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SMR.959 - 21

MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS
"Disorder and Interaction in Quantum Systems and Their Classical Analogs"

(1 - 19 July 1996)

"Photoemission Spectra of $(TaSe_4)_2I$: Evidence for One-dimensional Charge Density Wave Fluctuations"

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

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Photoemission Spectra of $(TaSe_4)_2I$

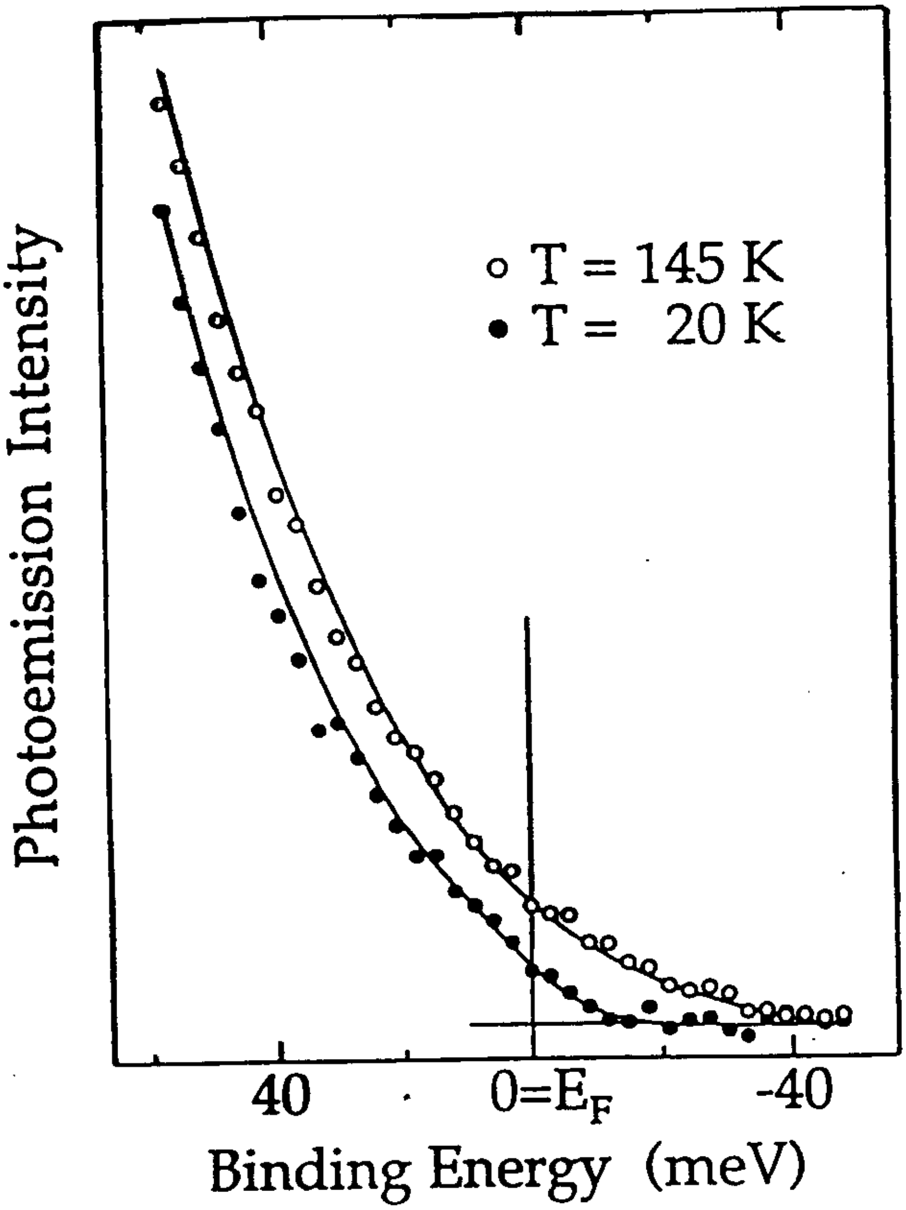
OUTLINE

- Review of data on some selected low-dimensional systems
- Overview of photoemission on $(TaSe_4)_2I$
- Fluctuating CDW picture of Lee, Rice, and Anderson (LRA)
- Calculations
- Comparison with experiment
- Conclusions

Nic Shannon, U. Warwick
Bob Joynt, U. Wisconsin

Angle-integrated photoemission

1464 (density of states) of $1T-TaS_2$



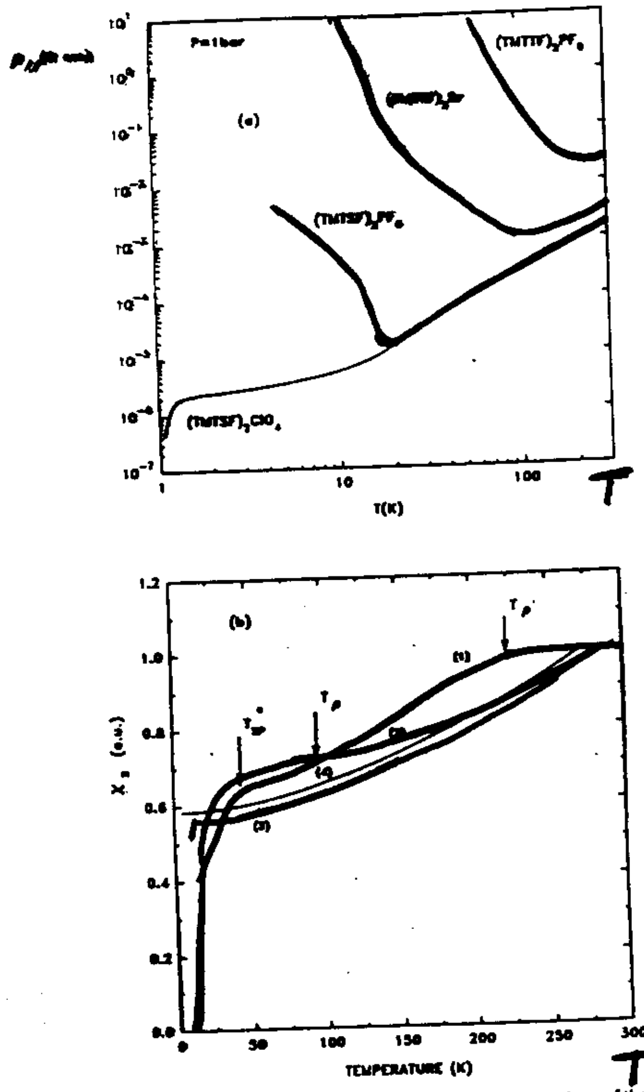
$\rho(\omega) \sim \omega^2$

Dardel et al.
Phys. Rev B 45, 1462 ('92)

Spin-charge separation (?) —
in organic chain compounds

$\rho_{\parallel}$

χ



T

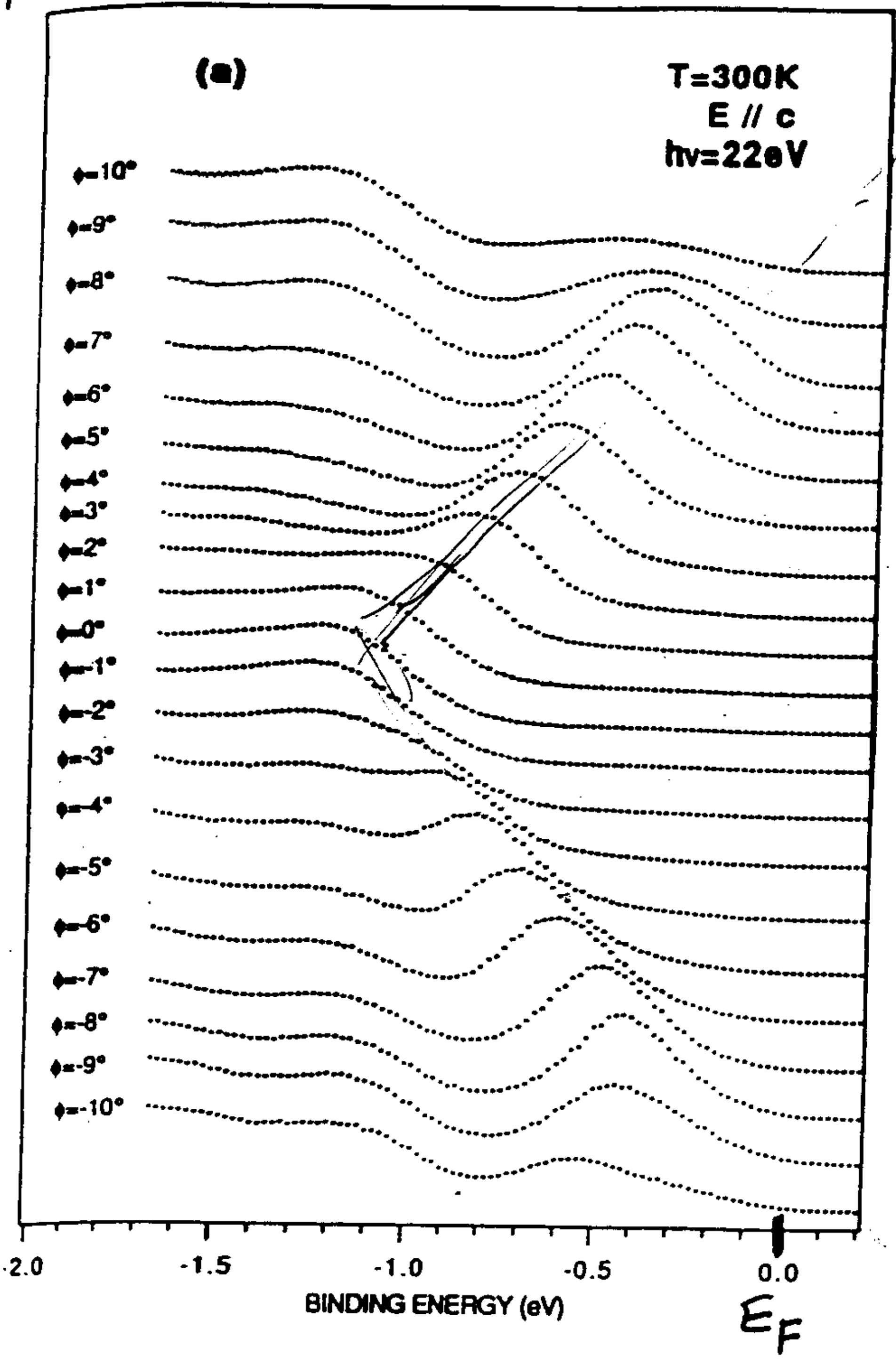
Red = $(TMTTF)_2PF_6$
Blue = $(TMTTF)_2Br$
Brown = $(TMTSF)PF_6$

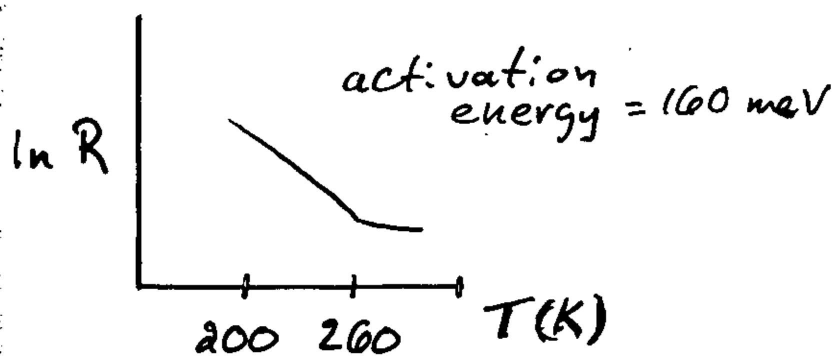
Fig. 2. (a) The temperature dependence of the resistivity for representatives of the Bechgaard salts and their sulphur analogs. After refs. [9,27,23]. (b) The temperature dependence of the magnetic susceptibility for $(TMTTF)_2PF_6$ (curve 1) (EPR), $(TMTTF)_2Br$ (curve 2) (EPR), $(TMTSF)_2PF_6$ (curve 3) (Faraday method), and $(TMTSF)_2ClO_4$ (curve 4) (Faraday method). After refs. [11–13].

Ground states are antiferromagnetic, spin-Peierls even superconducting.

Data reviewed by C. Bourbonnais, in "Strongly interacting fermions..." Les Houches, 1991 (Elsevier, 1995)

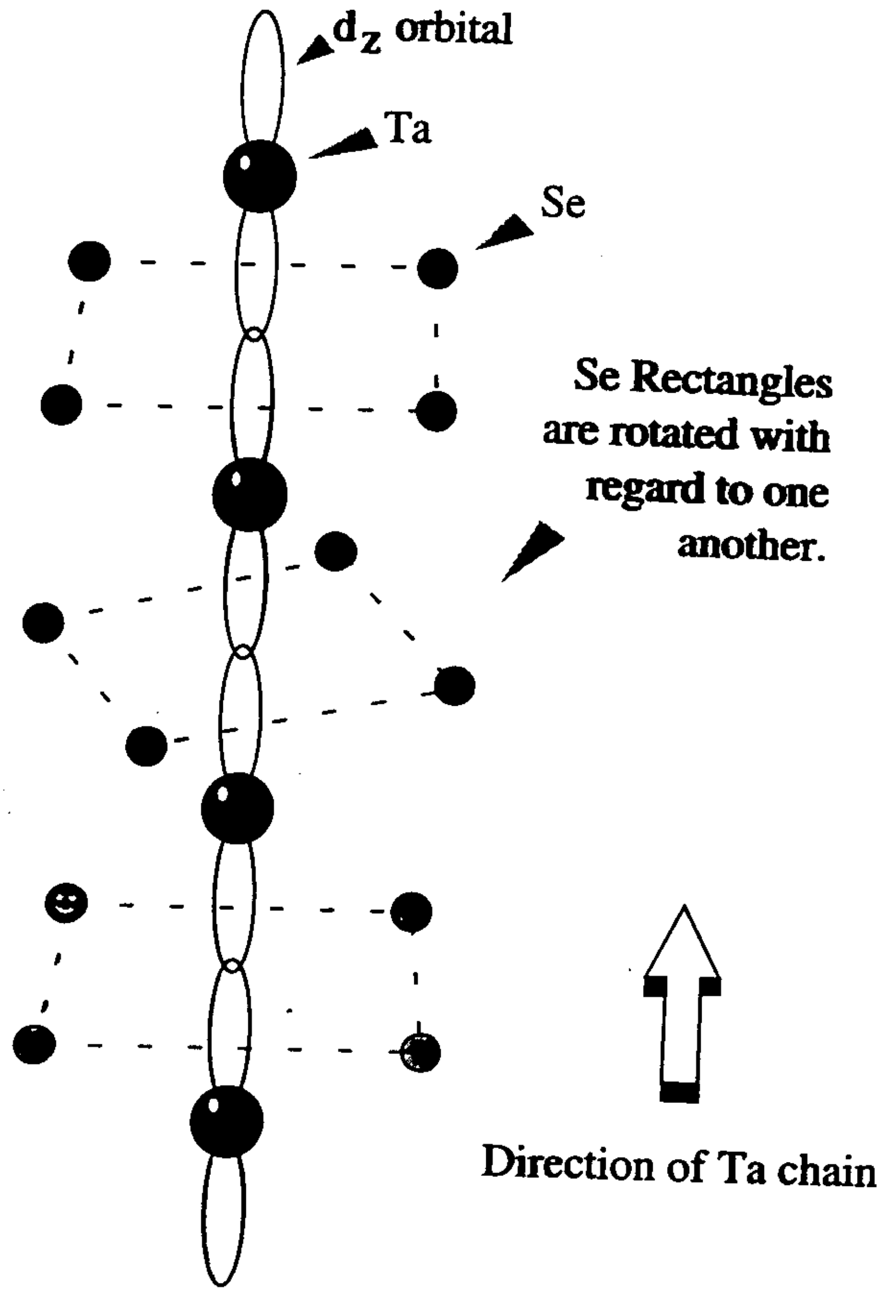
Angle-resolved photoemission (spectral function) of $(TaSe_4)_2I$





Terrasi et al. PRB 52, 5592 ('95)

Chains in $(TaSe_4)_2I$



One-dimensional single band, $\frac{1}{4}$-filled
$K_F = \pi/4a = 0.3\ Å^{-1}$

THE MODEL

(Fröhlich)

$$\mathcal{H} = \sum_{k\sigma} v_F k \, c^+_{k\sigma} c_{k\sigma} + \sum_q \omega(q) \, b_q^+ b_q + \frac{1}{\sqrt{L}} \sum g(q) \, c^+_{k+q} c_k \, u_q \,,$$

$$u_q = (2\omega(q))^{-1/2} (b_q^+ + b_{-q})$$

<u>non-interacting</u> electrons

The model is unstable, in mean-field theory, to a charge-density wave (CDW) with $Q = 2k_F$:

$$k_B T_c^{mf} = 1.13 \, E_F \, e^{-1/\lambda} \,, \quad \lambda = \frac{N_0 \, g(2k_F)}{|\omega(2k_F)|^2}$$

$$\Delta = \frac{1}{\sqrt{L}} \, g(2k_F) \, \langle u_{2k_F} \rangle$$

In a truly one-dimensional system, fluctuations destroy the transition

LEE-RICE-ANDERSON treatment

$$\mathcal{H} = \sum_{k\sigma} v_F k\, c^+_{k\sigma} c_{k\sigma} + \mathcal{H}_{e-p}$$

$$\mathcal{H}_{e-p} = \sum_{\substack{k>0\\ \sigma}} \psi^*_{-Q}\, c^+_{k-Q\sigma} c_{k\sigma} + \psi_Q\, c^+_{-k+Q\sigma} c_{-k\sigma}$$

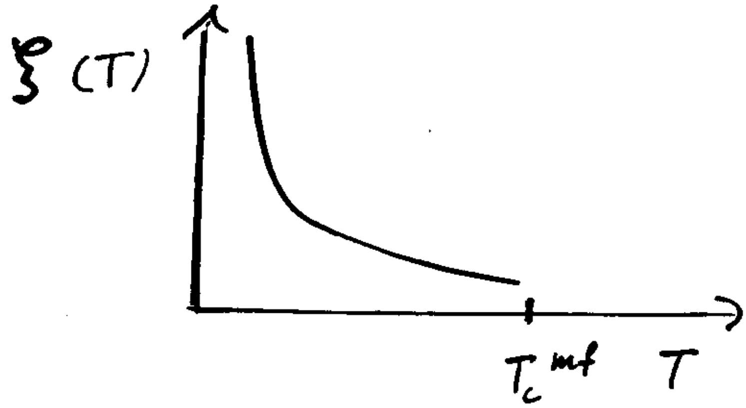
ψ_Q is taken to be a <u>static</u> field $\Rightarrow$

$$(\mathcal{G}(k, i\omega_n))^{-1} = i\omega_n - v_F k - \sum_Q \frac{\psi_Q \psi^*_{-Q}}{i\omega_n - v_F(k-Q)},$$

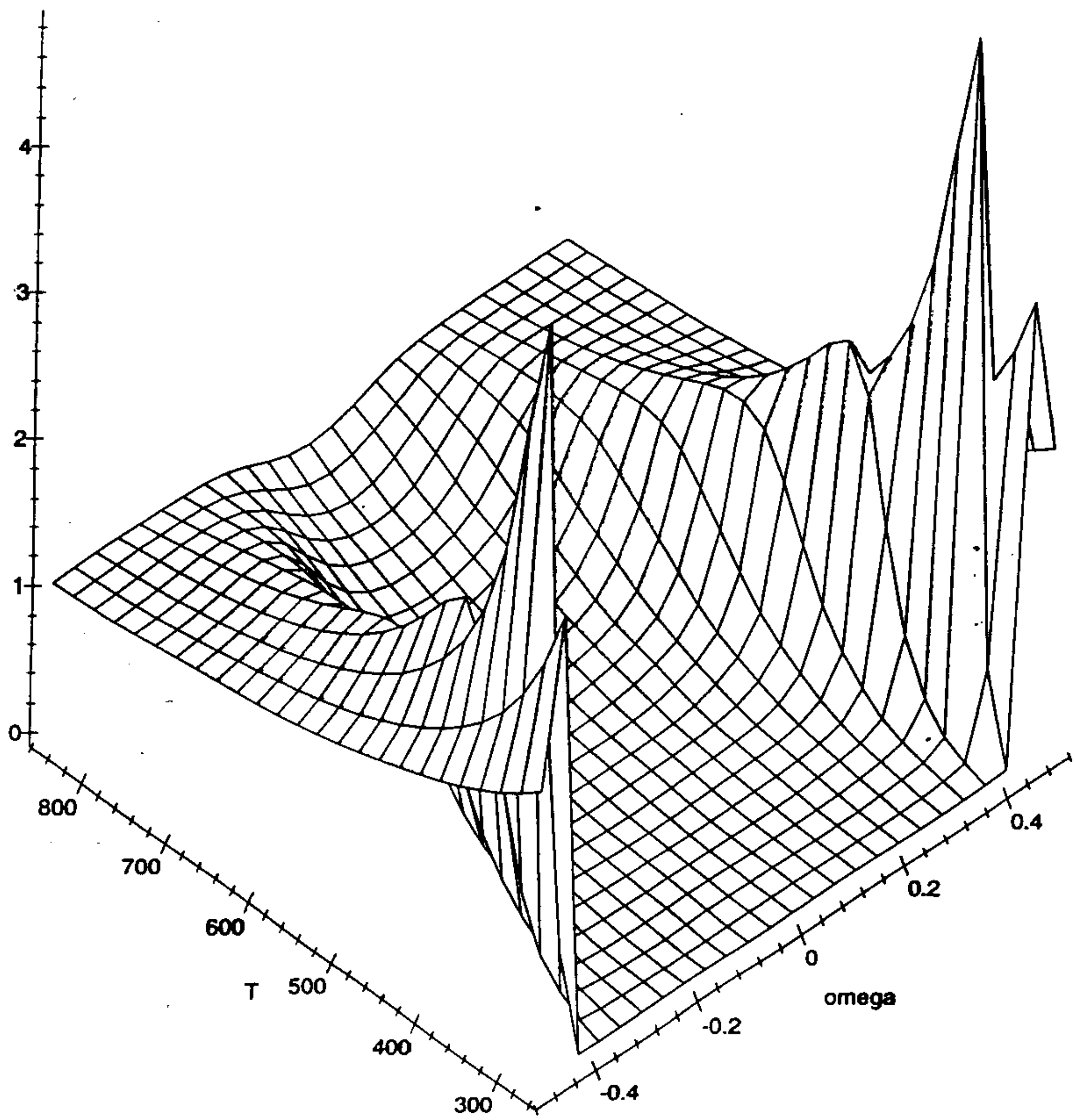
and ψ_Q is computed from the simplest possible field theory:

$$F[\psi_Q] = a(T)\,|\psi_Q|^2 + b(T)\,|\psi_Q|^4 + c(Q-2k_F)^2\,|\psi_Q|^2$$

$$\Rightarrow \langle \psi(x)\psi(x')\rangle = \langle \psi^2\rangle \exp -\left|\frac{x-x'}{\xi}\right| \cos(2k_F(x-x'))$$



$A(k_F,\omega)$



Comparison with experiment

$$A(K,\omega) \sim \mathrm{Im}\, \mathcal{G}(\omega + i\delta, k)$$

$$= \frac{2 v_F \xi^{-1} \langle \psi^2 \rangle}{[\omega^2 - v_F^2 k^2 - \langle \psi^2 \rangle]^2 + v_F^2 \xi^{-2} (\omega - v_F k)^2}$$

when: $T \gg T_c^{mf}$, $\langle \psi^2 \rangle < \frac{v_F^2 \xi^{-2}}{4}$

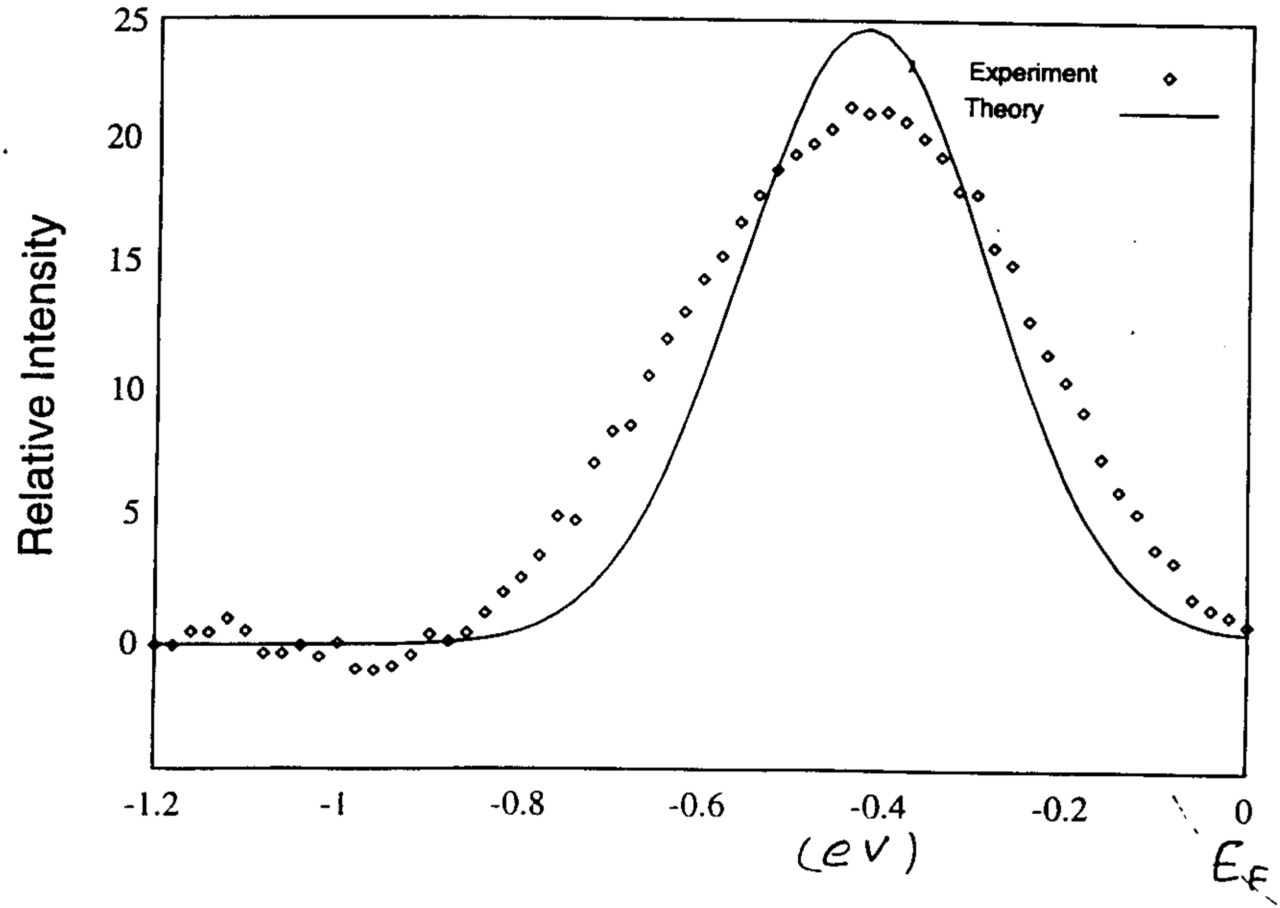
there is one peak

$T \lesssim T_c^{mf}$ $\langle \psi^2 \rangle > \frac{v_F^2 \xi^{-2}}{4}$

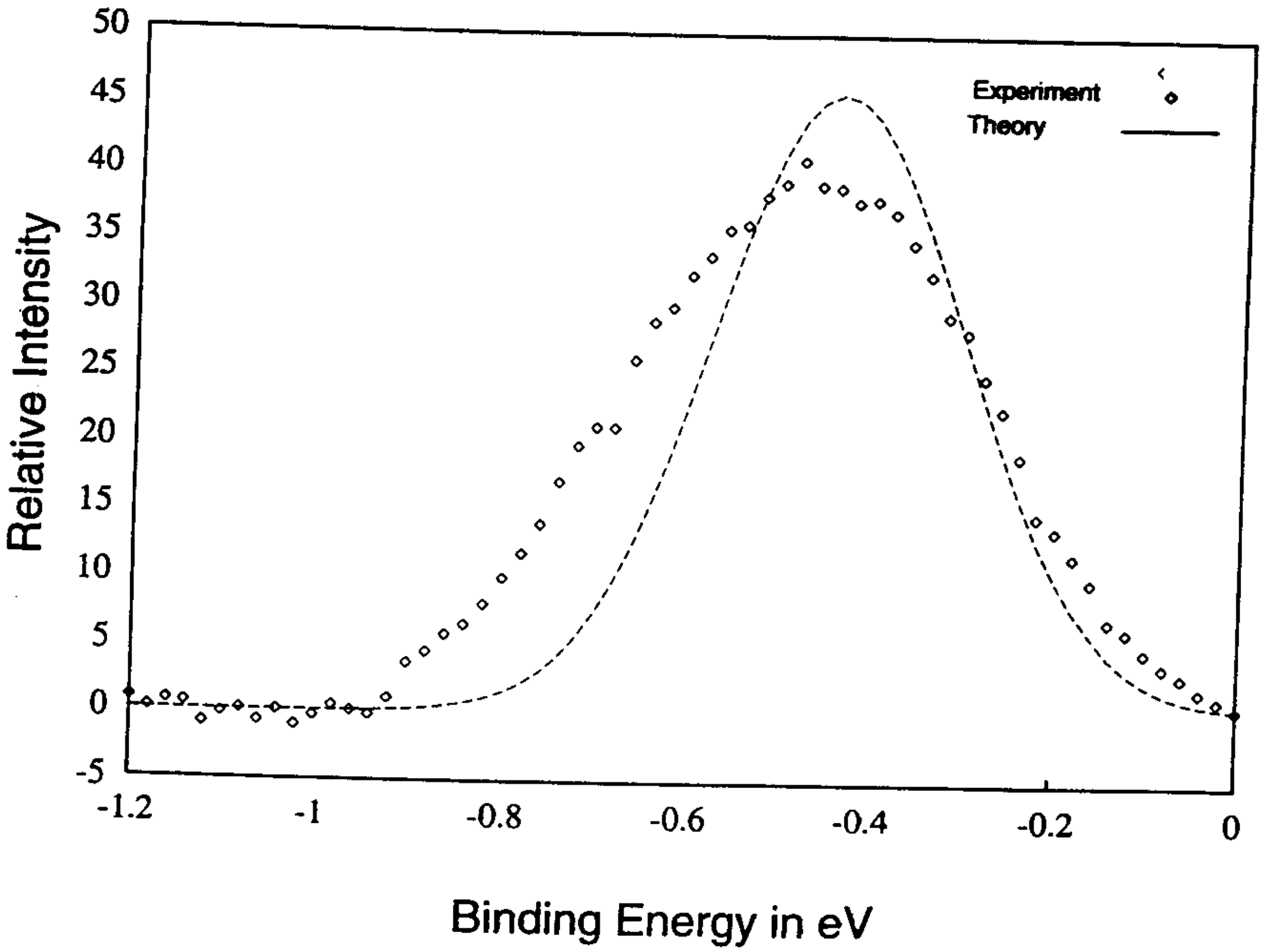
there are 2 peaks

Instrumental
resolution 160 meV:

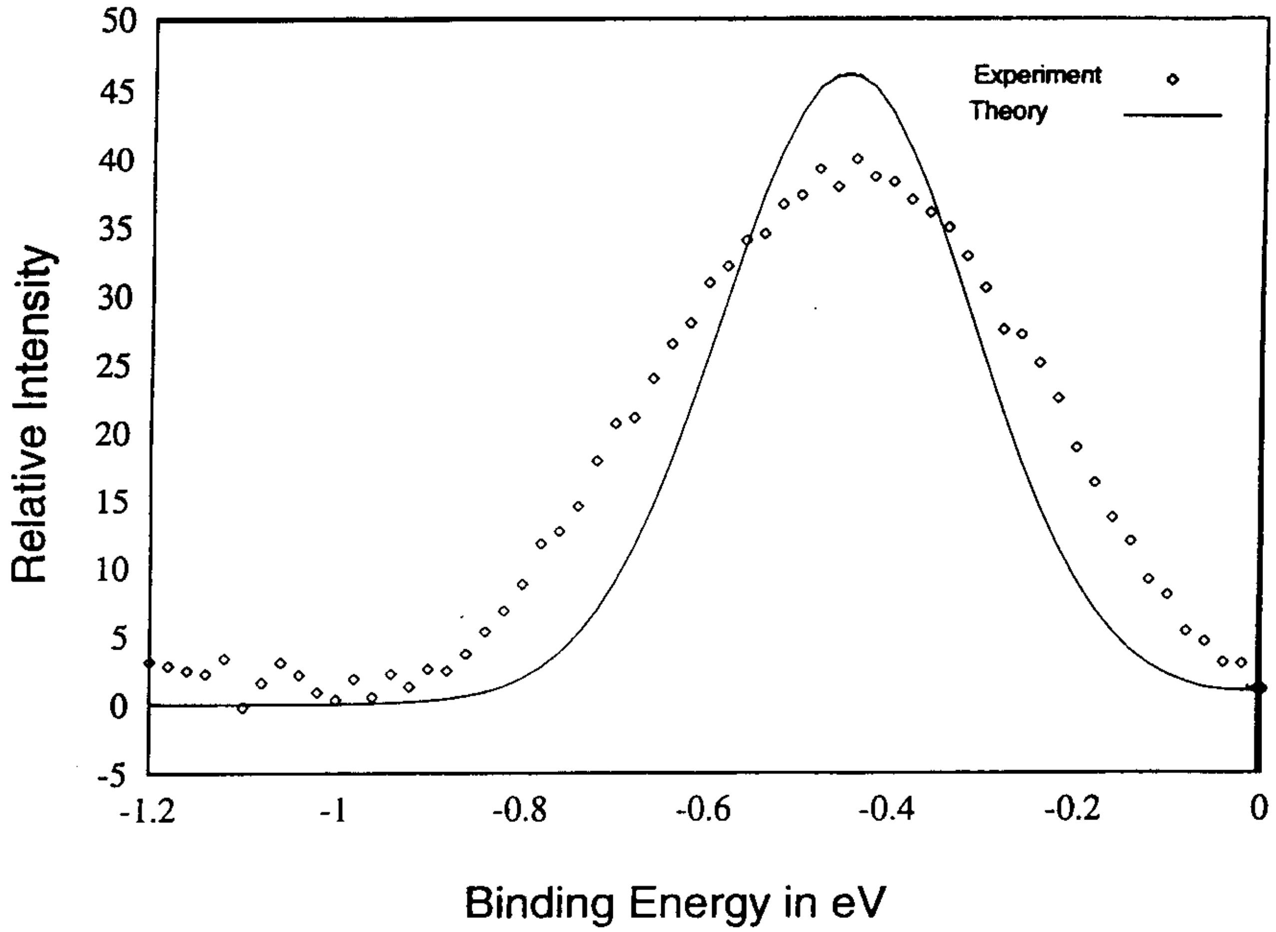
a) $k = k_f$



e) $k = -0.89\, k_f$

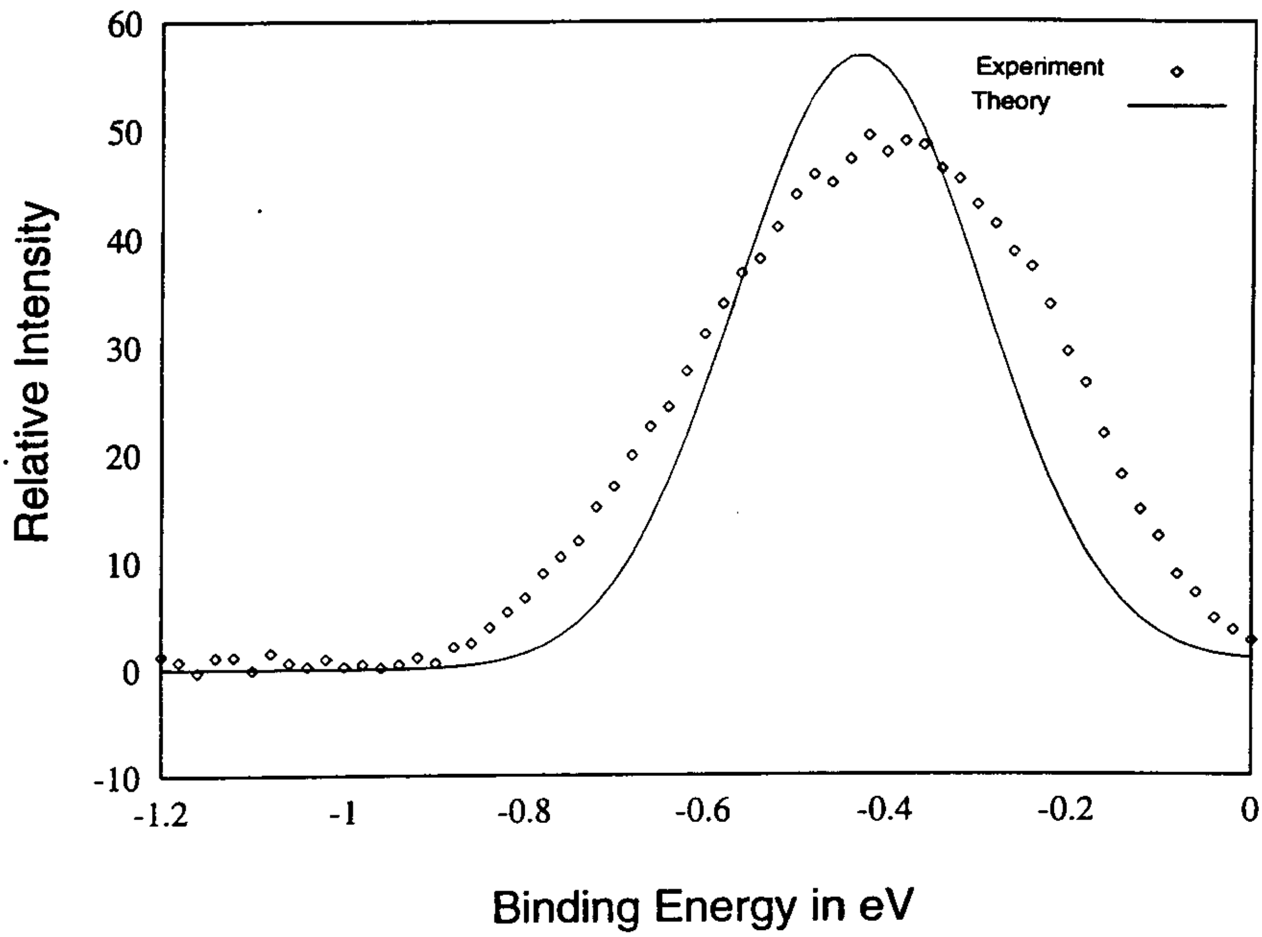

Experiment
Theory
Relative Intensity
50
45
40
35
30
25
20
15
10
5
0
-5
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
Binding Energy in eV

f) : k = - 1.15 k_f



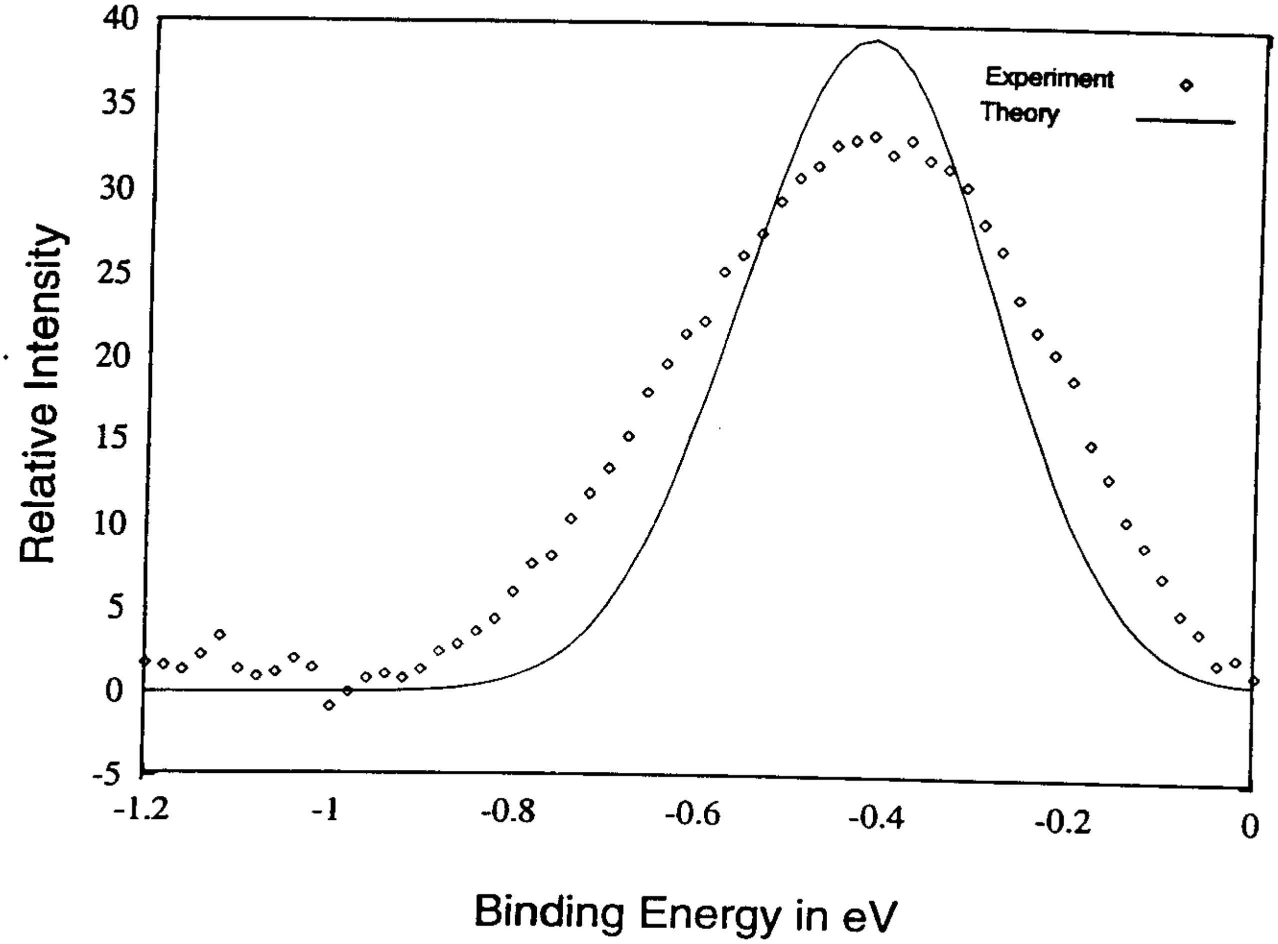
Experiment
Theory
Relative Intensity
50
45
40
35
30
25
20
15
10
5
0
-5
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
Binding Energy in eV

c) k = 0.93 k_f



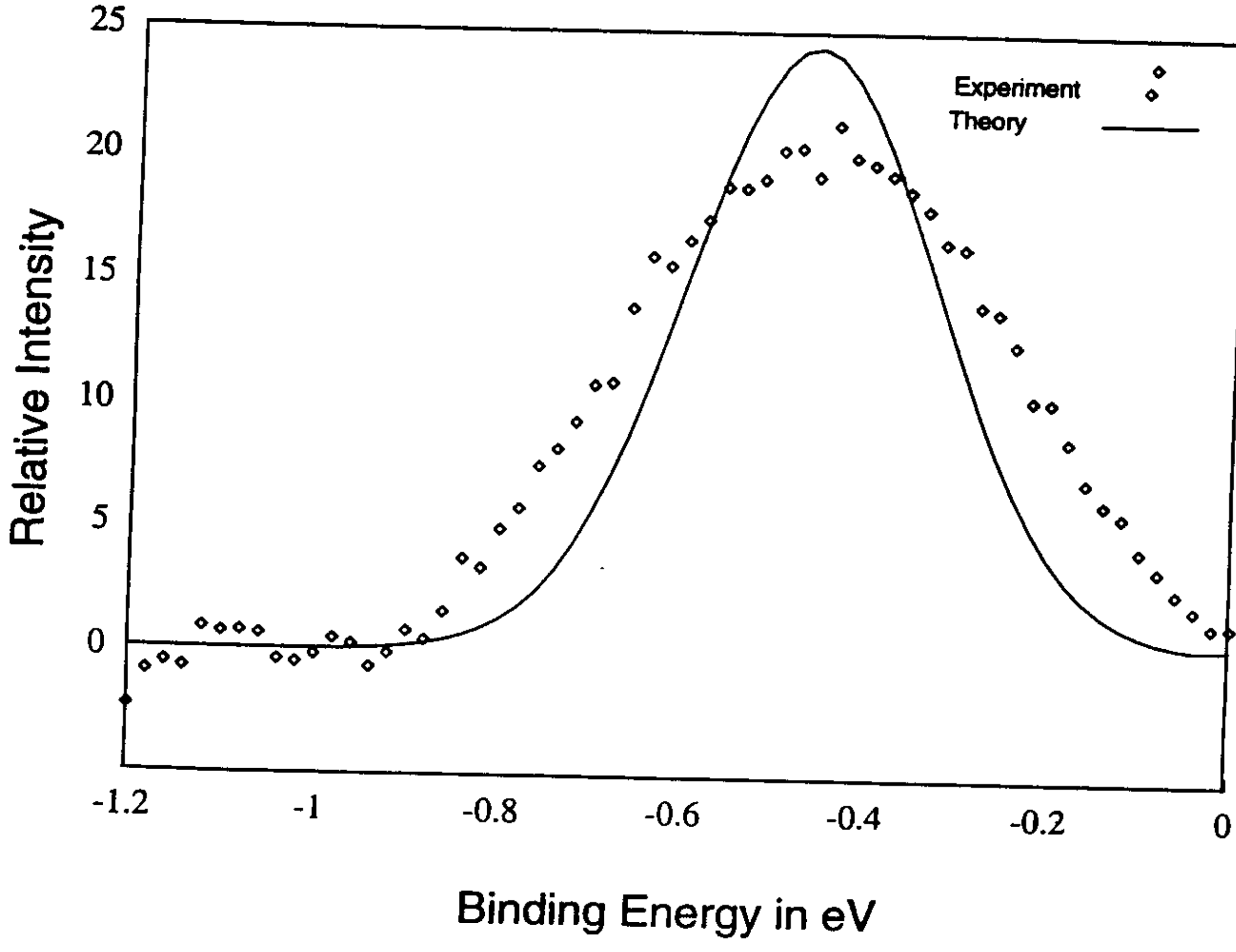
Experiment
Theory
Relative Intensity
60
50
40
30
20
10
0
-10
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
Binding Energy in eV

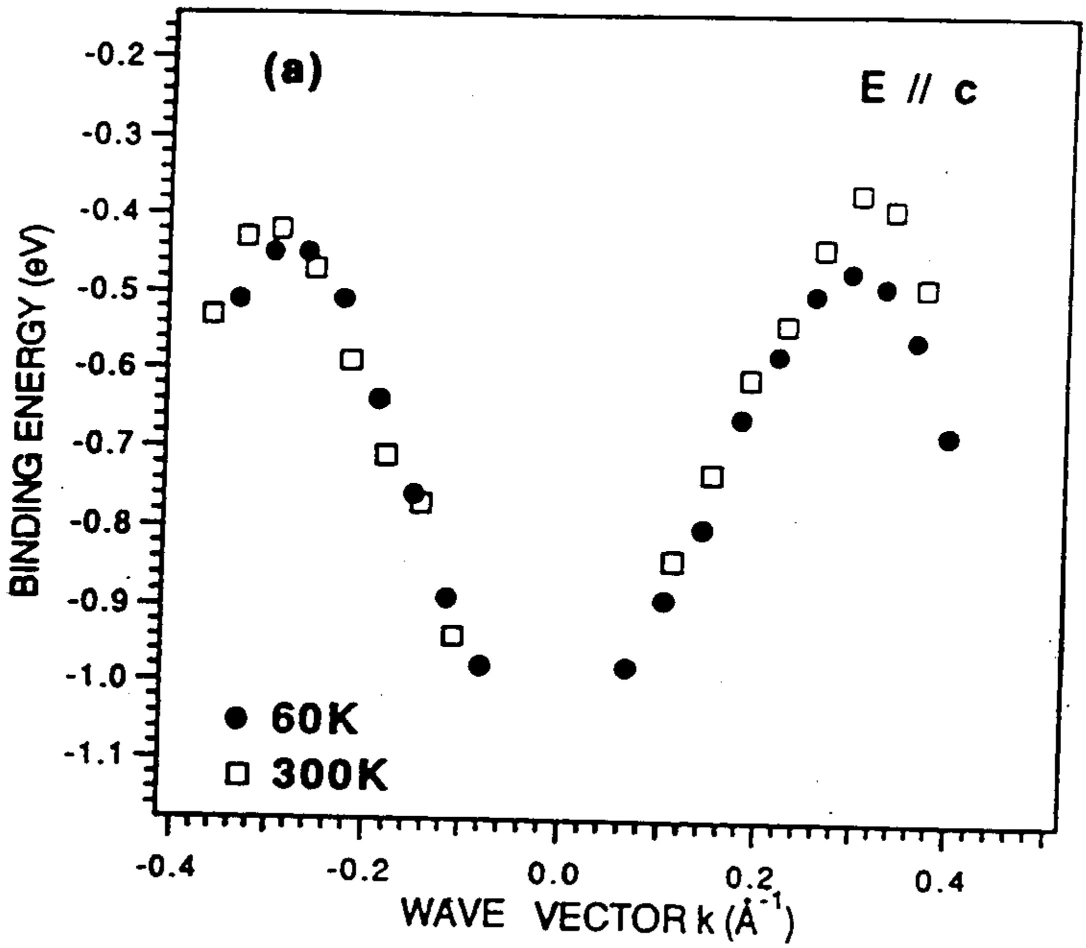
d) k = 1.03 k_f



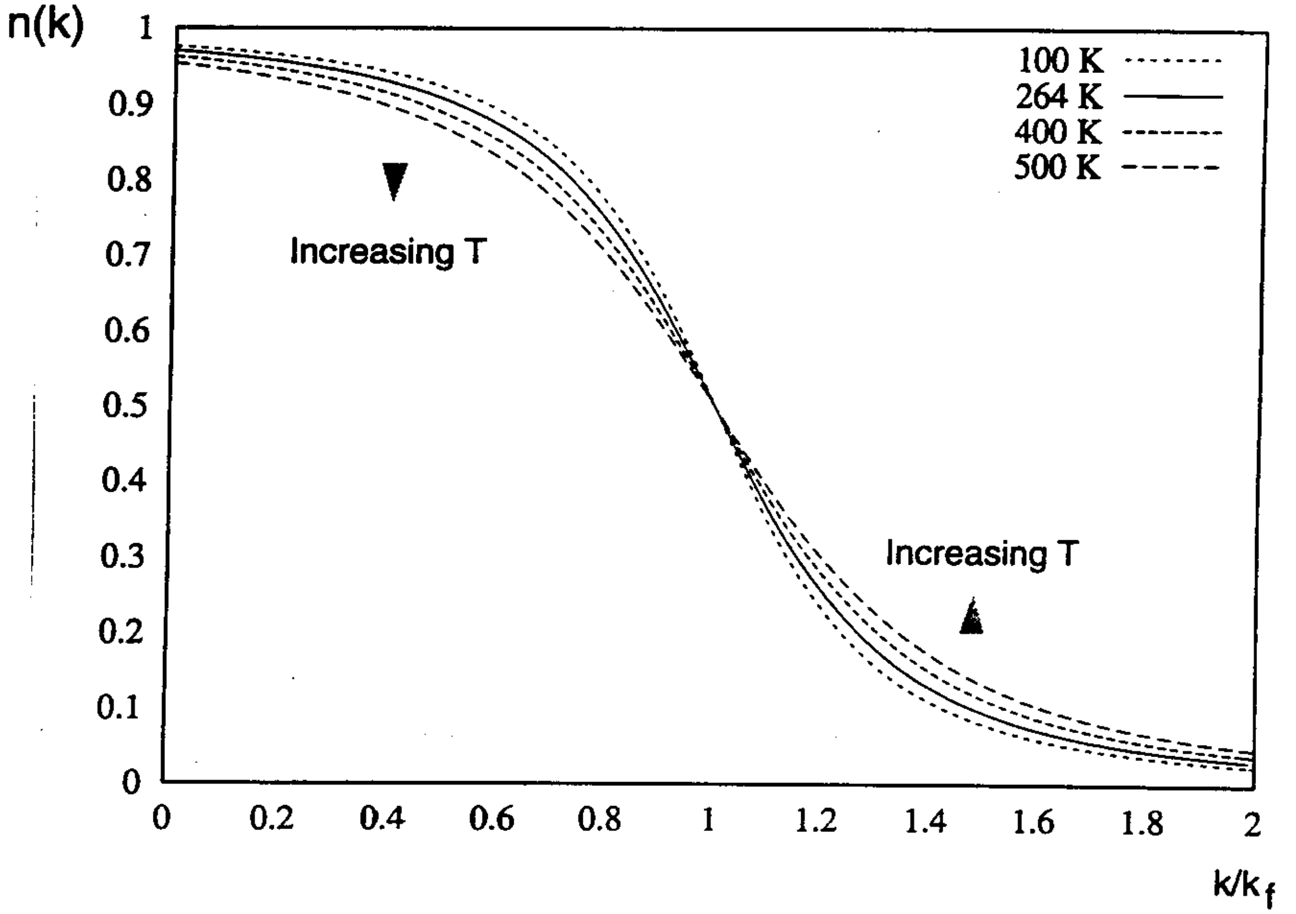
40
35
30
25
20
15
10
5
0
-5
Relative Intensity
Experiment
Theory
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
Binding Energy in eV

b) $k = 1.19\, k_f$


25
20
15
10
5
0
Relative Intensity
Experiment
Theory
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
Binding Energy in eV



(a)
E // c
BINDING ENERGY (eV)
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
-0.9
-1.0
-1.1
60K
300K
-0.4
-0.2
0.0
0.2
0.4
WAVE VECTOR k (Å^{-1})



n(k)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
k/k$_f$
100 K
264 K
400 K
500 K
Increasing T
Increasing T

Predictions of Luttinger liquid theory (with problems in italics)

- $A(k,\omega) \sim \Theta(\omega + \tilde{v}_f |k-k_F|)\,(-\omega + v_f(k-k_F))^{\gamma-1} \times$
  $(-\omega - v_f(k-k_F))^{\gamma}$, spinless case
- For $\gamma < 1$, the singularities (peaks) *disperse linearly* through the Fermi energy. (For $\gamma > 1$, they become diffuse.)
- The widths are not universal, but depend on the details of the interactions. Normally, however, the peaks are *asymmetric*.
- There is a pseudogap in the density of states. The exponent γ needed to fit the data is quite large ($\gtrsim 2$) and this is not consistent with most model interactions.
- There can be peaks for $\omega < 0$ and $|k| > k_F$. They are expected to be rather insignificant if $0 < \gamma < 1$.

Predictions of Fermi liquid theory (with discrepancies in italics).

- $A(k,\omega) \sim \delta(\omega - v_F(k-k_F))$
- Peaks should *disperse linearly* through the Fermi energy.
- Peaks should be symmetric, but should *broaden* as they get further from the Fermi energy.
- There is *no gap or pseudogap*, and the only energy scales are the Fermi energy (> 1 eV) and $k_B T \sim 30$ meV.
- There are *no peaks* when $|k| > k_F$.

LRA theory and experiment

- The "dispersion relation" (position of peak vs. momentum) has a quadratic maximum near k_F.
- The peaks are broad and symmetric. Their widths are not very momentum-dependent.
- There is a strong pseudogap at all momenta. This defines a distinct energy scale of about 500 meV. In the theory, this is essentially the zero-temperature CDW gap.

  $\frac{2\Delta}{k_B T_c^{mf}} \approx 3.9$
- There are "shadow bands". A clear peak is seen in the spectra even at $|k| > k_F$.
- Theory and experiment are in agreement on all four of these features.

Conclusions

- It appears to be very clear that ordinary Fermi liquid theory and Luttinger liquid theory are *not* appropriate for $(TaSe_4)_2I$
- A picture in which the electrons interact with the lattice degrees of freedom *only* seems to work very well
- This strongly suggests that, if the electron-phonon interaction is strong enough, the resulting pseudogap means that the electron-electron interactions may be treated in perturbation theory, and that this material at least is in that limit
- Other materials don't have to be !