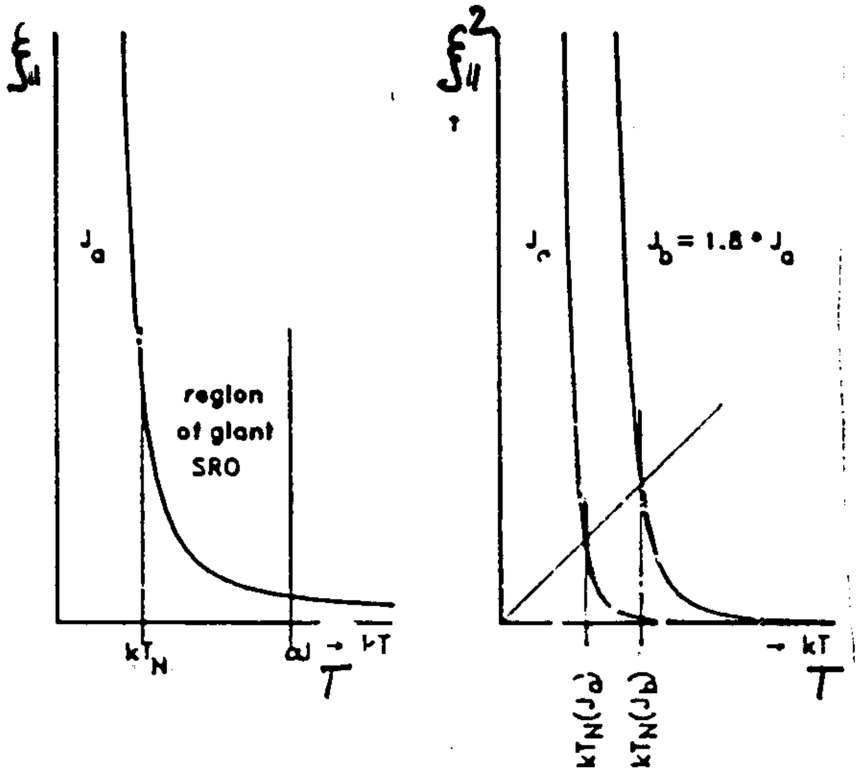
La_2CuO_4:

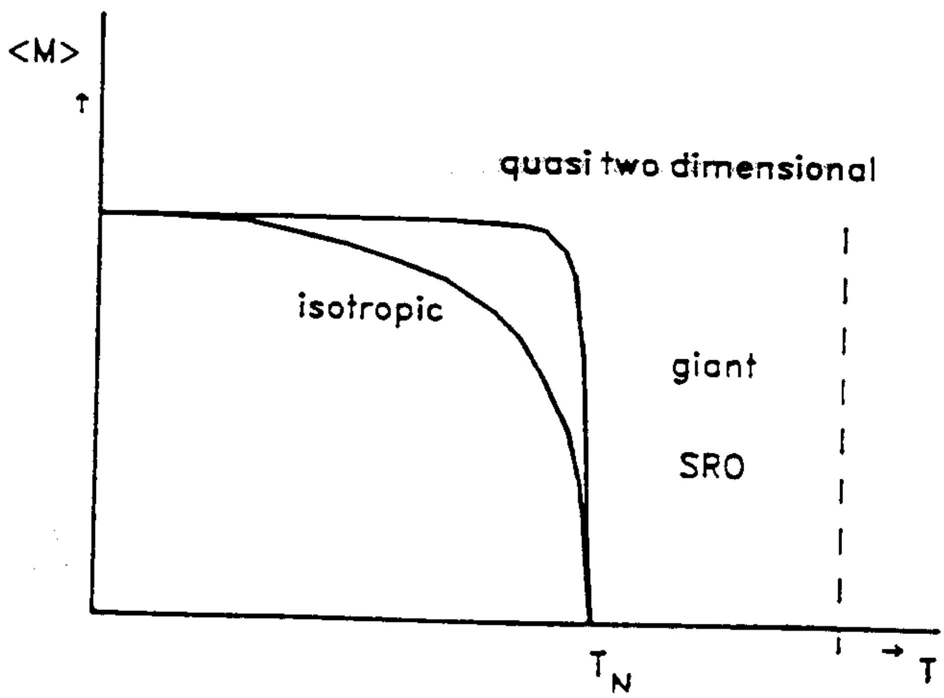
$$J_{\perp}/J_{\parallel} \approx 10^{-5}$$

$$J_{\parallel} \equiv J \sim 0.1\,eV \sim 1000\,K$$

3d-order at $T_N \approx 300\,K$

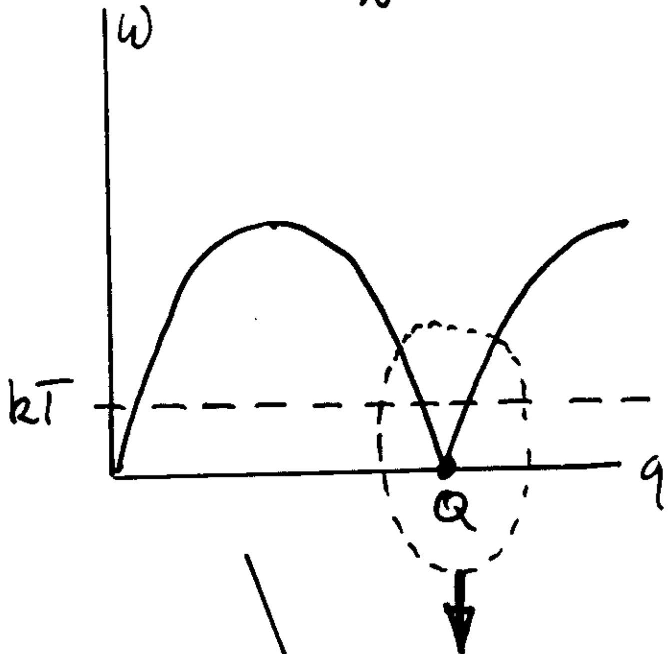
$$kT_N \sim \xi_{\parallel}^2 \cdot J_{\perp}$$

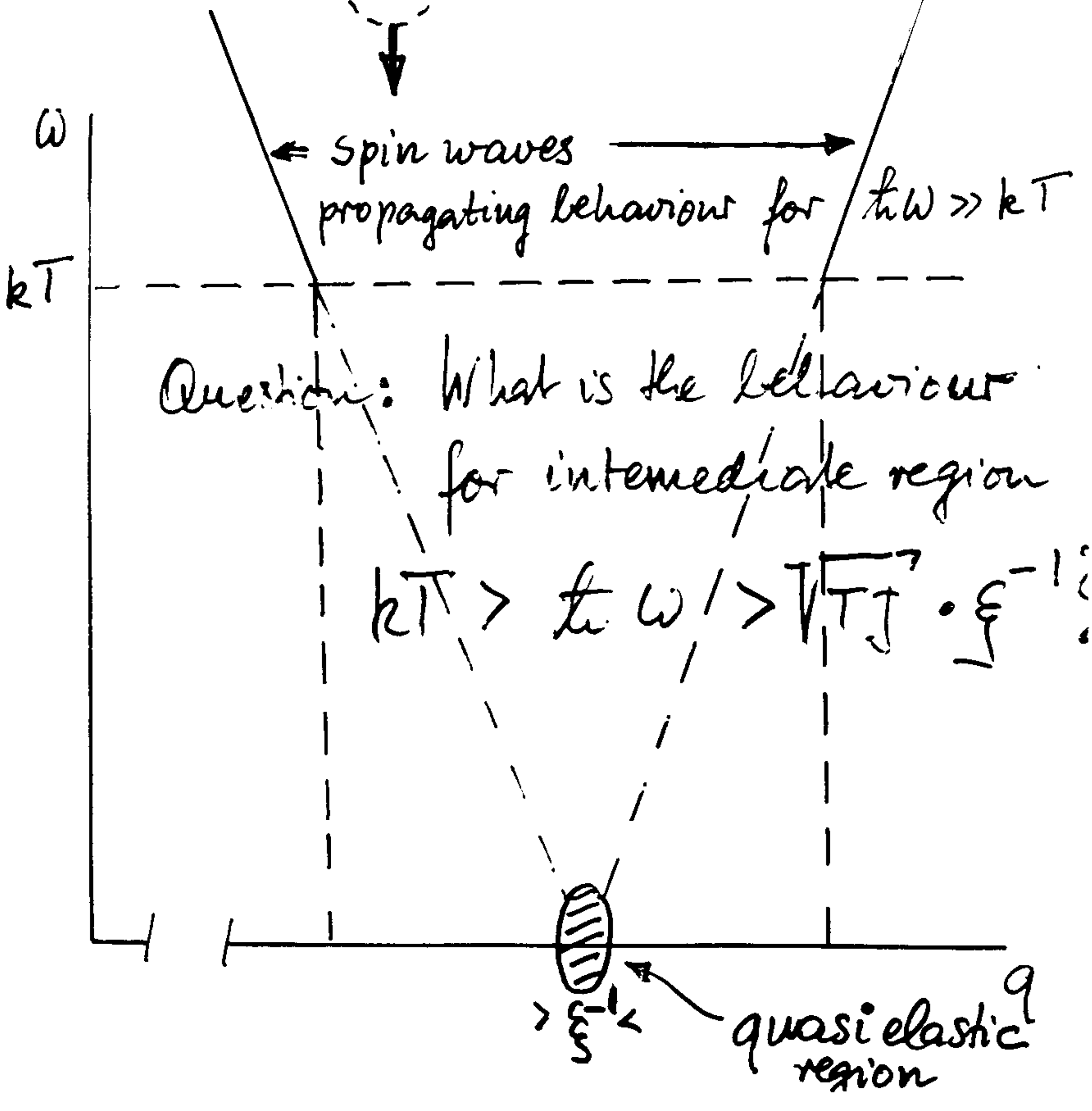




spectrum at finite T

$$T_N < T \ll J$$

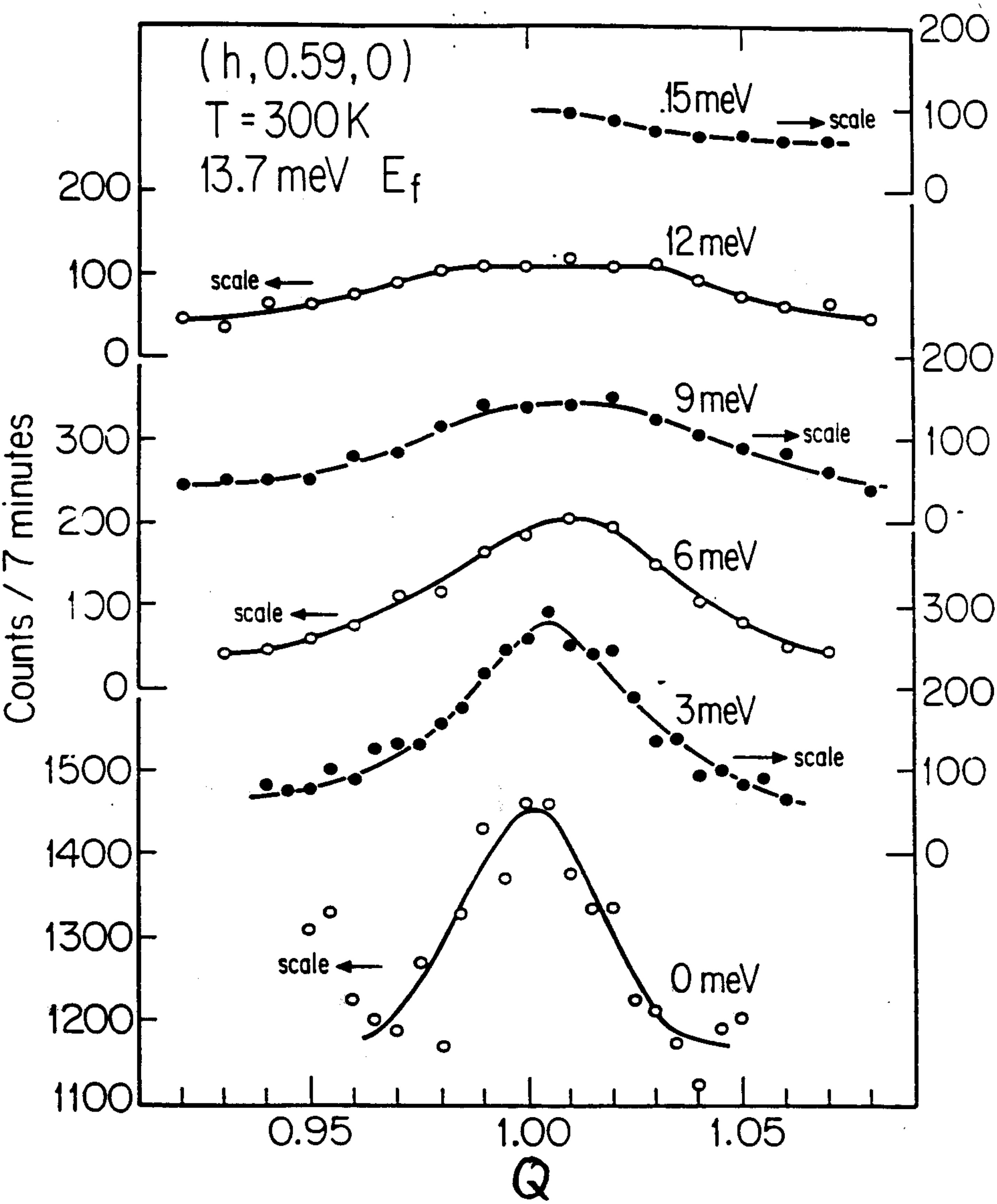




Question: What is the behaviour for intermediate region

$$kT > \hbar\omega > \sqrt{TJ}\cdot\xi^{-1} \,?$$

La_2CuO_4, Result from BNL, Shirane et al. [56]



Finite intensity in extremely narrow q-region,

→ very large correlation length $\xi \sim 200$ Å

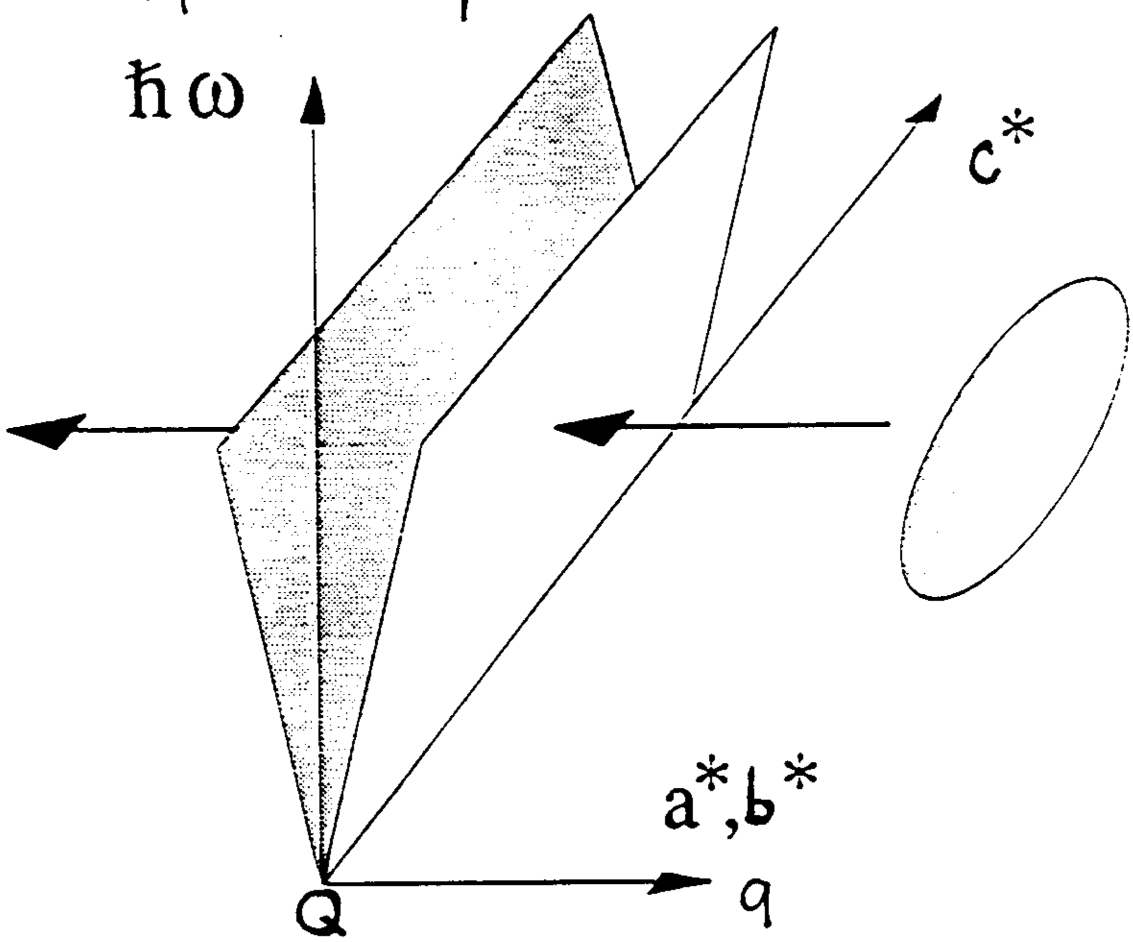
Interpretation: Spin waves for $q > \xi^{-1}$

$\hbar\omega_{\vec{q}} = c|\vec{q}_{\parallel}|$ independent of q_c.

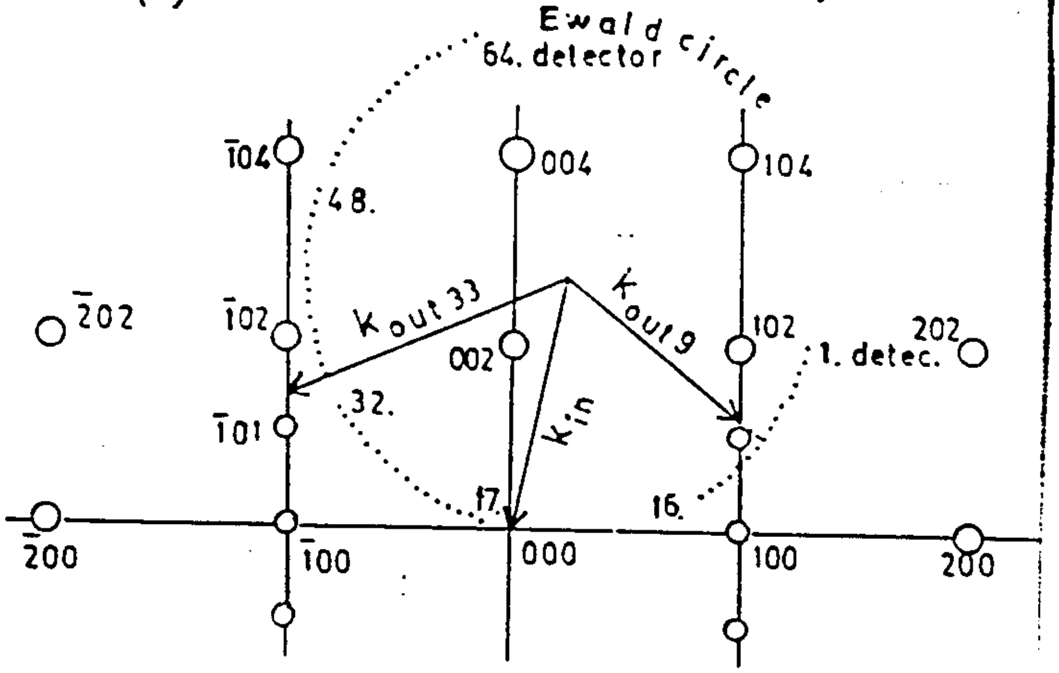
$\vec{q} = (q_a, q_b, q_c) = (\vec{q}_{\parallel}, q_c)$

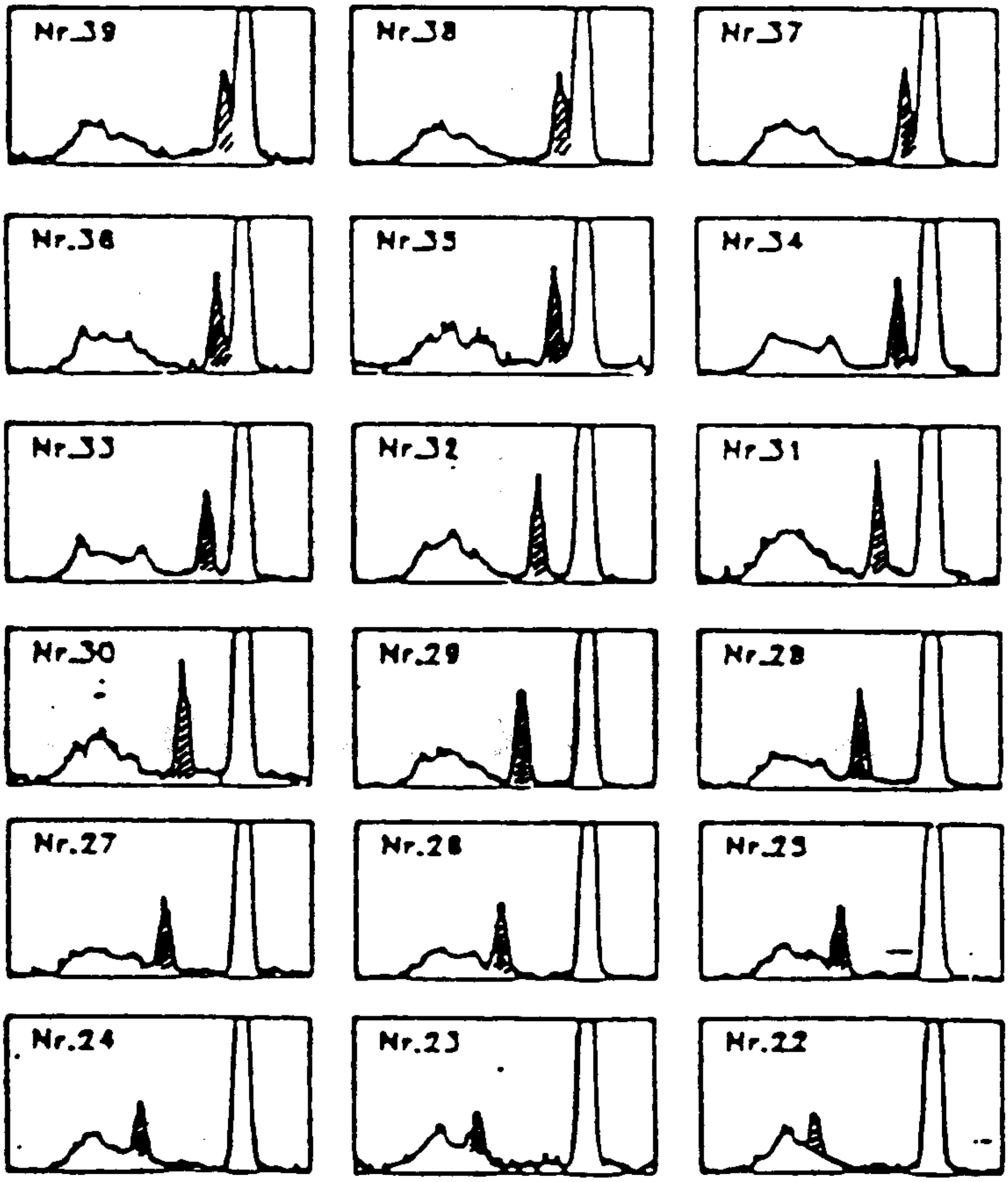
due to negligeable coupling $J_\perp$.

One experimental peak due to resolution.



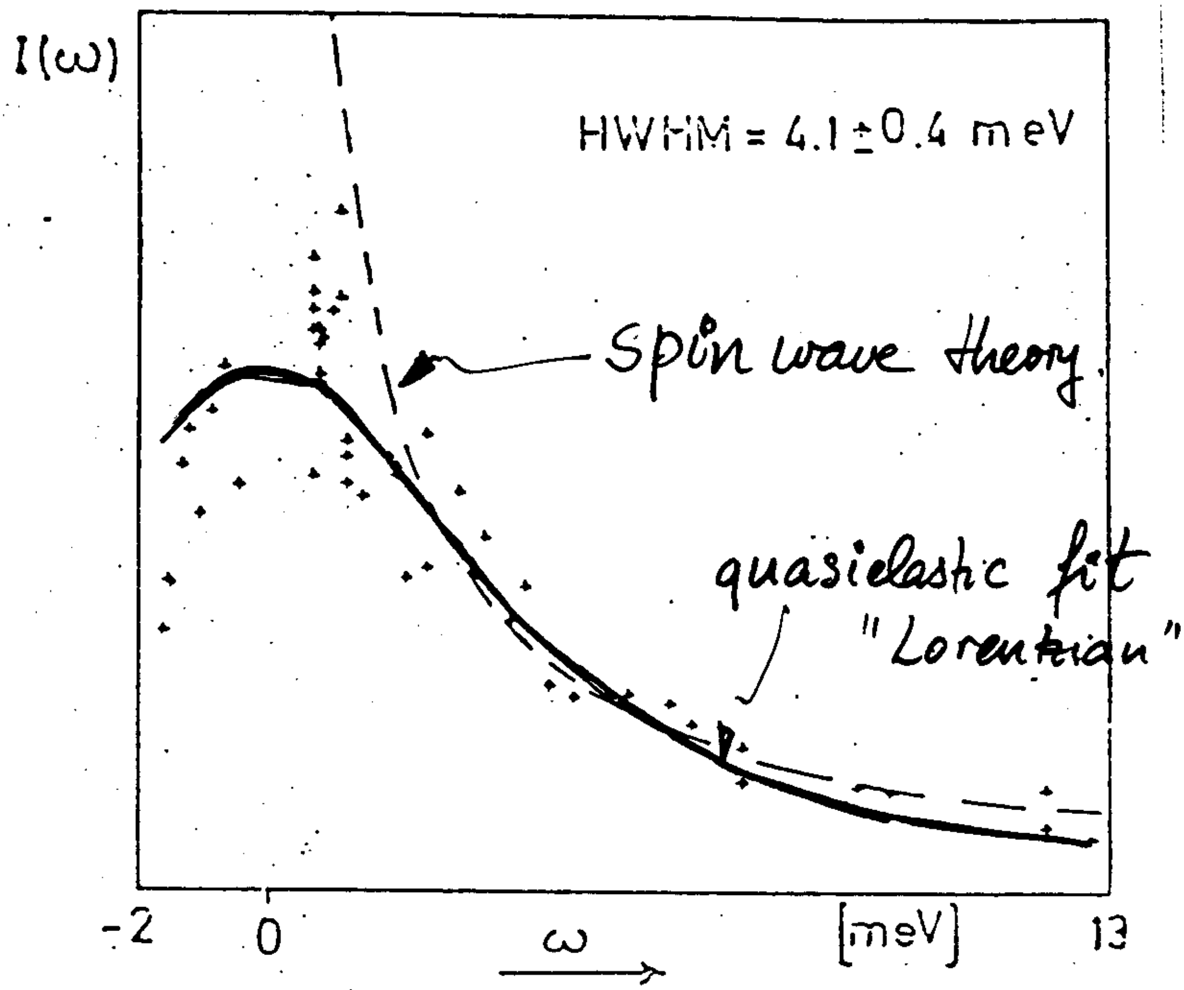
Problems: Where is the quasielastic peak?


Ewald circle
64. detector
48.
32.
17.
16.
1. detec.
K out 33
K out 9
K in
$\bar{1}04$
004
104
$\bar{2}02$
$\bar{1}02$
002
102
202
$\bar{1}01$
$\bar{2}00$
$\bar{1}00$
000
100
200


Nr.39
Nr.38
Nr.37
Nr.36
Nr.35
Nr.34
Nr.33
Nr.32
Nr.31
Nr.30
Nr.29
Nr.28
Nr.27
Nr.26
Nr.25
Nr.24
Nr.23
Nr.22

S

La_2CuO_4, (ILL: Schärpf et al.) , T = 300K



Theory: $H = \sum J_{ij} \vec{S}_i \cdot \vec{S}_j$; $S = 1/2$

$T = 0$; R.P.A.

$$\chi(\vec{q},\omega) = \frac{D}{4\pi}\sqrt{\frac{E_1}{E_2}}\left(\frac{1}{\omega - \sqrt{E_1 \cdot E_2} + i\varepsilon} - \frac{1}{\omega + \sqrt{} + i\varepsilon}\right)\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix}$$

where $D = |\langle S_{iz}\rangle| \cong 0.36$; $\Rightarrow M \cong .72\,\mu_B$

for 2d square lattice

$$E_1(q) = 2D\,(J_Q - J_{Q+q}) \quad \sim q^2$$

$$E_2(q) = 2D\,(J_{\vec{Q}} - J_{\vec{q}}) \quad \sim \frac{1}{(\vec{Q}-\vec{q})^2}$$

For 2d-system no long range order at finite T (Hohenberg, Marmin, Wagner) due to divergence of

$$\sum_q \int d\omega\, S(q,\omega) \quad \text{for } \vec{q} \to \vec{Q}$$

$$\sim \sum_q \int d\omega\, \frac{T}{\omega}\, \mathrm{Im}\,\chi(\vec{q},\omega)$$

→ No spin waves in small k-region
($\vec{k} = \vec{q} - \vec{Q}$)

– $T=0$ Bragg peak aquires finite width $\sim \xi^{-1}$
ξ = correlation length,
exponentially large!

⇒ 3 k-regions:

I: $k < \xi^{-1}$

II: $\xi^{-1} < k < \frac{k_B T}{c} = q_c$; c = spin wave velocity

III: $q_c < k < q_D$; $q_D \sim$ Brillouin zone boundary

I: quasielastic; relaxational behaviour

III: propagating spin waves; oscillating.

II: ?? question: relaxational or oscillating.

Simple argument: For $k > \xi^{-1}$ lack of long range order unimportant.
→ spin waves, oscillating.
(Too simple!!)

Discuss: $S(k) = \int d\omega\, S(k,\omega)$

Remember: $\sum_k S(k) = N\, S(S+1)$

1) For small k: quasielastic region

$$S_1(k) = A_1 \cdot N \frac{k_B T}{J} \frac{1}{q^2 + \xi^{-2}}$$

$\sum_k S_1(k) =$ total quasielastic intensity

$\approx$ Braggintensity at $T=0$

2) Define $\tilde{q}$ such that for $k > \tilde{q}$ spin wave behaviour:

$$S_2(k) = A_2 N \frac{ac}{\varepsilon(k)} g(k,\tilde{q}) \coth \frac{\varepsilon(k)}{k_B T}$$

where $\varepsilon(k) =$ spin wave energy

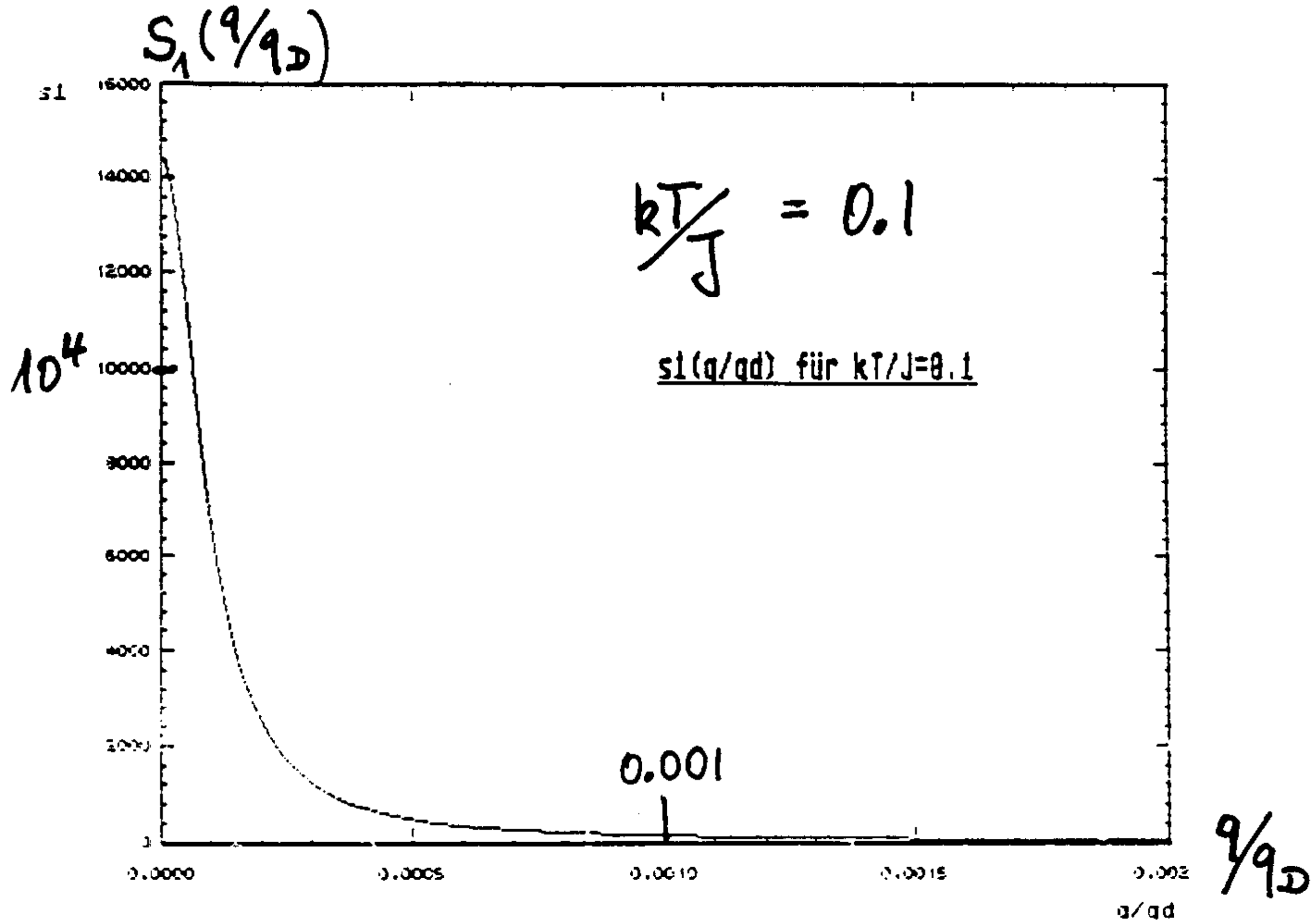
$$g(k,\tilde{q}) = \begin{cases} \to 1 & \text{for } k > \tilde{q} \\ \to 0 & \text{for } q < \tilde{q} \end{cases}$$

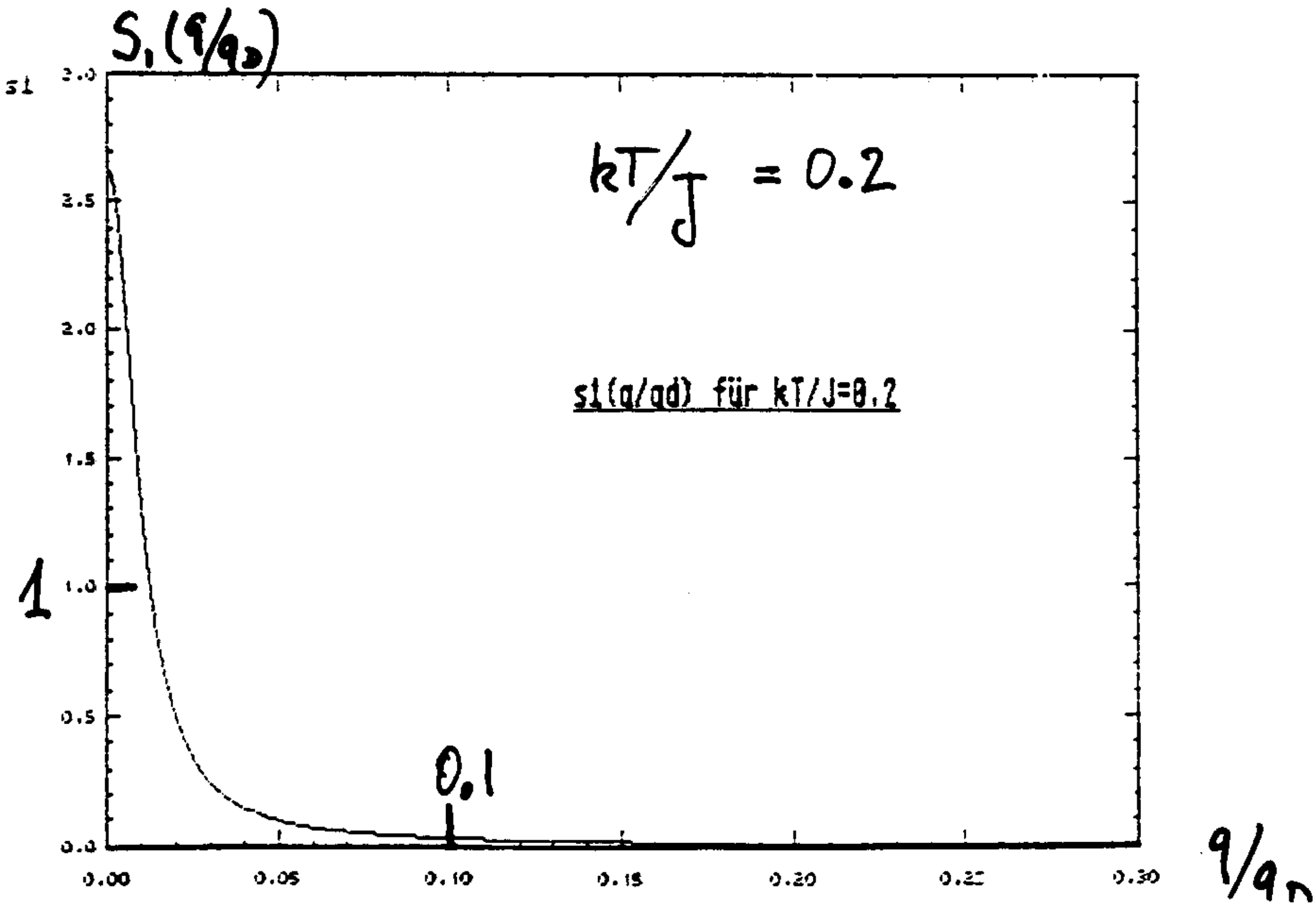
Ensure that $\sum_k \left(S_1(k) + S_2(k)\right) = N\, S(S+1)$

$$\Longrightarrow \quad \xi \simeq \frac{1}{q_D} \exp\left\{ \frac{(bS)^2}{2\pi A_1} \cdot \frac{J}{k_B T} \right\}$$

$\tilde{q} \simeq q_c(T) \simeq \frac{k_B T}{c}$: No spin waves for $\varepsilon(k) < k_B T$

Beschreibung des quasielastischen Anteils





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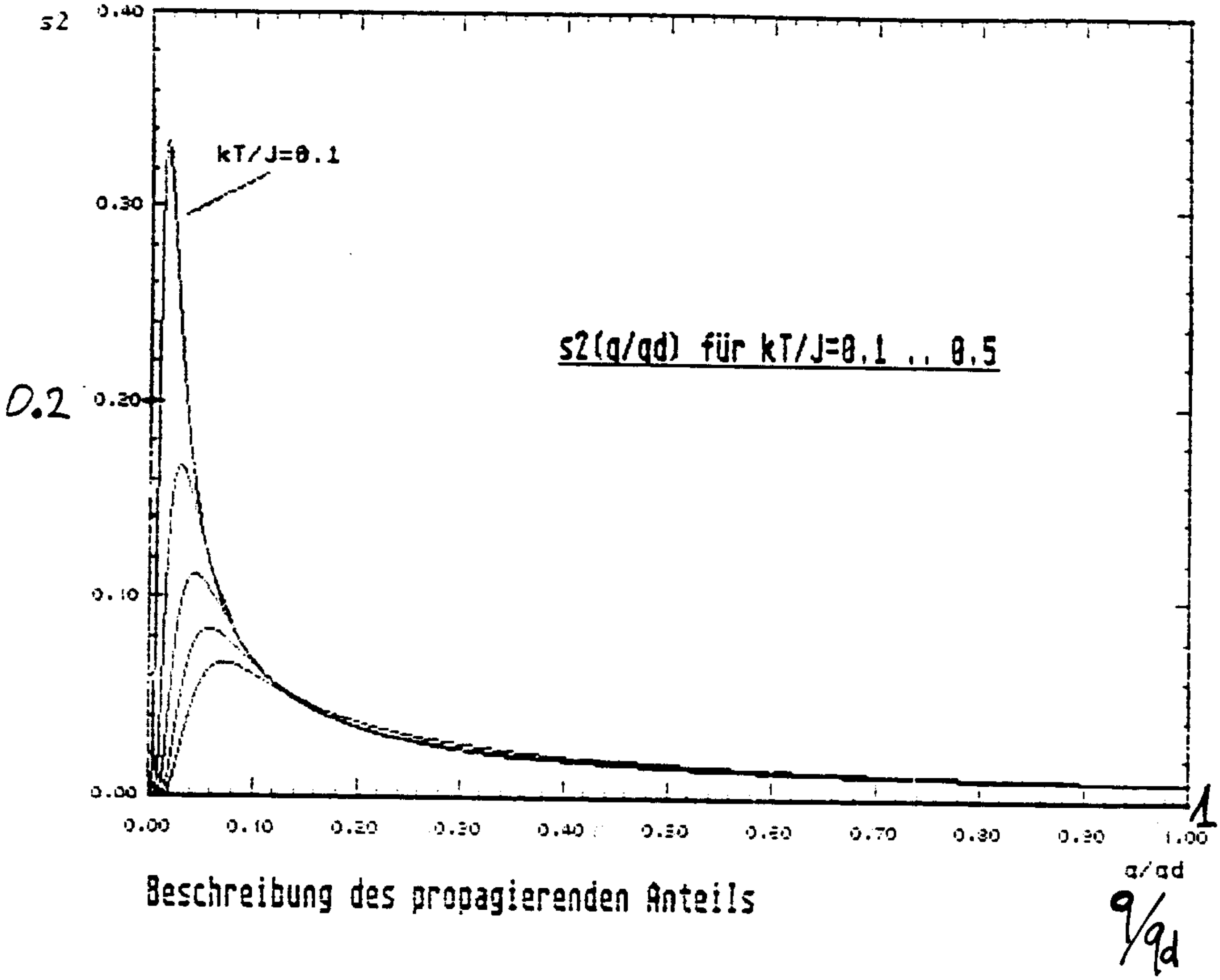
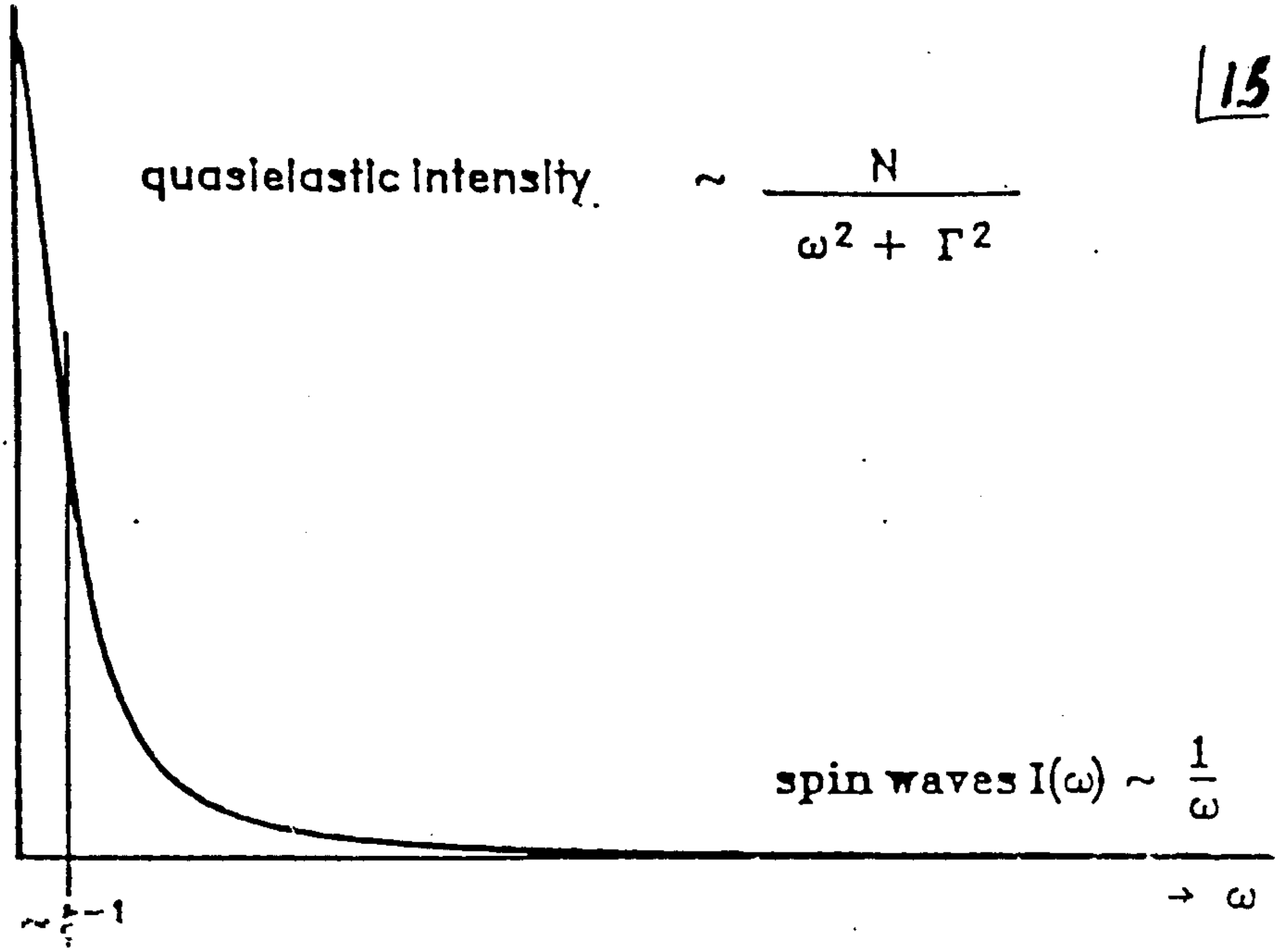
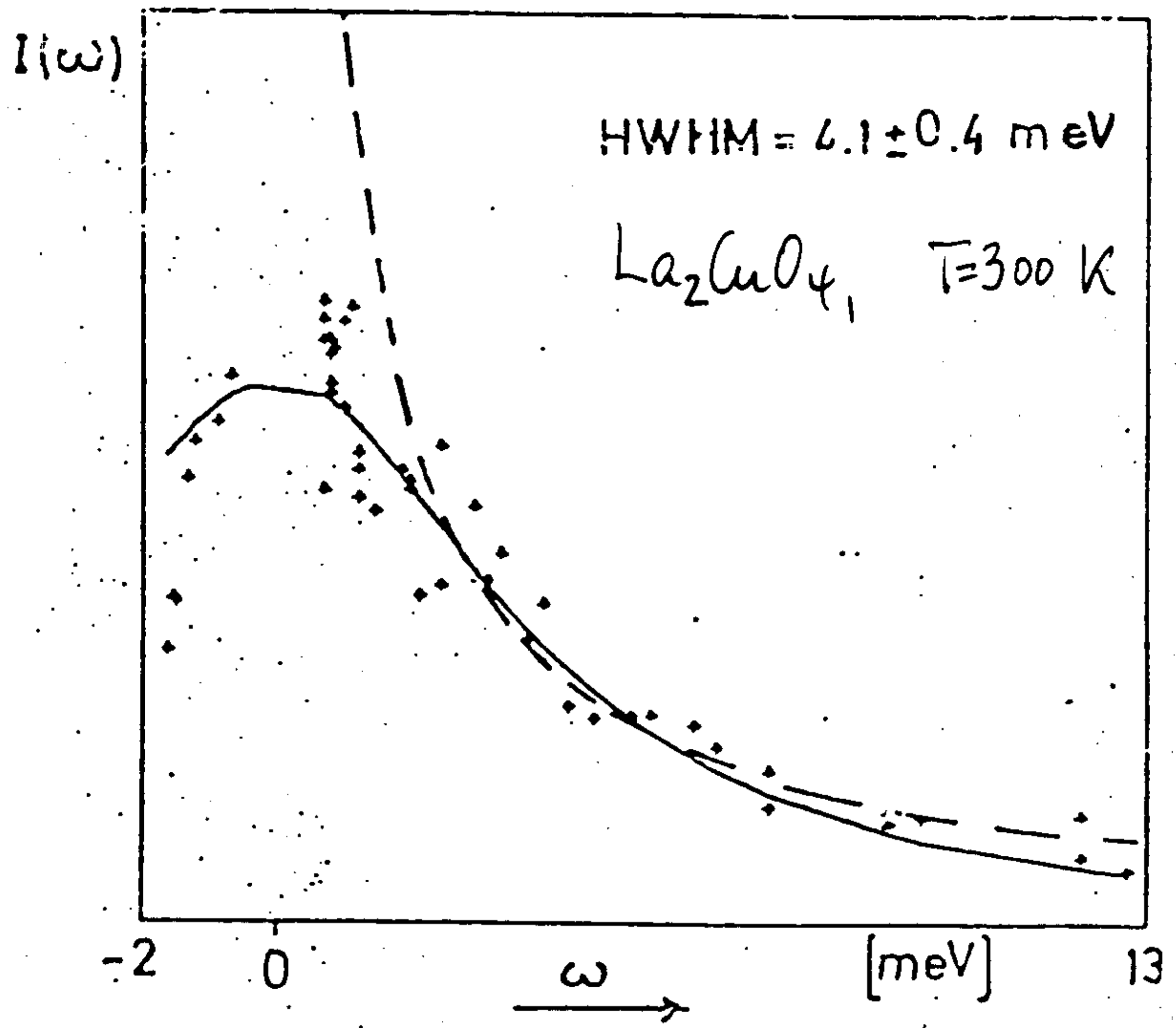


Beschreibung des propagierenden Anteils


quasielastic intensity $\sim \frac{N}{\omega^2 + \Gamma^2}$
spin waves $I(\omega) \sim \frac{1}{\omega}$
$\sim \xi^{-1}$
$\to \omega$


$I(\omega)$
HWHM = 4.1 ± 0.4 meV
La_2CuO_4, T=300 K
-2
0
ω
[meV]
13

quasielastic width : La_2CuO_4 , $T = 300\,K$

$$\Gamma_{exp} \simeq 4.1 \pm 0.4 \text{ meV}$$

mode-mode coupling theory (Grempel) : $\Gamma_G \cong 3.4$ meV

dynamic scaling (Tyc, Halperin, Chakravarty) : $\Gamma_H \cong 3$ meV

(No adjustable parameters for dynamics, all parameters determined from static properties).

$\Rightarrow$ Heisenberg model with stable $S = 1/2$ moments works well for La_2CuO_4

Similar properties for $YBa_2Cu_3O_6$.

Question: What happens for $La_{1.85}Sr_{.15}CuO_4$?
$YBa_2Cu_3O_7$.

Most detailed experiments for $YBa_2Cu_3O_{6+x}$

Rossat-Mignod et al. , ... Schärpf et. al ....

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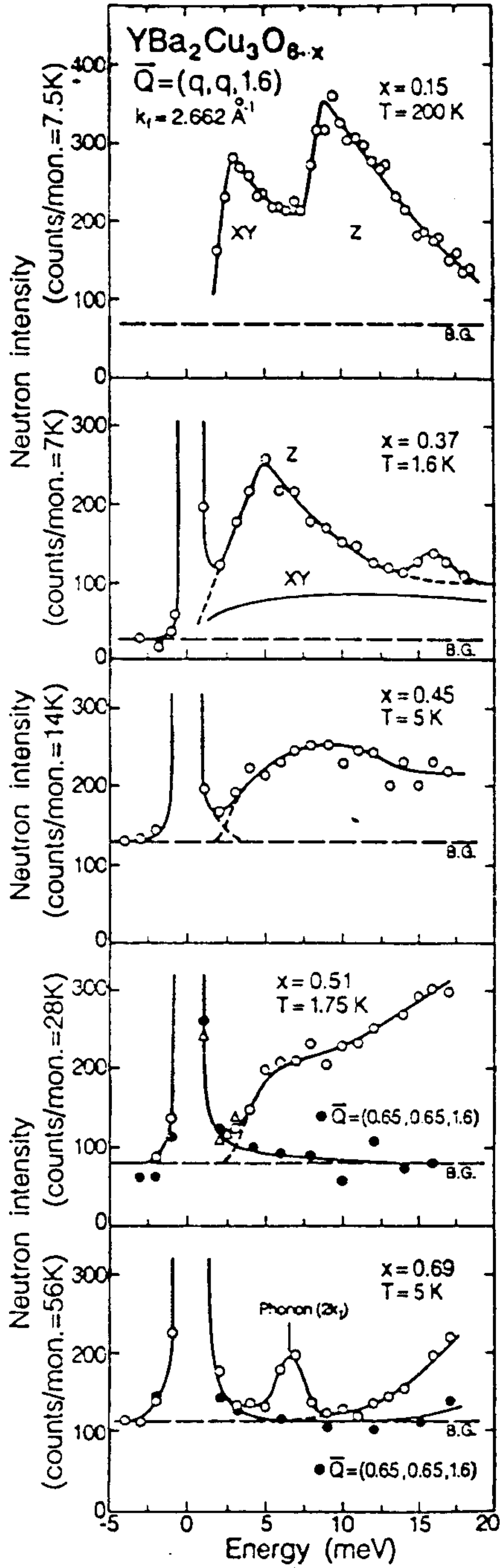
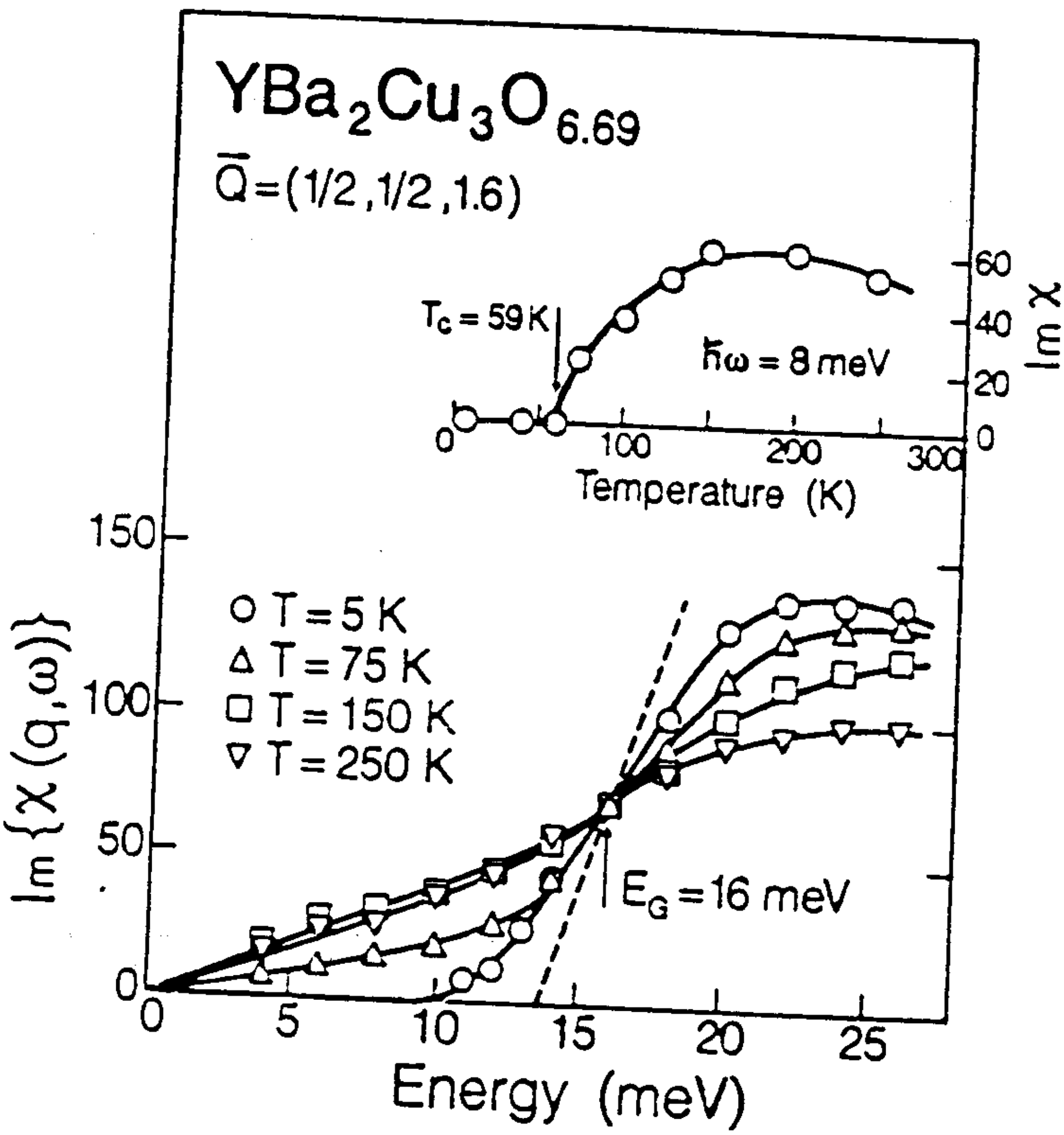
Rossat Mignod et al.

(ILL)



Rossat-Mignod et al. (ILL).



→ T21, T22

Magnetic properties, Summary:

La_2CuO_4 ; $YBa_2Cu_3O_6$ are quasi 2 dim. antiferromagnetic insulators.

"Quantum-Anti-Ferro-Magnetism - QAFM"

reasonably well described by spin ½ Heisenberg-m

Experimental facts

$YBa_2Cu_3O_7$ - superconducting - has <u>no</u> spin fluctuations in low energy region:

$$\int_{-30\,meV}^{+30\,meV} d\omega \sum_{\vec{q}} S(\vec{q},\omega) \text{ vanishingly small}$$

⇒ <u>no</u> slowly fluctuating, short range ordered magnetic background!

? Conclusions ? :

No moments, no pair breaking ⇒ Superconductivity possible

or

- superconductivity due to high energy spin fluct.

Anomalous lattice dynamics

(Experiments by Pintschovius, Reichardt, ...
Karlsruhe, Paris)

Materials studied

La_2CuO_4 (Ni_2CuO_4)

$La_{1.9}Sr_{0.1}CuO_4$

$YBa_2Cu_3O_6$

$YBa_2Cu_3O_7$

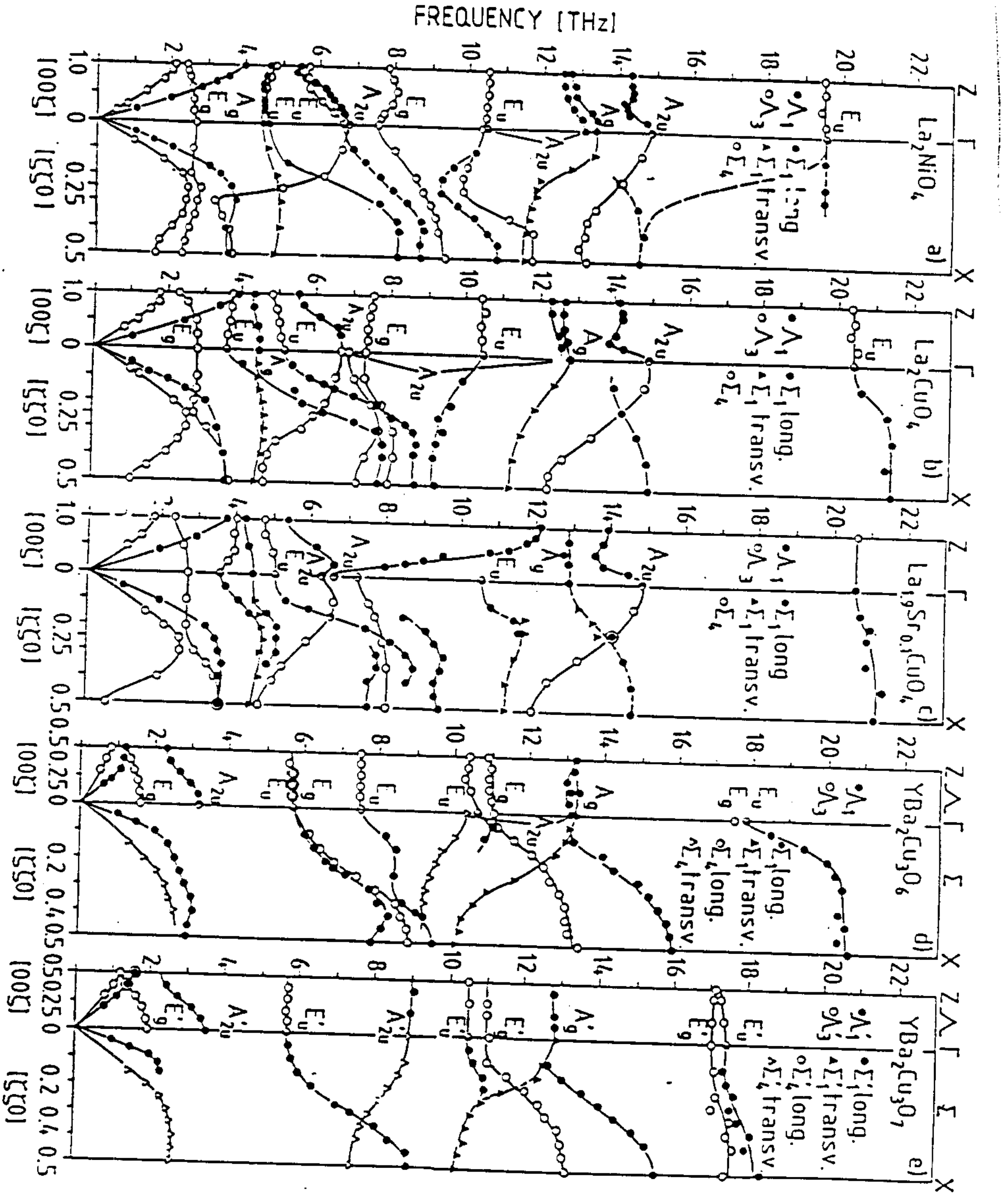
Measurements of <u>full</u> phonon spectra
in La_2CuO_4 (Ni_2CuO_4), $La_{1.9}Sr_{0.1}CuO_4$

$\Rightarrow$ Extra degree of freedom!

Partial information on $YBa_2Cu_3O_{6-7}$

$\Rightarrow$ Strong similarities to La_2CuO_4 ....

Pintschovius, Reichardt, et al.



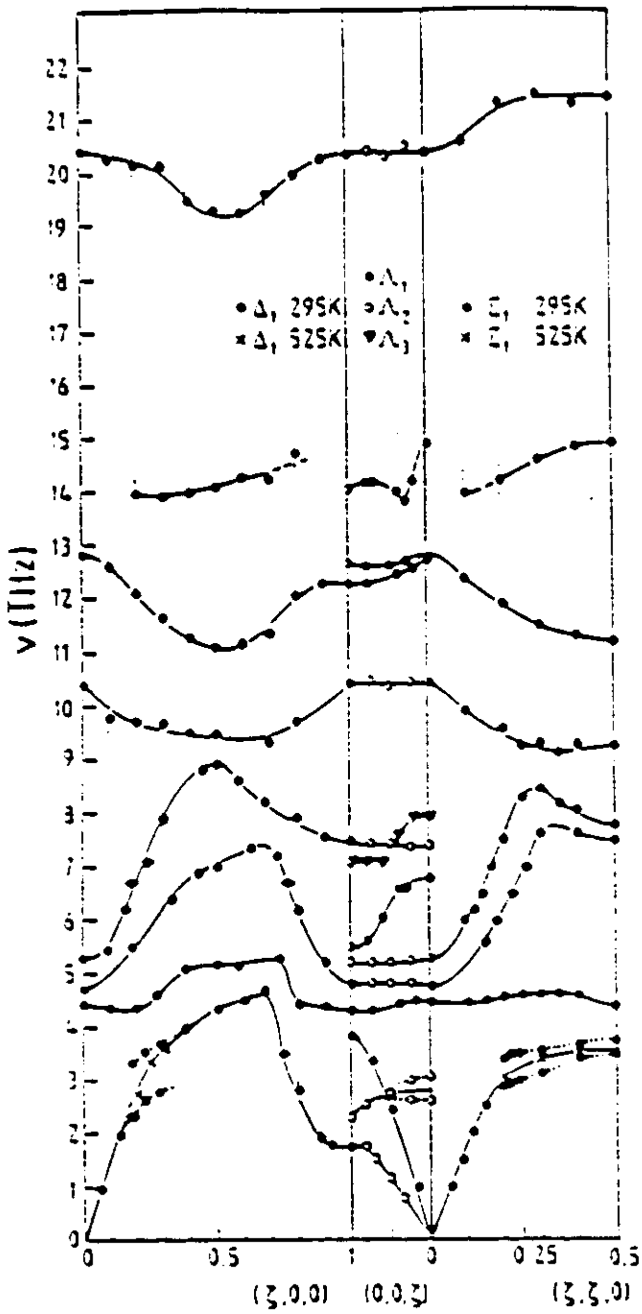


Fig. 3 continued

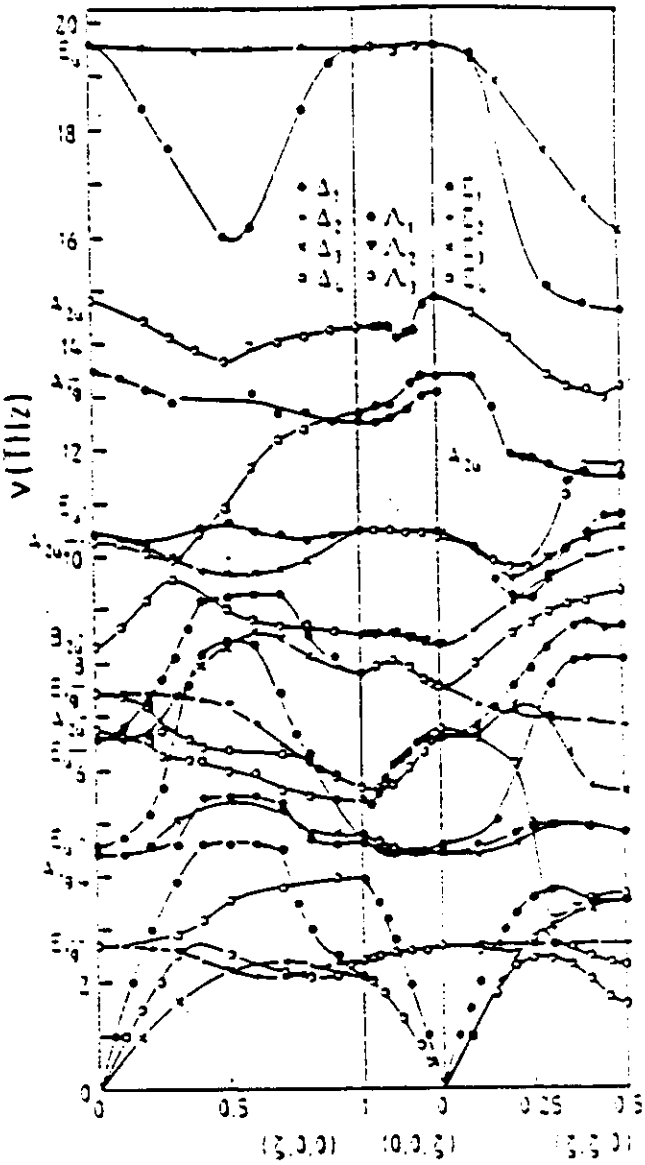
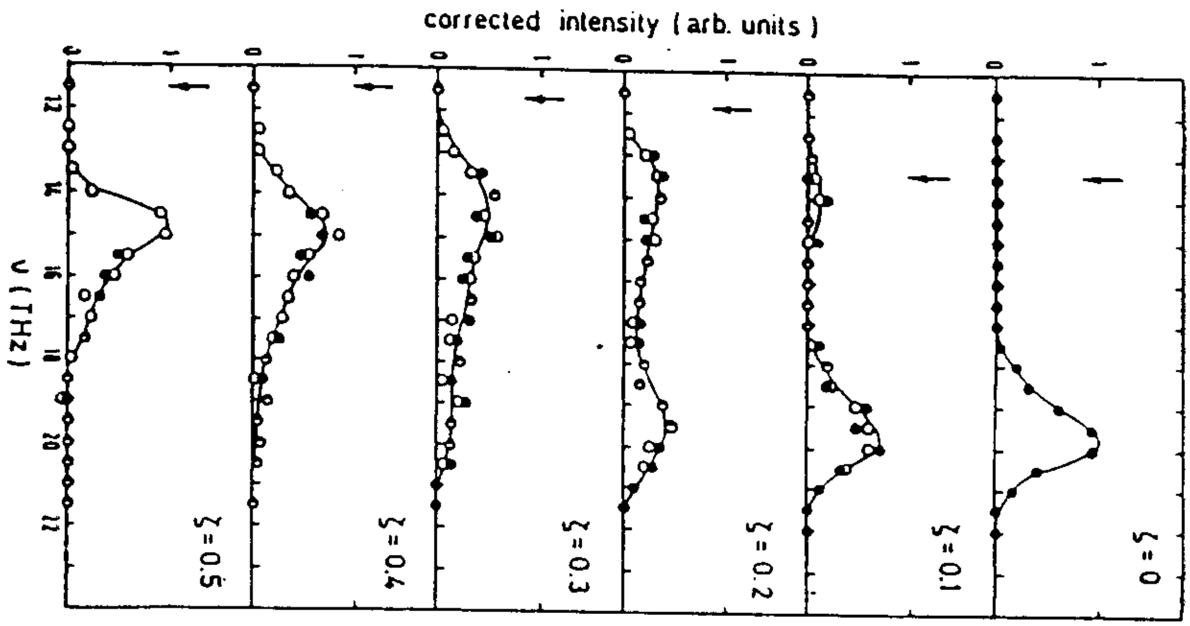
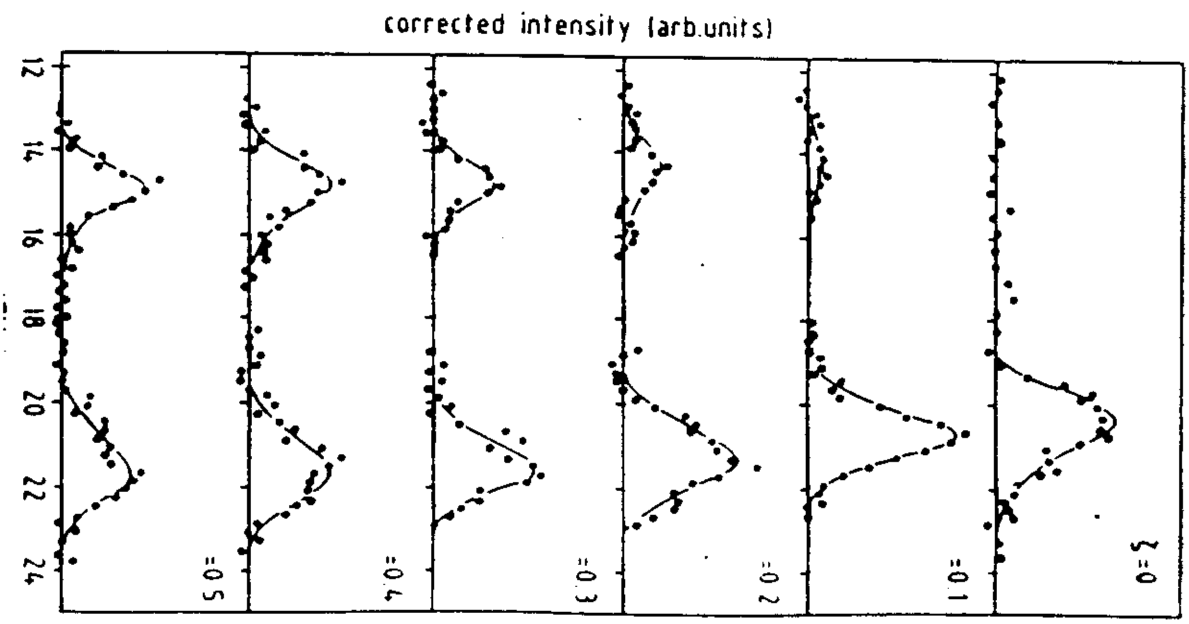


Fig.4: Phonon dispersion curves in La_2CuO_4 at room temperature (ref. 11). Lines are a guide to the eye.


corrected intensity (arb. units)
ν (THz)
12
14
16
18
20
22
0
1
ζ = 0.5
ζ = 0.4
ζ = 0.3
ζ = 0.2
ζ = 0.1
ζ = 0


corrected intensity (arb.units)
12
14
16
18
20
22
24
=0.5
=0.4
=0.3
=0.2
=0.1
ζ=0

• Possible explanation :

- Existence of "low energy" collective electronic charge excitation with $\hbar\omega < 100$ meV (instead of usual eV)

- hybridization with "high energy" oxygen vibrations (~ 80 meV) give mixed modes, ⇒ "extra mode" in neutron scattering.

Open questions: Origin of low $\hbar\omega$ charge excitation?

Consequences on superconductivity?