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SMR 1232 - 27

XII WORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

17 - 28 July 2000

1D SUPERCONDUCTING ORGANICS:

BEYOND THE FERMI LIQUID MODEL

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

1D Superconducting Organics: beyond the Fermi liquid model

Université Paris-Sud, Orsay

- P Auban-Senzier,D.Jérome, C.Pasquier,J.Moser,
- P.Wzietek and MGabay
- C.Jaccard and H.Wilhelm at Genève
- C.Bourbonnais at Sherbrooke
- J.M.Fabre at Montpellier
- K.Bechgaard at Risoe

and the cooperation of:
T.Giamarchi and A.George

Trieste 2000

[redacted]

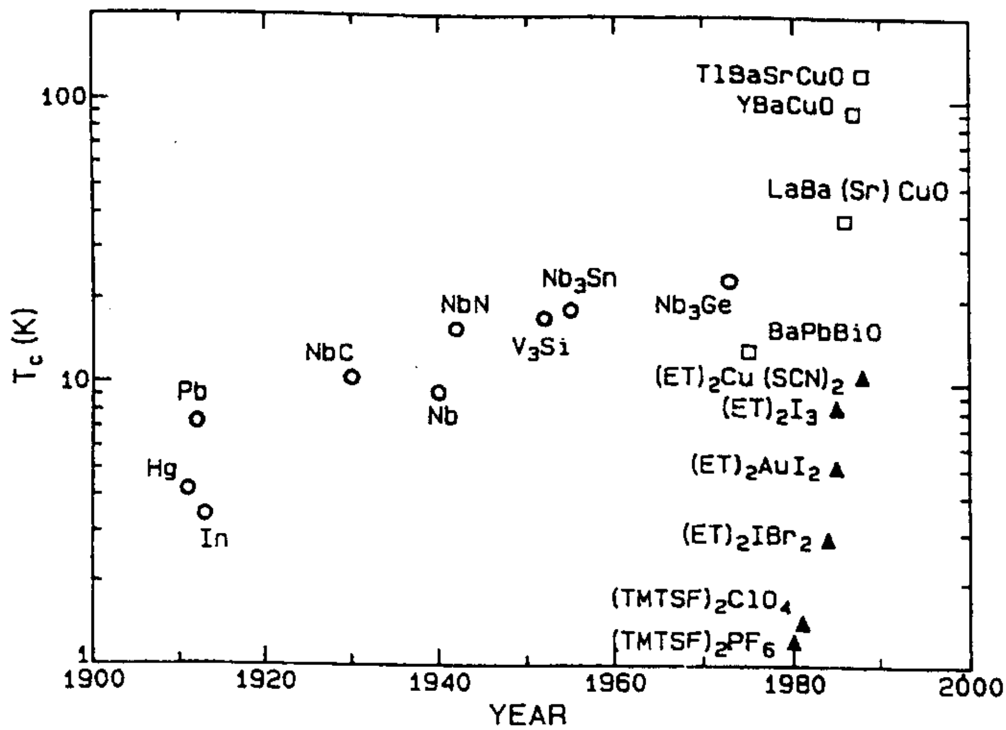

Fig.2: The evolution of T_c versus time in various inorganic and organic conductors.

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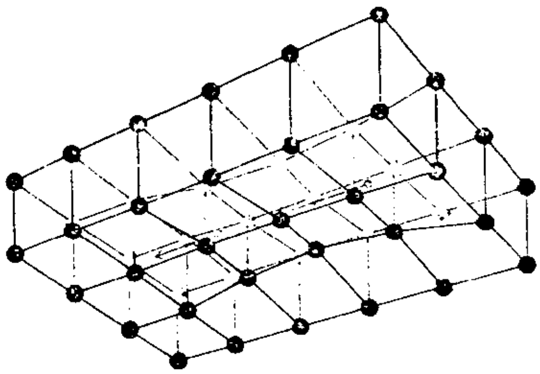


BCS theory, 1957

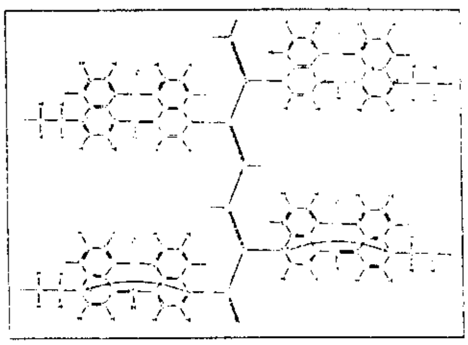
$$T_c \approx \theta_D \exp -\left(\frac{1}{\lambda}\right)$$

$$\lambda = N_F V \approx 0.1 - 0.4$$

λ is mass independent

$$\theta_D \approx 100K \propto 1/\sqrt{M}$$ → Isotopic effect in the BCS theory

Molecule of Little, 1964



Lattice polarization → Electronic polarization

$$\theta_D \Rightarrow E_F$$

[redacted] ??

Problems !! 1-D Conductor →

- ★ No long range order and
- ★ Coexistence of BCS and Peierls correlations

[redacted]

Can one synthesize an organic conductor?
conduction through the overlap of π-orbitals?

If yes, are they one dimensional conductors?

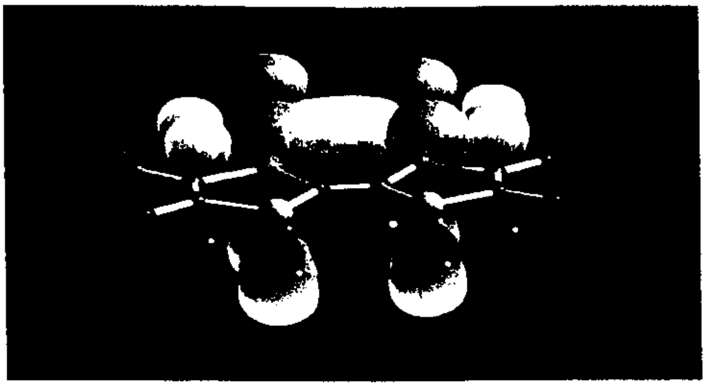
Role of transverse coupling?

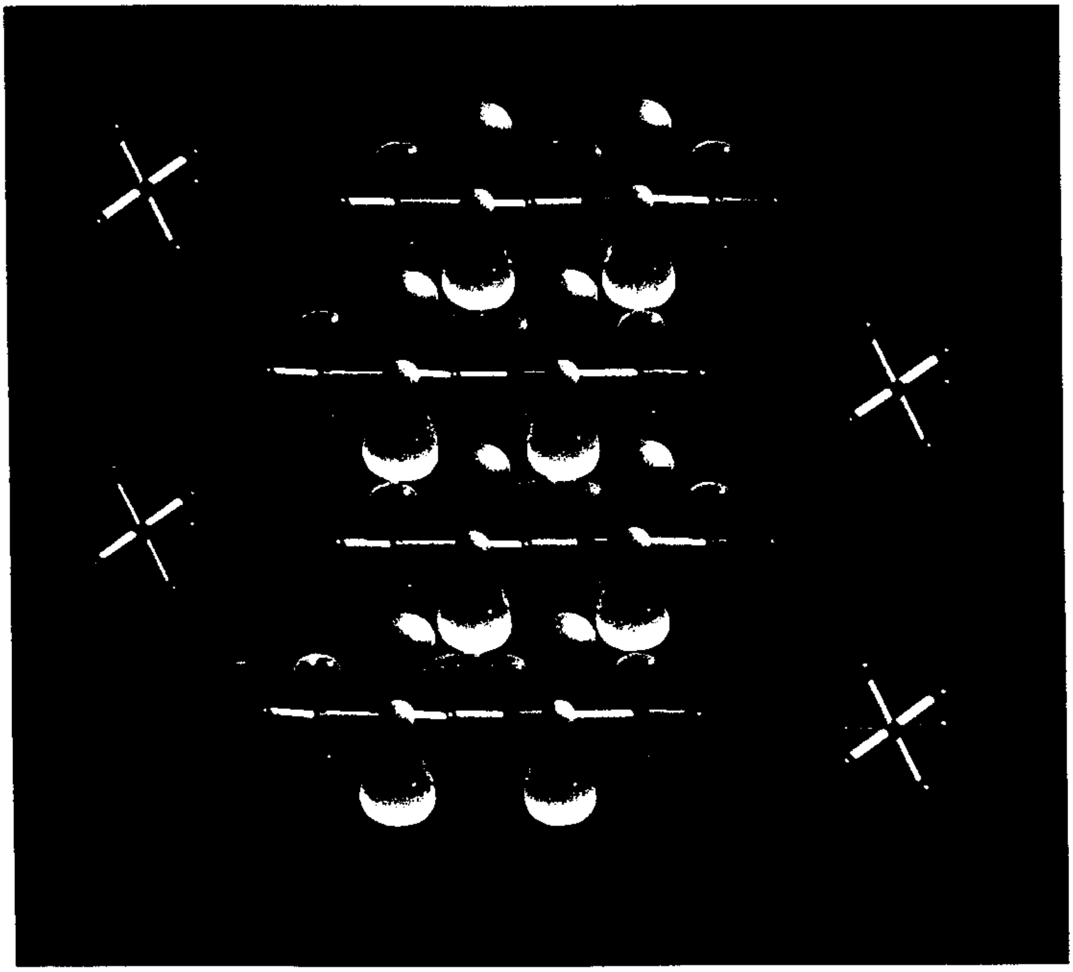
Relation between their physical properties and the prediction of 1D theory

Can one extend BCS theory to organic superconductivity?

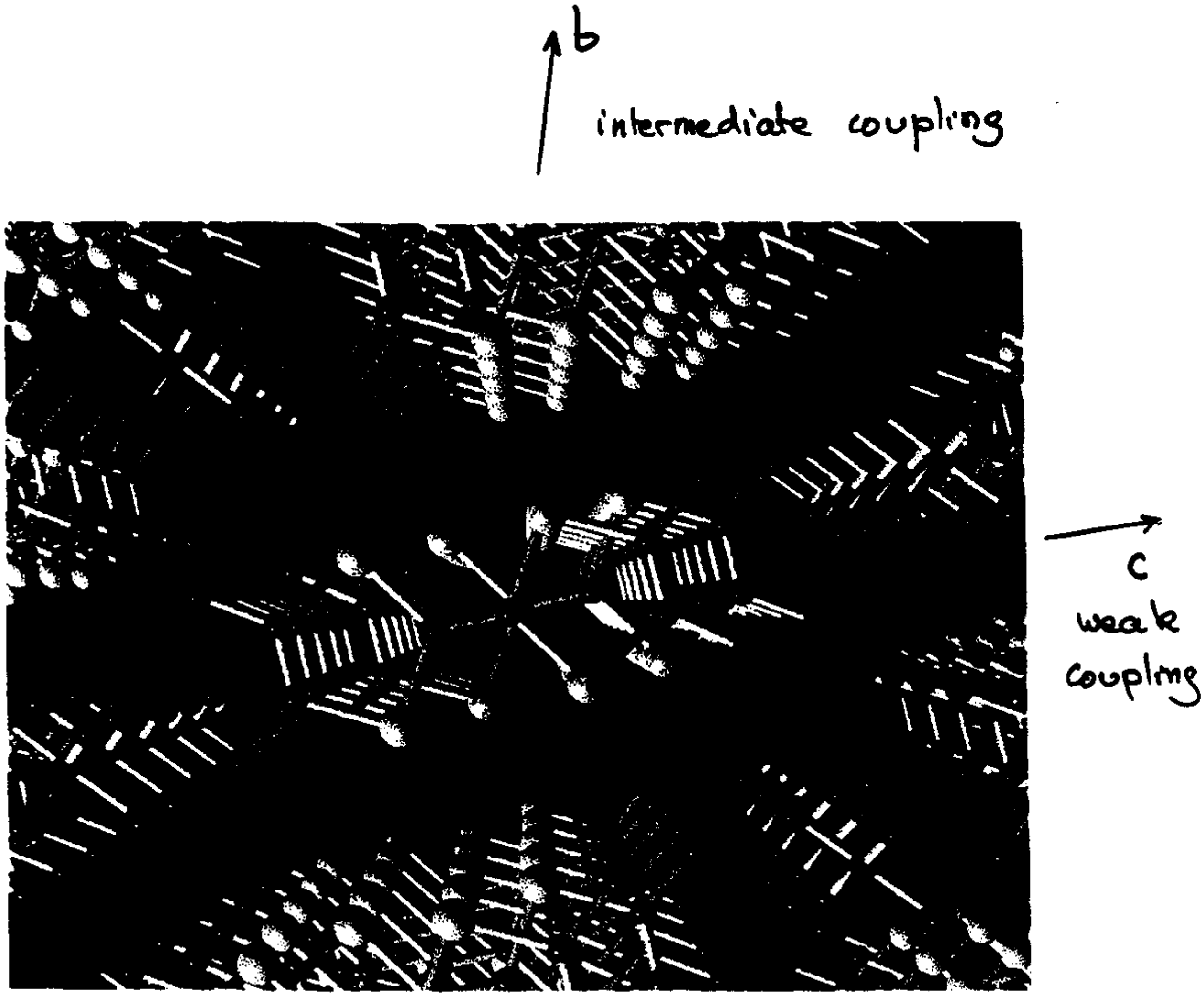
La molécule de Bechgaard

TMTSF





$(TMTSF)_2X$ $X=(PF_6)^-$,,,,,



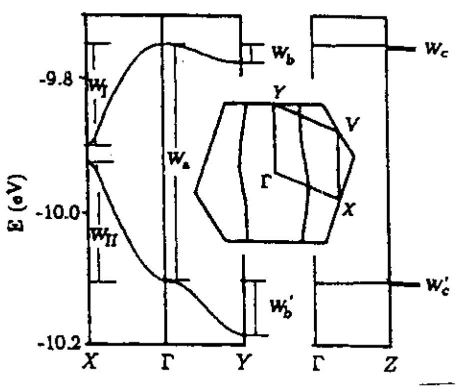
TM_2X

A big family : TM = TMTSF (Bechgaard salts)

Triclinic TM = TMTTF (Fabre, Giral salts)

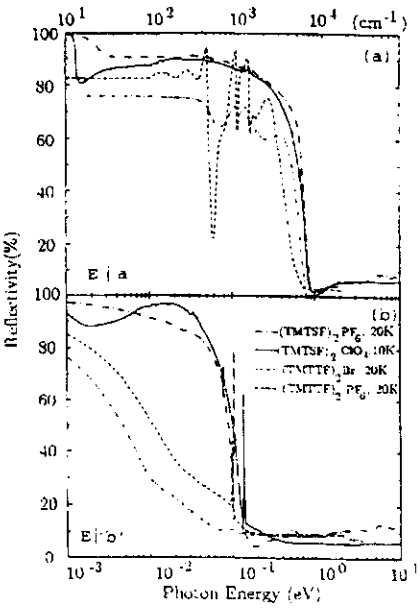
$X = PF_6$, ClO_4 , NO_3 , SCN

[redacted]

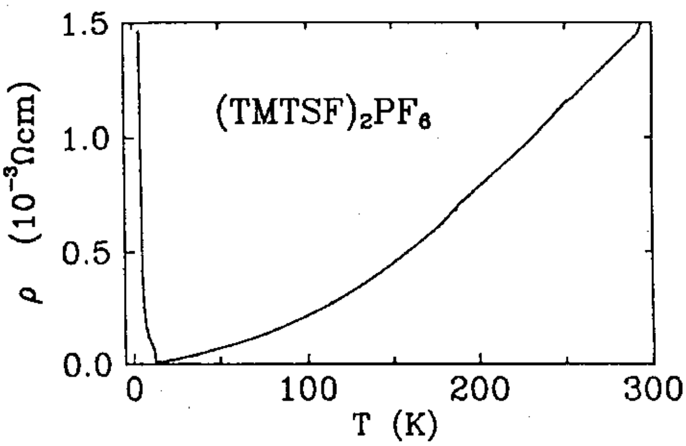


S	$(TMTTF)_2PF_6$	$(TMTSF)_2PF_6$
d_1(Å)	3.52	3.68
d_2(Å)	3.62	3.66
t_1(meV)	137	252(395$_b$)
t_2(meV)	93	209(334$_b$)
W_a(meV)	463	884(495$_a$)
W_b(meV)	55(52$_a$)	130(70$_a$)
W'_b(meV)	49	206
W_c(meV)	2*	
W'_c(meV)	2*	

$$\rho_{//} : \rho_b : \rho_c = 1: 200: 3*10^4$$



Optical anisotropy



Metal insulator at 12K!!

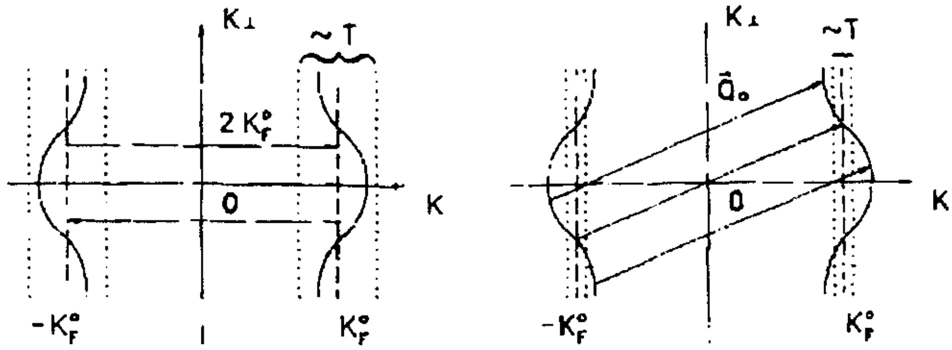
$$\omega_{p//} = 8000\ cm^{-1}$$

$$\omega_{p//} / \omega_{p\perp b} = t_{//} / t_{\perp b} = 10$$

No coherence along b at high T

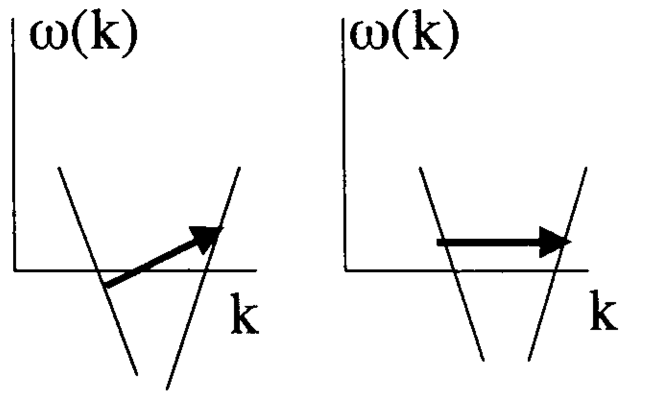
No coherence along c at any temperature

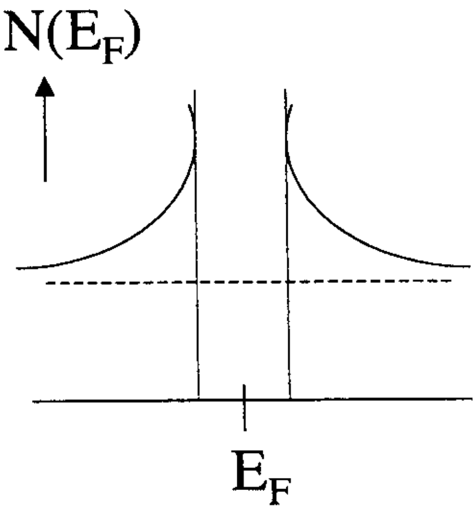
[redacted]



Nesting properties : $\varepsilon(k) = -\varepsilon(k + 2k_F)$

Mixture of Peierls(CDW,SDW) and BCS channels





$\chi(T)=\ln E_F/T$

~~Fermi liquid theory~~

Quasiparticle pseudo gap at Fermi level

Decoupled collective modes, spin and charge

[redacted]

1D Fermi liquids

$$\chi_S(T) = \frac{\chi_0(T)}{1 - U\chi_0(T)} \qquad \chi_0(T) \propto \ln\frac{E_F}{T}$$

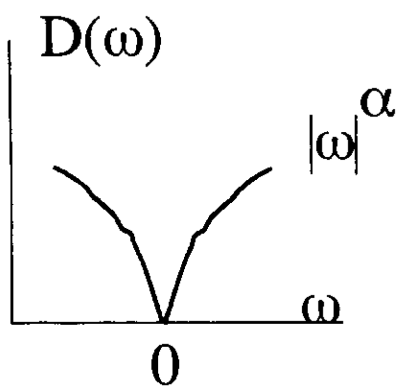
If U>0 -> ~~Finite~~ T_c ??

1D Luttinger liquids

$$\chi_{SDW,CDW} = \cos(2k_F x)\, x^{-1-K_\rho} + ..$$

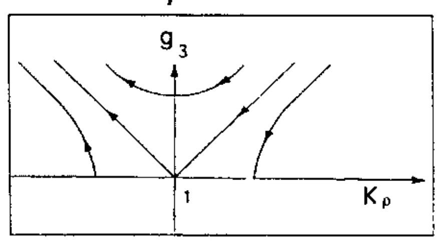
$$\chi_{SC} = x^{-1-\frac{1}{K_\rho}} + ..$$

Power laws



$$D(\omega) = |\omega|^\alpha$$

$$\alpha = \frac{1}{4}(K_\rho + \frac{1}{K_\rho} - 2)$$



$$K_\rho < K_{\rho_{critic}} \Rightarrow \textit{Mott insulator}$$

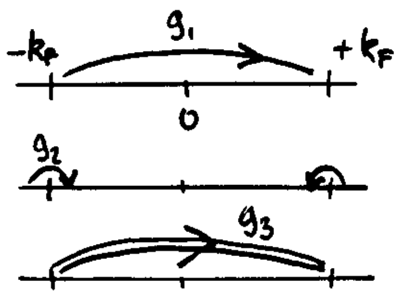
Commensurability 2

$$K_{\rho_{critic}} = 1$$

Commensurability 4 ➡ (case of TM_2X)

$$K_{\rho_{critic}} = 0.25$$

Renormalization in a 1-D commensurate conductor



Scaling equations (2nd order)

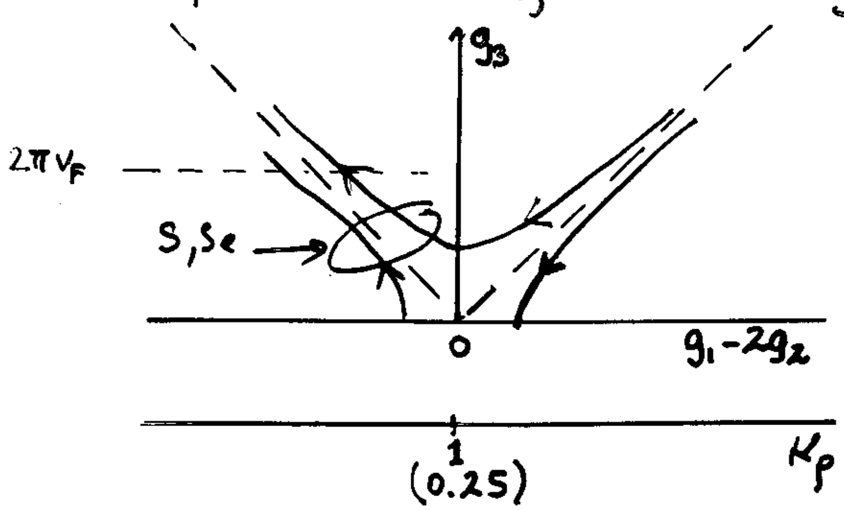
$$l = \ln E_F/T$$

$$\frac{dg_1}{dl} = -g_1^2 + \cdots \qquad \Big\}\text{spin DOF}$$

$$2k_F = \begin{cases} G/2 & \tfrac{1}{2}\text{-filled} \\ G/4 & \tfrac{1}{4}\text{-filled} \end{cases}$$

$$\left.\begin{aligned} \frac{d\,g(2g_2 - g_1)}{dl} &= g_3^2 + \cdots \\ \frac{d g_3}{dl} &= g_3(2g_2 - g_1) + \cdots \end{aligned}\right\}\text{charge DOF}$$

Flow of interactions for the charge



$$K_\rho \sim 1 + \frac{g_1 - 2g_2}{2\pi v_F}$$

Fixed point at low T :

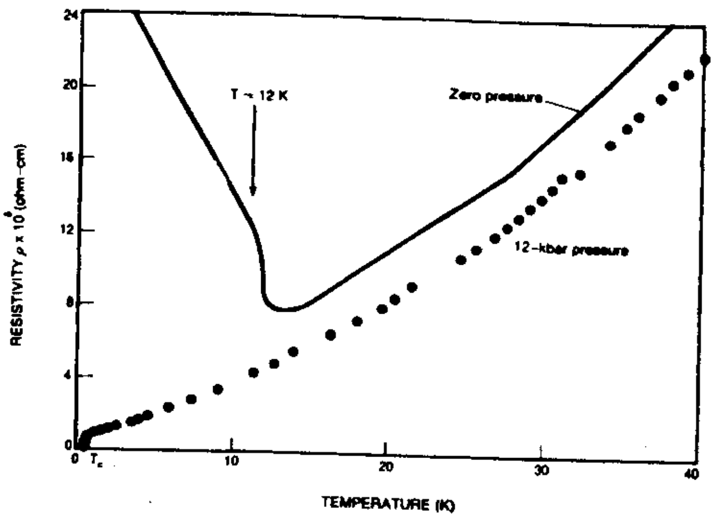
$$\left.\begin{aligned} g_3^* &= 2\pi v_F \\ g_1^* &= 0 \\ g_2^* &= \pi v_F \end{aligned}\right\} \quad K_\rho^* = 1 - \frac{g_2^*}{\pi v_F} = 0$$

Strong coupling
= Mott insulator

<u>Question</u> : Is the fixed point reached before or after the cross-over (1-D → 2-D) temperature ?

[redacted]

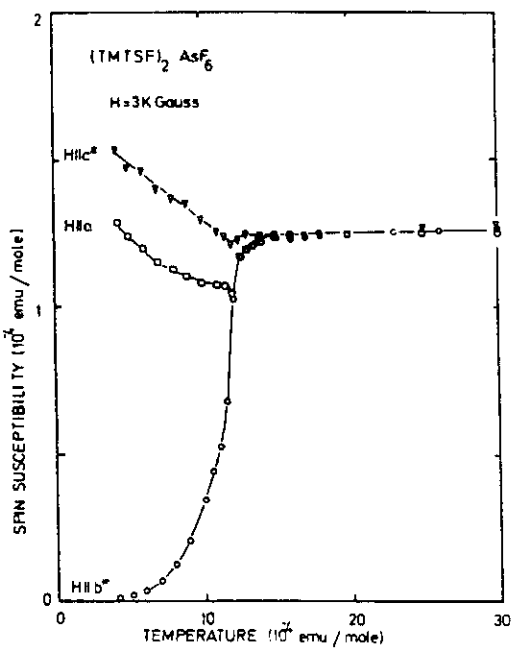
Transport



Metal insulator transition at 12K

Superconducting at 1K under pressure
Déc 1979

Susceptibility



Insulator =
itinerant antiferromagnet
=(excitonic transition)

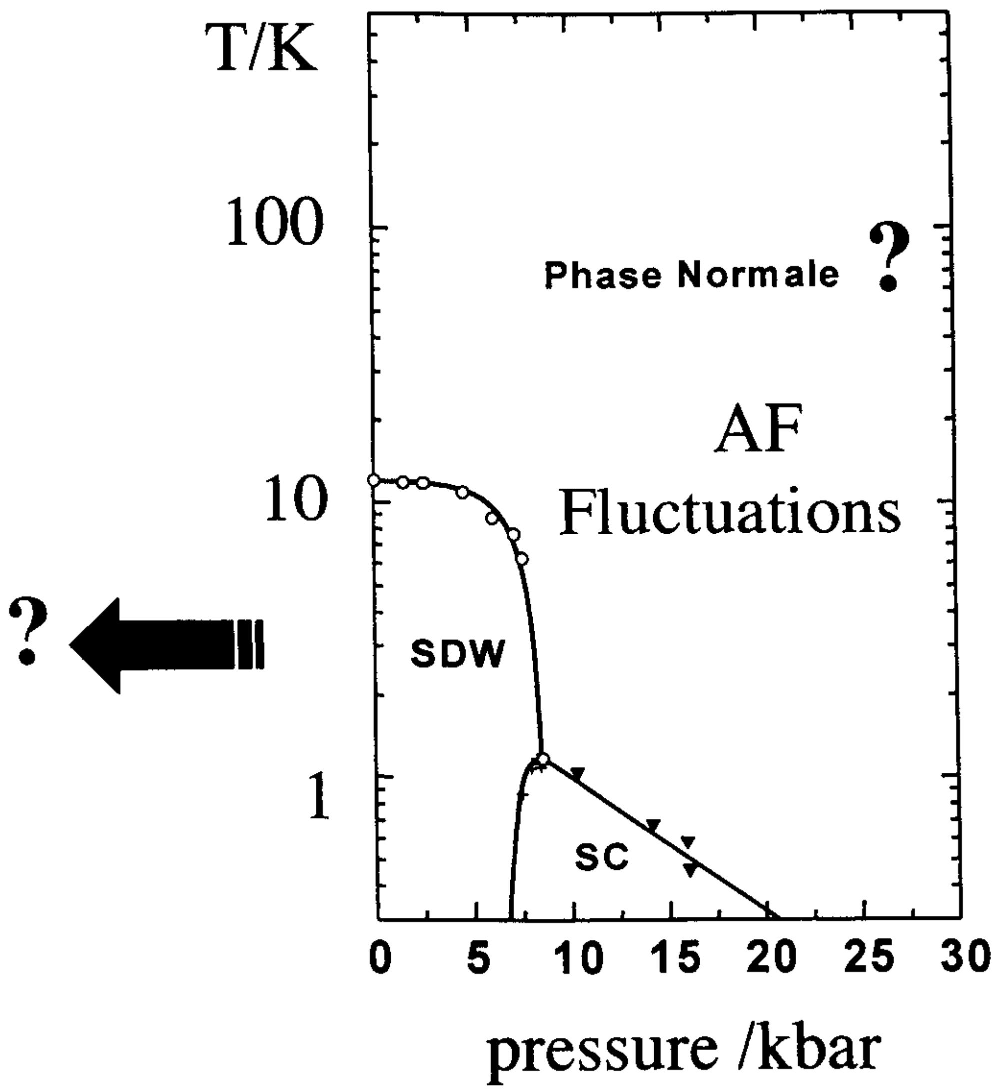
spin-flop field 5 kGauss //b*

Easy axis for the magnetization

[redacted]

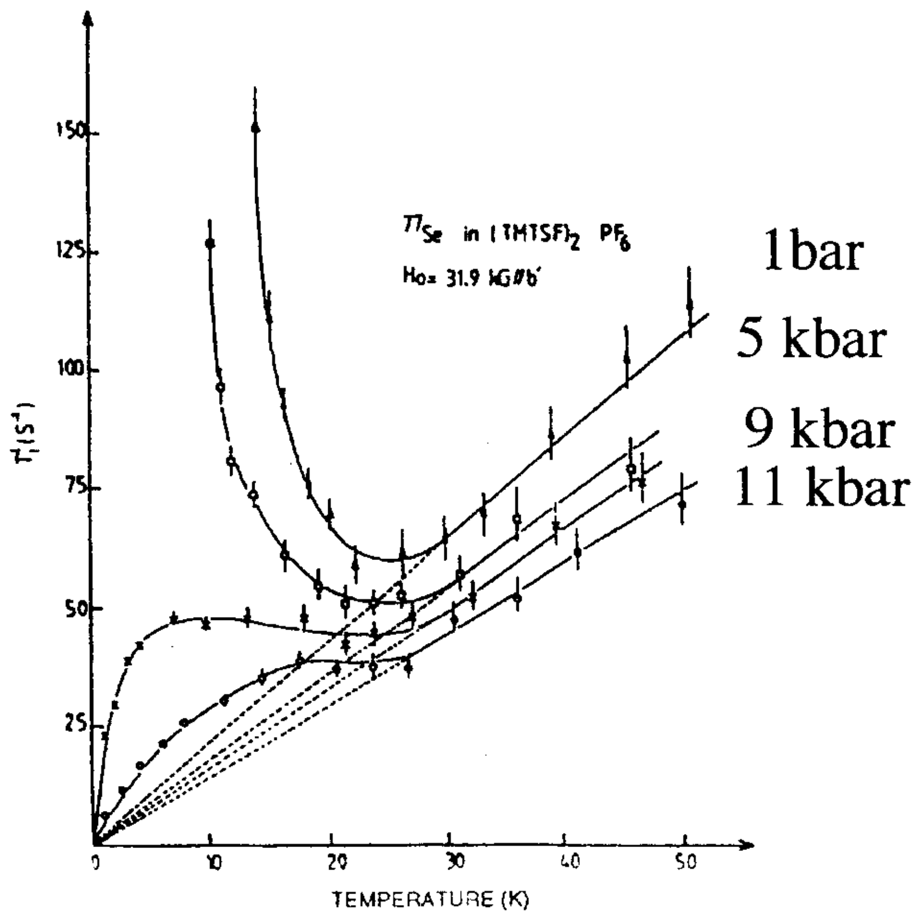
The prototype for quasi 1-D organic conductor

➡ Conduction due to the oirganic stack only
No role played by the anions



Common border SC/SDW
Coexistence SC/SDW
AF Fluctuations

Antiferromagnetic fluctuations



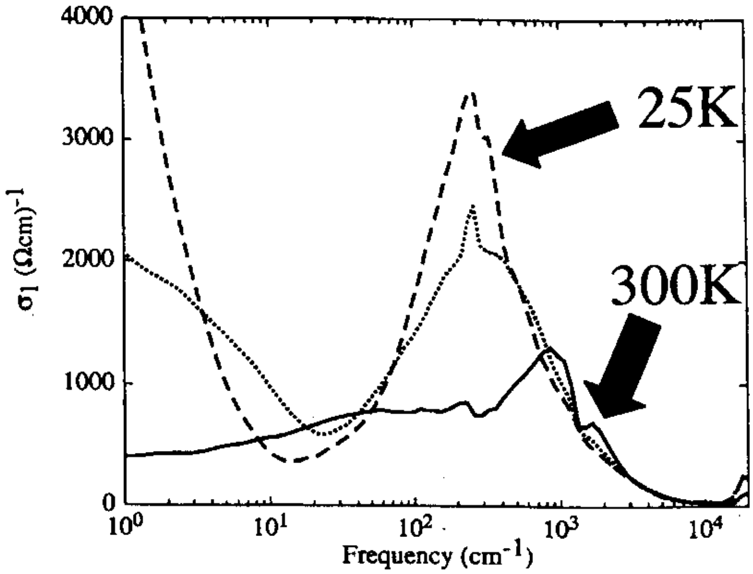
RMN Relaxation

$$\frac{1}{T_1} = A^2 T\, \chi_{SDW}(2k_F, T) \quad + \quad A^2 T\, \chi_S^2(T)$$

[redacted]

$$1/T_1 = \text{constant}, \quad K_\rho \Rightarrow \quad 0$$

[redacted]



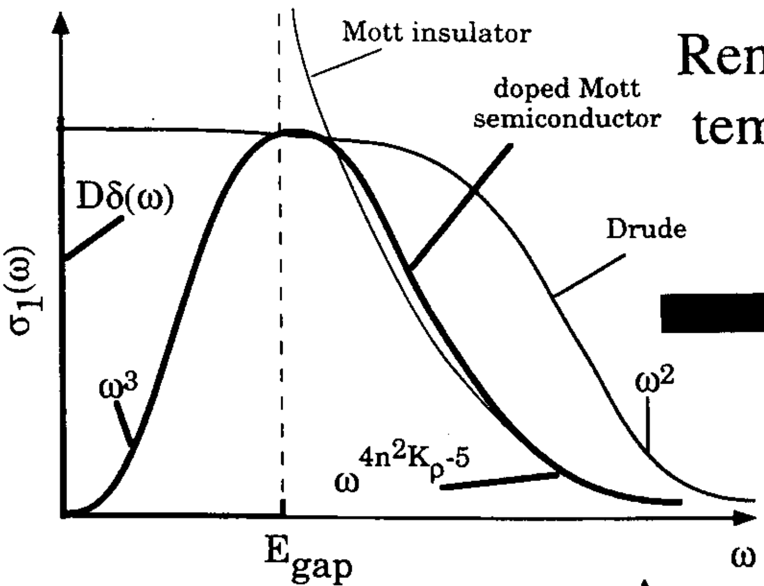
Correlation gap at $170\ cm^{-1}$

and

Zero frequency mode 1% of the total oscillator strenght

$$\omega_p^2$$

Theory:doped Mott insulator



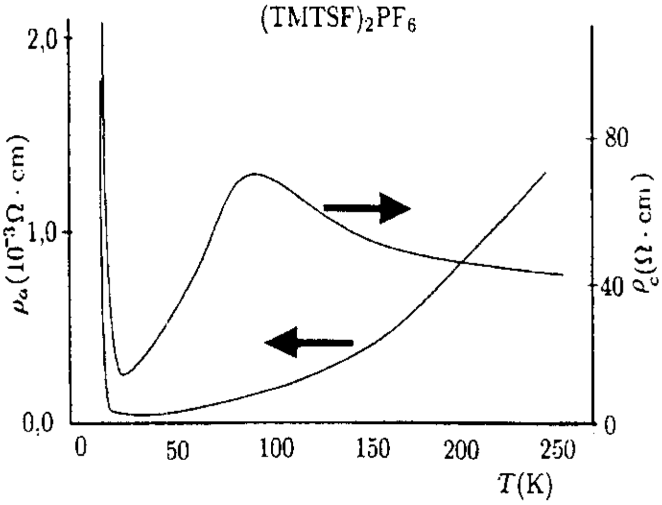
Remnence of the high temperature 1-D physics

$$\Rightarrow K_\rho \approx 0.23$$

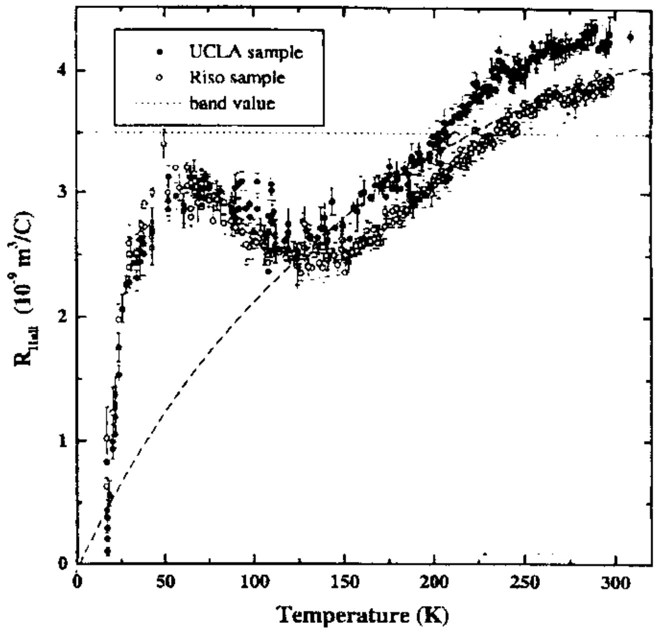
Agrees with DC transport

1D/2D dimensionality cross-over at T*=120K

Transport



Hall effect



High temperature regime (1D) T>T*

$$\rho_c \propto T^{-2\alpha} \quad , \quad \rho_a \propto T^{16K_\rho - 3} \qquad \text{at}(T \geq \Delta_\rho)$$

R_H α power law T $^{0.7}$ according to theory?

$$\Longrightarrow \quad K_\rho \approx 0.23$$

In agreement with optics and photoemission

Cross over around 130K

Recovers Hall effect of a 2D liquid at low T

$$\boxed{t_c \ll t_b < T \ll t_a} \tag{1}$$

- Kubo formula

$$j_z = -i\frac{t_c ec}{\hbar}\sum_{ix\sigma} C^+_{i+1,\sigma}(x)C_{i,\sigma}(x) + H.c. \tag{2}$$

$$\sigma_c(\omega) = \frac{4e^2ct_c^2}{\hbar}\int dx' \int \frac{d\varepsilon}{2\pi}\frac{f(\varepsilon)-f(\varepsilon+\hbar\omega)}{\hbar\omega}A_e(x',\varepsilon)A_h(x',\varepsilon+\hbar\omega) \tag{3}$$

A_e (A_h) is the spectral function of the *real* electron (hole) in the Luttinger liquid.

- Tunneling formalism approach

$$t_c\sum_{ix\sigma} C^+_{i+1,\sigma}(x)C_{i,\sigma}(x) + H.c. \tag{4}$$

$$I = \frac{4ect_c^2}{\hbar}\int dx' \int \frac{d\varepsilon}{2\pi}\left(f(\varepsilon)-f(\varepsilon+\hbar\omega)\right)A_e(x',\varepsilon)A_h(x',\varepsilon+\hbar\omega) \tag{5}$$

The conductance g in the z direction is then

$$\boxed{g \sim \frac{4e^2ct_c^2}{\hbar}\int dx' \int \frac{d\varepsilon}{2\pi}\frac{f(\varepsilon)-f(\varepsilon+\hbar\omega)}{\hbar\omega}A_e(x',\varepsilon)A_h(x',\varepsilon+\hbar\omega)} \tag{6}$$

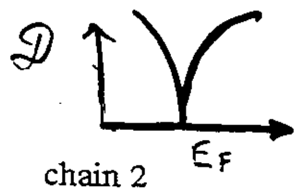
$$A(x,\varepsilon) = \frac{1}{v_c}\left(\frac{\varepsilon}{\hbar v_c}\right)^{\alpha}\tilde{h}\left(\frac{\omega x}{v_c}\right) \tag{7}$$

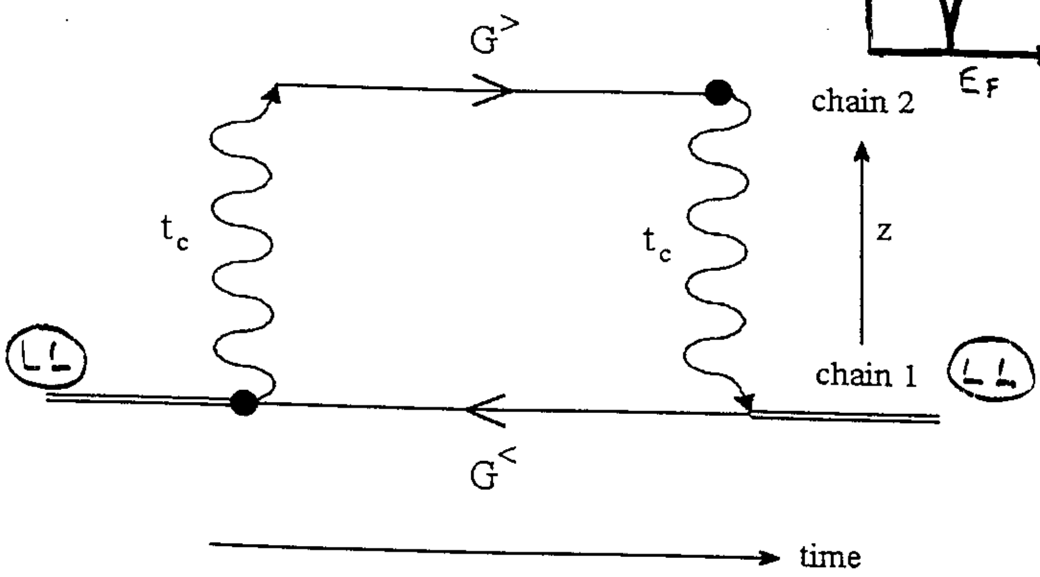
$$\sigma_c(\omega) \sim t_c^2\frac{e^2}{\hbar}\frac{ac}{v_c^2}\left(\frac{\omega}{v_c}\right)^{2\alpha} \tag{8}$$

Accordingly, the dc-conductivity $\sigma_c(T)$ is such that

$$\boxed{\sigma_c(T) \sim T^{2\alpha}} \tag{9}$$

$\mathcal{D}(\epsilon) = \epsilon^{\alpha}$





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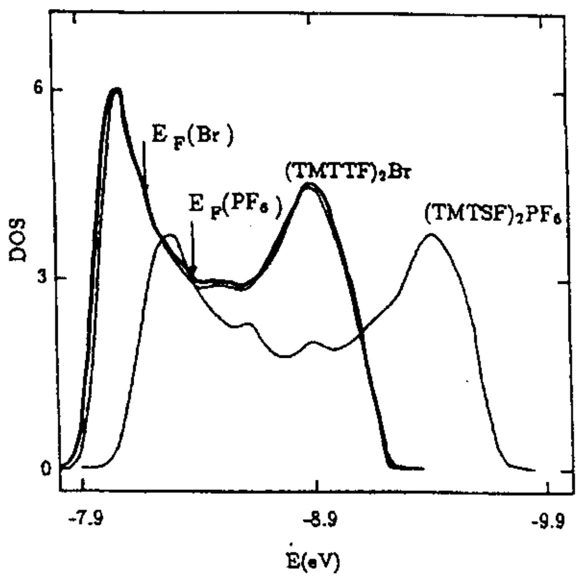
Isostructural to$TMTSF_2X$

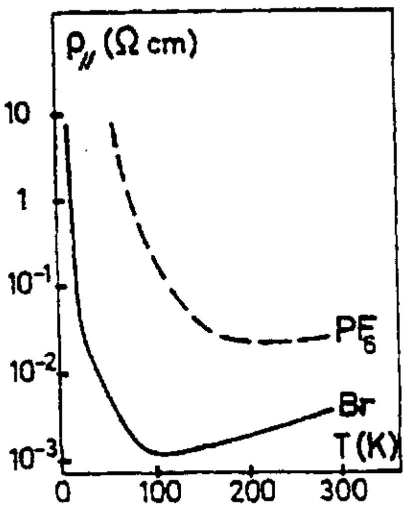


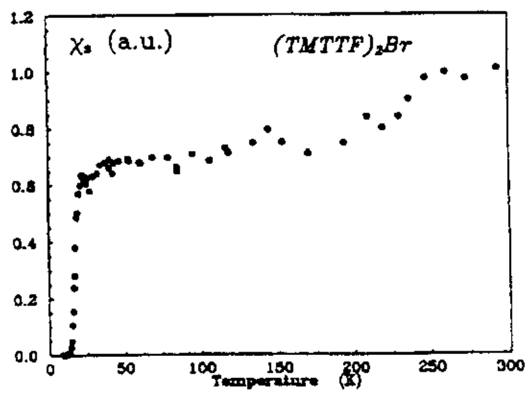
W=0.8 eV (Se)
0.4 eV (S)

U≈ 0.8 eV

Identical in both series

spin-charge separation
A textbook exemple





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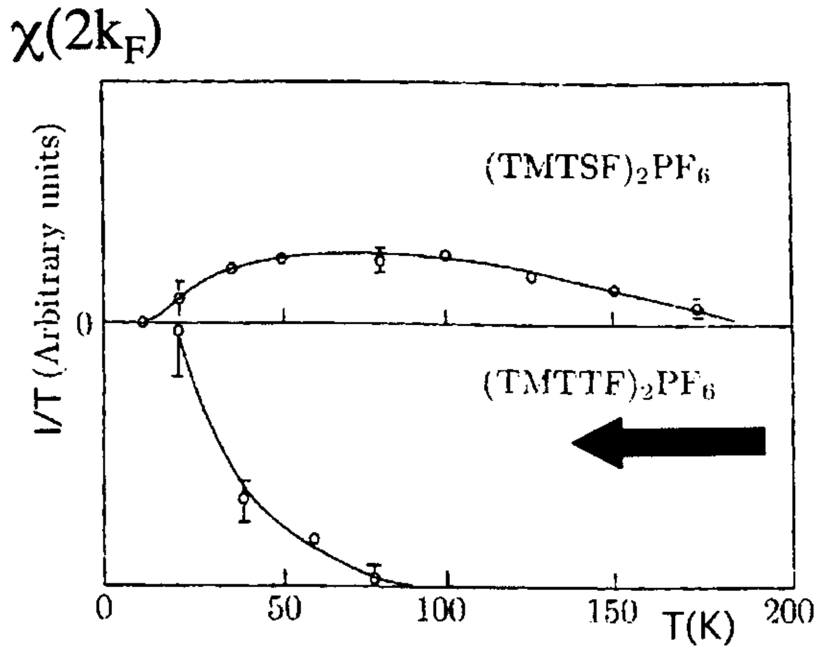
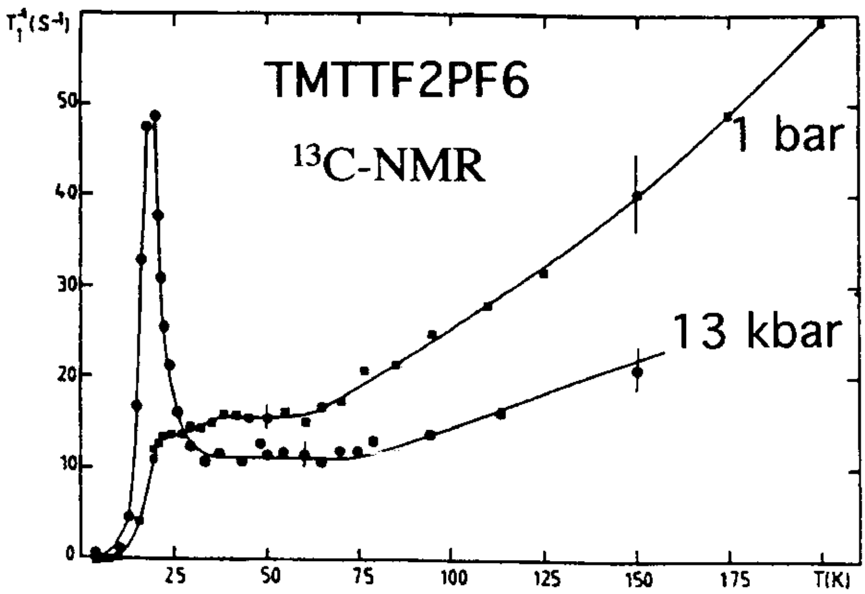


Onset of a $2k_F$ lattice modulation below 100K



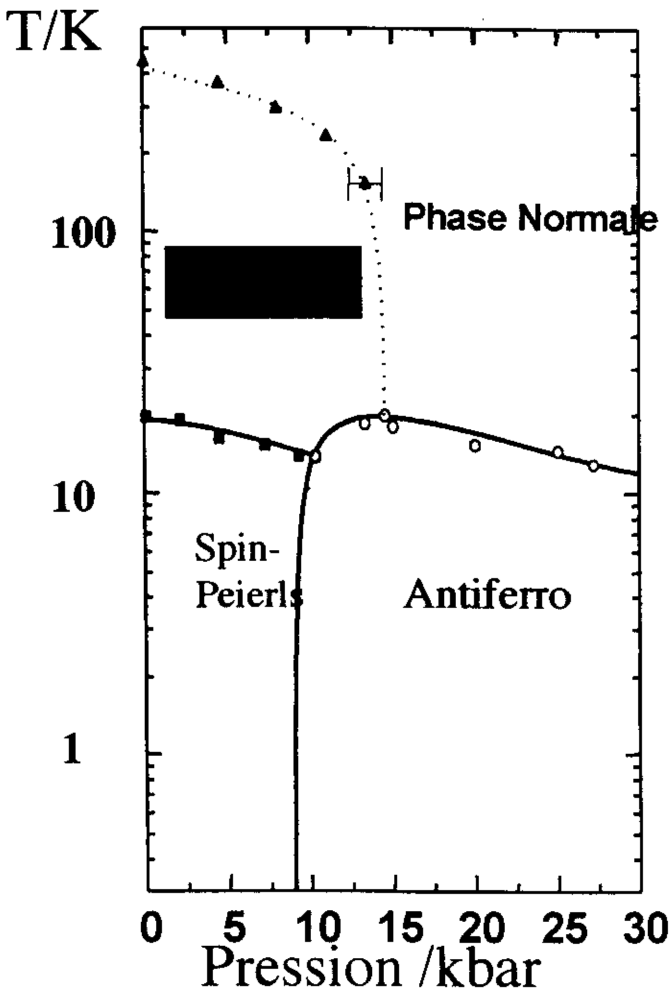
[redacted]

Pseudo gap in the density of spin excitations at P=1 bar
Precursor to spin Peierls ordering, (S=0 ground state)

[redacted]

Prototype for a 1D commensurate Mott insulator

Charge gap, $2\Delta_\rho \approx 900K$ at 1 bar



Pertinence of the interchain exchange (Superexchange)

$$J_\perp \approx t_\perp^2 / \Delta_\rho$$

$\longrightarrow$ $T_N \Delta_\rho = const$

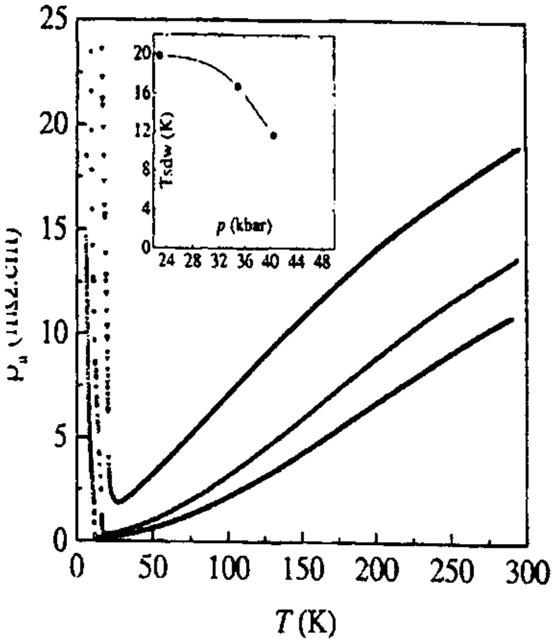
$\Rightarrow$ [redacted]

Theory of Spin Peierls ordering, Bourbonnais and Caron

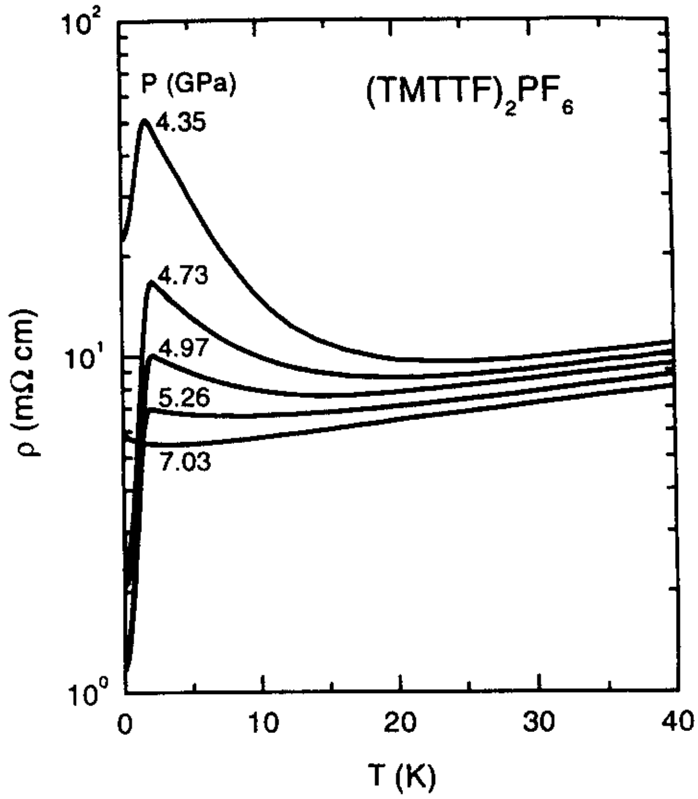
g_{ph}=-0.15 $\longrightarrow$ -0.05 à 40 kbar Supercon ??

According to T_{SP} under pressure

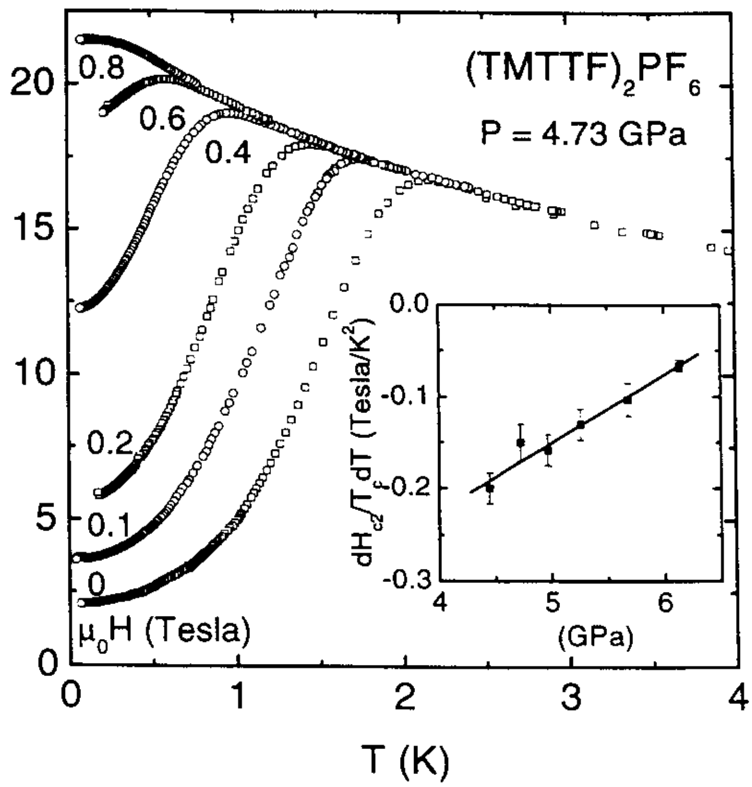
Superconductivity in TMTTF2PF6



Orsay

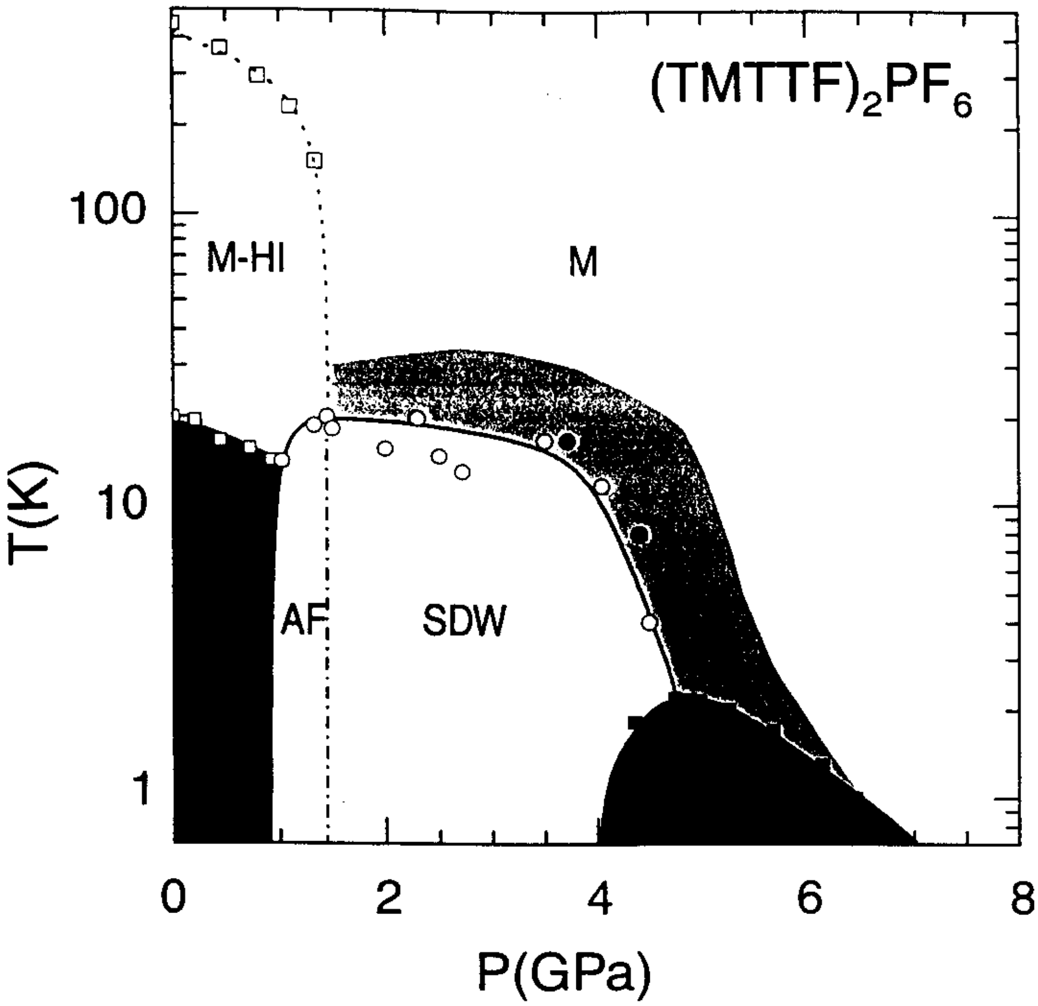


Genéve

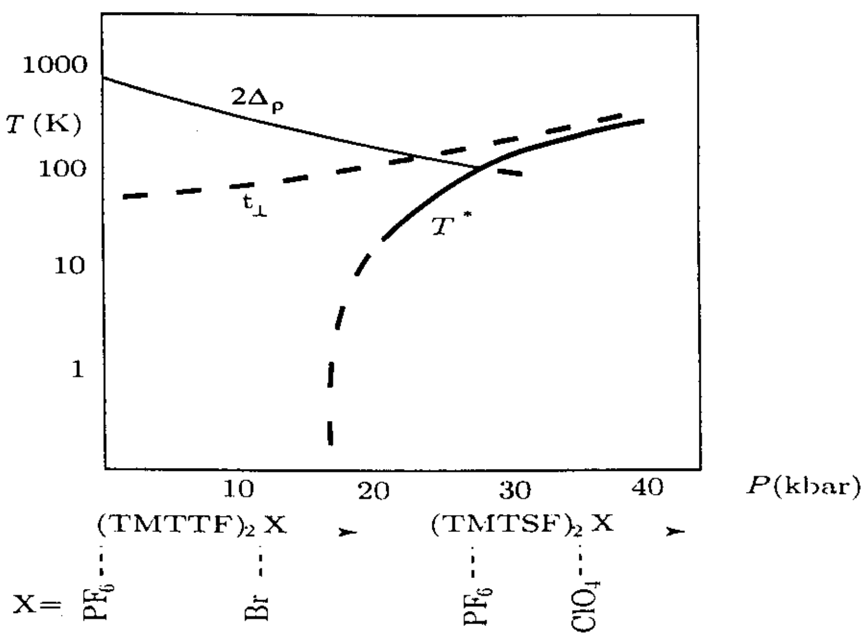


Precursor fluctuations and coexistence between SC and SDW in a narrow pressure range

Universal phase diagram for TM2X



Correlation gap and dimensional cross-over



Mott insulator gap. $[K_\rho < 1, (0.25)]$

$$\frac{2\Delta_\rho}{W} = \left(\frac{g_u}{W}\right)^{\frac{1}{2-2n^2K_\rho}}$$

H.J. Schulz
T. Giamarchi

$$g_u = \begin{cases} g_{1/2} = g_1 \dfrac{\Delta_D}{W} \\ g_{1/4} = g_1 \left(\dfrac{g_1}{W}\right)^2 \end{cases}$$

Energy scale for renormalization is $\simeq E_F/2$

$(TMTSF)_2PF_6$ $E_F/2 \sim 1500K > \Delta_D \sim 500K$

$1/4$ renormalization is plausible (also for $TMTTF_2PF_6$)

$$\frac{2\Delta_\rho}{W} = \left(\frac{g_1}{W}\right)^{\frac{3}{2-8K_\rho}}$$

$TMTSF_2X$ $W \sim 12000\ K$ $g_1/W \sim 0.6-0.7$

$2\Delta_\rho \sim 200K$

$\Rightarrow K_\rho = 0.22$

$TMTTF_2X$ $W = 6000K$ $g_1/W \sim 0.75$

$2\Delta_\rho \sim 1000K$

$\Rightarrow K_\rho = 0.18$

Pressure dependence of K_ρ

All TM_2X compounds are Mott insulators.

in $(TMTSF)_2X$ cross-over is reached before strong coupling limit.

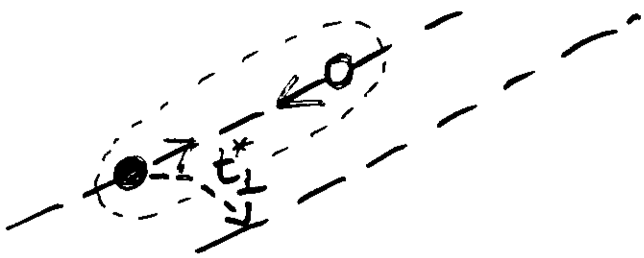
not in $TMTTF_2PF_6$!

1-D confinement in a strongly correlated 1-D gas

Renormalization of the interchain cross-over.

$$t_\perp^\circ \longrightarrow t_\perp^* = t_\perp^\circ \left(\frac{t_\perp^\circ}{t_{//}}\right)^{\frac{1-K_\rho}{K_\rho}}$$

Bourbonnais Caron 86



Spin fluctuations (el-hole) $\Longrightarrow$ 1-D confinement

[redacted]

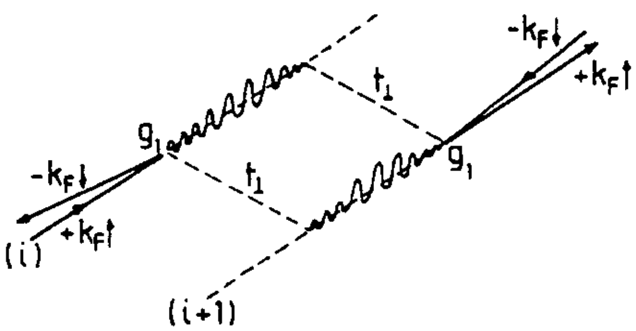
What must be taken into account in a model for the SC coupling:

High energy excitations are 1D-like
Strong AF fluctuations before SC
Weak lattice response at $2k_F$
Repulsive BCS response

Suggestions:

If AF fluctuations are included in the 2D regime at T<T*
No SDW transition because of the bad nesting but BCS interaction is always repulsive, Emery 1983

1D history and strong AF fluctuations contribute to an interchain exchange coupling J_{perp}(IEX)
In case of bad nesting > attractive SC coupling
Boubonnais and Caron, 1986



$$Tc \approx T_{SDW} \exp - \frac{1}{\lambda^*}$$

$$\Delta(k_\perp) = \Delta_0 \sin k_\perp d$$

Consequences: singlet pairing
anisotropic gap
zeros in the gap
sensitive to non magnetic defects

[illegible]

[illegible]

Spin and charge decoupling [illegible]

[illegible] 1000K [illegible]

High energy physics (high temperature) is 1-D

Competition between the Mott localization
and the dimensionality cross over

The low temperature metal is not straightforward

Remnence of the high temperature history

[illegible]

Superconducting coupling

Non phonon mediated

Singlet coupling (d-like)

Zeros in the gap

Much more in the organics

Collective motion of the SDW

Magnetic field induced SDW and Quantum Hall effect

Coexistence of SC and SDW near P_c

Further readings

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