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SMR 1232 - 14

XII WORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

17 - 28 July 2000

DO WE KNOW EVERYTHING ABOUT THE MAGNETISM OF CUPRATES?

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

Do we know everything about the magnetism of cuprates?

Beyond Heisenberg

R.Coldea(ORNL,RAL)

P.Dai(ORNL)

H.A.Mook(ORNL)

S.M.Hayden(Bristol)

Z.Fisk(NHMFL)

S-W.Cheong(Lucent/Rutgers)

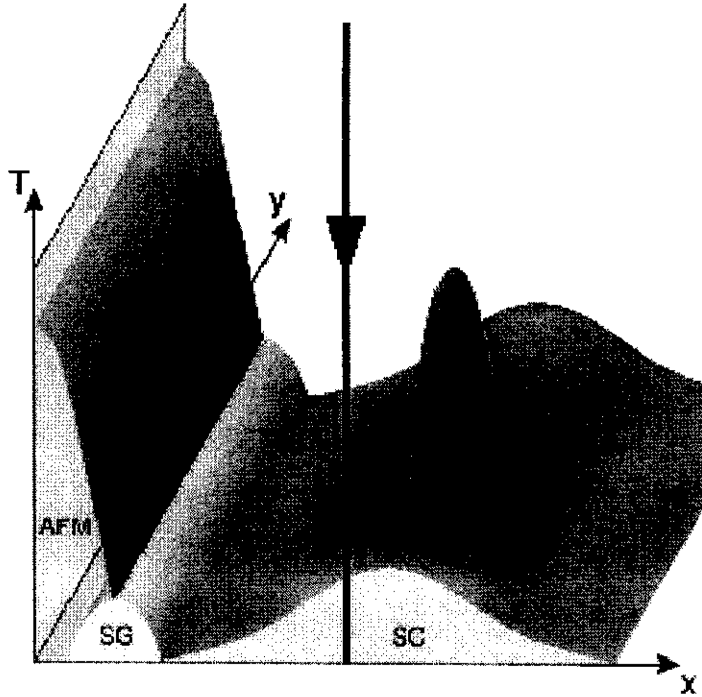
T.G. Perring(RAL)

F.Dogan(UW)

T.E.Mason(ORNL)

Things we know

- 2-dimensionality
- phase diagram
- Heisenberg model with strong nearest neighbor exchange



From "Nearly Singular Magnetic Fluctuations in the Normal State of a High-T_c Cuprate Superconductor", G. Aeppli, T. E. Mason, S. M. Hayden, H. A. Mook, J. Kulda, *Science* **278**, pp. 1432-1435 (1997)

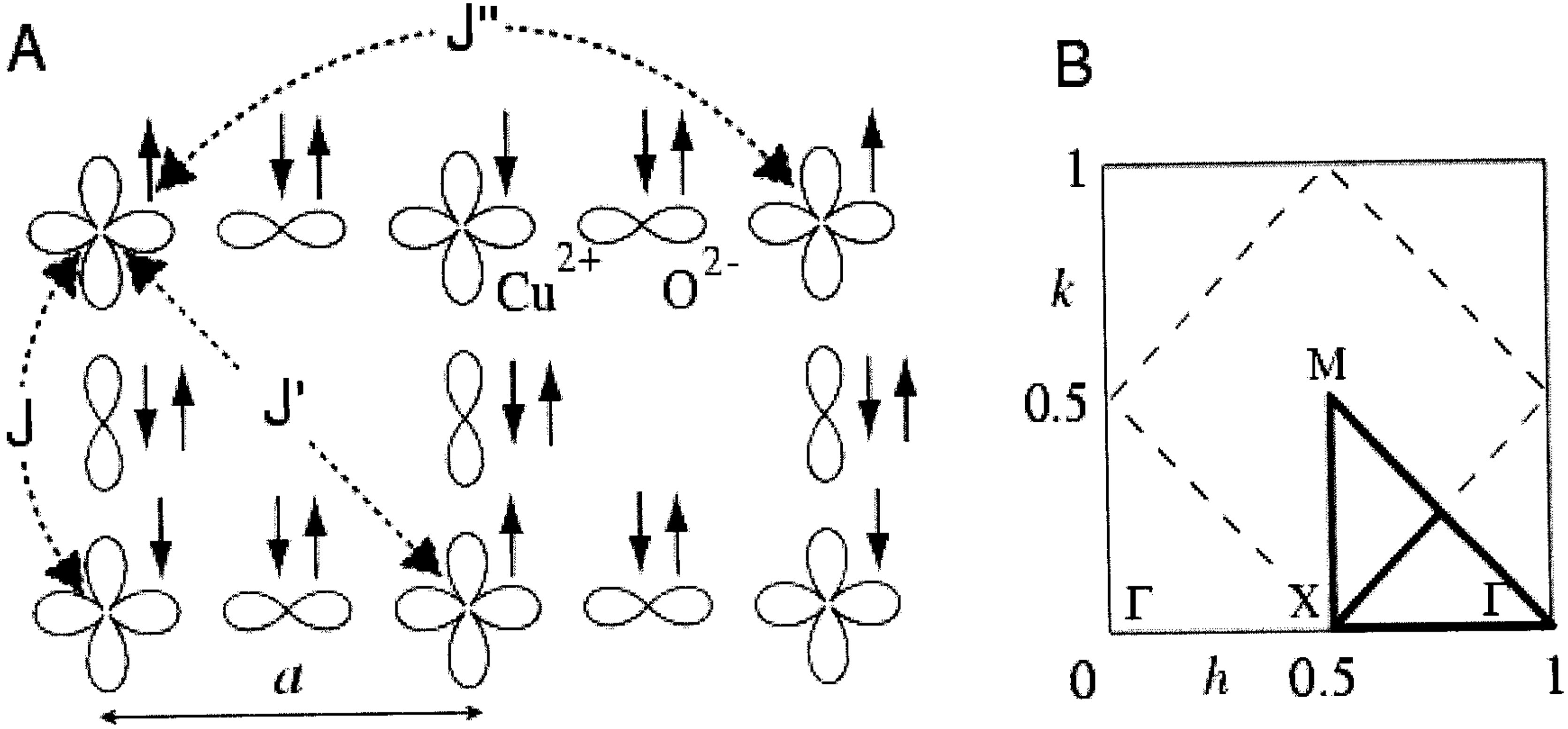
Naïve(Heisenberg)picture of spin physics in hi-T_c materials

- Starting point is AFM Heisenberg Hamiltonian
- a QCP between AFM and Spin Fluid phases with pairing built in
- damping to take account of metallicity
- appropriate embellishments for spare ground states(e.g. black mountain) found in some alloy series

Is Heisenberg picture all we need to understand spin sector of hi-T_c problem?

- Revisit insulator(Dai et al,Cond Mat 2000)
- look at excitations in the s.c.(Coldea et al,Cond Mat 2000)

La_2CuO_4



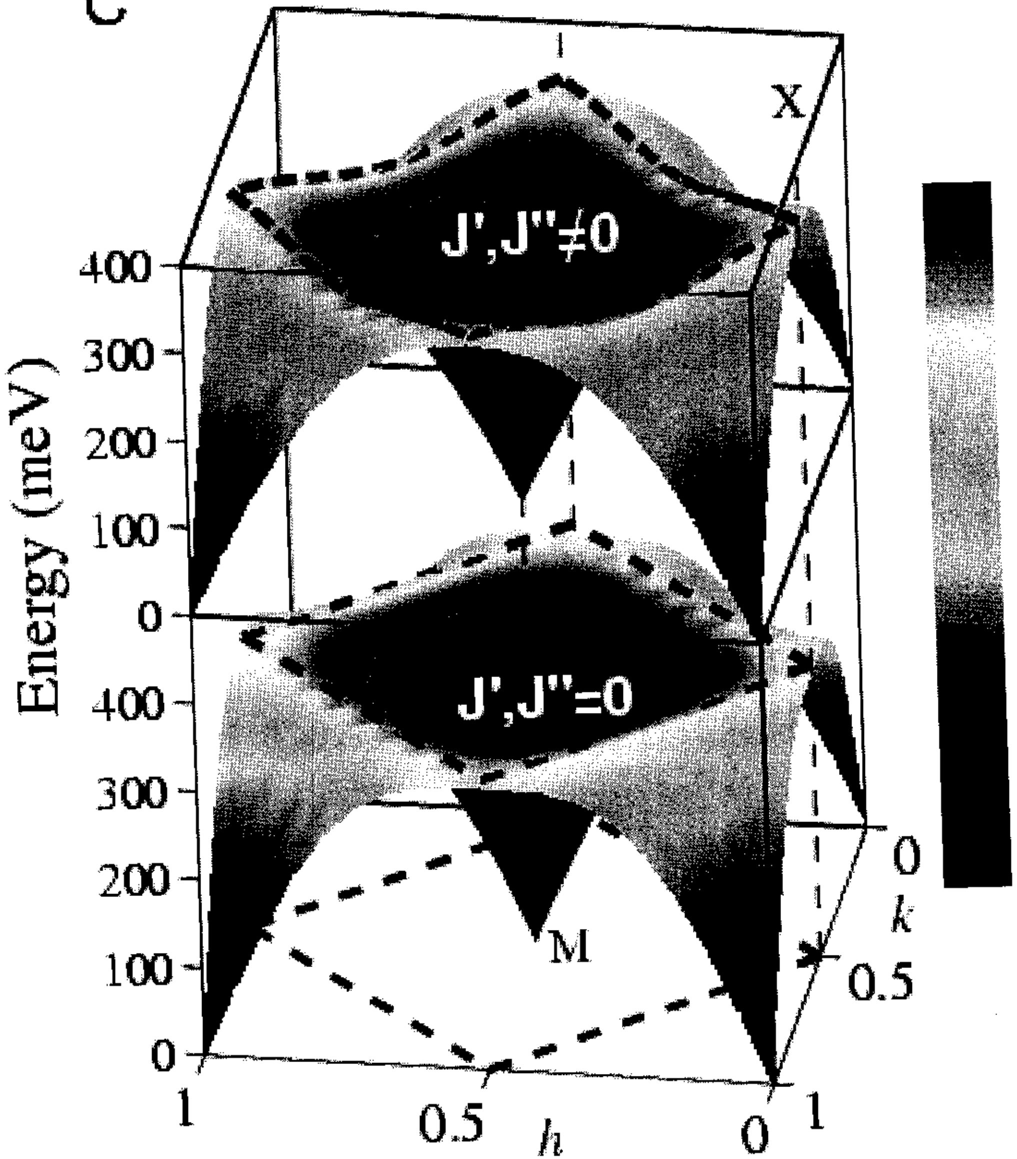
Spin wave theory

$$\mathcal{H} = \sum_{i,\delta} J\mathbf{S}_i \cdot \mathbf{S}_{i+\delta} + \sum_{i,\delta'} J'\mathbf{S}_i \cdot \mathbf{S}_{i+\delta'} + \sum_{i,\delta''} J''\mathbf{S}_i \cdot \mathbf{S}_{i+\delta''}$$

$$\begin{aligned}
\hbar\omega_Q &= 2Z_c J\sqrt{A_Q^2 - B_Q^2} \\
A_Q &= 1 - \frac{J'}{J}\left(1 - \cos(2\pi h)\cos(2\pi k)\right) - \frac{J''}{J}\left(1 - \frac{\cos(4\pi h) + \cos(4\pi k)}{2}\right) \\
B_Q &= \frac{\cos(2\pi h) + \cos(2\pi k)}{2}
\end{aligned}$$

Z_c=quantum renormalization factor =1.18

C


X
J',J''≠0
J',J''=0
Energy (meV)
400
300
200
100
0
400
300
200
100
0
M
1
0.5
h
0
1
0.5
k
0

Why neutrons?

- Electrons have charge and spin, many excellent probes of charge sector(e.g.electron & photon spectroscopies described elsewhere in this meeting), many interesting properties of solids in spin sector(e.g. magnetism)
- want neutral & easily interpretable probe of spin sector

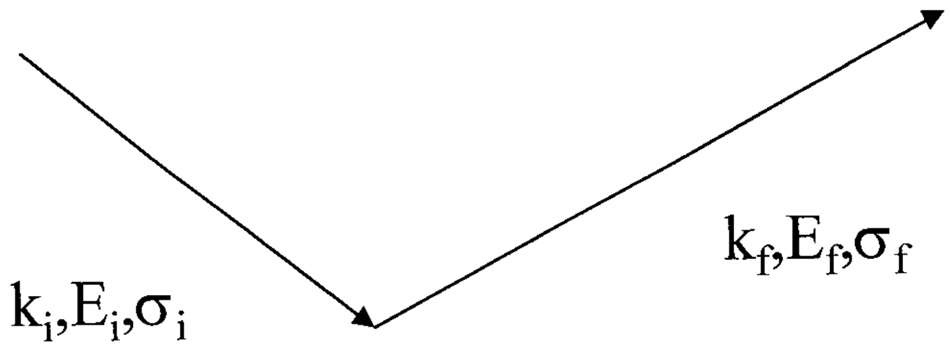
Neutrons are an ideal probe because-

- they carry spin(1/2) but not charge
- $E=hk^2/2m$ with m=mass of proton=mass of hydrogen so that
  λ=interatomic spacings
- wide spectral range with modern sources
  1meV<E<1eV
- weak coupling, so simple expressions for cross-sections

Some useful facts

- $h^2/2m$=2.07meV-A^2
- 1meV=11.6K
- 4.14meV=1THz=10^{12}Hz
- a 5 meV neutron has a wavelength of 4.05A & velocity of 976m/sec
- m=$1.82 \times 10^3 m_e$

Scattering experiments



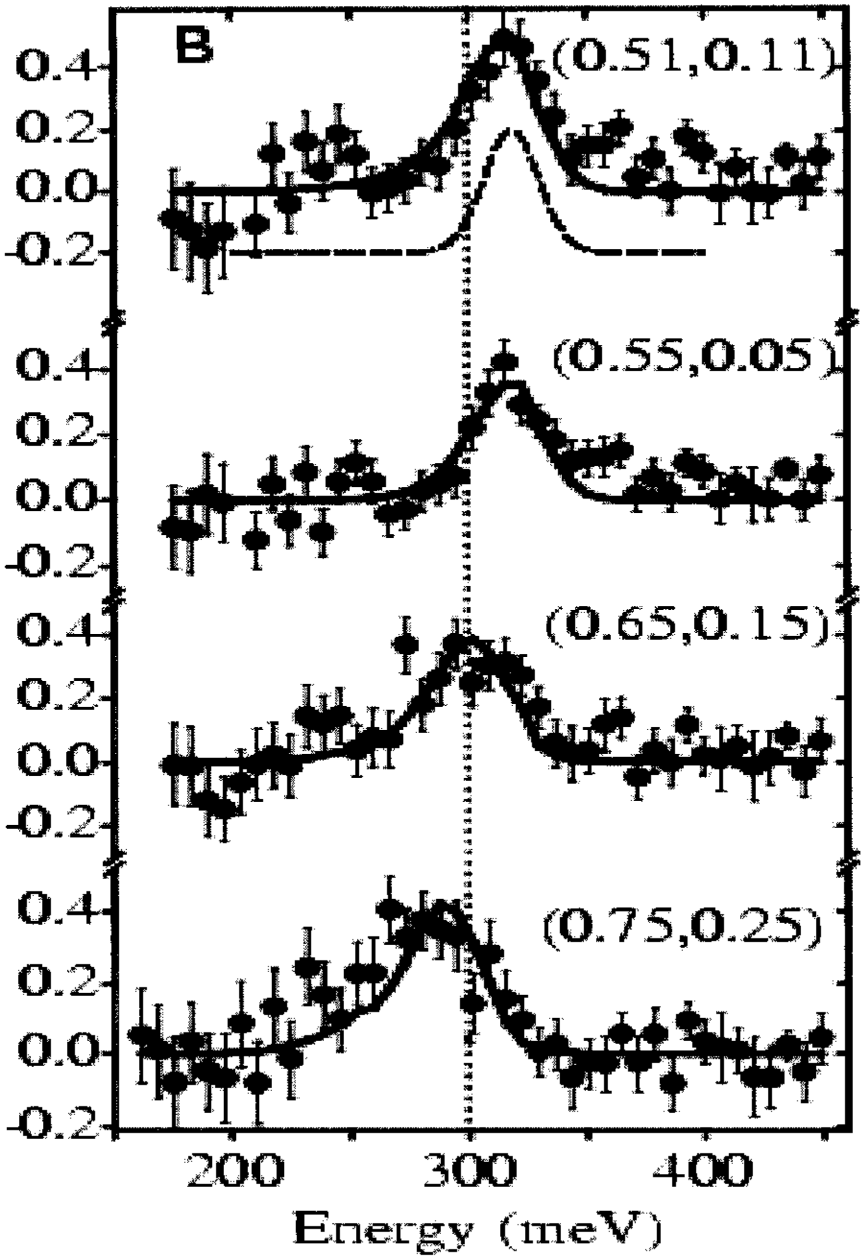
$$Q = k_i - k_f$$

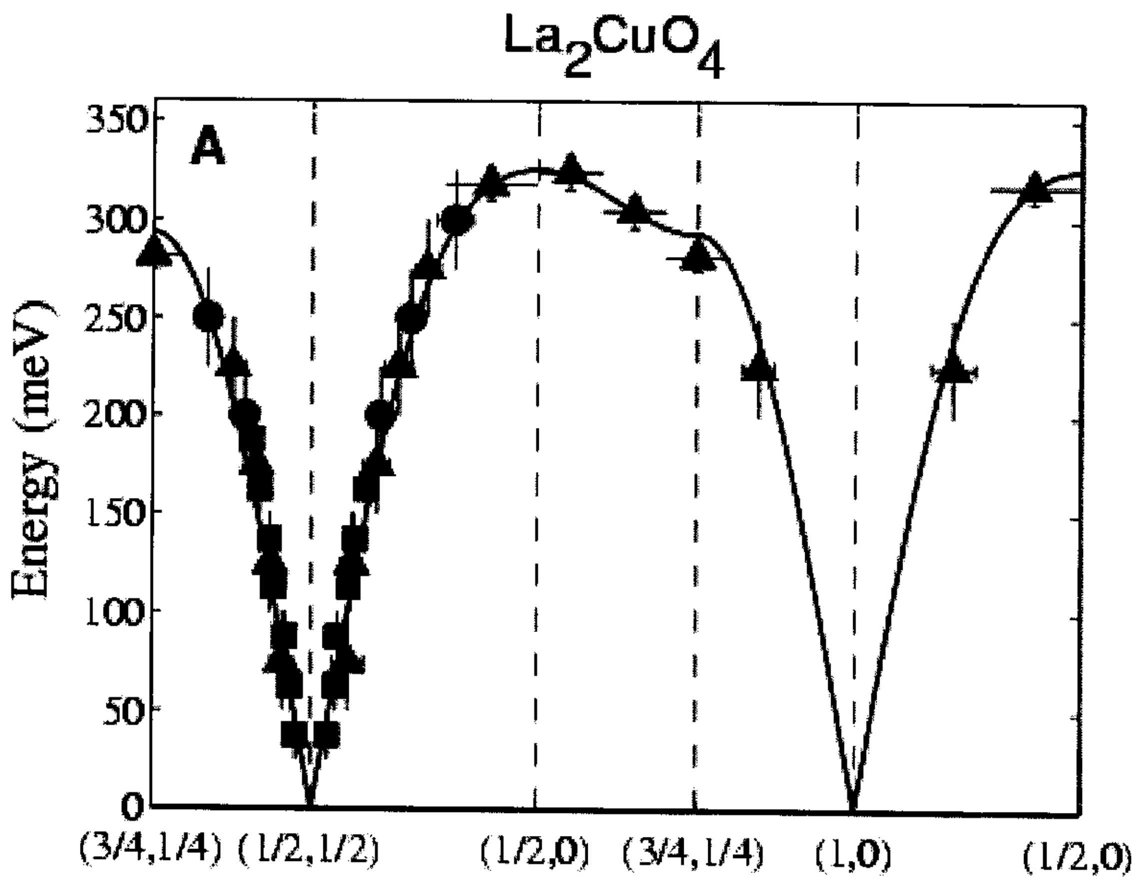
$$h\omega = E_i - E_f$$

Measure differential cross-section=ratio of outgoing flux per unit solid angle and energy to ingoing flux=$\delta^2\sigma/\delta\Omega\delta\omega$

inelastic neutron scattering Fermi's Golden Rule

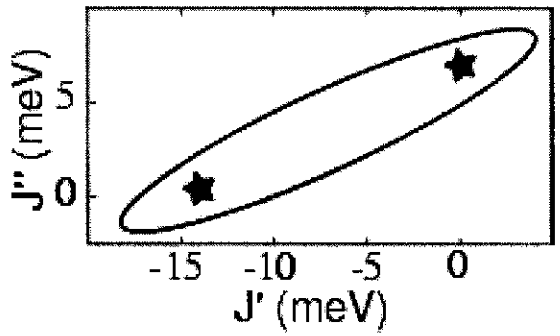
- at T=0,
  $\delta^2\sigma/\delta\Omega\delta\omega=\Sigma_f|<f|S(Q)^+|0>^2\delta(\omega-E_0+Ef)$ where
  $S(Q)^+ =\Sigma_m S_m{}^+ \exp iq.r_m$
- for finite T, $\delta^2\sigma/\delta\Omega\delta\omega= k_f/k_i\ S(Q,\omega)$ where
  $S(Q,\omega)=n(\omega+1)\mathrm{Im}\chi(Q,\omega)$


B
(0.51,0.11)
(0.55,0.05)
(0.65,0.15)
(0.75,0.25)
0.4
0.2
0.0
-0.2
200
300
400
Energy (meV)


La2CuO4
A
Energy (meV)
350
300
250
200
150
100
50
0
(3/4,1/4)
(1/2,1/2)
(1/2,0)
(3/4,1/4)
(1,0)
(1/2,0)

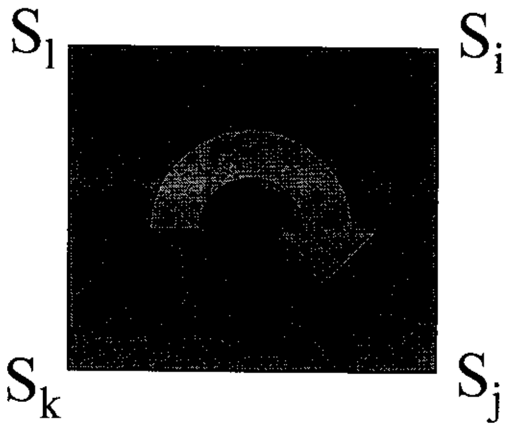
$$\mathcal{H} = \sum_{i,\delta} J\mathbf{S}_i \cdot \mathbf{S}_{i+\delta} + \sum_{i,\delta'} J'\mathbf{S}_i \cdot \mathbf{S}_{i+\delta'} + \sum_{i,\delta''} J''\mathbf{S}_i \cdot \mathbf{S}_{i+\delta''}$$

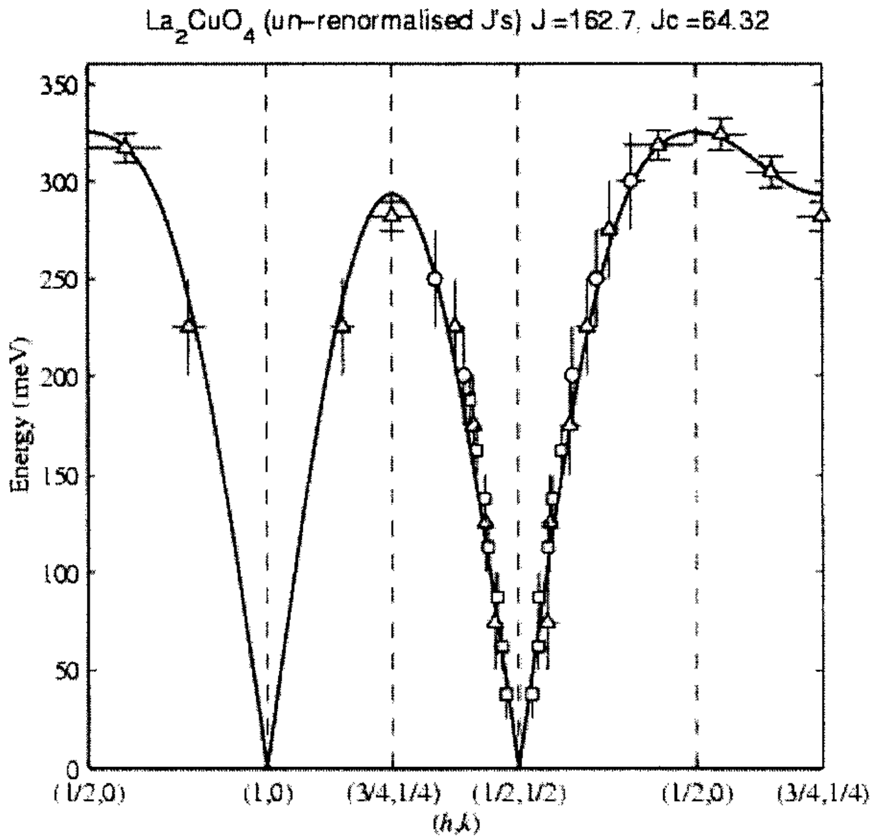
J=0.11eV(J”=0),0.14eV(J’=0)



A ferromagnetic next nearest neighbor coupling

- Not expected
- are we using the wrong Hamiltonian?
- consider ring exchange terms which provide much better fit to small cluster calculations and explain light scattering anomalies , i.e.
  $H = \Sigma J S_i S_j + J_{ring} S_i S_j S_k S_l$





La_2CuO_4 (un–renormalised J's) J =162.7, Jc =64.32
Energy (meV)
350
300
250
200
150
100
50
0
(1/2,0)
(1,0)
(3/4,1/4)
(1/2,1/2)
(1/2,0)
(3/4,1/4)
(h,k)

More detail on J_c

$$H = J \underset{i,j}{\;} \mathbf{S}_i ? \mathbf{S}_j + J' \underset{i,i'}{\;} \mathbf{S}_i ? \mathbf{S}_{i'} + J'' \underset{i,i''}{\;} \mathbf{S}_i ? \mathbf{S}_{i''}$$

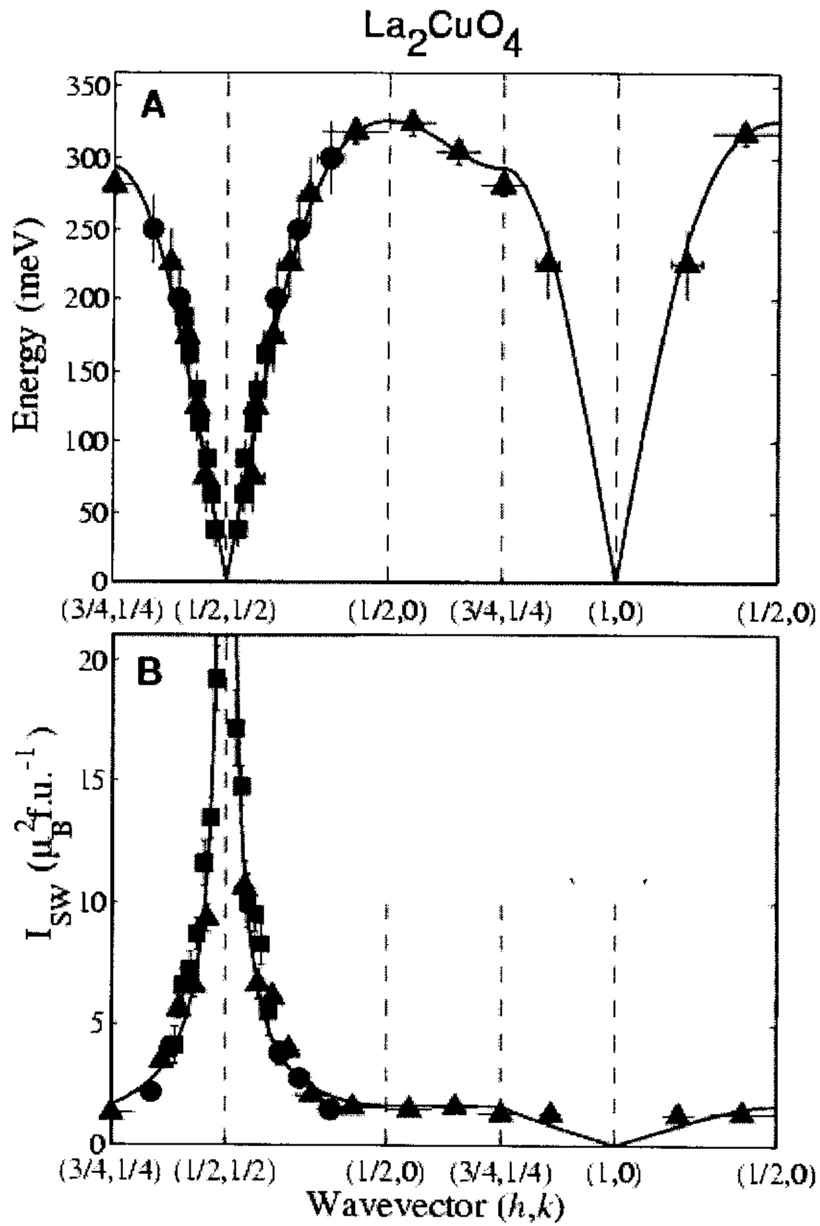
$$+ J_c \underset{i,j,k,l}{\;} \left[(\mathbf{S}_i ? \mathbf{S}_j)(\mathbf{S}_k ? \mathbf{S}_l) + (\mathbf{S}_i ? \mathbf{S}_l)(\mathbf{S}_k ? \mathbf{S}_j) - (\mathbf{S}_i ? \mathbf{S}_k)(\mathbf{S}_j ? \mathbf{S}_l) \right]$$

J=143.3±5 meV and J_c =48.4±9 meV.

$$H = -t \underset{i,j,\sigma=-)}{\;} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.} \right) + U \underset{i}{\;} n_{i-} n_{i)}$$

$$J = 4t^2/U - 24t^4/U^3 \quad J_c = 80t^4/U^3 \quad \text{and} \quad J' = J'' = 4t^4/U^3$$

t=0.32±0.02 eV and U=2.6±0.3 eV


La2CuO4
A
Energy (meV)
350
300
250
200
150
100
50
0
(3/4,1/4) (1/2,1/2) (1/2,0) (3/4,1/4) (1,0) (1/2,0)
B
20
15
10
5
0
(3/4,1/4) (1/2,1/2) (1/2,0) (3/4,1/4) (1,0) (1/2,0)
Wavevector (h,k)

Conclusions- parent insulator- need to go beyond Heisenberg

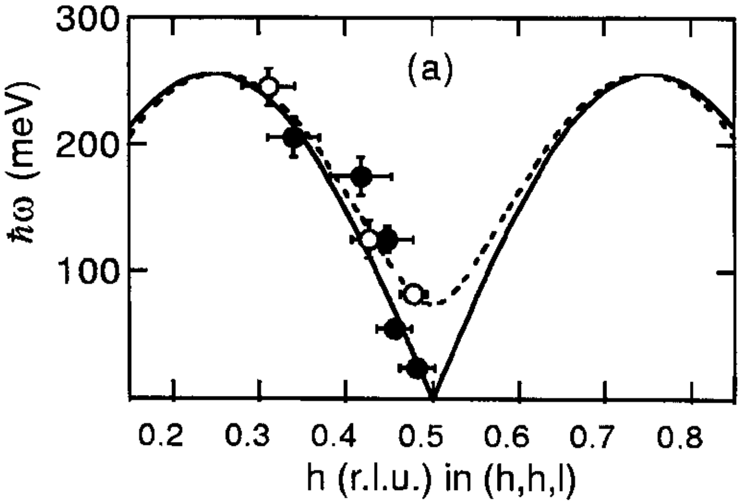
- Substantial(on scale of T_c) further neighbor interactions
- **J_{ring} a term to worry about** - data most consistent with cluster calculations with cyclic(4-spin) interactions(e.g. Schmidt '90 with $J_{ring}/J=30\%$)
- remarkable consistency also with Hubbard model parameters from electronic spectroscopies - **charge neutral low energy probe gives independent estimate of effective electronic parameters t & U**
- once further neighbor interactions are taken into account, spin wave theory gives excellent account of absolute amplitudes as well as dispersion

What happens for Y123

- Higher Tc
- ‘Cleaner’
- easier to adjust stoichiometry
- many more data of other types

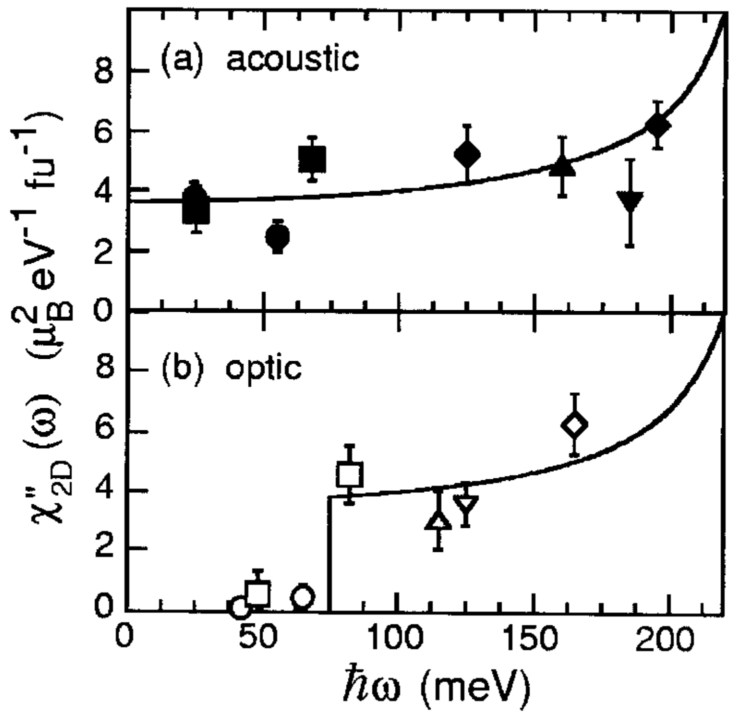
Y123 is a bilayer AFM -bilayers give rise to acoustic(in-phase) & optic(out-of-phase) spin waves

"High-Frequency Spin Waves in $YBa_2Cu_3O_{6.15}$", S. M. Hayden, G. Aeppli, T. G. Perring, H. A. Mook, F.Dogan, *Phys. Rev. B* **54(10),** pp. R6905-6908, (1996)



Q-averaged spin wave spectral weights

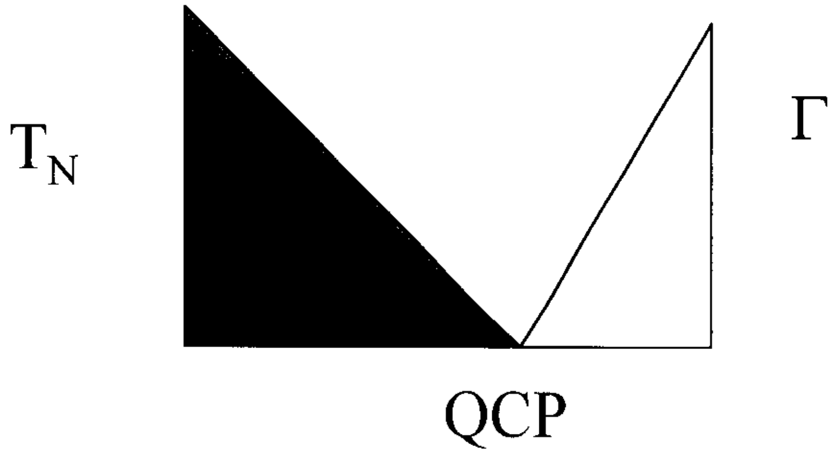
"High-Frequency Spin Waves in $YBa_2Cu_3O_{6.15}$", S. M. Hayden, G. Aeppli, T. G. Perring, H. A. Mook, F.Dogan, *Phys. Rev. B* **54(10),** pp. R6905-6908, (1996)



- Spin wave dispersion for $Y123O_{6.15}$ & *amplitudes* very well described by conventional theory with significant coupling between planes in bilayers and in-plane J slightly less than for La_2CuO_4
- acoustic DOS is flat for low E, gap in optic DOS
- what happens on doping?

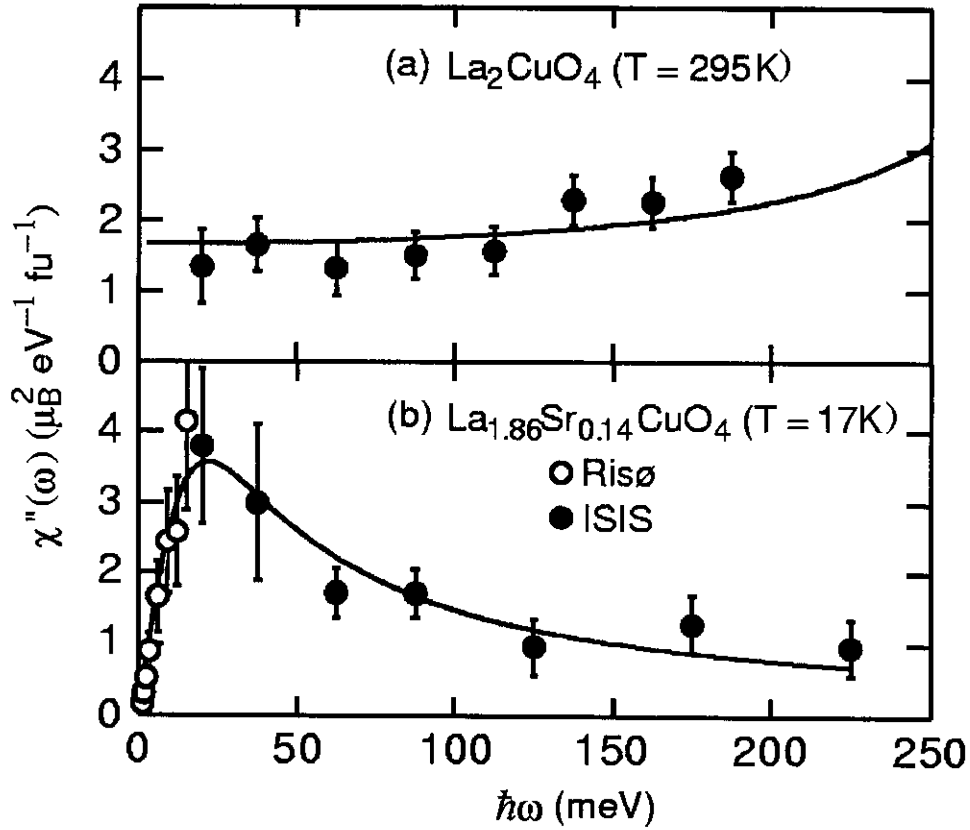
Might expect(simple quantum critical point for a metal emerging from an AFM)-

- Replacement of AFM Bragg peaks and SW peaks by quasielastic acoustic term and damped optical term, i.e. $\delta(\omega)$+SW--->
$\mathrm{Im}\chi_{acoustic}=\Gamma\omega/(\omega^2+\Gamma^2)$ and
$\mathrm{Im}\chi_{optic}=\Gamma\omega[1/((\omega-\omega_o)^2+\Gamma^2)+1/(\omega+\omega_o)^2+\Gamma^2)]$

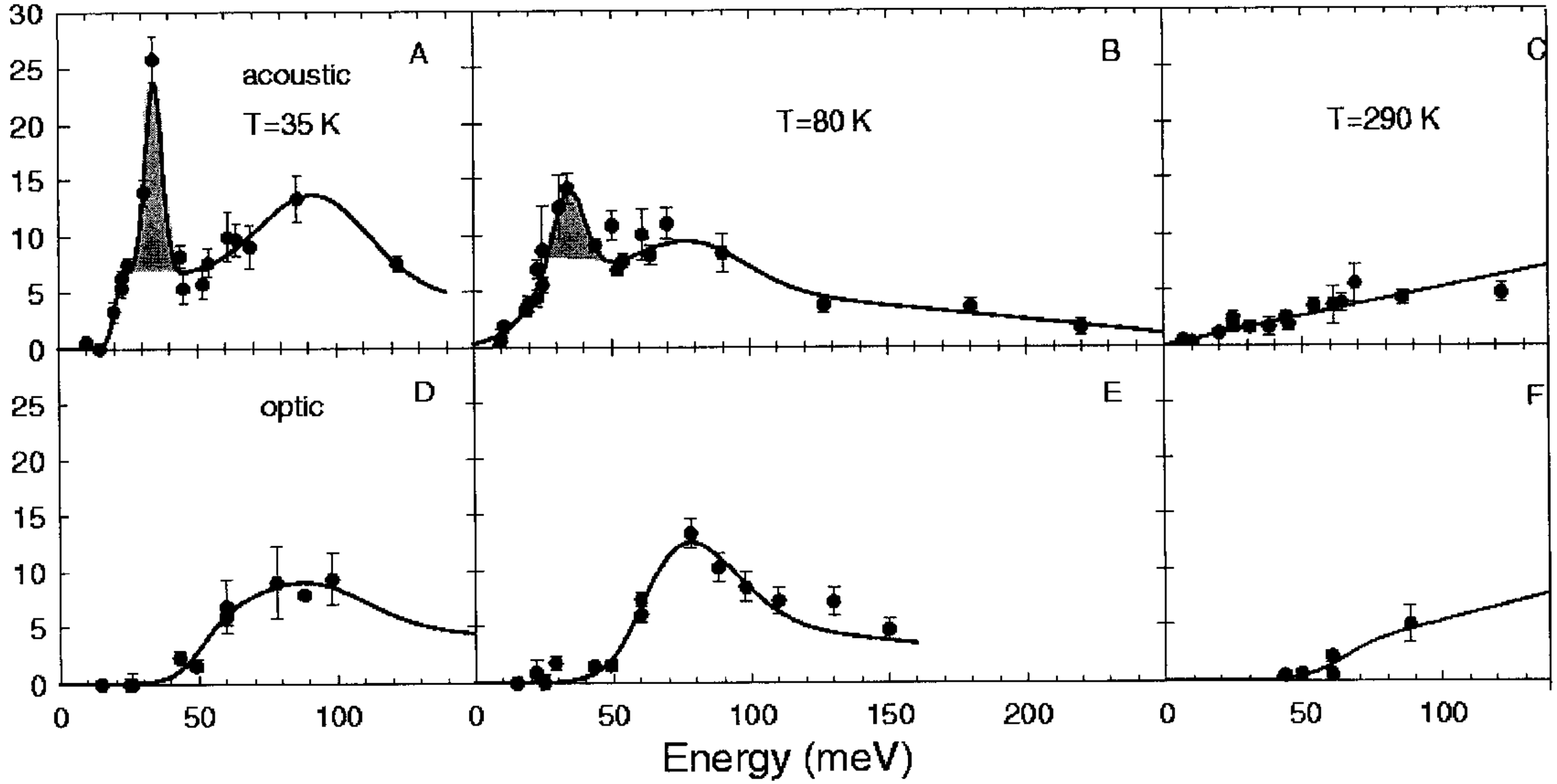


This is actually what seems to happen for $La_{2-x}Sr_xCuO_4$

"Comparison of the High-Frequency Magnetic Fluctuations in Insulating and Superconducting $La_{2-x}Sr_xCuO_4$", S. M. Hayden, G. Aeppli, H. A. Mook, T. G. Perring, T. E. Mason, S-W. Cheong, Z. Fisk, *Phys. Rev. Letts.* **76(8),** pp. 1344-1347 (1996).



$YBa_2Cu_3O_{6.6}$ (T_c=62.7 K)

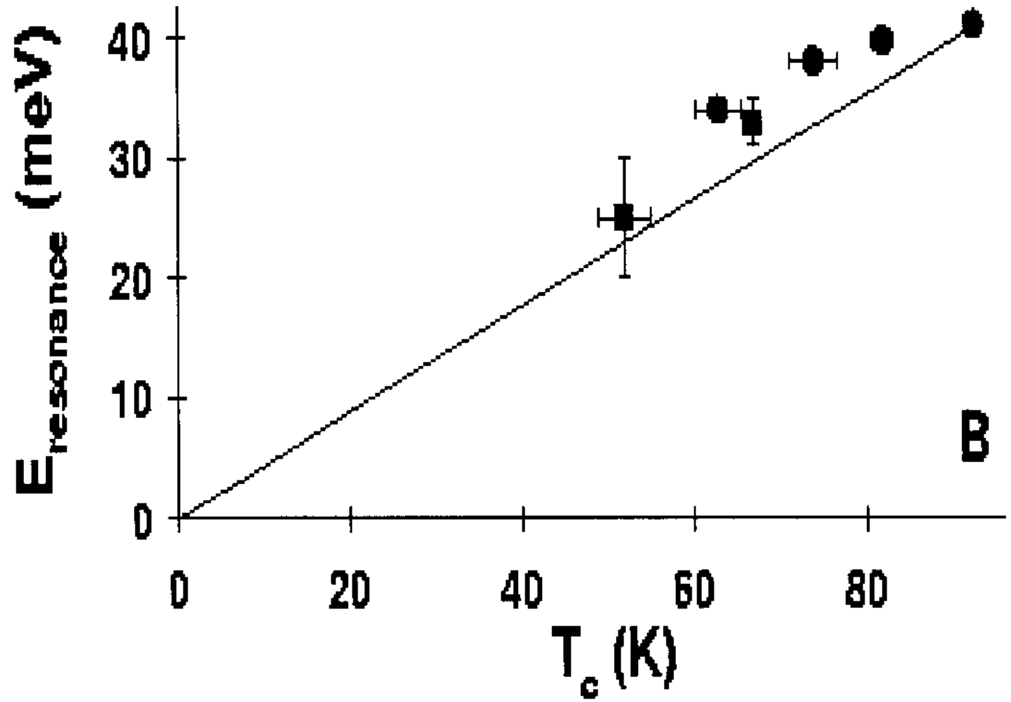


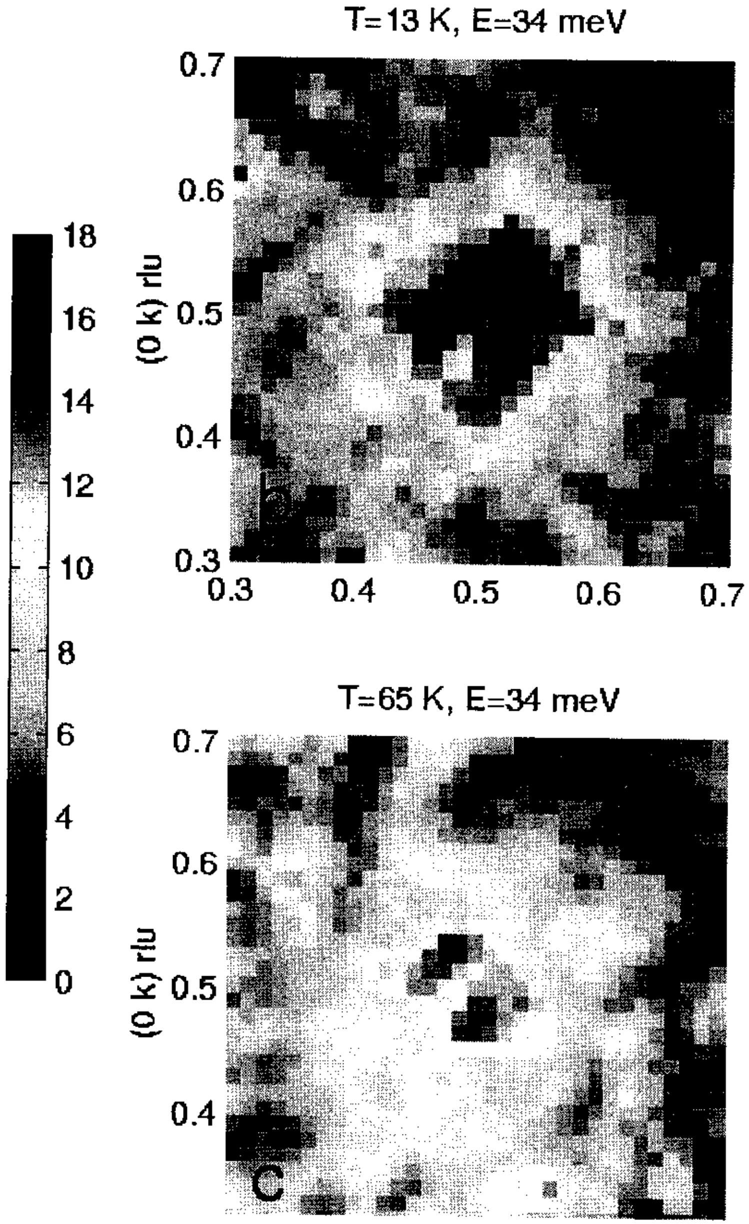
"The Magnetic Excitation Spectrum and Thermodynamics of High-T_c Superconductors", P. Dai, H. A. Mook, S. M. Hayden, G. Aeppli, T. G. Perring, R. D. Hunt, F. Dogan, *Science* **284**, pp. 1344-1347, (1999).

Y123 seems much more complicated

- Optic mode(expected)
- spin gap in SC phase(expected because of spin singlet pairing in BCS-type states)
- pseudogap in normal phase, with onset T*(not expected)
- ‘resonance’ (not expected)

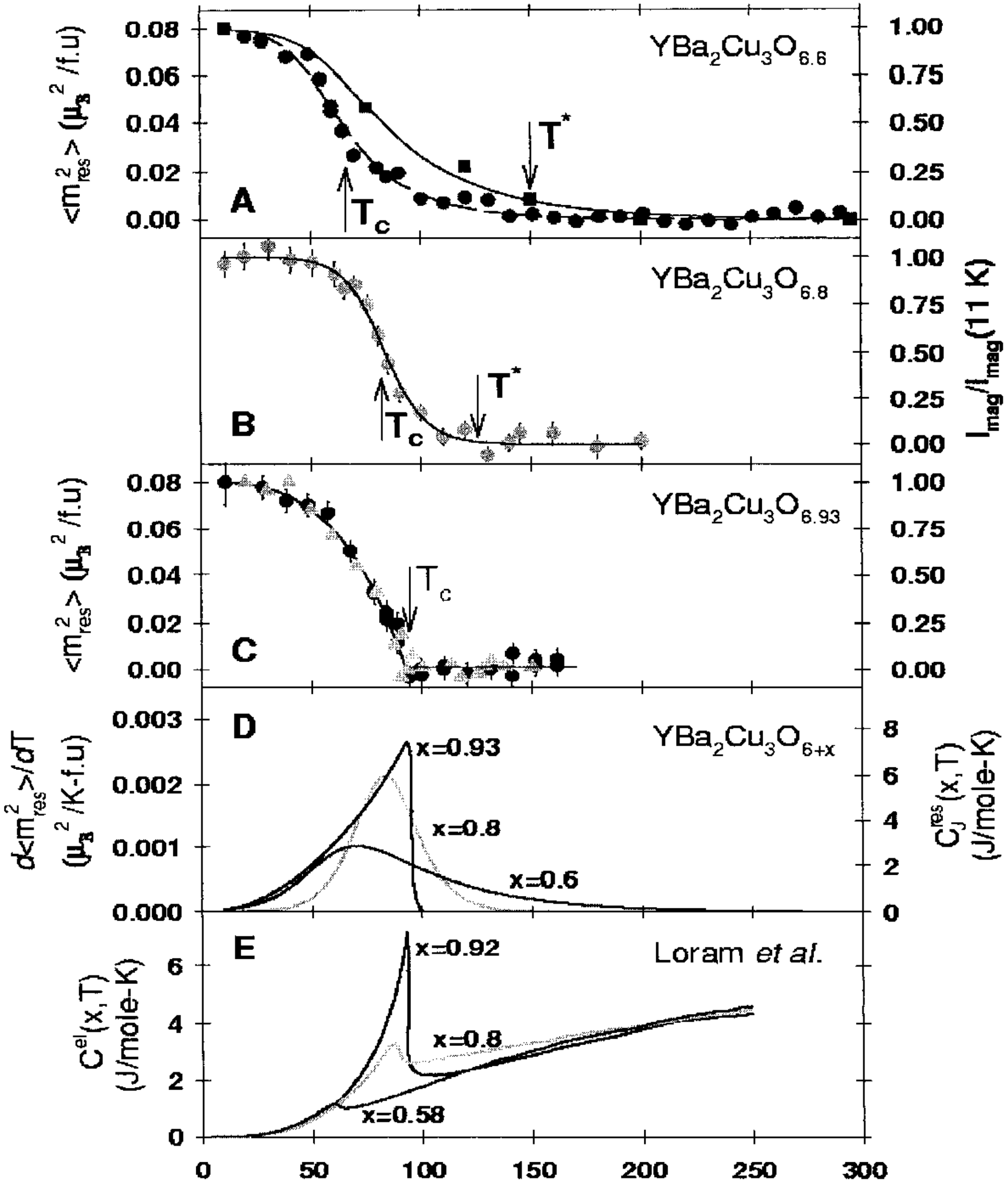
Focus on 'resonance' because it is easy to see(but beware that it contains only ~1% of S(S+1))



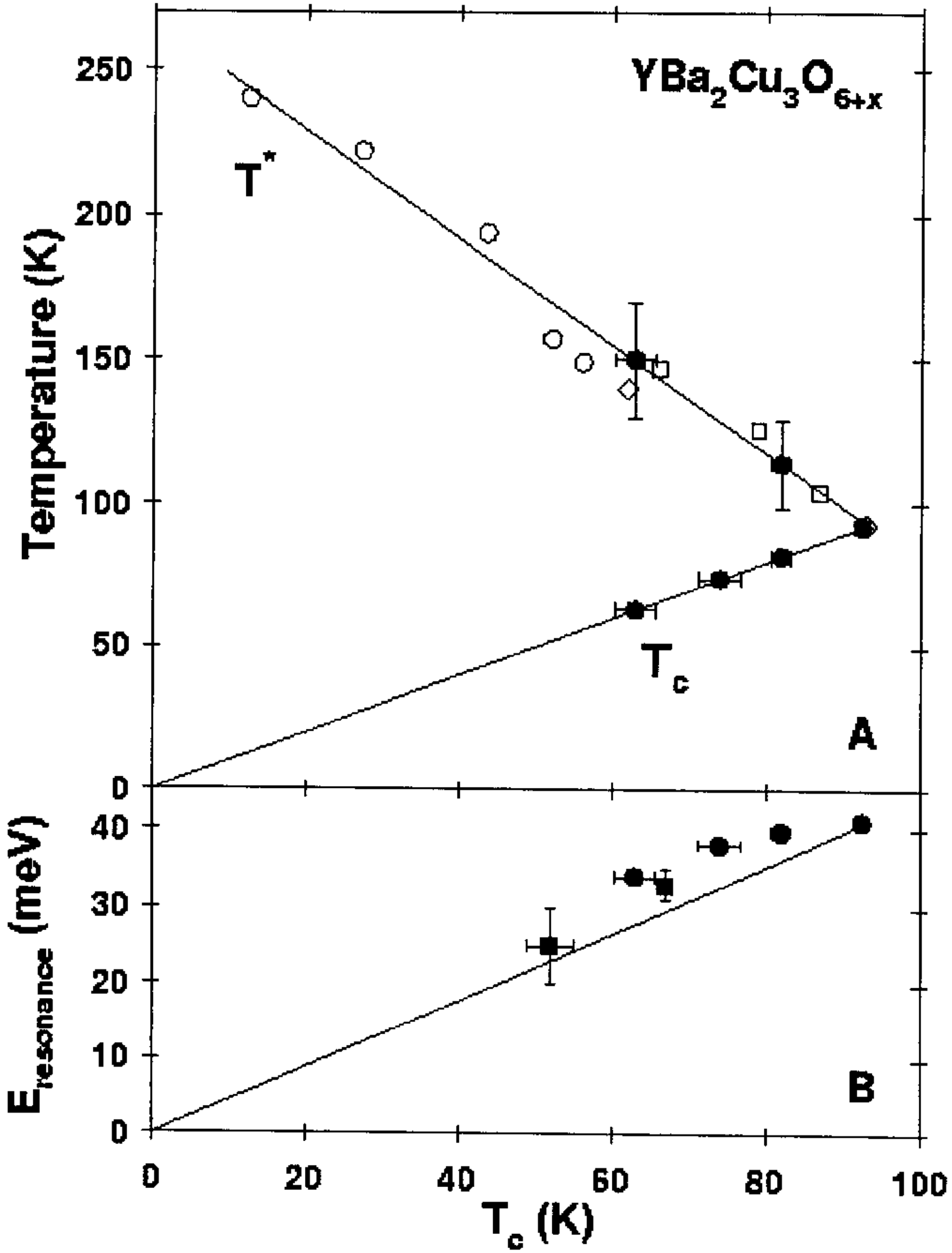


"Spin Fluctuations in $YBa_2Cu_3O_{6.6}$ – A New Picture", H. A. Mook, P. Dai, S. M. Hayden, G. Aeppli, T. G. Perring, F. Dogan, *Nature* **395**, pp. 580-582, (1998)

"The Magnetic Excitation Spectrum and Thermodynamics of High-T_c Superconductors", P. Dai, H. A. Mook, S. M. Hayden, G. Aeppli, T. G. Perring, R. D. Hunt, F. Dogan, *Science* **284**, pp. 1344-1347, (1999).



"The Magnetic Excitation Spectrum and Thermodynamics of High-T_c Superconductors", P. Dai, H. A. Mook, S. M. Hayden, G. Aeppli, T. G. Perring, R. D. Hunt, F. Dogan, *Science* **284**, pp. 1344-1347, (1999).

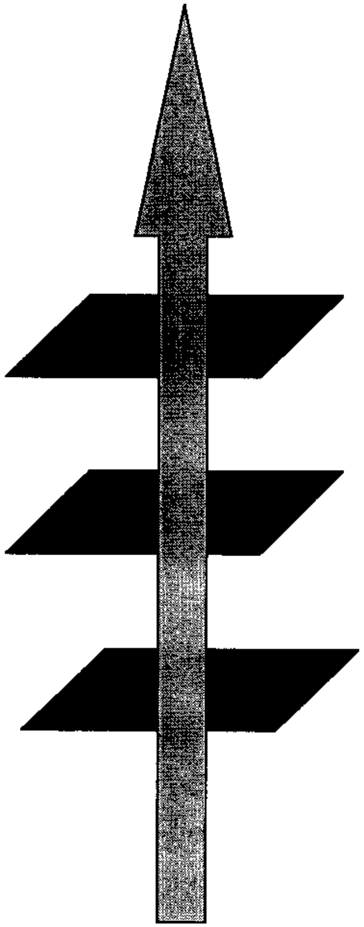


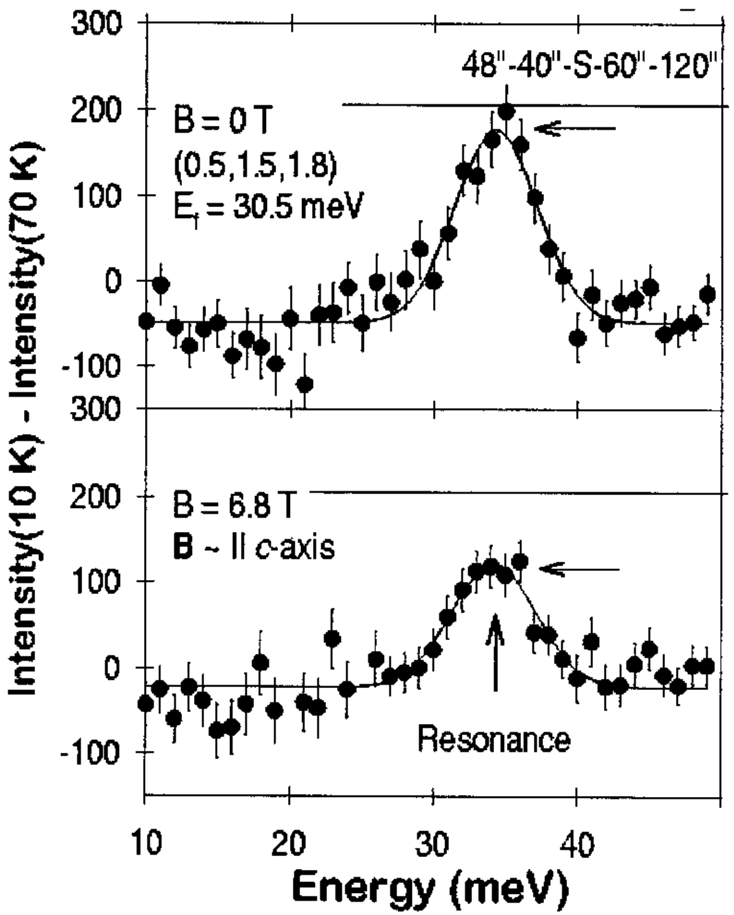
resonance

- an extra feature in the *acoustic* mode spectrum beyond spin gap
- seems connected with s.c., and pseudogap regime above Tc
- dI(resonance)/dT~C as doping, T is varied
- sharper in Q,E in s.c. phase than in normal state

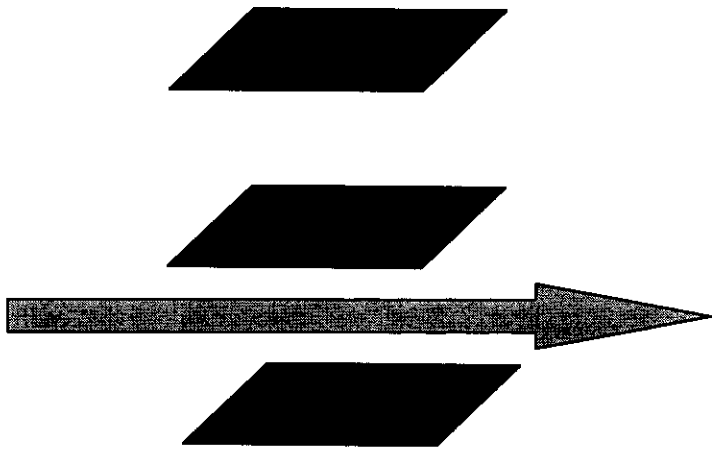
Are all of these properties simply related to spin pairing(from some underlying Heisenberg picture) or is there something more profound?

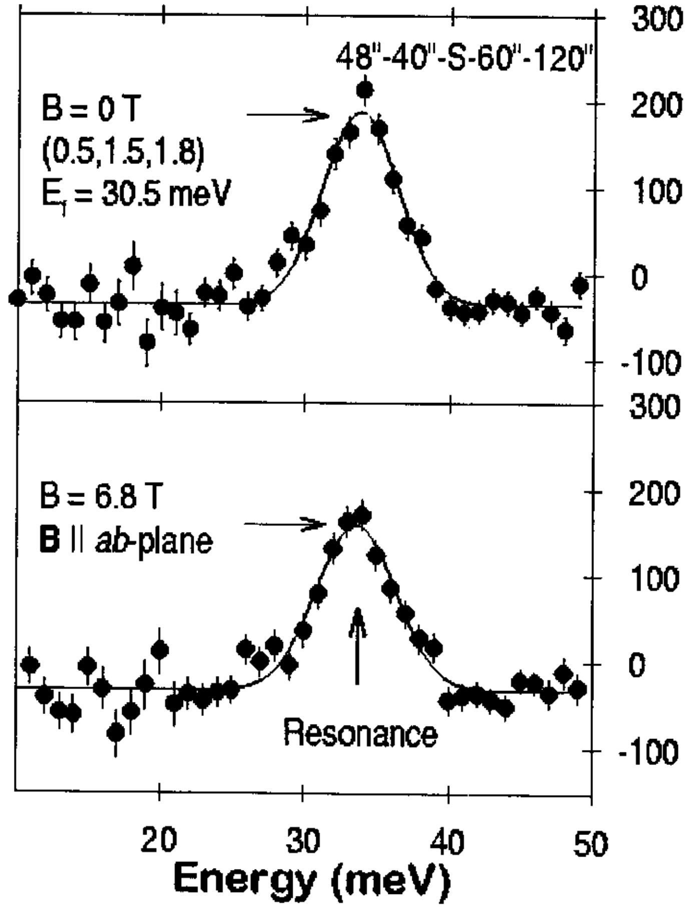
- test by applying a magnetic field - if spin pairing is the only physics, expect Zeeman effect(which should be isotropic) to dominate, if orbital effects matter, will see anisotropic effects at energy scales different from $g\mu_B H$ (Dai et al., Cond Mat 2000)



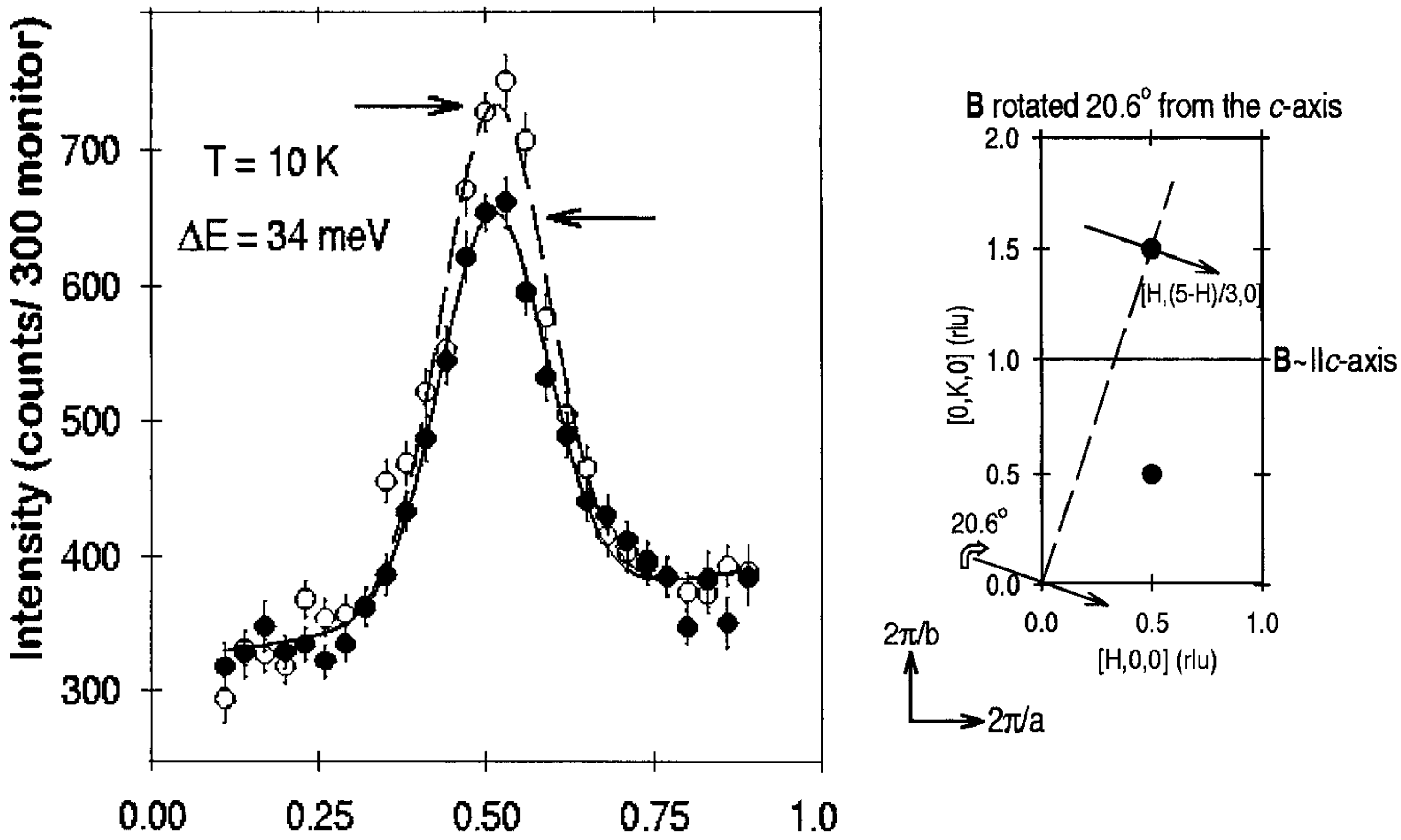


48"-40"-S-60"-120"
B = 0 T
(0.5,1.5,1.8)
E_f = 30.5 meV
B = 6.8 T
B ~ ll *c*-axis
Resonance
Intensity(10 K) - Intensity(70 K)
Energy (meV)





48''-40''-S-60''-120''
B = 0 T
(0.5,1.5,1.8)
E_f = 30.5 meV
B = 6.8 T
B || ab-plane
Resonance
300
200
100
0
-100
20
30
40
50
Energy (meV)



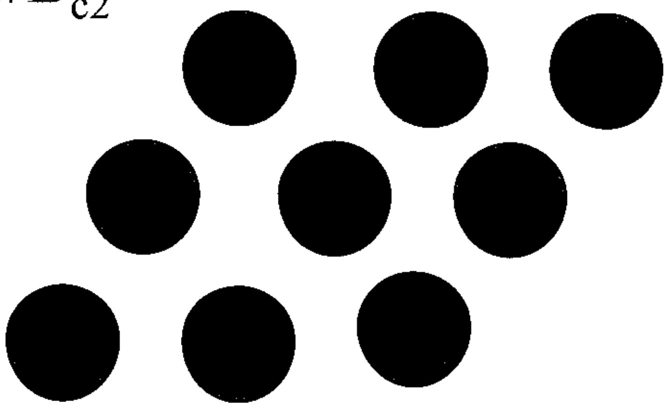
Intensity (counts/ 300 monitor)
T = 10 K
ΔE = 34 meV
300
400
500
600
700
0.00
0.25
0.50
0.75
1.0
B rotated 20.6° from the c-axis
2.0
1.5
1.0
0.5
0.0
[0,K,0] (rlu)
[H,(5-H)/3,0]
B~IIc-axis
20.6°
0.0
0.5
1.0
[H,0,0] (rlu)
2π/b
2π/a

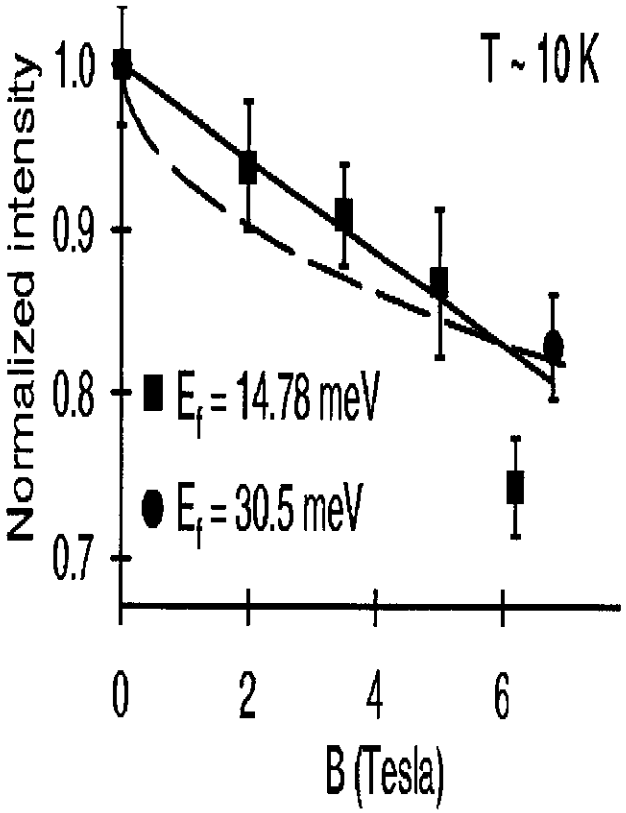
Very modest field, very strong effect

- 30% effect at 34meV for H=6.5T along c
$6.5T \sim 0.7meV \sim 7K << T_c \sim 60K << E_{res} \sim 360K$
- much smaller effect for H=6.8T along CuO_2 planes
- conclude that not a spin(Zeeman) effect, but an orbital effect

In a superconductor, most natural 'orbital' effect is from vortex inclusions

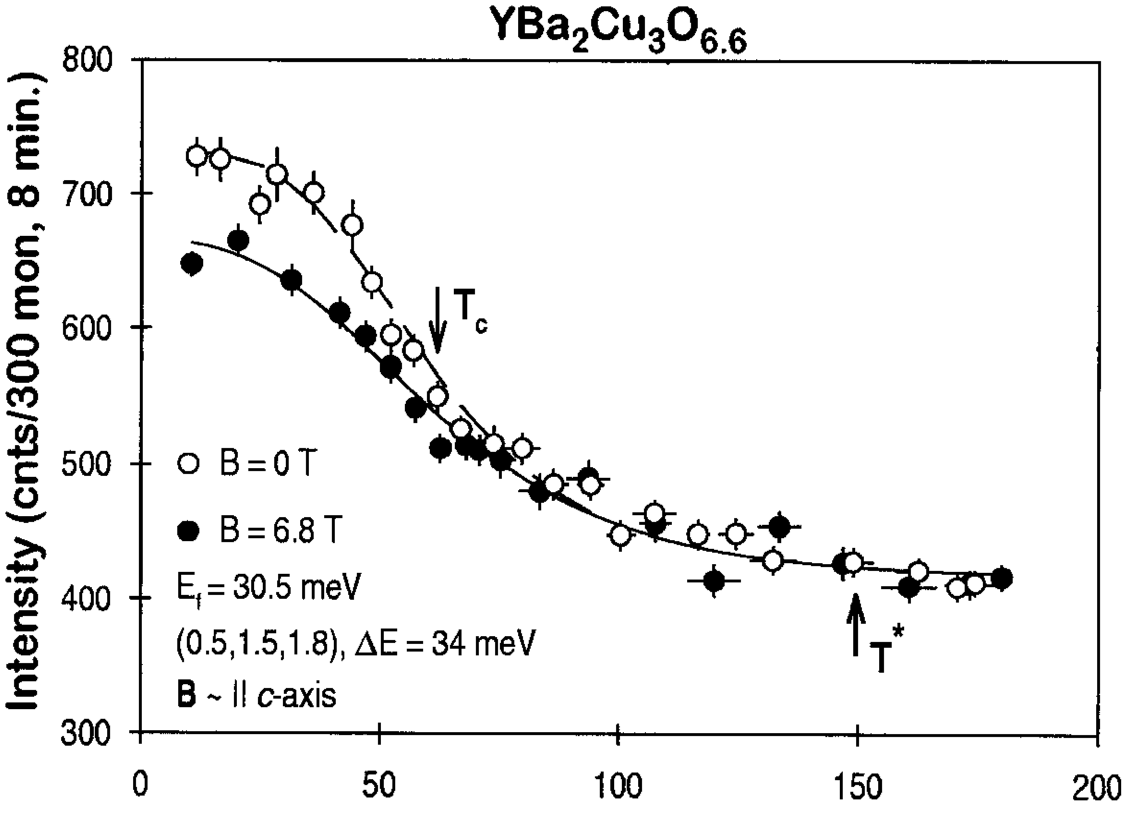
- vortices~normal state inclusions
- sc state has sharp resonance and normal state has no sharp resonance
- resonance intensity~1-volume fraction for normal state inclusions~1-B/B_{c2}





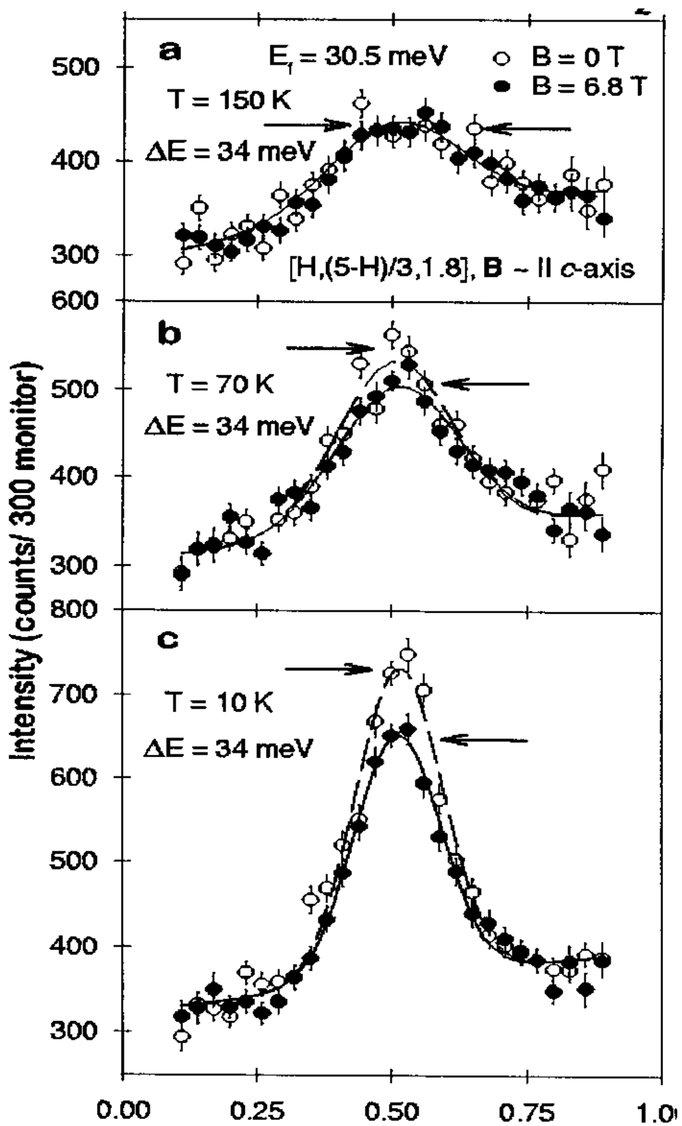
$I/I_0 = 1 - B/B_{char}$ where

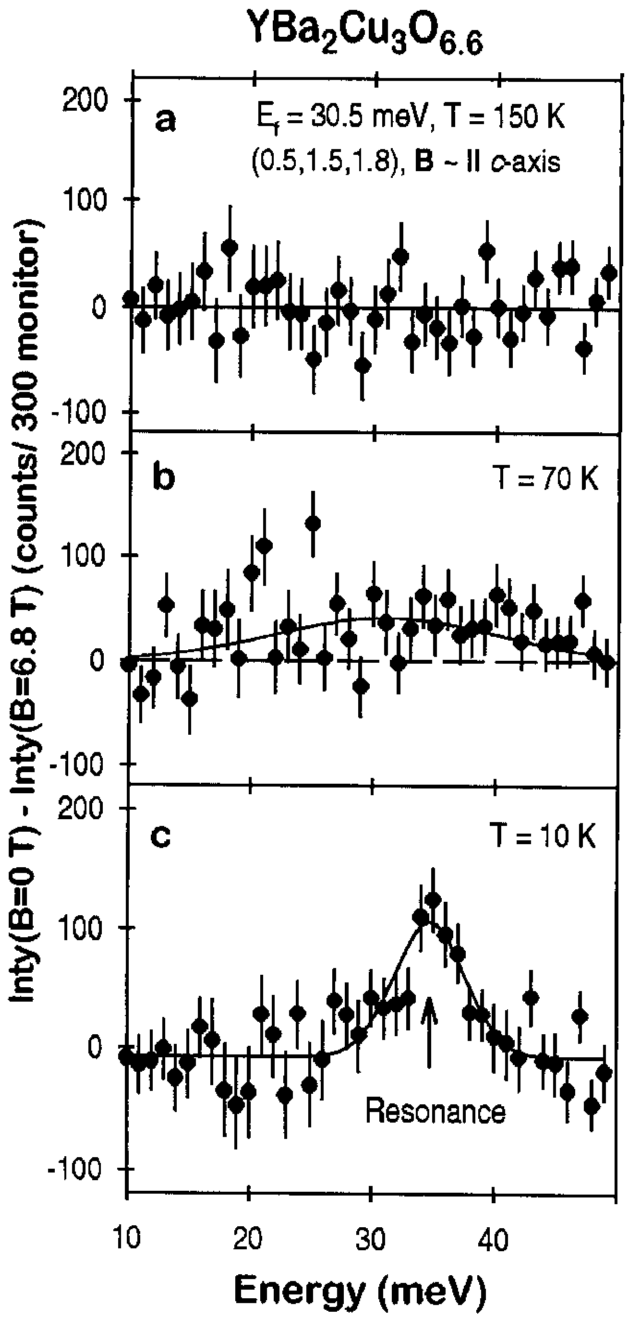
$B_{char} = 36T \sim B_{c2} = 45T$



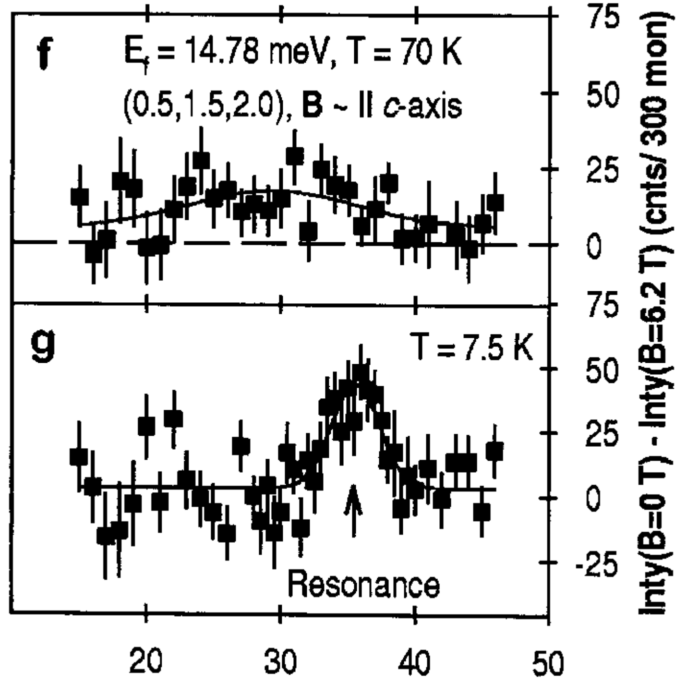
Temperature(K)

Is there really life above T_c?

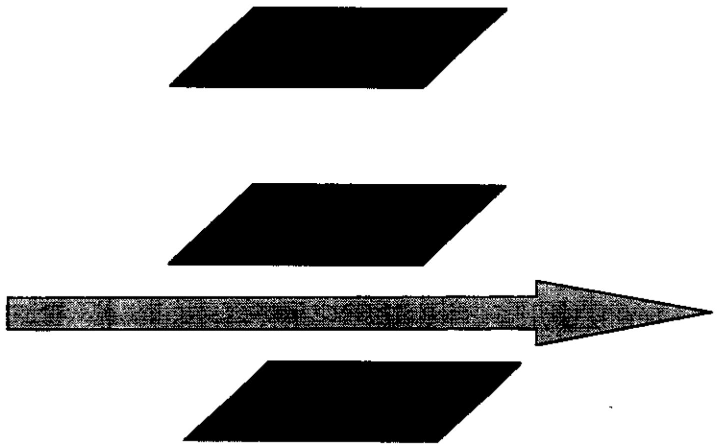


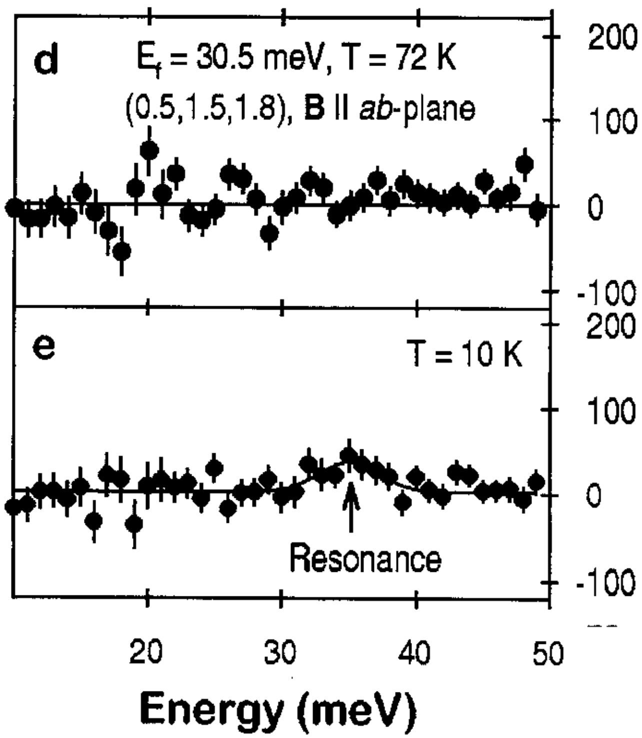

YBa2Cu3O6.6
a
Ef = 30.5 meV, T = 150 K
(0.5,1.5,1.8), B ~ II c-axis
b
T = 70 K
c
T = 10 K
Resonance
Inty(B=0 T) - Inty(B=6.8 T) (counts/ 300 monitor)
200
100
0
-100
10
20
30
40
Energy (meV)

Yes,but let's change instrument configuration to make sure



What about anisotropic response to field?





Orbital effect for T>Tc

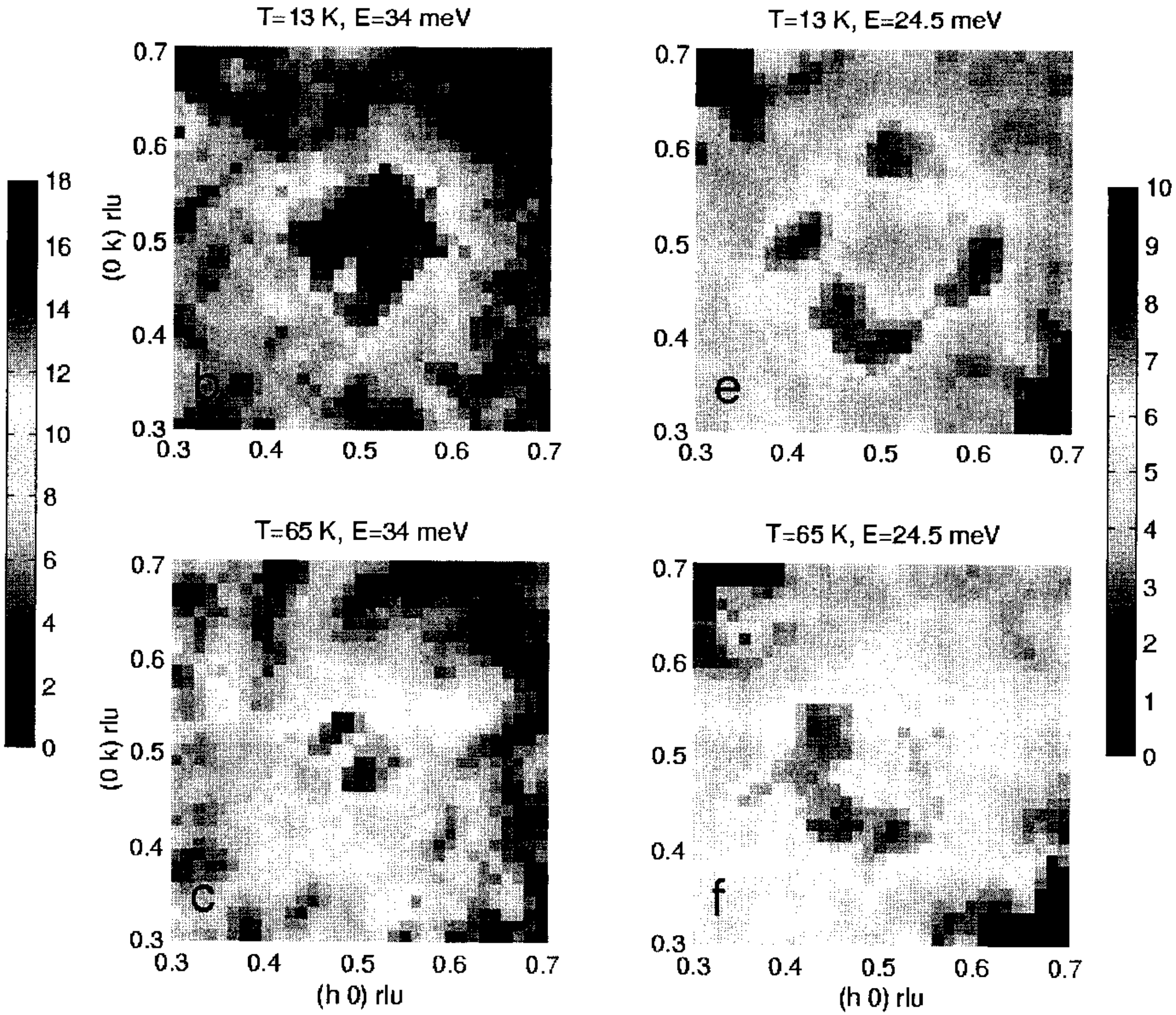
- $I \sim |\langle \psi_f | S^+ | \psi_0 \rangle|^2$
- Wavefunctions giving rise to resonance contain non-trivial orbital as well as spin terms - contrast with spin-Peierls where we also have sharp singlet-triplet excitation but only a Zeeman response to field
- one natural explanation is to invoke short range s.c. phase coherence as well as spin pairing

The ‘resonance’ as a measure for s.c. order

- Integrated weight~# of pairs
- width in frequency~1/(phase coherence time)
- width in k-space~1/(phase coherence length)
- T-dependence in agreement with LBL(Orenstein) optical data showing s.r. phase coherence showing up for T<T**<T* ----> 2-stage pre-s.c. regime involving pseudogap formation followed by onset of phase coherence

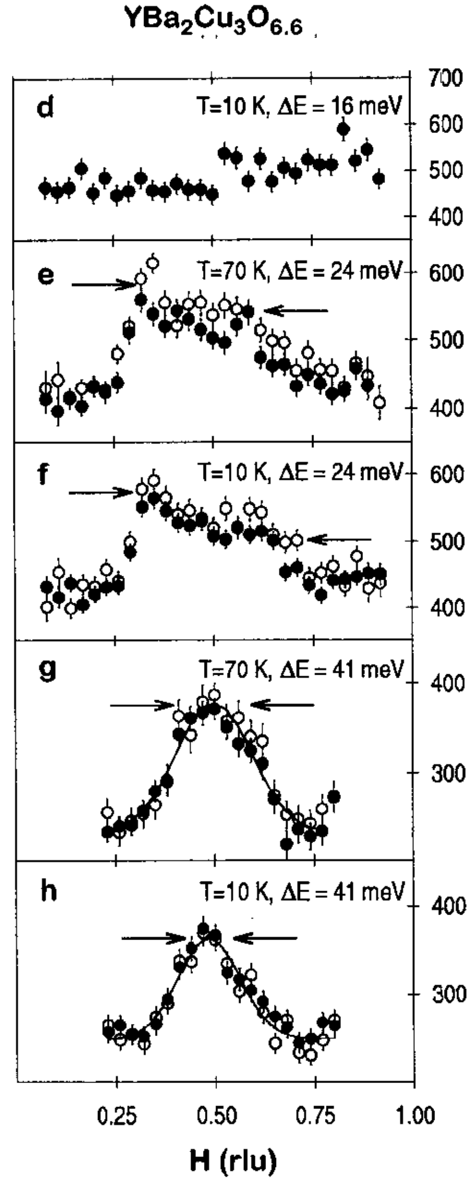
An oddity- seeming non-conservation of spectral weight when field is varied at fixed T

- even though at fixed B, S is conserved
- reminiscent of STM data - loss of 'coherence peaks' at gap edge but no obvious compensating changes
- because Q,E is a huge place, search for missing weight...

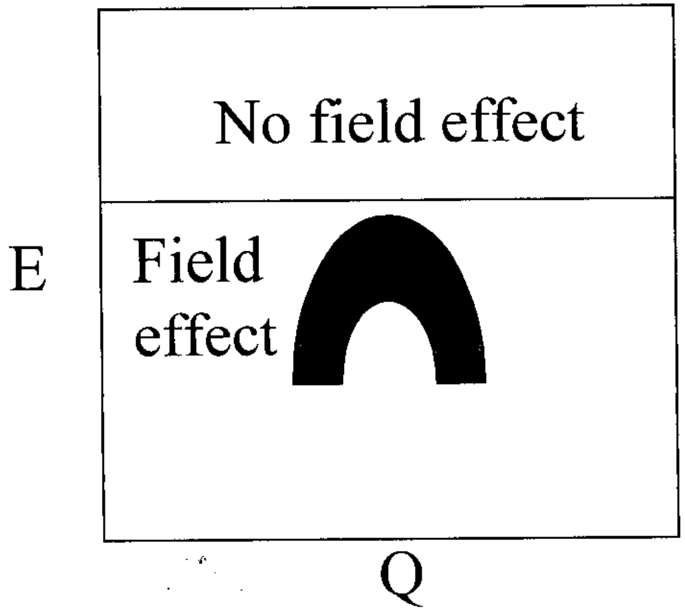


T=13 K, E=34 meV
T=13 K, E=24.5 meV
T=65 K, E=34 meV
T=65 K, E=24.5 meV
(0 k) rlu
(h 0) rlu
b
e
c
f
0.3
0.4
0.5
0.6
0.7
0
2
4
6
8
10
12
14
16
18
1
3
5
7
9

Hunting for missing spectral weight



- no luck in hunt - no increasing signals so far anywhere
- decreasing incommensurate signals for $E=24meV<E_{res}$, but no decrease in signal for $E=41meV>E_{res}$ ---> is Eres the top of an 'excitation band' sensitive to pairing & s.c. phase coherence



Is Heisenberg picture(perhaps with some damping and disordered ground states) all we need to understand spin sector of hi-Tc problem? -**NO**

- Revisit insulator - find ring exchange term
- look at excitations in the s.c. - discover that resonance is sensitive to orbital effects, most likely due to orbital aspect of s.c.pairing