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H4.SMR/1001-5

IX TRIESTE WORKSHOP ON OPEN PROBLEMS IN STRONGLY CORRELATED SYSTEMS

14 - 25 July 1997

EXPERIMENTAL PHYSICS AND STRONGLY CORRELATED SYSTEMS: ARE WE SIMPLY AT THE MERCY OF THE CHEMISTS AND THE THEORISTS?

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SOLID STATE PHYSICS (> 1920's)

electrons $\{ p_i, r_i \}$

nuclei $\{ P_j, R_j \}$

(1) $$\mathcal{H} = \sum \frac{\hbar^2}{2m} p_i^2 + \sum \frac{\hbar^2}{2M} P_j^2 + \sum V_{ee}(r_i, r_e) + \sum V_{eN}(r_i, R_j) + \sum V_{NN}(R_j, R_m)$$

Want to solve for Ψ, E in $\mathcal{H}|\Psi\rangle = E|\Psi\rangle$,

where generally

$\langle R_j \rangle$ form a periodic array

(1) nearly impossible to solve

(but ⚠ Carr-Parinello

⊕ computing power)

Even so, BAND THEORY

≡ COUNTING + SOLUTION OF SINGLE é PROBLEM IN PERIODIC POTENTIAL

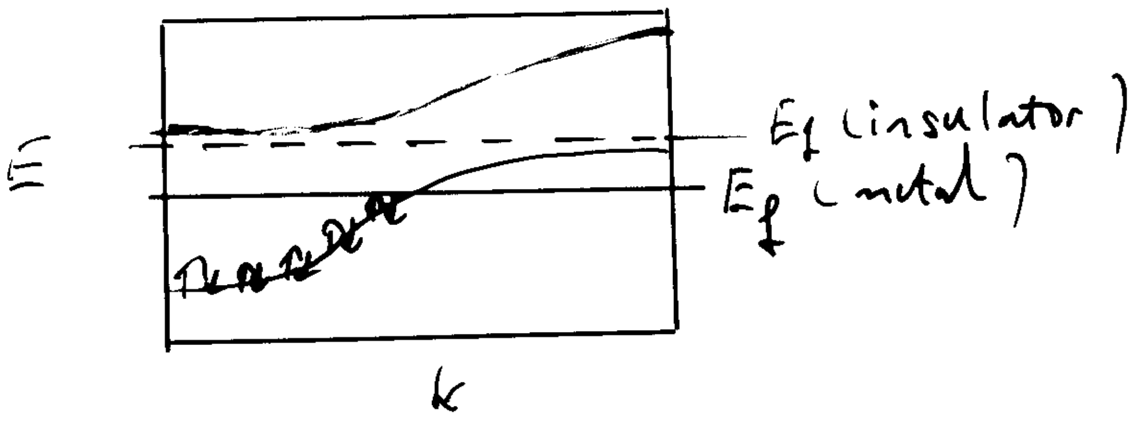
$$\left(\mathcal{H} = \frac{\hbar^2}{2m} p^2 + \sum_{R_i \in \text{rg. lattice}} V(r-R_i)\right)$$

accounts for –

metals

insulators

semiconductors (doping phenomena)



TRIUMPH OF 50'S & EARLY 60'S -

KEEP BAND PICTURE INTACT
(a.k.a. FERMI LIQUID THEORY)

& ACCOUNT FOR 'FERMI SURFACE INSTABILITIES'

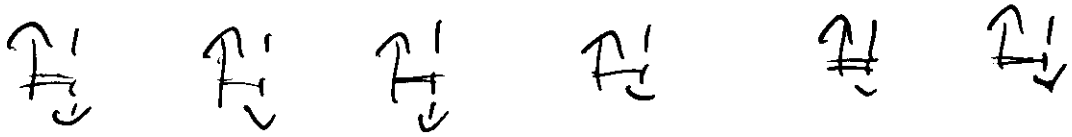
- (BCS) SUPERCONDUCTIVITY

- CHARGE & SPIN DENSITY
WAVES (OVERHAUSER)

A PARALLEL DEVELOPMENT,
LARGELY IN REAL SPACE

Curie - Weiss, Heisenberg

unfilled d & f shells localised electrons



(e.g. $Cu^{2+} \equiv d^9$, Ni^{2+} d^8 ...)

$$\mathcal{H} = \sum_{i,j} S_i \cdot S_j \, J_{ij}$$

Successes - mean field theory
}
Onsager solution
}
Renormalization group
crystal fields
spin waves (Goldstone modes)

\+ METHOD TO CHECK ALL OF THE ABOVE

a.k.a. MAGNETIC NEUTRON SCATTERING

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \sim \frac{k_f}{k_i} S(Q,\omega)$$

and
$$S(Q,\omega) = \int dt \sum_{i,j} \langle S_l(t) S_j(0) \rangle \exp (R_l - R_j) \cdot Q i \; \exp -it\omega$$

(F.T. in space & time of 2-spin correlation fcn)

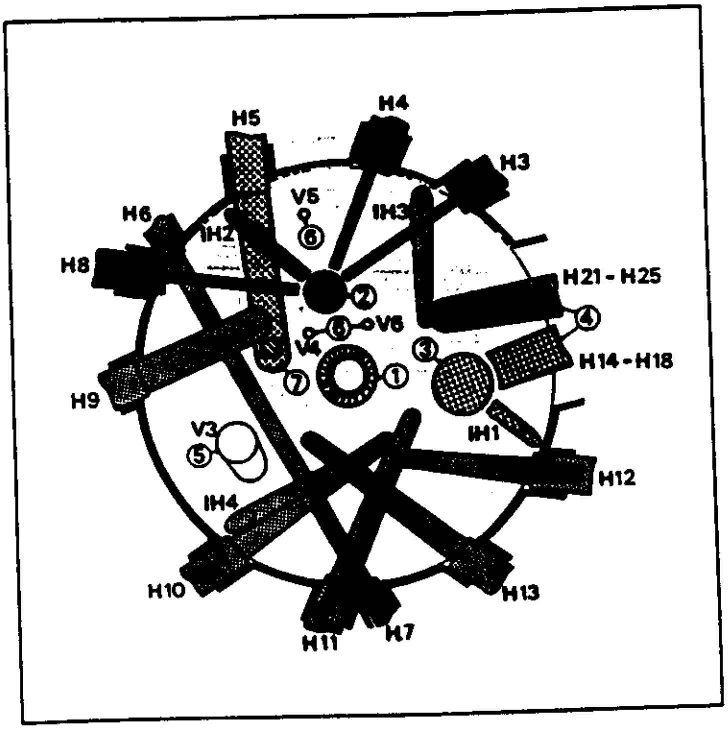
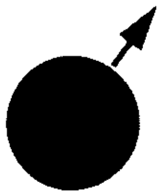

H5
H4
H3
V5
⑥
IH3
H6
IH2
H8
H21 - H25
②
⑧
V6
④
V4
③
H14 - H18
H9
⑦
①
IH1
V3
⑤
H12
IH4
H10
H13
H11
H7

FIGURE 1

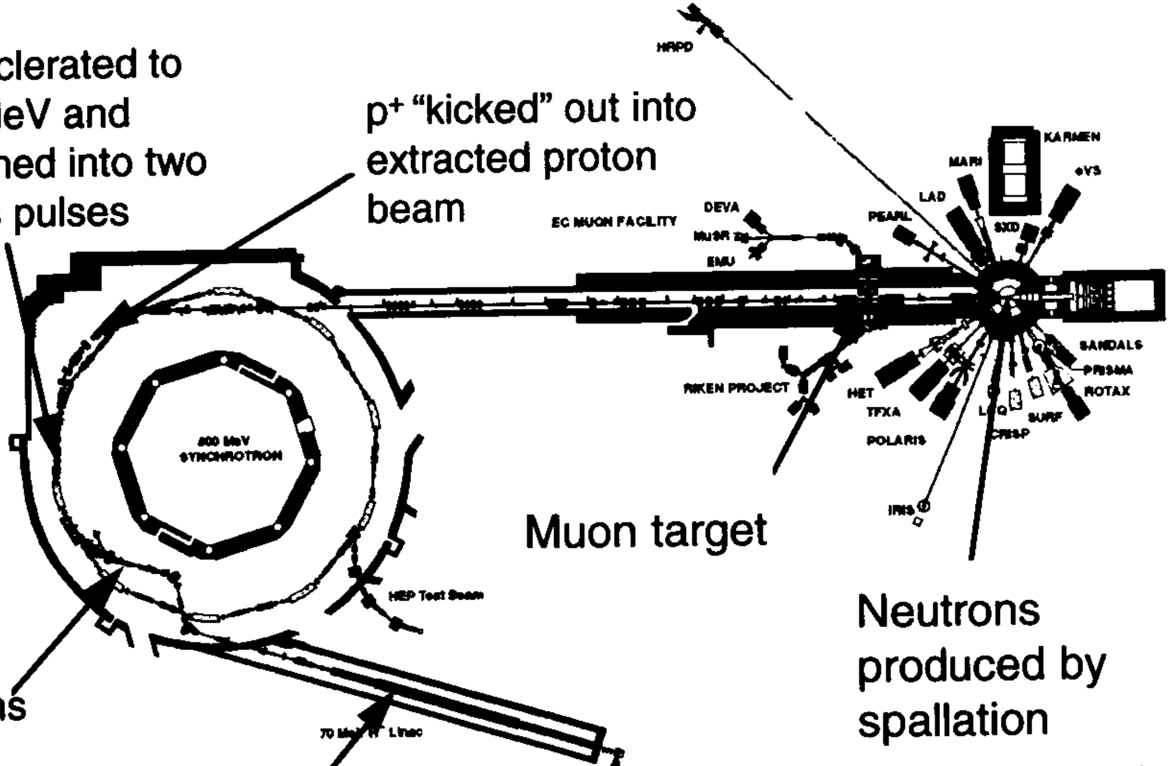
Why Neutrons?



Mass	**$m = 1.67 \times 10^{-27}$ kg**
Charge:	**0**
Spin:	**1/2**
Magnetic Moment	**$\mu = -1.9\mu_N$**

λ similar to atomic spacings.	☞	diffraction
Energy similar to atomic and electronic processes	☞	spectroscopy
Scatter from the nuclei	☞	scattering amplitude does not vary linearly with z ➢ can see Hydrogen ➢ contrast variation
	☞	no form factor
Magnetic moment	☞	magnetic structures and excitations
Highly penetrating	☞	study sample bulk, complex sample environment
Non-destructive	☞	delicate samples

Producing Neutrons and Muons



p^+ acclerated to 800MeV and bunched into two 0.3μs pulses

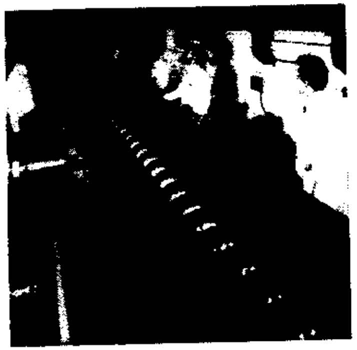
p^+ "kicked" out into extracted proton beam

Muon target

Neutrons produced by spallation

Stripped of electrons
$H^- \Rightarrow p^+$

H^- ions produced at -665kV



H^- ions accelerated to 70MeV in LINAC

ISIS Spectrometers for Magnetic Studies

HET - **High Energy Transfer Chopper Spectrometer**

- Optimised for the measurement of magnetic excitations
- $15meV < E_i < 2000meV$
- $3 < \phi < 32$ and matched high angle banks

PRISMA -

-
-
-
-

[illegible]

- 10 < [illegible]
- [illegible]

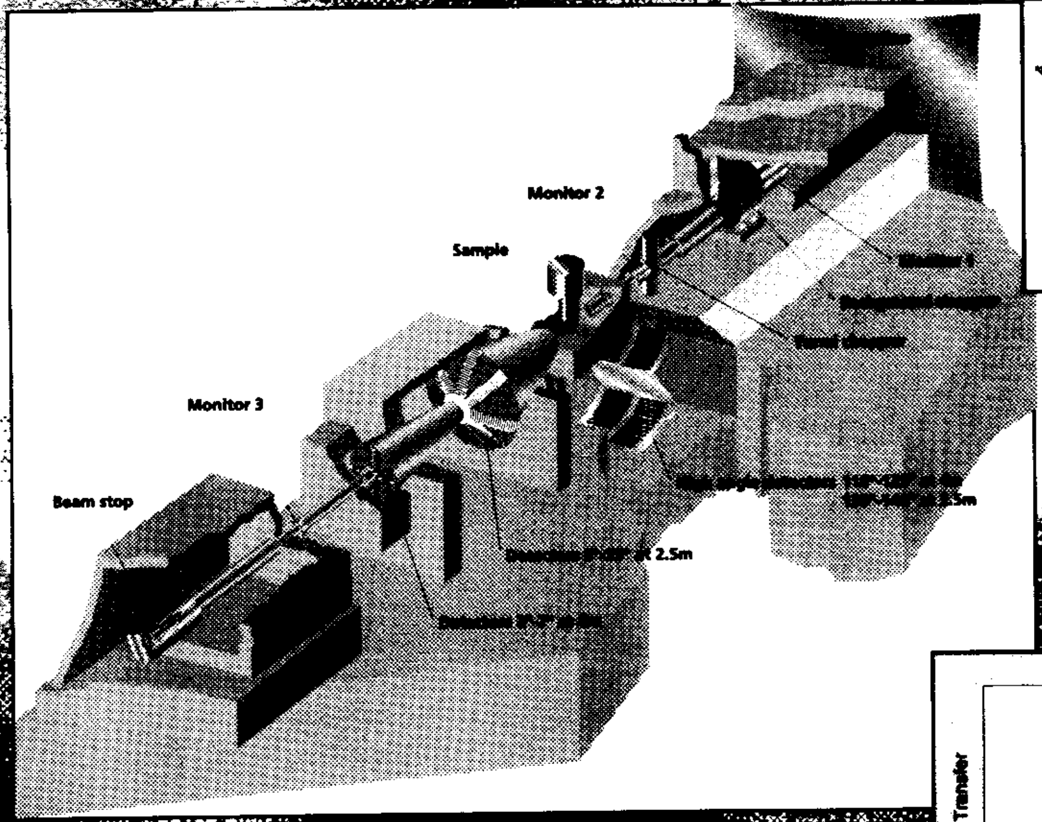
IRIS- **Low Energy Spectroscopy and Long Wavelength Diffraction**

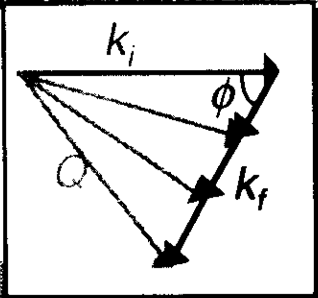
- $1\mu eV < \Delta E < 50\mu eV$
- $-3.5meV < \hbar\omega < 4meV$
- $1Å < d < 12Å$

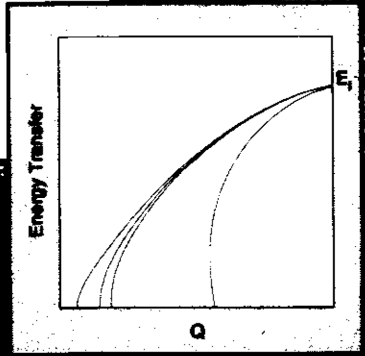
TFXA- **Molecular Spectroscopy and Crystal Fields**

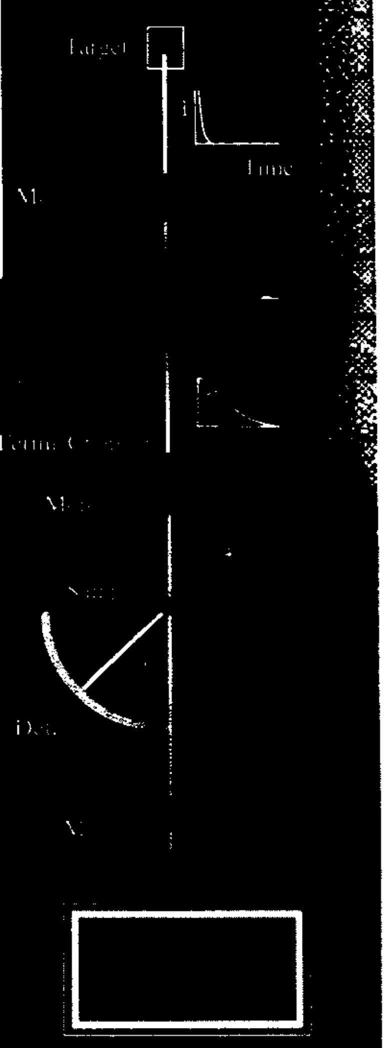
- Wide energy range indirect geometry spectrometer
- $2meV < \hbar\omega < 1000meV$

HET – High Energy Transfer Chopper Spectrometer







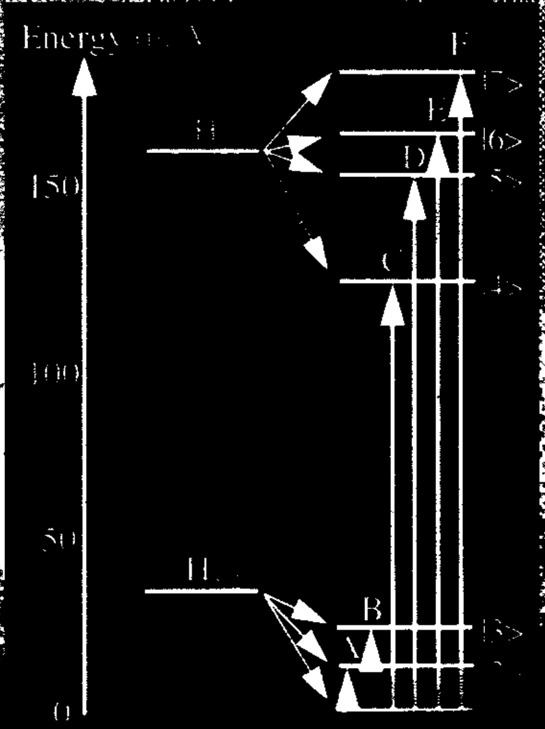


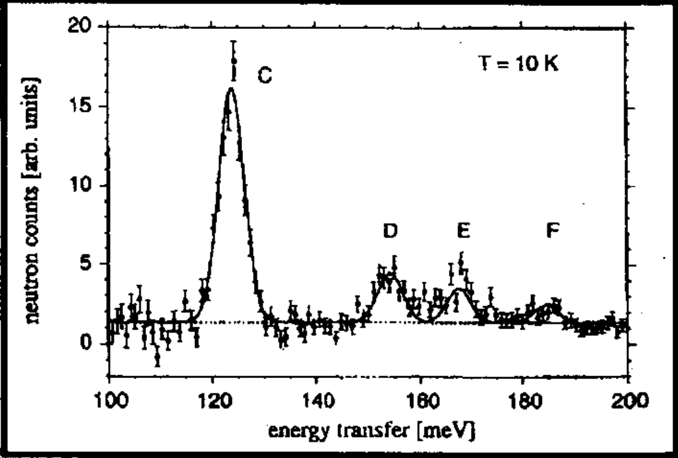
$$\frac{\hbar^2 Q^2}{2m} = 2E_i - \hbar\omega - 2\cos\phi\left[E_i(E_i - \hbar\omega)\right]^{1/2}$$

5

Crystal-[illegible] Transitions in [illegible]Ba$_2$Cu$_3$O$_7$

[illegible] [illegible]eller, A Furrer, [illegible] and V Trounov





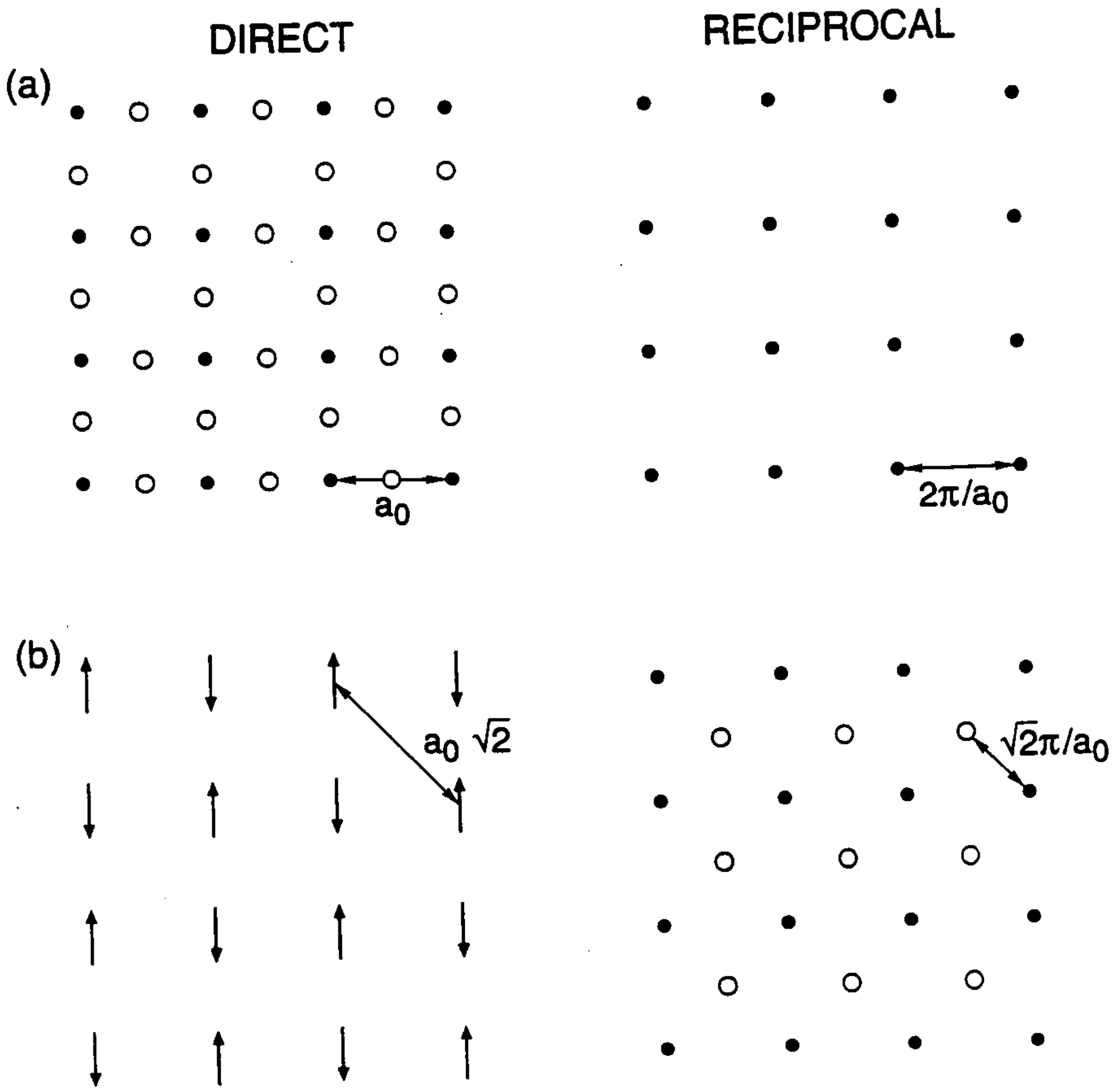


FIGURE 8

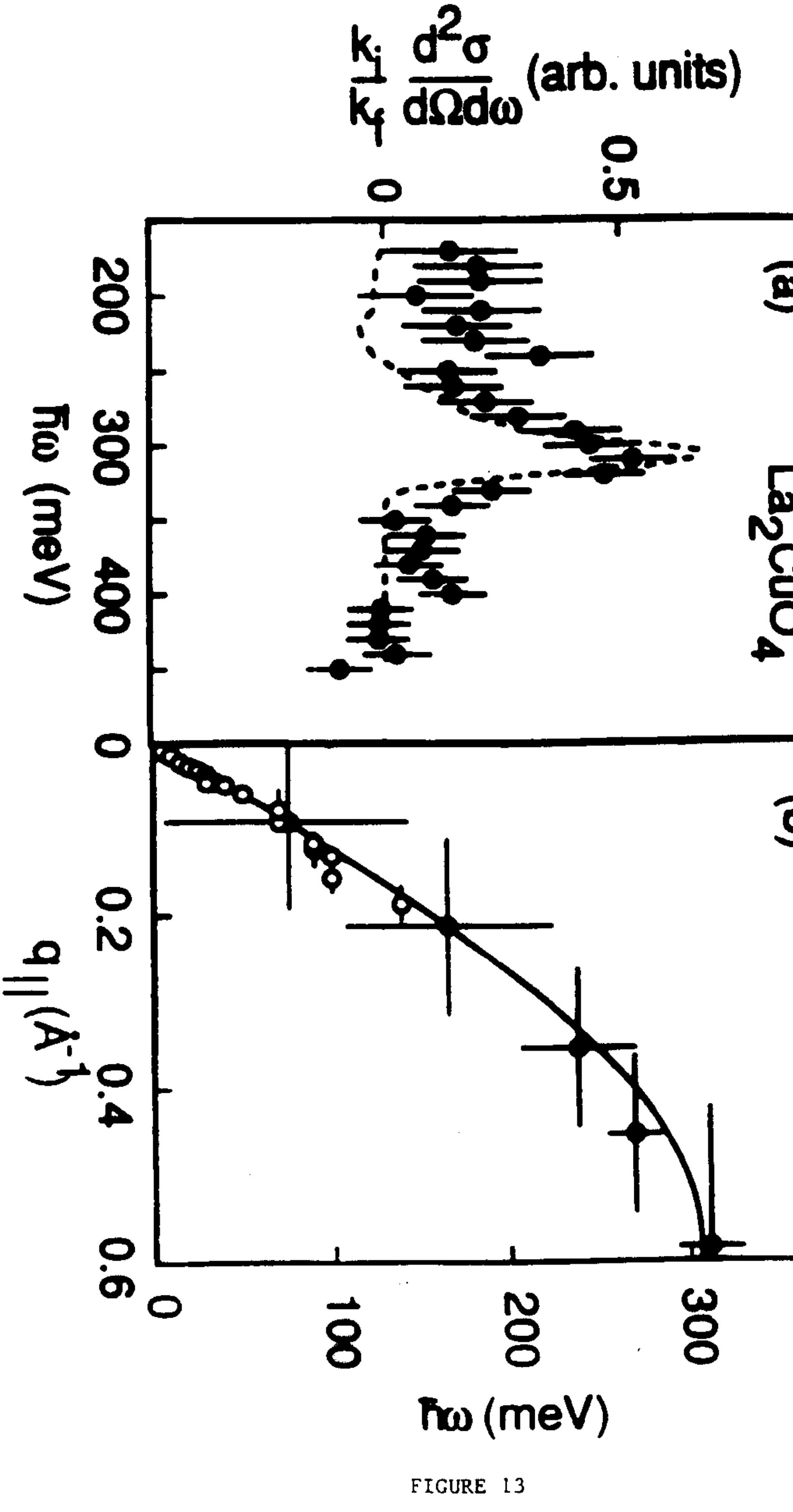
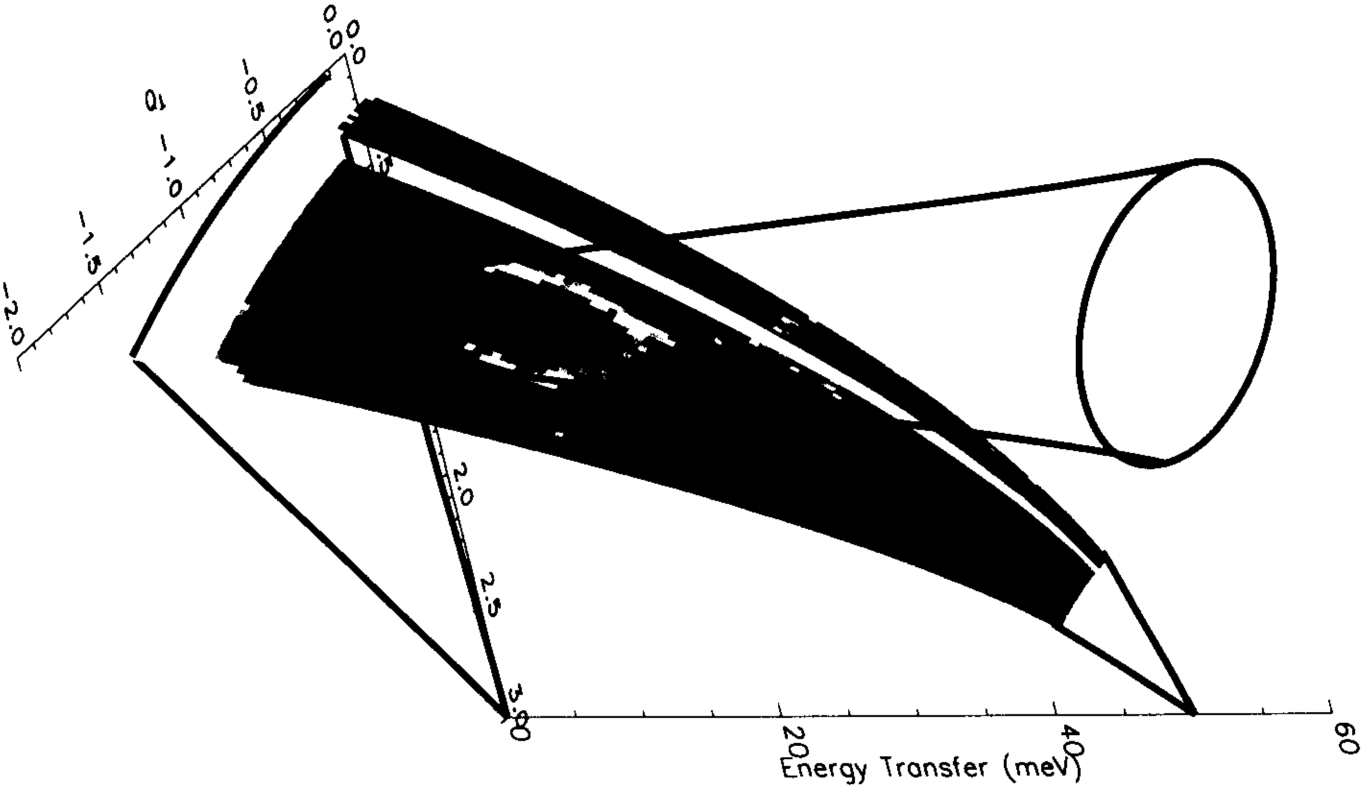

$\frac{k_i}{k_f} \frac{d^2\sigma}{d\Omega d\omega}$ (arb. units)
0
0.5
(a)
La$_2$CuO$_4$
200
300
400
ħω (meV)
(b)
0
0.2
0.4
0.6
$q_{||}$ (Å^{-1})
0
100
200
300
ħω (meV)

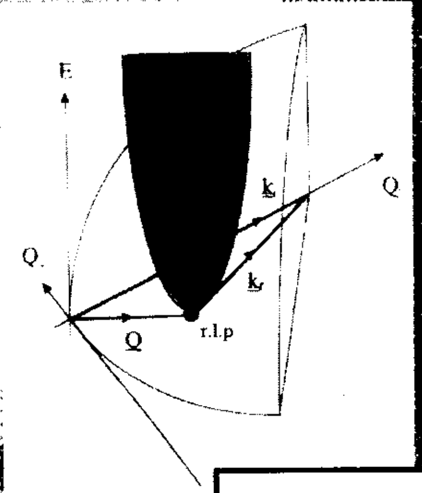
FIGURE 13

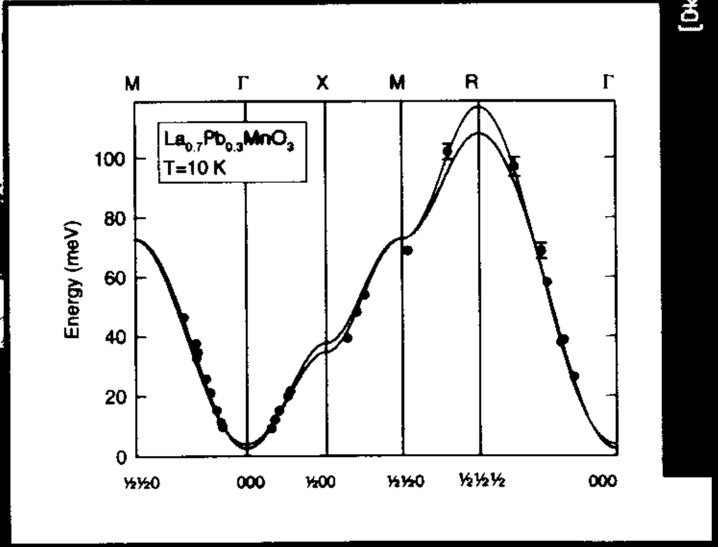

0.0
0.0
Q
-0.5
-1.0
-1.5
-2.0
2.0
2.5
3.0
0
20
40
60
Energy Transfer (meV)

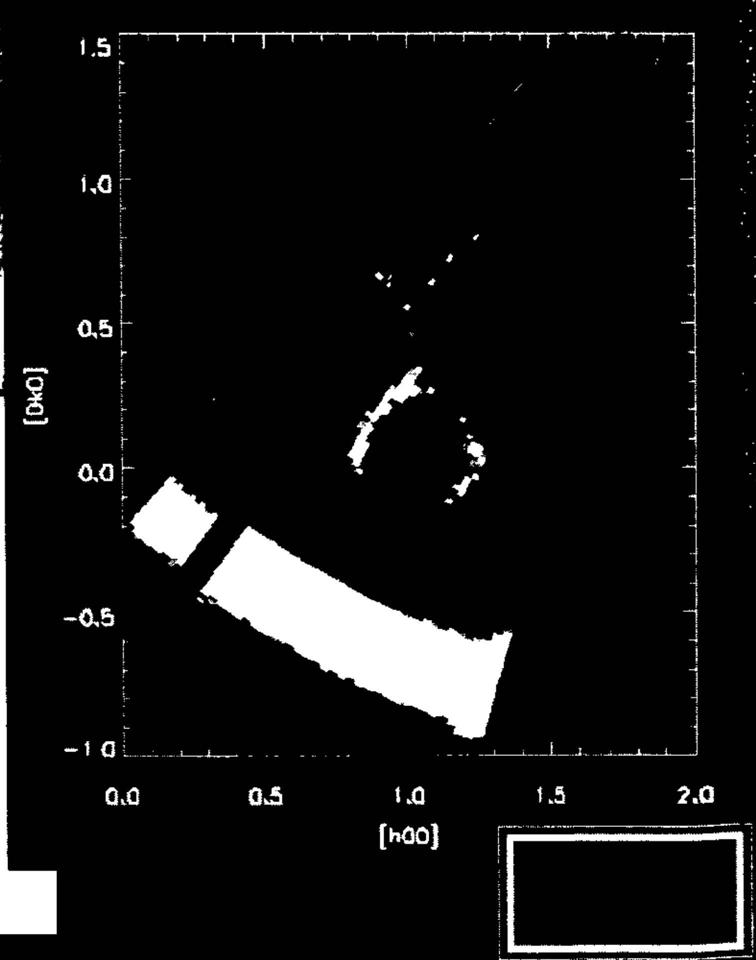
6

Spin Waves in the CMR Material La$_{0.7}$Pb$_{0.3}$MnO$_3$

Perring [illegible]







Since 60's, increased interest in local moments interacting with band electrons –

KONDO PROBLEM $\sum a_i^+ a_i + \underset{\substack{\uparrow \\ \text{d or f} \\ \text{electron}}}{S} \cdot \underset{\substack{\uparrow \\ \text{s or p} \\ \text{electron!}}}{\sigma(0)}$

ANDERSON HAMILTONIAN

↓

KONDO LATTICE

heavy fermions

Kondo insulators

↳ Renormalized Fermi liquids (even near metal-insulator transition*) but with unusual superconducting ground states & ubiquitous proximity to antiferromagnetism

* as shown for FeSi:Al

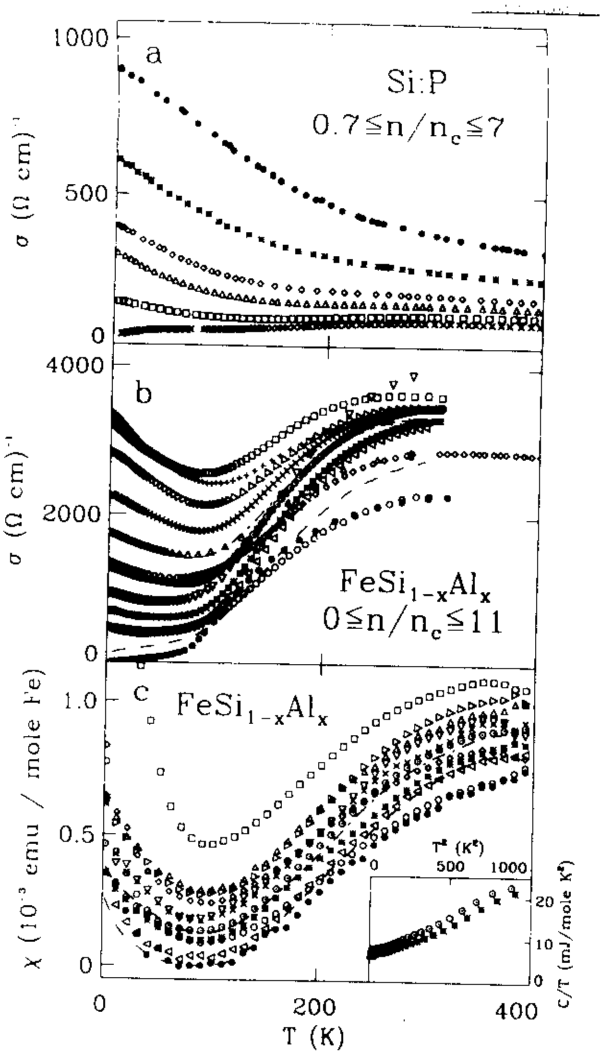
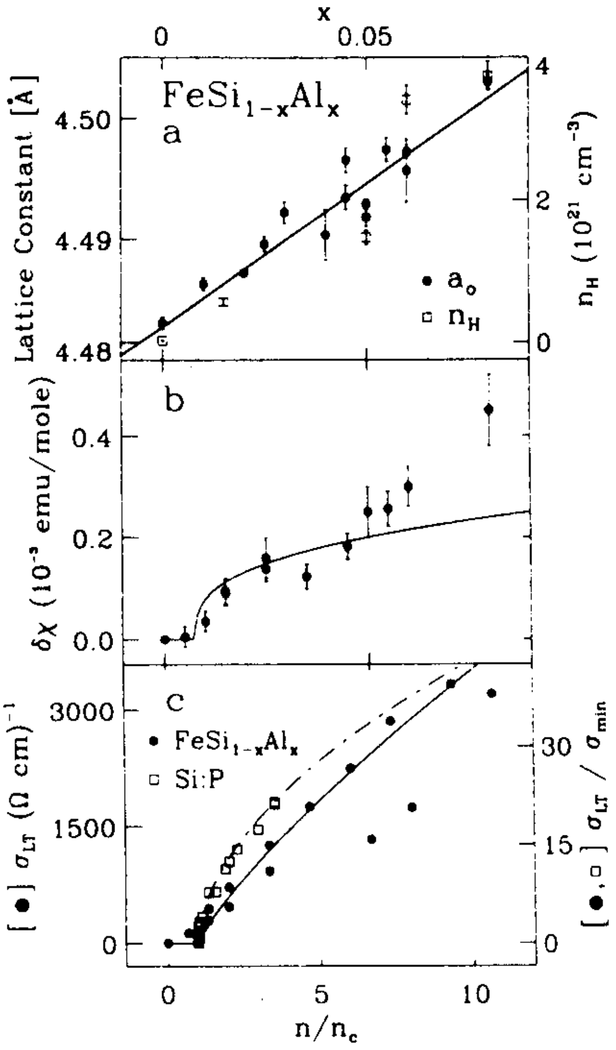


FIG. 2. (a) $\sigma(T)$ for Si:P with P concentrations of 2.7×10^{19} (●), 1.6×10^{19} (*), 1.1×10^{19} (◇), 7.8×10^{18} (△), 4.9×10^{18} (□), 2.8×10^{18} (×) data of Chapman *et al.* [11]. (b) $\sigma(T)$ for $FeSi_{1-x}Al_x$ with x of 0.0 single crystal (●), 0.0 (solid line), 0.005 (dashed line), 0.01 (◁), 0.015 (○), 0.015 (*), 0.025 single crystal (▽), 0.025 (⊙), 0.035 (dashed dotted line), 0.045 (×), 0.05 (◇), 0.055 (▷), 0.06 (△), 0.07 (+), 0.08 (□). (c) $\chi(T)$ for $FeSi_{1-x}Al_x$ with symbols same as in (b). Inset: $C(T)/T$ plotted as a function of T^2 for $x = 0.015$ (*) and $x = 0.025$ (⊙).


x
0
0.05
$FeSi_{1-x}Al_x$
a
Lattice Constant [Å]
4.50
4.49
4.48
n_H (10^{21} cm^{-3})
4
2
0
● a_o
□ n_H
b
$\delta\chi$ (10^{-3} emu/mole)
0.4
0.2
0.0
C
● $FeSi_{1-x}Al_x$
□ Si:P
[●] σ_{LT} $(\Omega$ $cm)^{-1}$
3000
1500
0
30
15
0
[●, □] σ_{LT} / σ_{min}
0
5
10
n/n_c

Metal-Insulator Transitions in the Kondo Insulator FeSi and Classic Semicondutors are Similar
[Phys. Rev. Lett. 78, 2831 (1997)]

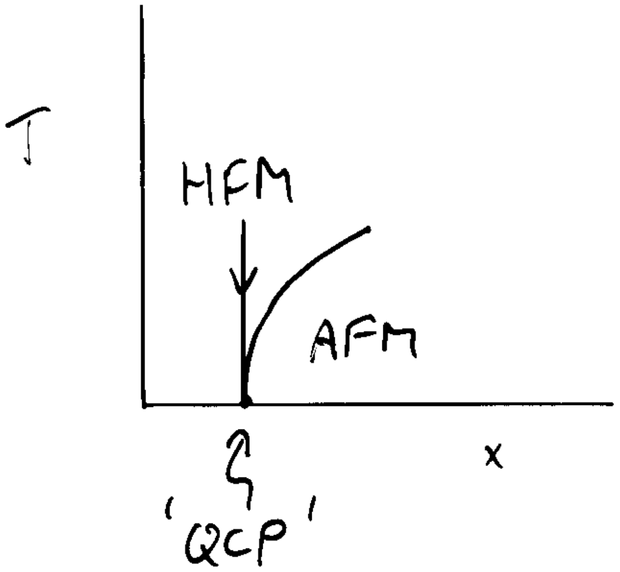
J. F. DiTusa, K. Friemelt, E. Bucher, G. Aeppli, and A. P. Ramirez

[S0031-9007(97)03287-0]

In Table I, the left hand column identifying the rows of the table was inadvertently removed during the production process. The correct table and caption are shown below.

TABLE I. Values of the energy gap in the undoped systems (E_g), critical concentration n_c, the effective carrier mass m^*/m_e, the dimensionless diffusion constant ($k_F l/3$) for $n = 2n_c$ calculated using the dopant density as the nominal carrier concentration, a valley degeneracy of 8 for FeSi, 6 for Si, and 4 for Ge, and the free electron formula for σ [1] (the value for La$_{2-x}$Sr$_x$CuO$_4$ was scaled from a high temperature estimate given in Ref. [13]), σ_0, and ν obtained from fits of the data to the form $\sigma = \sigma_0(n/n_c - 1)^\nu$, a from fits to the form $\sigma = \sigma_0(n) + aT^{1/2}$ to the low temperature conductivity at zero field, and the parameter b from fits to the linear temperature dependent conductivity to the form $\sigma(T,n) = \sigma_1(n) + bTn/n_c$. Data for Si:P were taken from Refs. [1,11,14], for Si:B from Refs. [1,11,14], for Si:As from Refs. [14,15], for Ge:Sb from Refs. [14,16], and for La$_{2-x}$Sr$_x$CuO$_4$ from Refs. [13,17].

System	E_g (eV)	n_c (10^{18} cm^{-3})	m^*/m_e	$k_F l/3$	σ_0 (1/Ω cm)	ν	a (Ω cm K$^{1/2}$)$^{-1}$	b (Ω cm K)
FeSi$_{1-x}$Al$_x$	0.06	330 ± 110	14 ± 2	0.23	600 ± 150	0.85 ± 0.1	−10.0	−1.1 ± 0.2
Si:P	1.17	3.74	0.26	0.46	260 ± 30	0.55 ± 0.1	−3.0	−0.41 ± 0.07
Si:B	1.17	4.06	0.38	0.20	152 ± 18	0.65 ± 0.14	−7.0	0.062 ± 0.005
Si:As	1.17	8.2	0.31	0.34	381	0.64 ± 0.2	−11.0	−8 ± 2
Ge:Sb	0.75	0.15	0.22	0.51	26 ± 10	0.9 ± 0.1	−12.0	0.073 ± 0.008
La$_{2-x}$Sr$_x$CuO$_4$	1.8	260	2	~3				−1.5 ± 0.3



At QCP, $\rho \sim T^{x}$ where $x \simeq 1$ & $x \neq 2$ (FLT)

$C \sim \ln T$

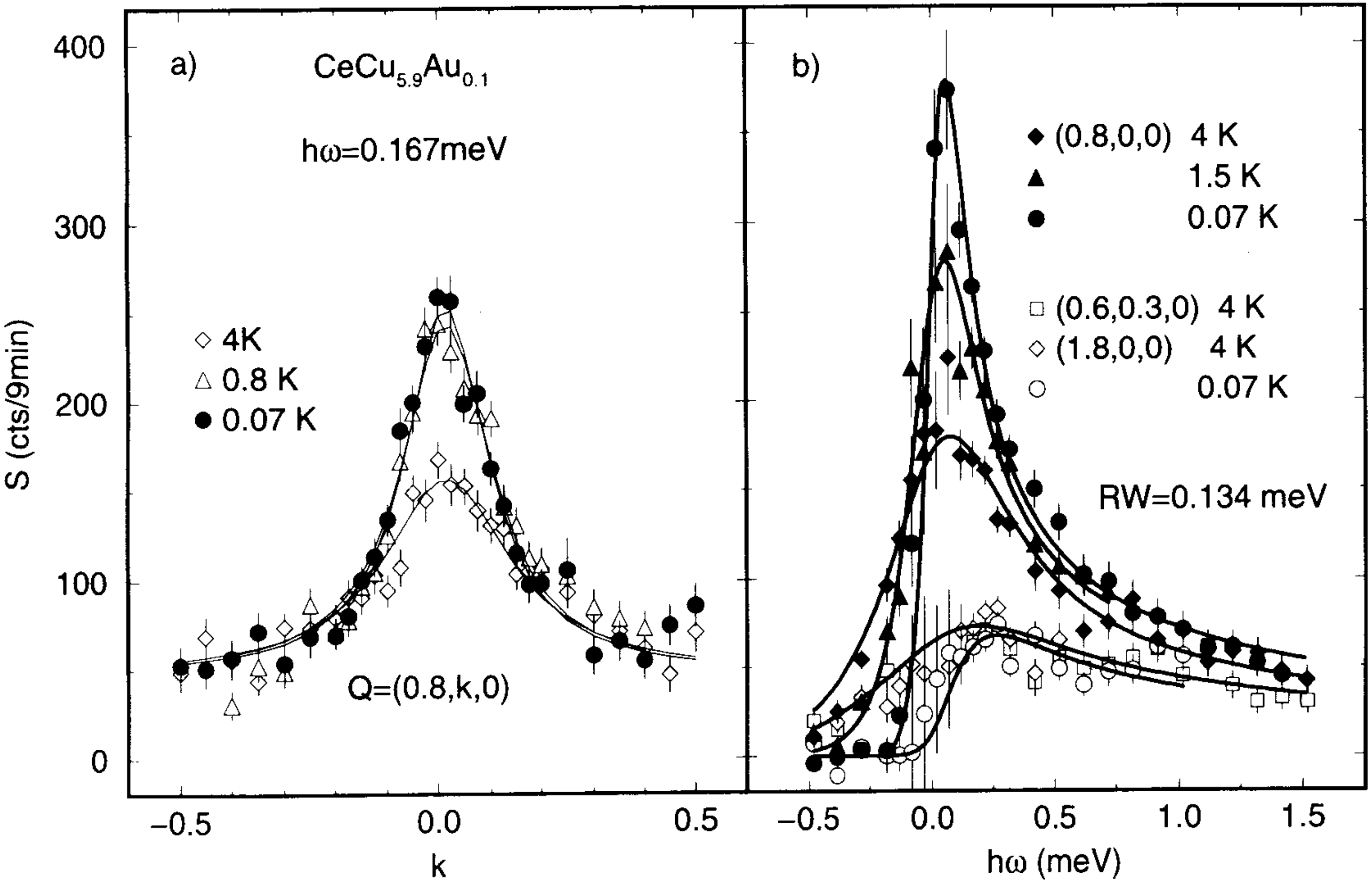
Examples of x :

ρ

H

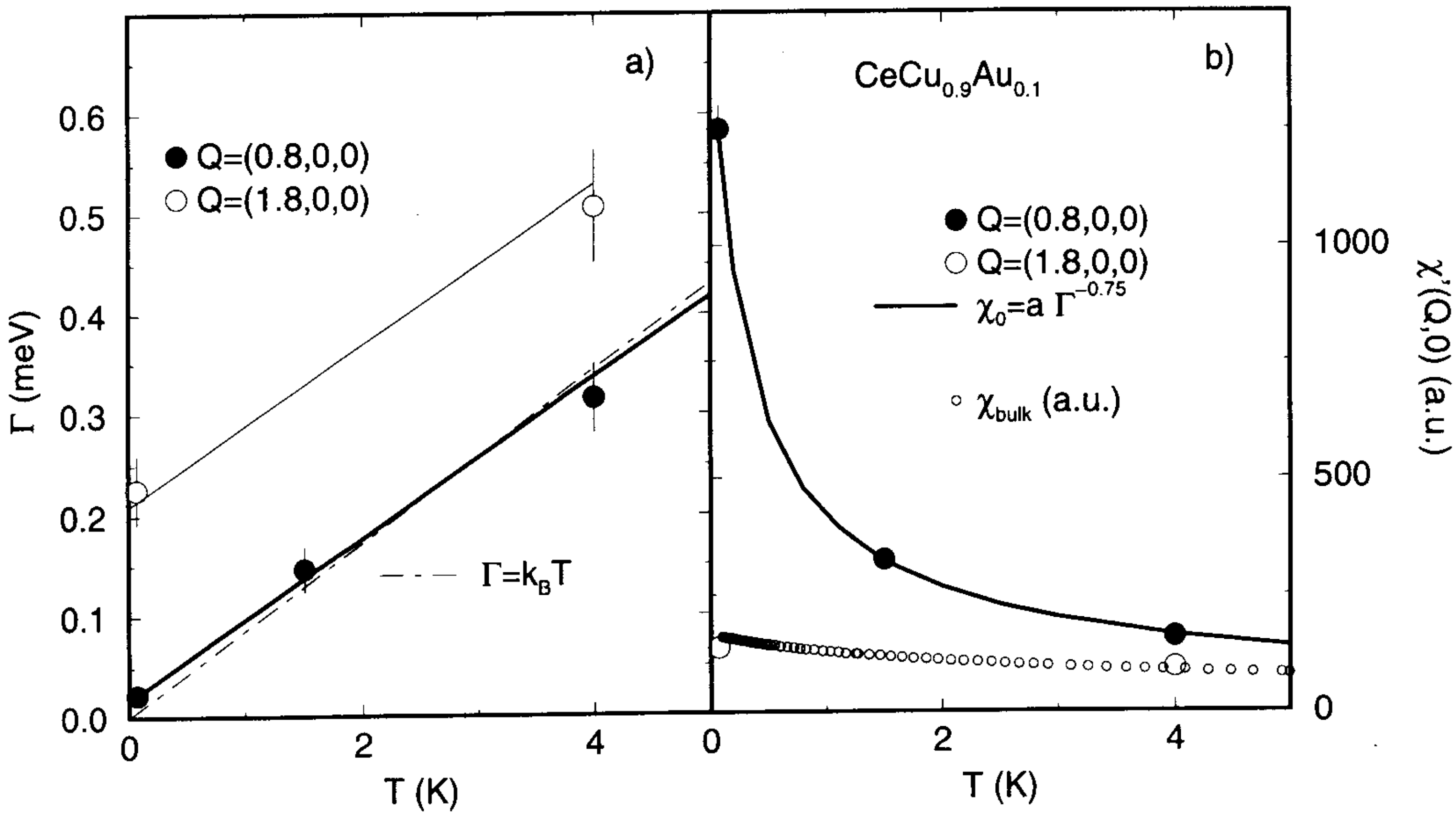
composition $CeCu_{5.9}Au_{0.1}$

icnsfig1ab.plo



$S(\omega) \sim \omega^{-3/4}$

icnsfig2.plo



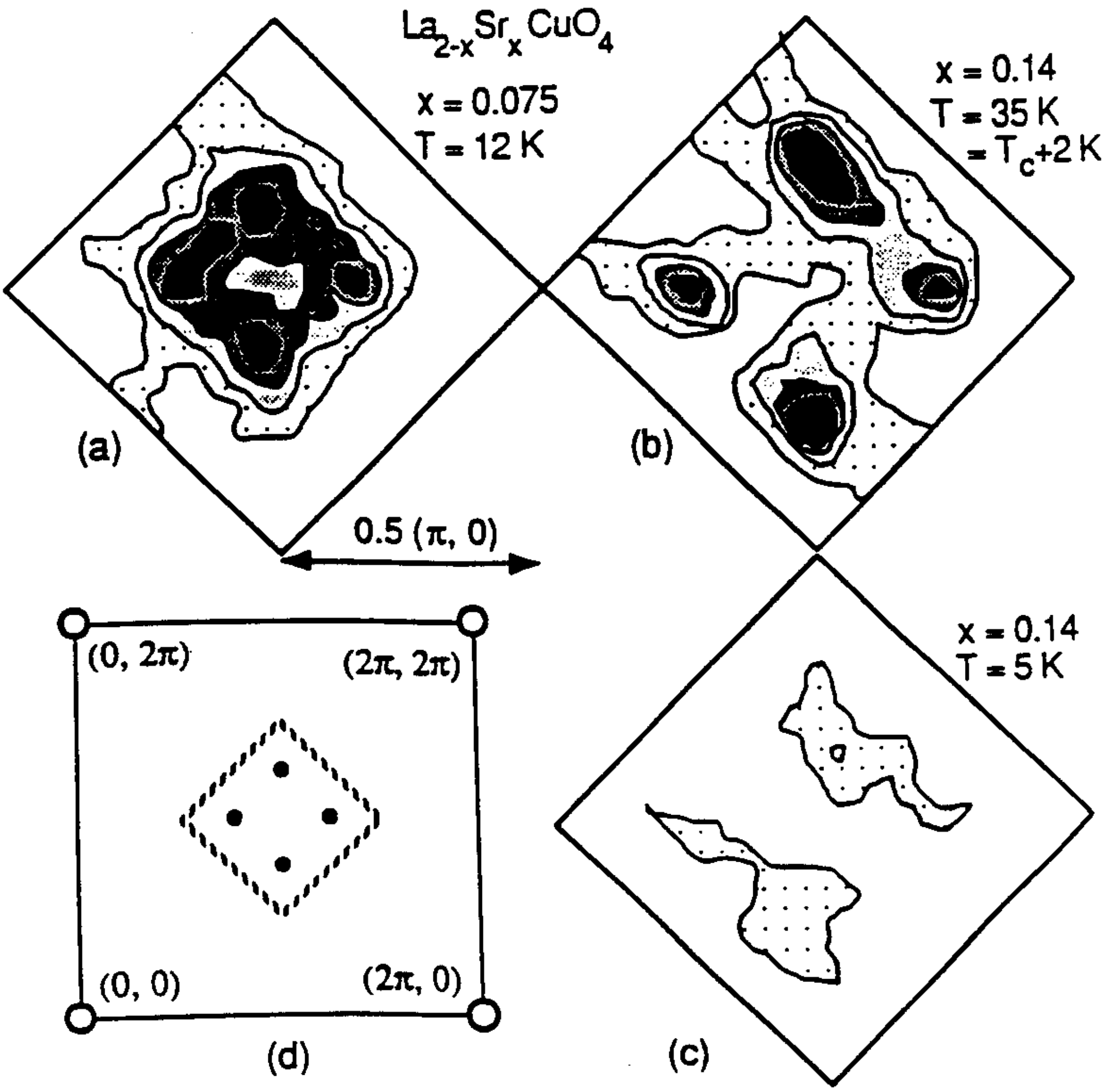
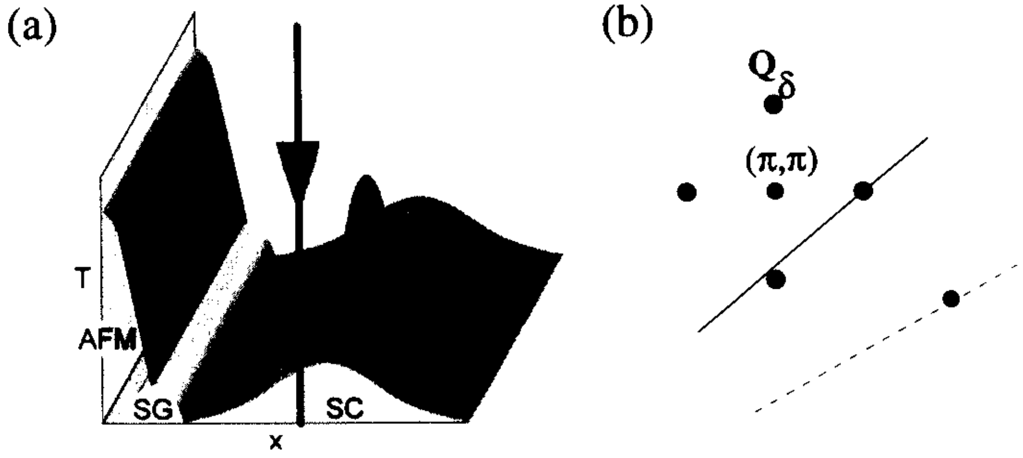
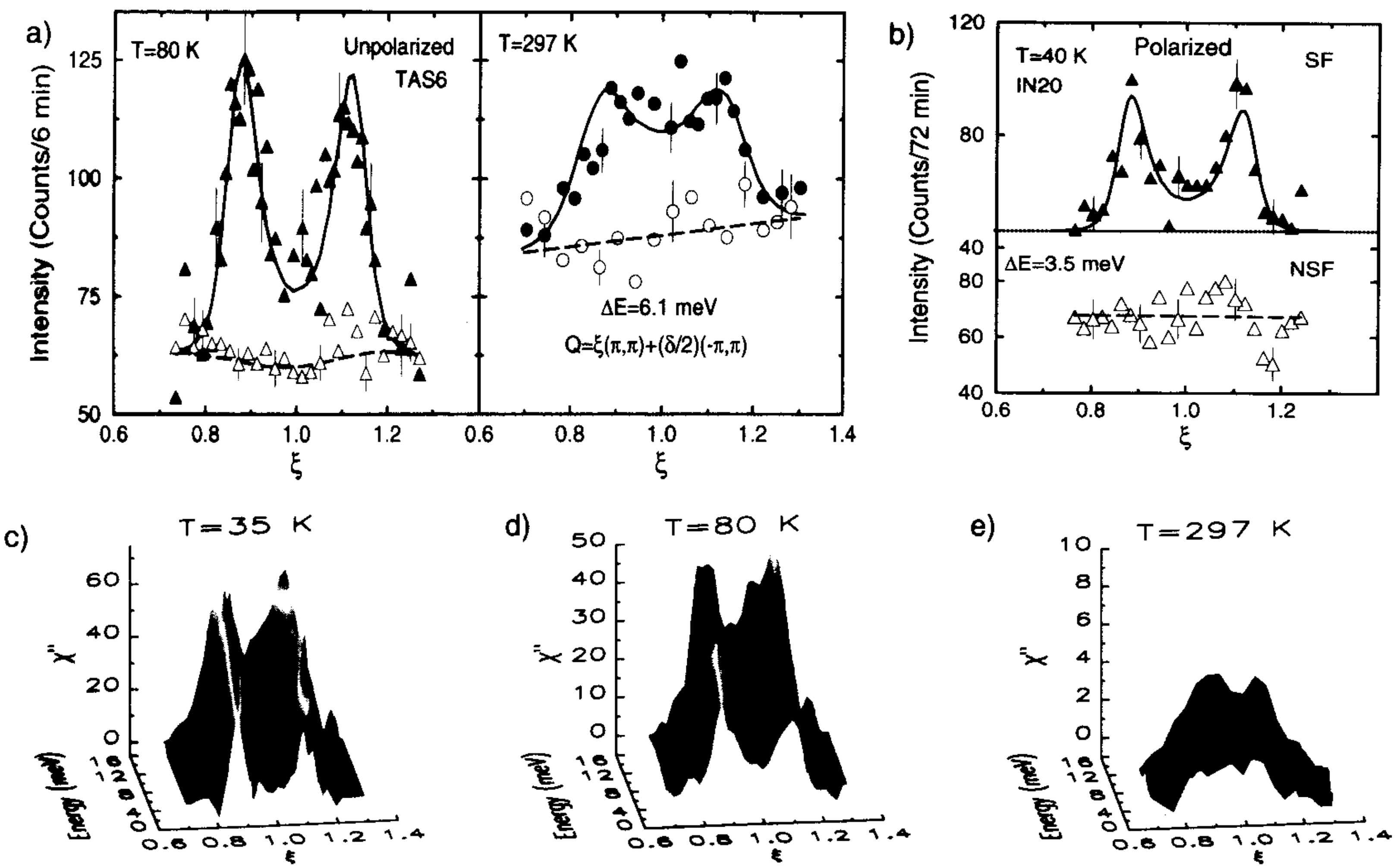
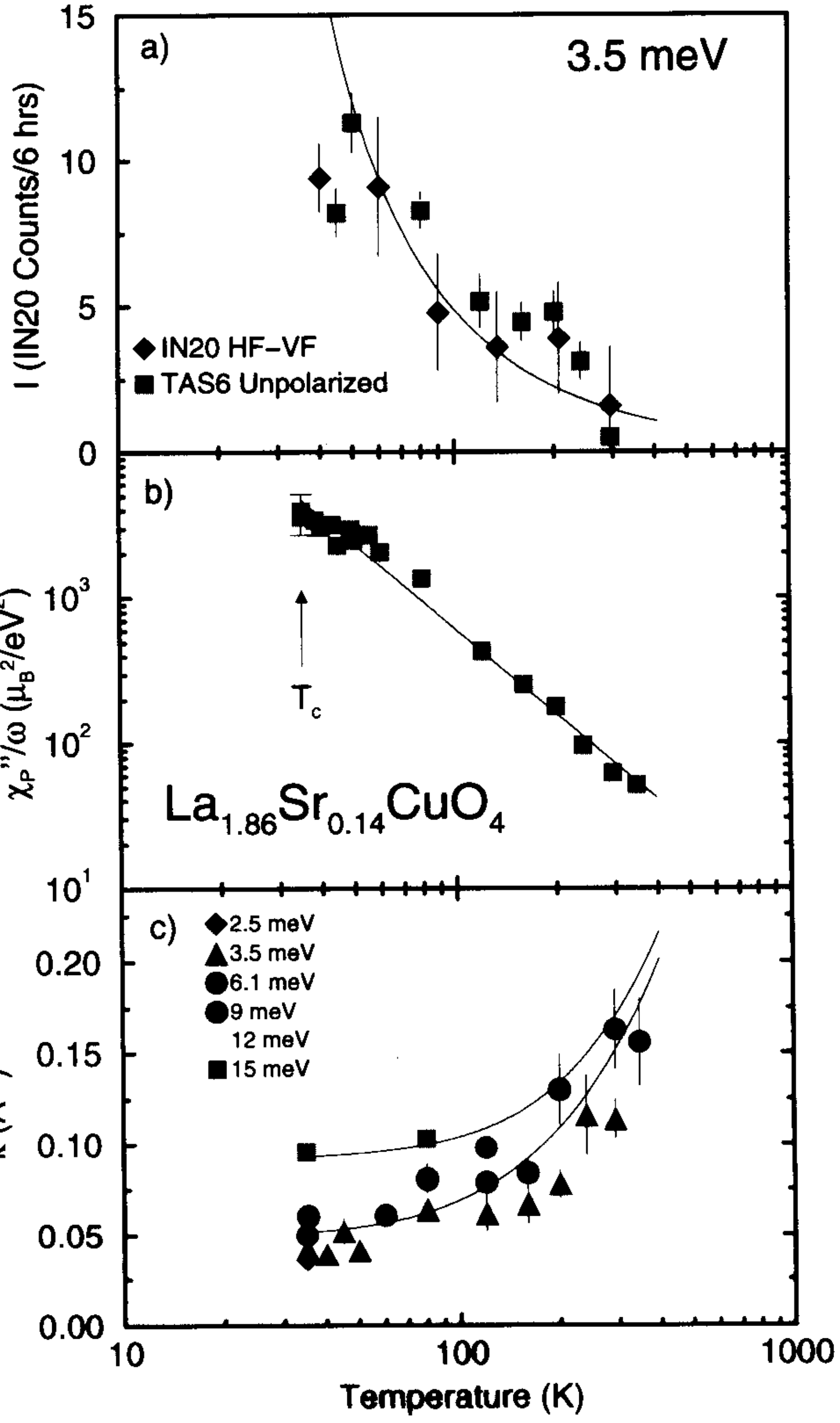

La$_{2-x}$Sr$_x$CuO$_4$
x = 0.075
T = 12 K
(a)
x = 0.14
T = 35 K
= T$_c$+2 K
(b)
0.5 (π, 0)
x = 0.14
T = 5 K
(c)
(0, 2π)
(2π, 2π)
(0, 0)
(2π, 0)
(d)

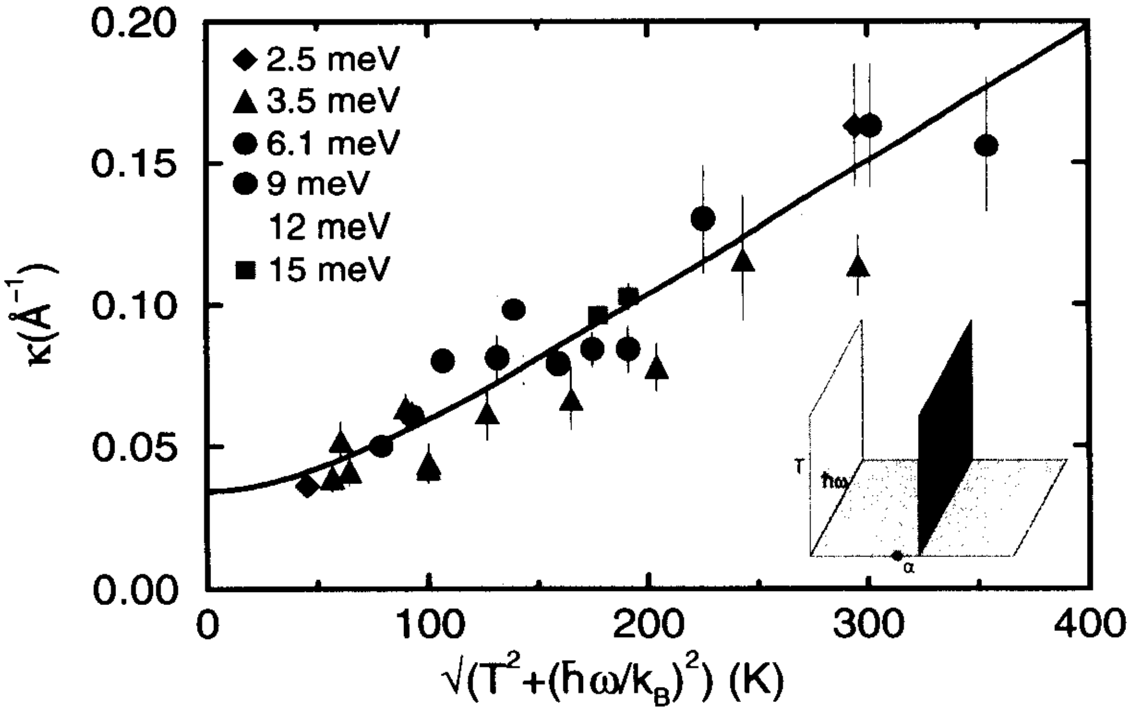
FIGURE 15


(a)
T
AFM
SG
SC
x
(b)
Q_δ
(π,π)


a)
T=80 K
Unpolarized
TAS6
T=297 K
ΔE=6.1 meV
Q=ξ(π,π)+(δ/2)(-π,π)
Intensity (Counts/6 min)
125
100
75
50
0.6
0.8
1.0
1.2
1.4
ξ
b)
T=40 K
IN20
Polarized
SF
NSF
ΔE=3.5 meV
Intensity (Counts/72 min)
120
80
40
60
ξ
c)
T=35 K
d)
T=80 K
e)
T=297 K
χ''
60
40
20
0
50
30
10
8
6
4
2
Energy (meV)
16
12
ξ



a)
3.5 meV
I (IN20 Counts/6 hrs)
15
10
5
0
◆ IN20 HF−VF
■ TAS6 Unpolarized
b)
χ_P''/ω (μ_B^2/eV^2)
10^3
10^2
10^1
T_c
$La_{1.86}Sr_{0.14}CuO_4$
c)
◆ 2.5 meV
▲ 3.5 meV
● 6.1 meV
● 9 meV
12 meV
■ 15 meV
κ (Å^{-1})
0.20
0.15
0.10
0.05
0.00
10
100
1000
Temperature (K)



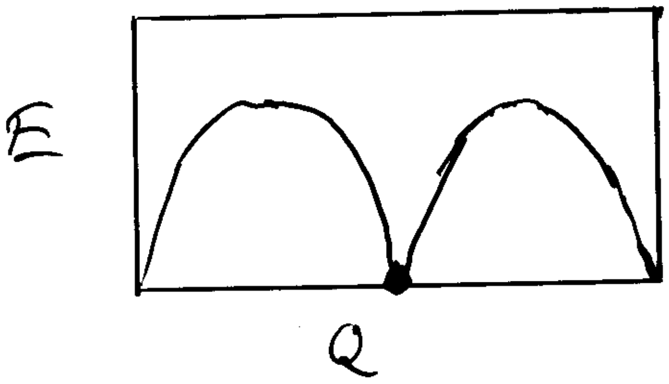
0.20
0.15
0.10
0.05
0.00
κ(Å^{-1})
◆ 2.5 meV
▲ 3.5 meV
● 6.1 meV
● 9 meV
12 meV
■ 15 meV
T
ħω
α
0
100
200
300
400
$\sqrt{(T^2+(\hbar\omega/k_B)^2)}$ (K)

HEAVY FERMIONS, $\overset{?}{=}$ LANDAU FERMI LIQUID
HIGH T_c (BAND) THEORY
COMPOUNDS ⊕ RENORMALIZED
PARAMETERS

LOCAL MOMENT $\overset{?}{=}$ SPIN WAVES (RENORMALIZED
MAGNETS
⊕ RG THEORY
FOR PARAMETERS

– TRUE FOR D=2 BUT FOR D=1,

PROBLEMS KNOWN FOR LONG
TIME –



FOR AFM

$$\langle S^+ S^- \rangle = \int |\langle q | S^+ | 0 \rangle|^2 \, d^d q$$

$$= \int_{L^{-1}} \frac{1}{q} \, d^d q = \ln L \text{ for } d=1$$

because $\langle q | S^+ | 0 \rangle = 1/\sqrt{q}$

where $|0\rangle = \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow \ldots$

FROM THEORISTS :

DRAMATIC PREDICTIONS

$S = 1/2$ CHAIN $\equiv$ 1-D LIQUID OF FERMIONS w/o CHARGE

$S = 1$ CHAIN $\equiv$ GAPPED QUANTUM LIQUID WITH ONLY SHORT-RANGED MAGNETIC CORRELATIONS

FROM CHEMISTS :

REALIZATIONS OF $S=1$ & $S=1/2$ CHAINS

FROM EXPERIMENTALISTS :

TOOLS TO MEASURE $S(Q,\omega)$

$S = 1/2$

Dispersion for spinons

Pair-production continuum $\sim S(Q,\omega)$

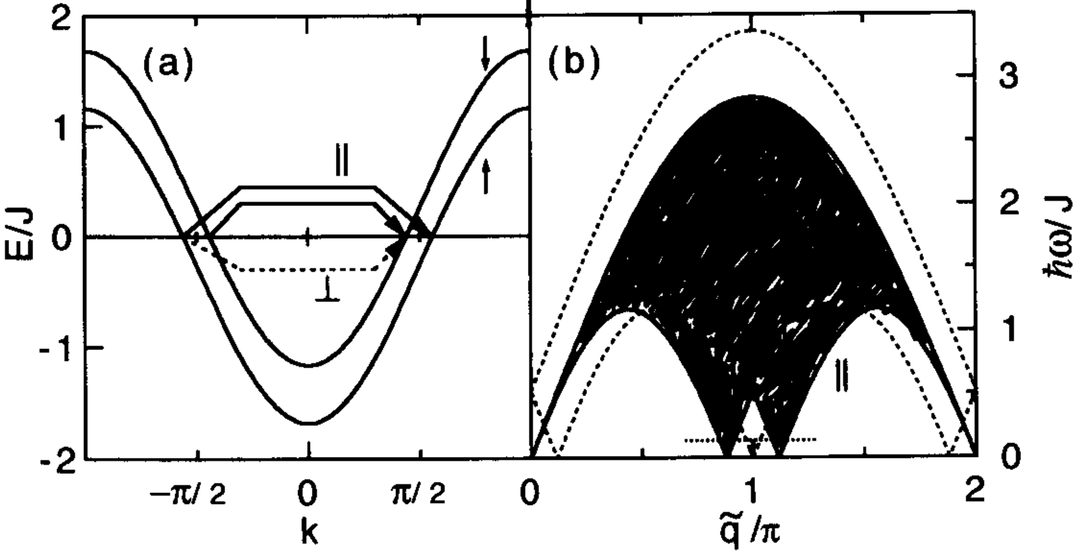
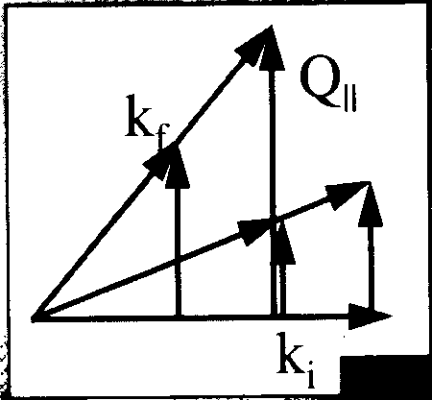
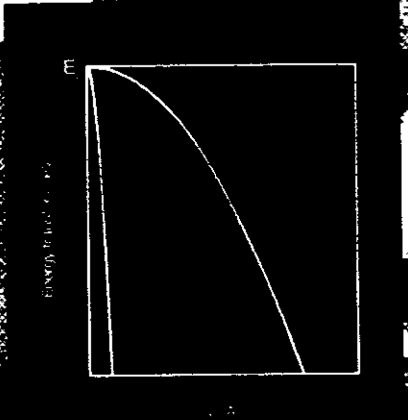
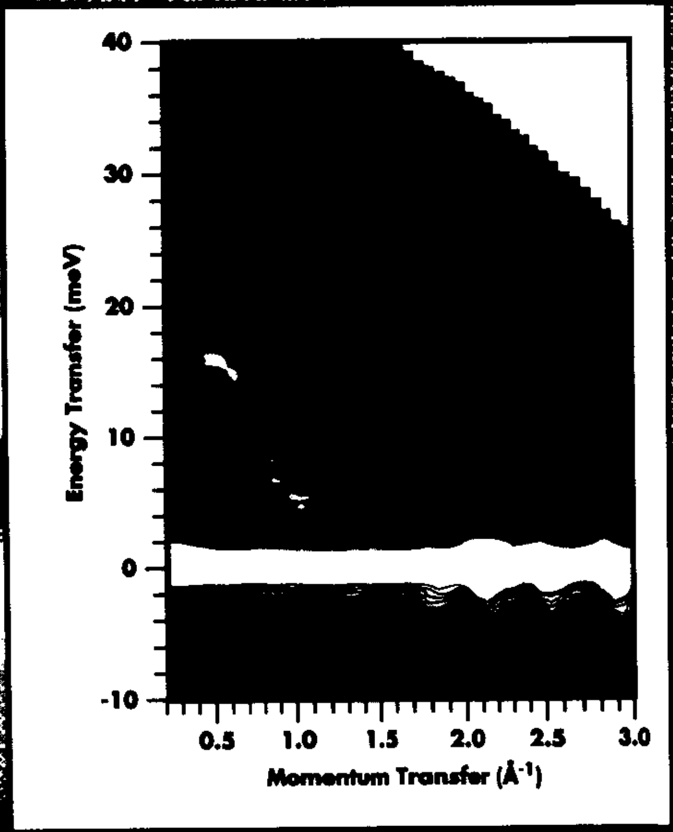


Fig. 1 Dender et al.

The Spin Peierls system CuGeO$_3$







(17)

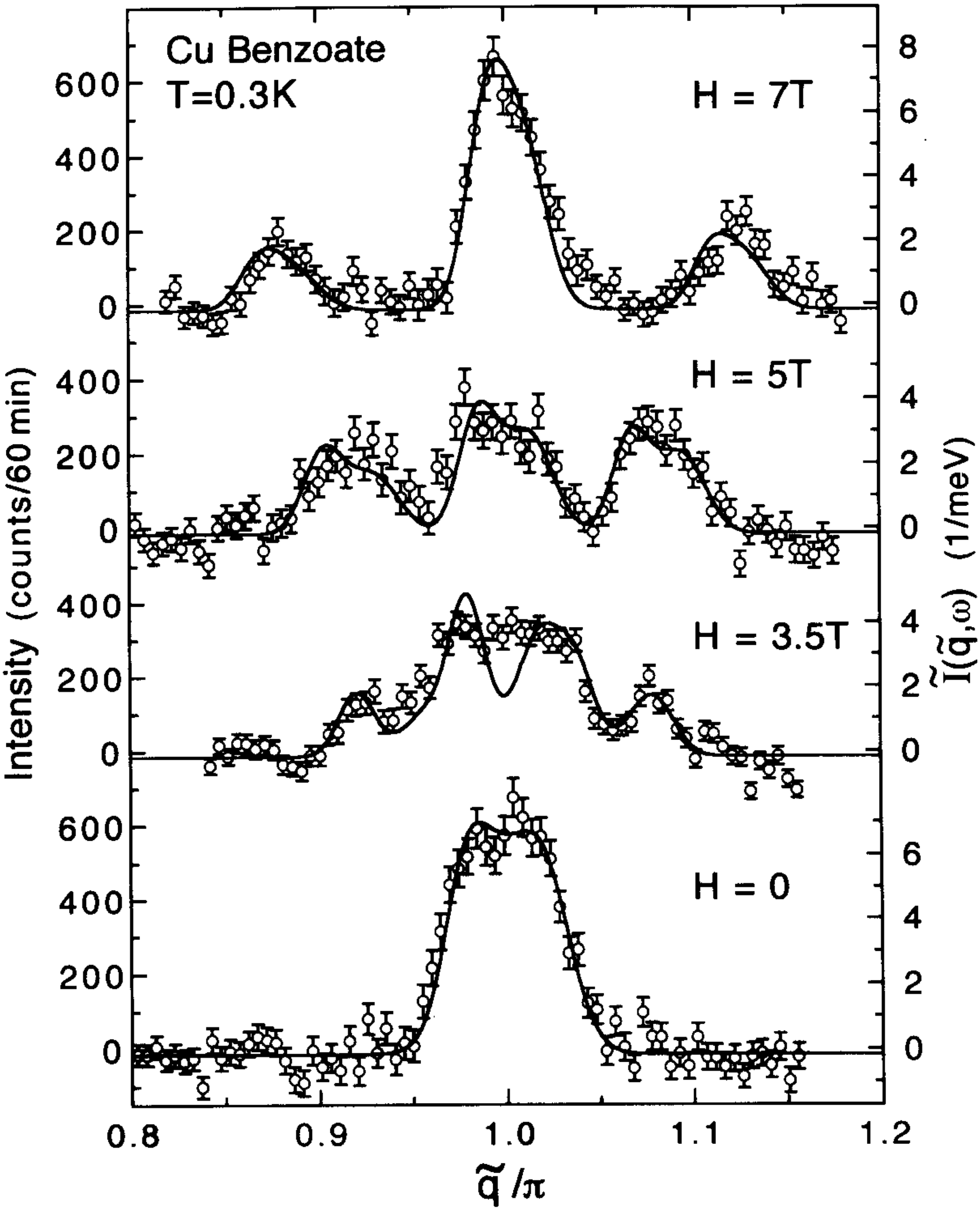
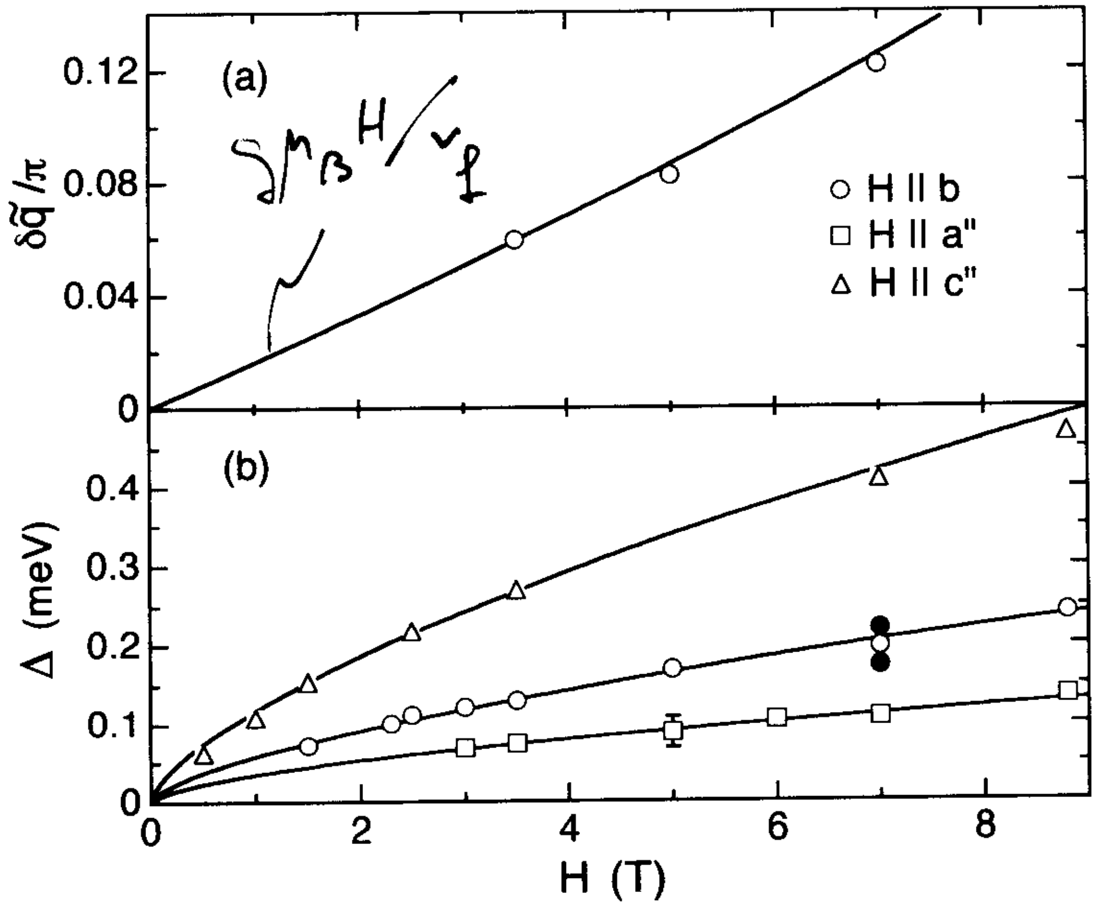


Figure 2. Dender et al.



$g\mu_B H / v_f$

Fig. 5 Dender, et al.

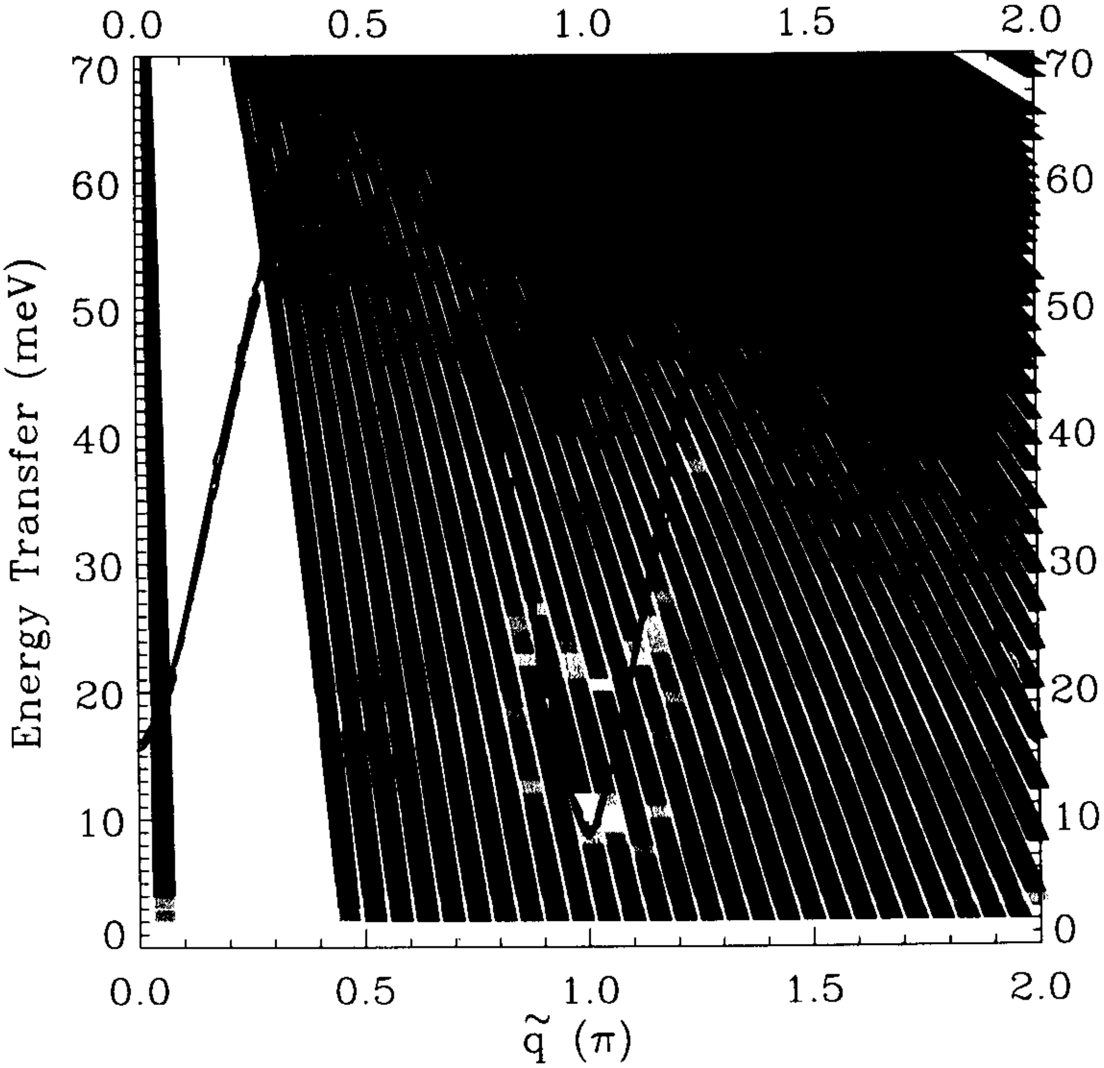
Fermionic character of underlying excitations in $S = 1/2$ verified in extraordinary detail ... what about incompressible Quantum Fluid for $S = 1$ (Haldane conjecture

Y_2BaNiO_5

$\ldots$ Ni - O - Ni - O - Ni - O $\ldots$

↑

d^8 $S=1$



Single-mode (Feynman) approx works!

$$S(Q) \sim \frac{1}{E(Q)}$$

Add 'Q' to "conventional"
AFM

$\rightsquigarrow$ high T_c

Add 'Q' to Spin Liquid

- Akimitsu, Takagi

  (spin ladders ...)

CONCLUSIONS

BAND THEORY (aka LFLT)
STARTING TO COLLAPSE WHEN
APPROACHING AFM METAL STATE

S.W. THEORY HOPELESS IN 1-D

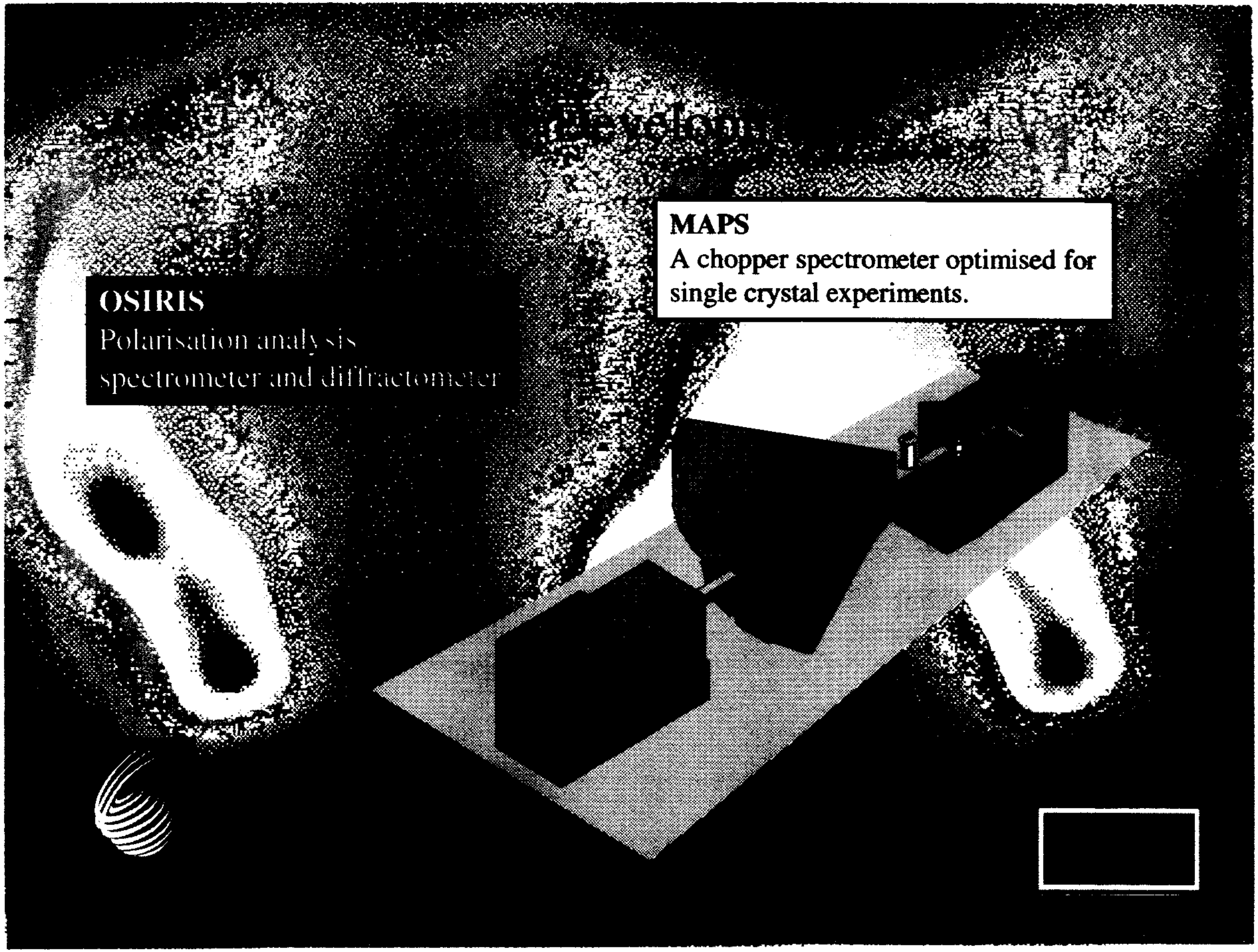
→ CURIE WEISS / SPIN WAVE
⊕ BAND THEORY

PARADIGM FOR SOLID STATE
PHYSICS IS BREAKING DOWN
IN VERY OBVIOUS WAYS

QUESTION -

IS 1-D SPECIAL & ALL WE NEED FOR $D \geq 2$ IS TO PROPERLY UNDERSTAND QCP, IN ANALOGY WITH WHAT KADANOFF/WILSON/FISHER DID FOR CLASSICAL CRITICAL POINTS 30 YRS AGO ?

FOR ANSWERS -



OSIRIS
Polarisation analysis
spectrometer and diffractometer

MAPS
A chopper spectrometer optimised for
single crystal experiments.

A Next Generation Neutron Source

5 MW
~ 1μs pulse
50Hz and 10Hz Targets
30 x ISIS

Better Resolution
True from astronomy to microscopy

Smaller Systems
crack tip
dilute solutions
new materials

Shorter Experiments
kinetics
extreme environments

Complex Systems
wide Q,ω range
high signal-to-noise

Advanced Techniques
polarisation analysis