INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONE: 2240-1
CABLE: CENTRATOM - TELEX 460392 - I

SMR/459 - 24

SPRING COLLEGE IN CONDENSED MATTER
ON
'PHYSICS OF LOW-DIMENSIONAL SEMICONDUCTOR STRUCTURES'
(23 April - 15 June 1990)

QUASI 1 DIMENSIONAL CHARGE DENSITY WAVE SYSTEMS

Andras JANOSSY
Hungarian Academy of Sciences
Central Research Institute for Physics
P.O. Box 49
H-1525 Budapest
Hungary

Quasi 1D materials:

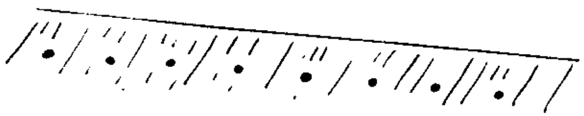
here: crystals with chainlike structure

1D electronic structure: overlap between chains small

(1D atomic displacement also exists), 1D magnets: J-P. Boch

Interest of it: unstable against periodic distortion,
collective excitations
fluctuations

Ground state: charge density waves
spin density waves
superconductor



uniform chain

$\mathcal{H}$ = electron (kinetic) + phonon + electron-phonon + electron-electron

ε_k^0 $\quad$ ω_q^0 $\quad$ g

– structural properties
materials

– dynamics

Perturbation theory

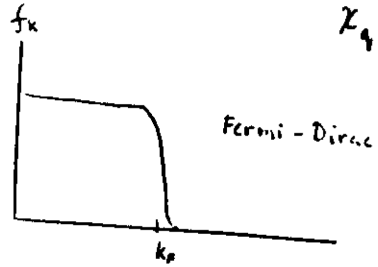
mean field: electron and phonon spectra

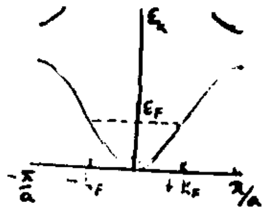
displacement: $u = u_q \cos qx$

electronic potential: $V = gu = V_q \cos qx$

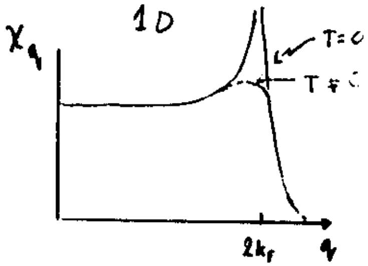
charge density $\delta\rho = \chi_q e^2 V$

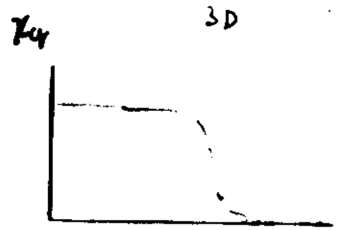
$$\chi_q = \sum_k \frac{f_k - f_{k+q}}{\varepsilon_k^0 - \varepsilon_{k+q}^0}$$



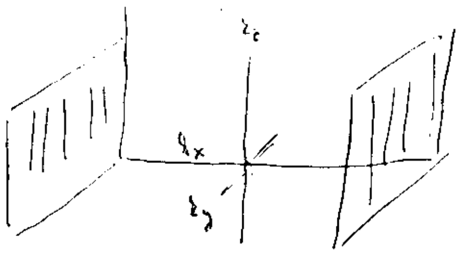


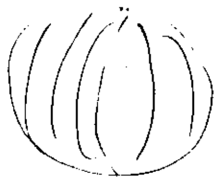
$q = 2k_F$ gives large perturbation especially in 1D



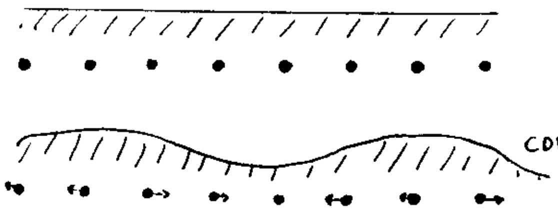


Lindhard function





Formation of CDWs



high temp.:

$\rho =$ const

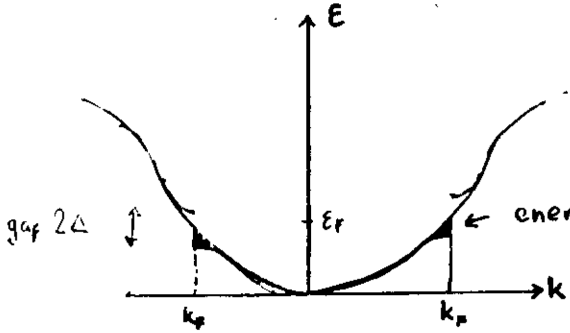
lattice uniform

low temp.:

CDW: $\rho = \rho_0 + \rho_1 \cos(2k_F x + \varphi)$

lattice distortion:

PLD: $a = a_i + u_{2k_F} \cos(2k_F x + \varphi)$



energy gain balanced by lattice distortion

$\Delta \ll \varepsilon_F$ (Δ typically ...)

$\Delta = 2D\, e^{-1/\Lambda}$ $\qquad \Lambda = g^2 \dfrac{N(\varepsilon_F)}{\omega_{2k_F}^2 / m}$

$\rho_1 = \Delta \rho_0 / \Lambda v_F k_F$

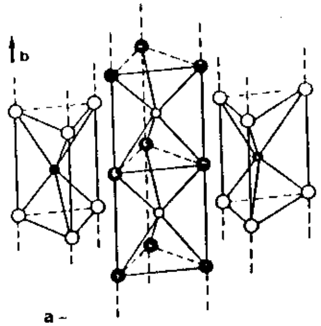
$u_{2k_F} = 2\Delta / g$

at $T = 0$ $\quad \sum_k (\varepsilon_k - \varepsilon_k^0) >$ elastic energy at some u_q

$T > 0$ in mean field $\Delta = \Delta(T)$

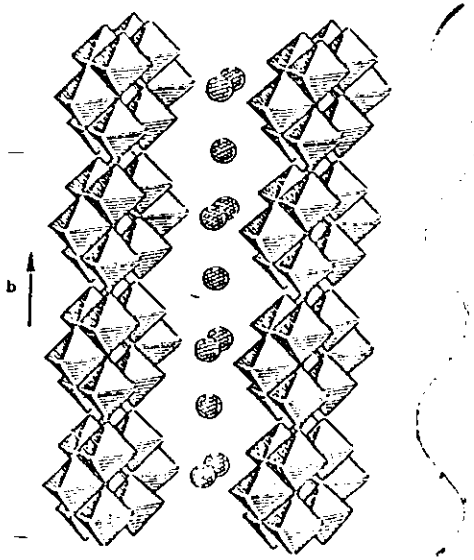
φ: undetermined (at the moment)

$NbSe_3$



$K_{0.3}MoO_3$

"blue bronze"



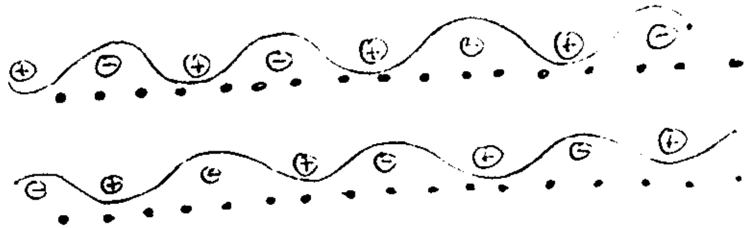
Real materials:

3D ordering of CDW at finite T

coupling $\begin{cases} \text{coulomb} \\ \text{overlap} \end{cases}$

$$q = (q_x, q_y, q_z)$$

$q_x = 2k_F$ Coulomb: $q_y, q_z = \pi/c$



Many atoms in unit cell:

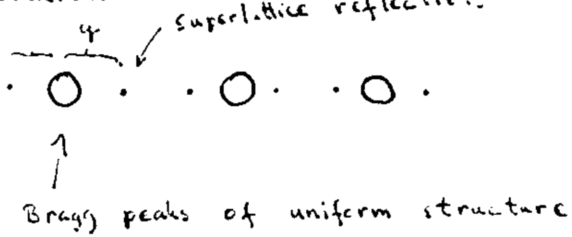
$$a_i^{(\ell)} = a_{i0}^{(\ell)} + \underline{U}_1^{(\ell)} \cos(q\, a_i^{(\ell)}) + \underline{U}_2^{(\ell)} \sin(q\, a_i^{(\ell)})$$

simple $U \cos(q a_i)$ is only approximation!

determination of CDW structure:

X-ray or neutron diffraction:

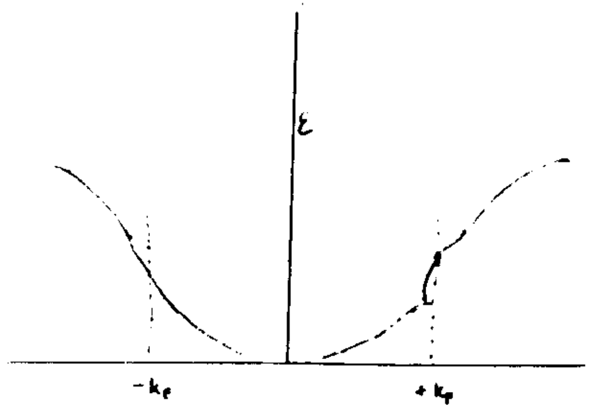
Ordered:



Temperature dependence of Δ

1 D order only at $T = 0$

3 D coupling $\rightarrow$ finite T_P

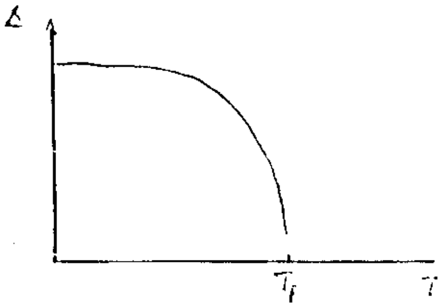


$W_{electronic} = \sum_k (\varepsilon_k - \varepsilon_k^0)\, f_k(T)$ balanced by elastic energy

"Peierls transition"

second order phase transition

order parameter : $\Delta e^{i\varphi}$



CDW : $\rho_1 \cos(2k_F x + \varphi)$

PLD : $u_1 \cos(2k_F x + \varphi)$

$k_B T_P = \alpha\, \Delta(0)$

$\alpha \sim 1$

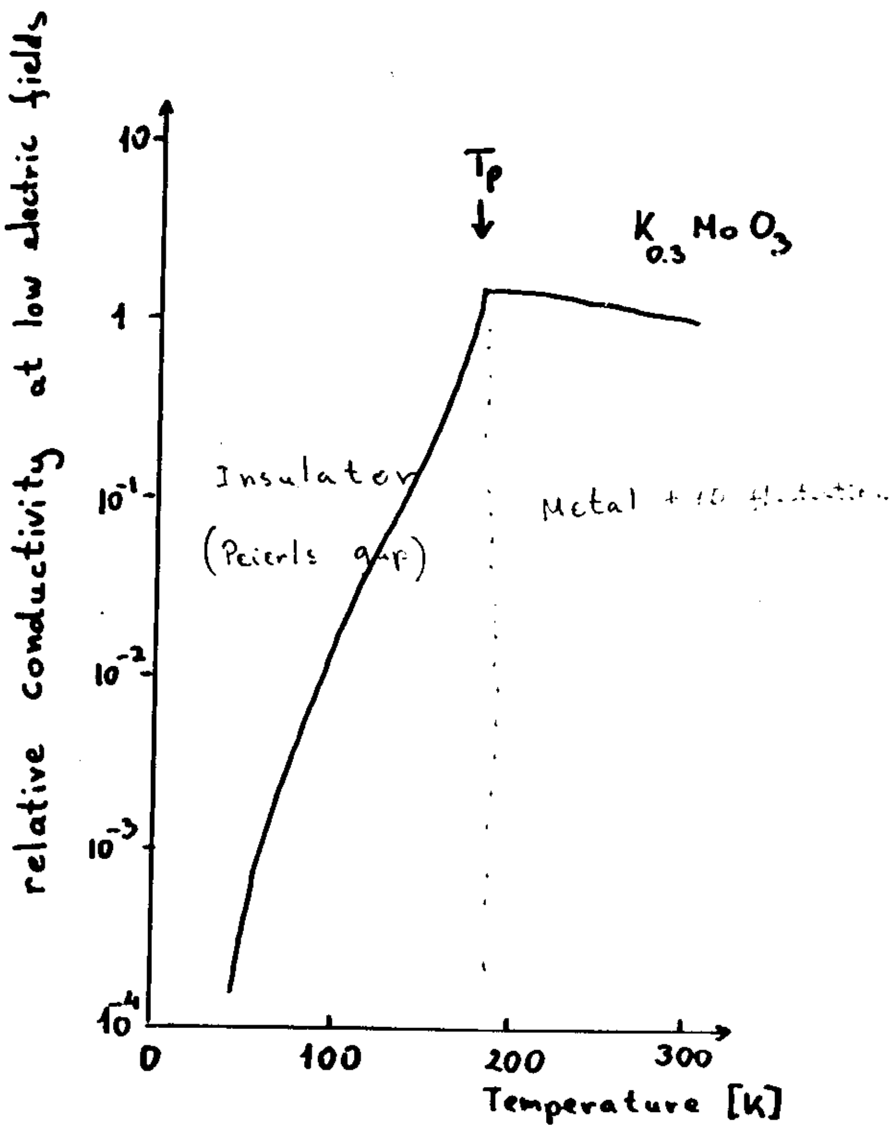
$\rho_1\, ,\, u_1 \sim \Delta(T)$

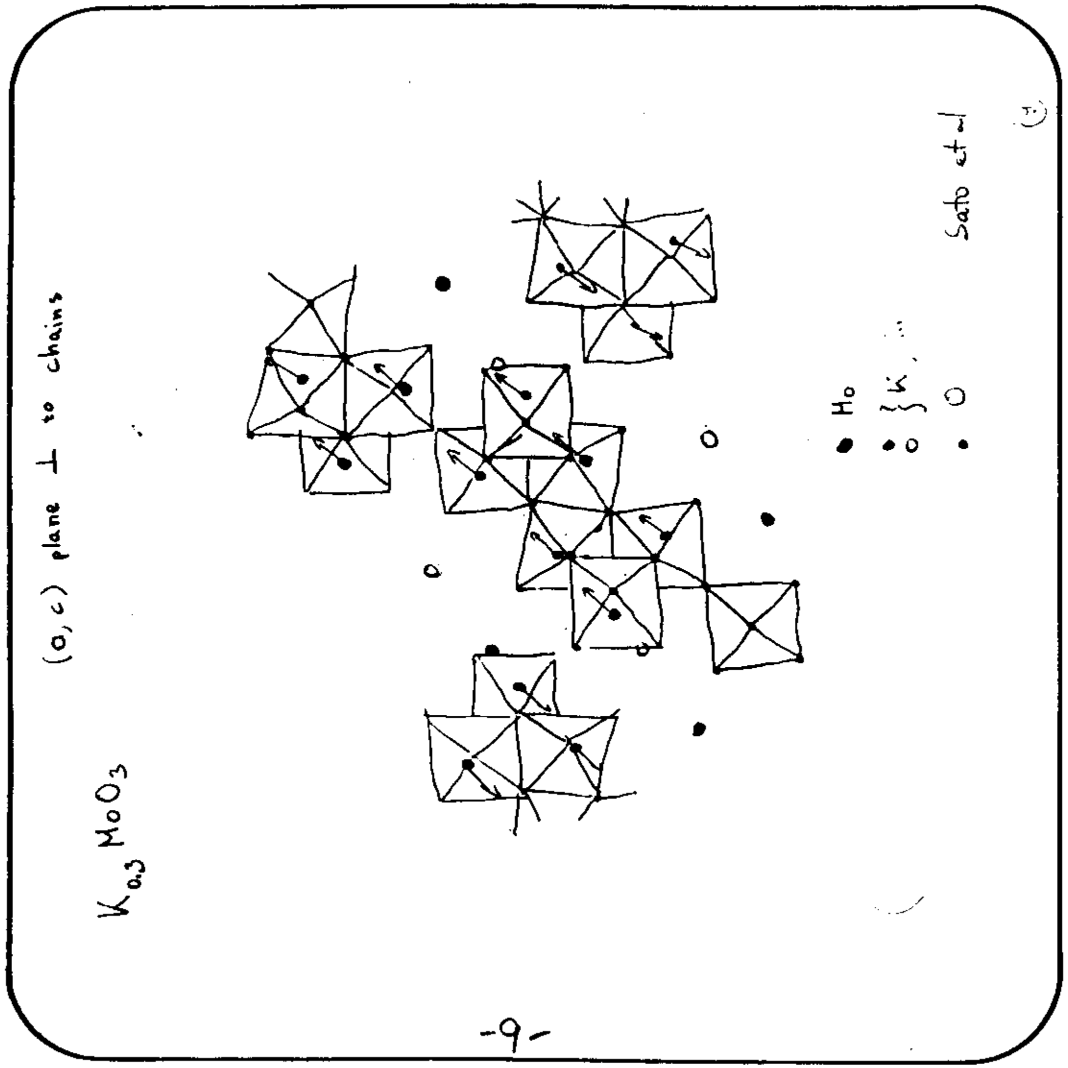
X-ray intensity

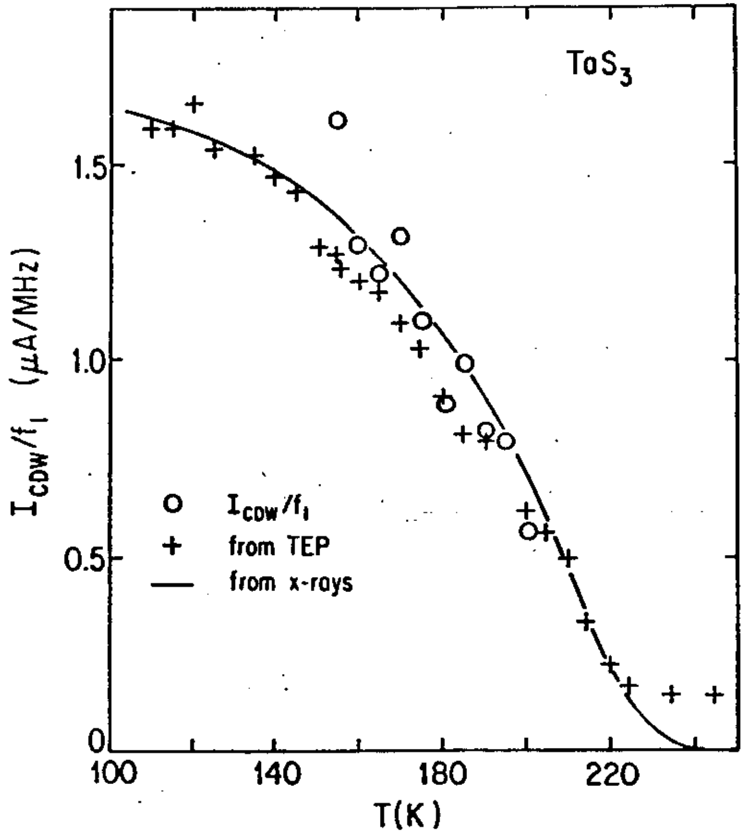
NMR

conductivity

TEP

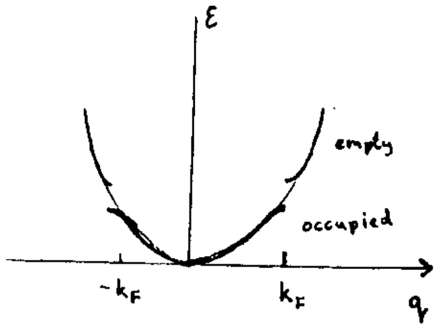






ZETTL AND GRÜNER
FIG. 11

Interaction with lattice

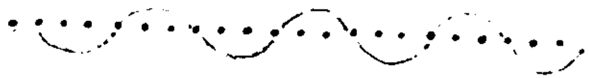


Instability of a quasi 1d metal. $T << T_p$

electron density:

$$\rho = \rho_0 + \rho_1 \cos(2k_F x + \varphi)$$

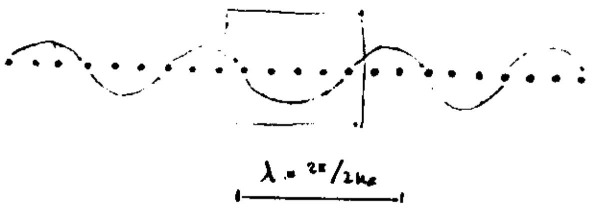
lattice potential
periodicity: $a = 2\pi/a$



commensurate

$k_F = \frac{n}{m}\frac{\pi}{a}$

n, m small integer



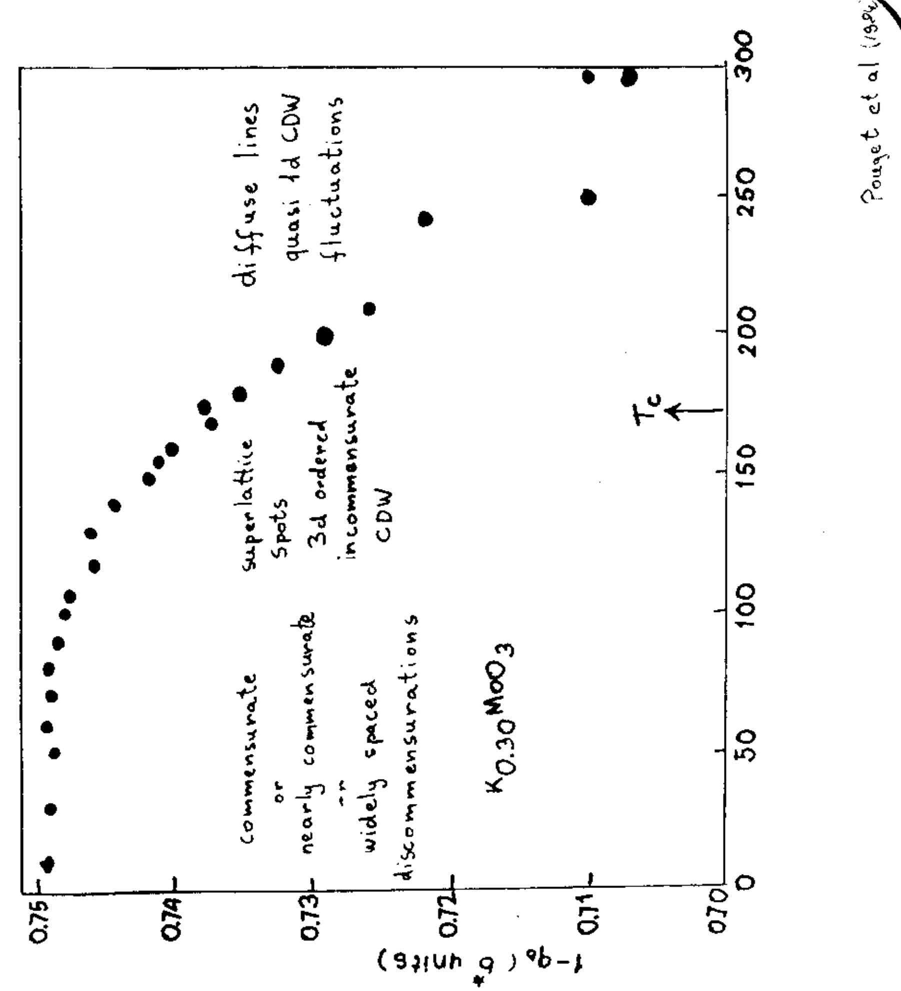
nearly commensurate

$k_F \approx \frac{n}{m}\frac{\pi}{a}$

incommensurate CDW

$k_F \neq \frac{n}{m}\frac{\pi}{a}$

depinned CDW : coupled oscillations of atoms and translation of electrons : $\boxed{j_{CDW} = \rho_0 v \;;\; v = \frac{\lambda}{2\pi}\frac{d\varphi}{dt}}$



$K_{0.3}MoO_3$ at low temperatures:

thought commensurate by

R. M. Fleming und L. F. Schneemeyer (1984)
Bell Lab. X-ray

incommensurate by

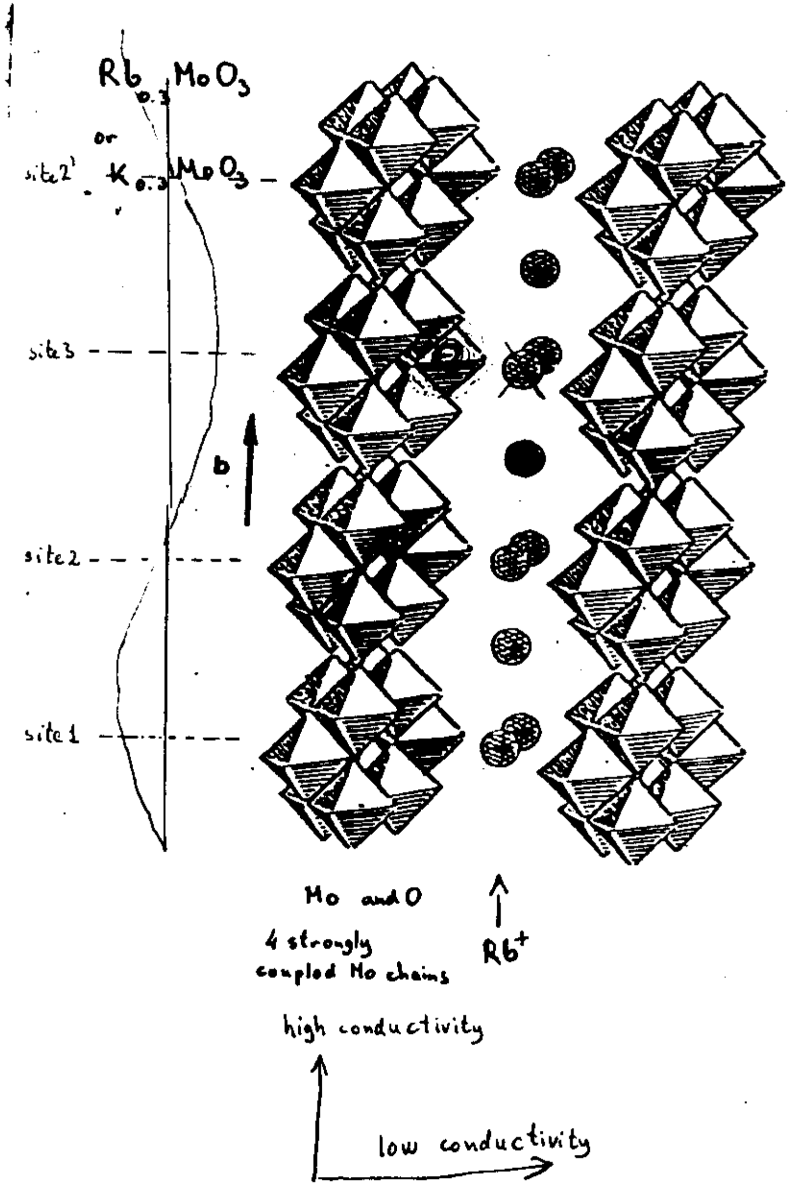
M. Sato, H. Fujishita and S. Hoshino (1983)
neutron scattering $q_b = 0.748$

J. Pouget et al. (1984)
Orsay X-ray

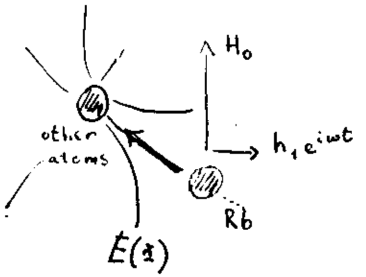
C. Berthier et al. (1985-6)
Grenoble NMR

incommensurate and commensurate regions:

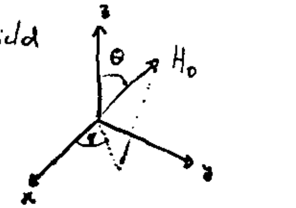
A. Jánossy, G. L. Dunifer, S. Payson (1987)
Wayne State U. ESR



Nuclear magnetic resonance

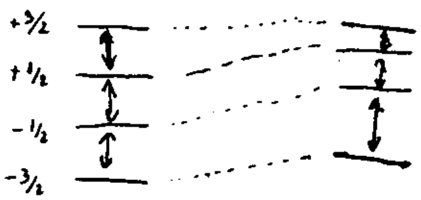


magnetic field



$g_N \mu_N \underline{S}\,\underline{H}$ $\qquad$ $e^2 q Q\,[3S_z^2 - S(S+1) + \eta(S_+^2 + S_-^2)]$

Zeeman interaction + quadrupole

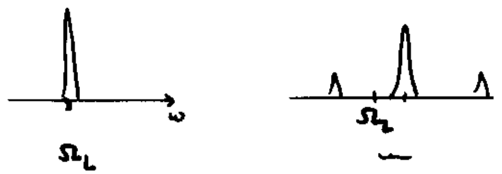


$g_N \mu_N$ nuclear magnetic moment

$q = \frac{\partial E_z}{\partial z}$ EFG

η asymmetry par.

Q nuclear quadrupole moment



$\nu_Q^2/\Omega_L \cdot f(\theta, \varphi, \eta)$

Electric field gradient tensor $\frac{\partial \vec{E}}{\partial r} \sim q_{ij}$ but only 2 independent parameters: q_{zz}, η

(15)

NMR lineshape

Static CDW

$1/2 \to -1/2$ ^{87}Rb spin transition, axial EFG, second order pert.

$\Omega_L = \Omega_L^0 + \nu_Q^2/\Omega_L^0\, f(\theta)$

$\nu_Q \sim q_{zz} Q$ $\qquad$ $q_{zz} = \partial E_z/\partial z$

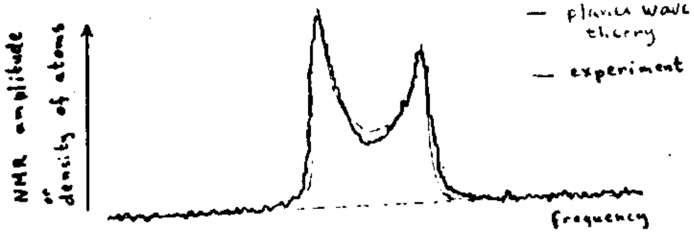
Change due to CDW: $q_{zz}^{(r)} - q_{zz}^0 = \Delta q_{zz}(r)$

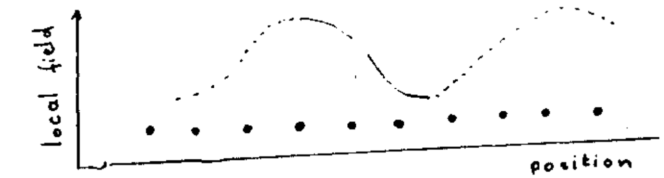
$\Delta\Omega_L \sim \Delta\nu_Q^2 \sim \Delta q_{zz}$

local field approx.:

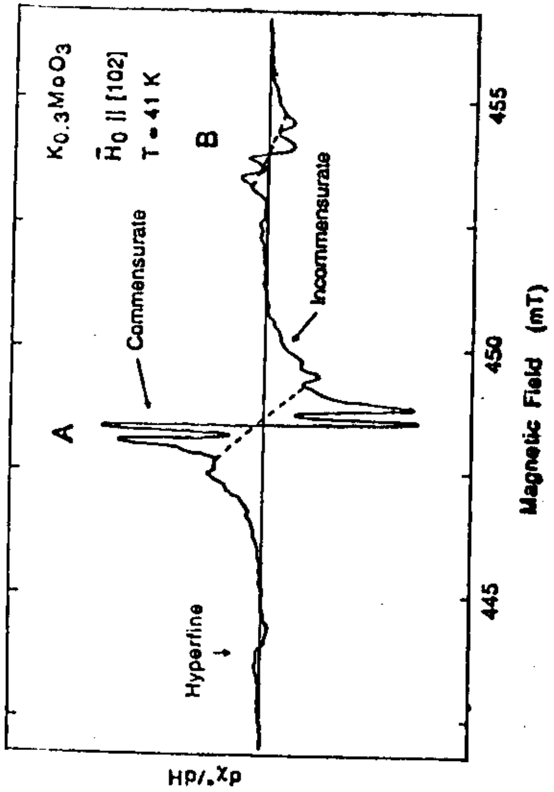
$\Delta q_{zz} = A_1 n(T) \cos(2k_F r) + A_2 n^2(T) \cos^2(2k_F r) + \ldots$

incommensurate k_F





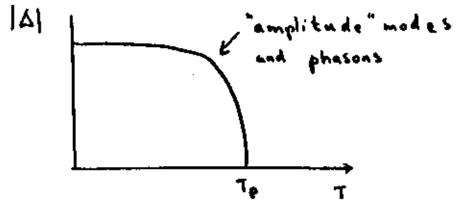
(17)



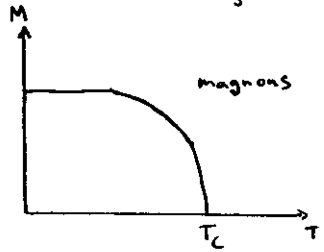
A. JÁNOSSY, G.L. DUNIFER, J.S. PAYSON 1988

(13)

Excitations of the CDW

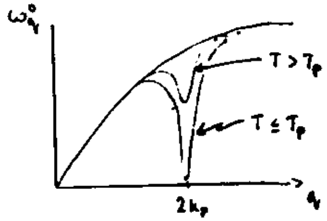


Ferromagnet



At finite T	at low T
$\Delta(x,t)$	$\Delta_0 + \delta\Delta(x,t)$
$\varphi(x,t)$	$\varphi_0 + \delta\varphi(x,t)$

pinned mode

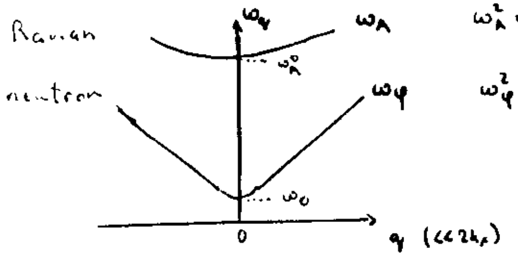


" giant Kohn anomaly "

phasons :
restoring force diminished
by e-ph coupling

T = 0 order complete
T > 0 thermal fluctuations

excitation spectrum



$$\omega_A^2 = \lambda^2(\omega^0_{2k_F})^2 + \frac{1}{3}\frac{m}{m^*}(v_F q)^2$$

$$\omega_\varphi^2 = \frac{m}{m^*}(v_F q)^2 + \omega_0^2$$

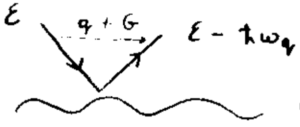
phason velocity: $c_0 = \left(\frac{m}{m^*}\right)^{1/2} v_F$

$\frac{m}{m^*} \sim 1/100 - 1/1000$
at low T

conductivity
$\sigma(\omega)$

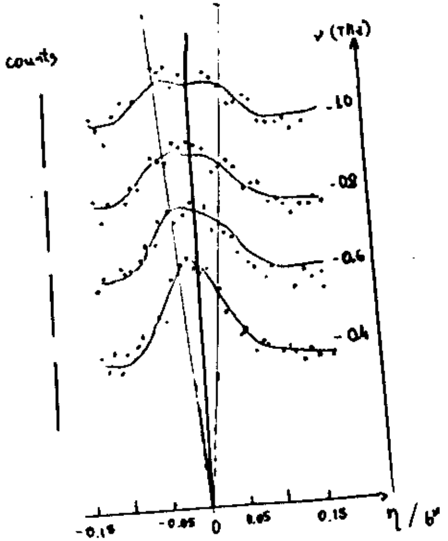
(20)

inelastic neutron scattering



CDW + phason (amplitudon)

$T = 175\,K \quad (T_P - 8\,K)$



$\vec{Q} = (5,\ 0.73+\eta,\ 2.5)$

$V_{phason} = 3\cdot 10^5\ cm/s$

Escribe-Filippini, Pouget,
Hennion, Sato
Synthetic Metals 19 931 (1987)

Frequency dependent conductivity

$$\frac{d^2\varphi}{dt^2} + \frac{1}{\tau}\frac{d\varphi}{dt} + \omega_0^2\varphi = \frac{2k_F e E}{m^*}$$

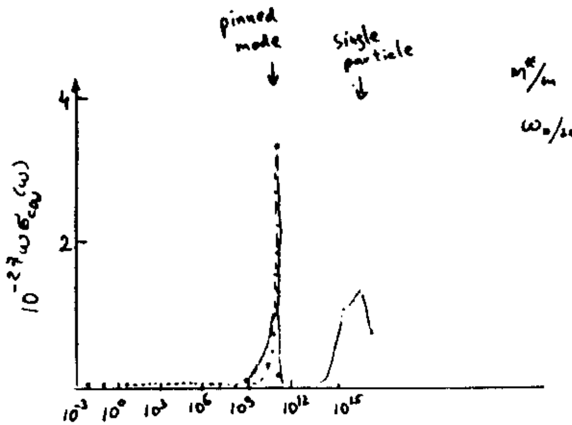
M. Rice and S. Strässler

$$\sigma(\omega) = \frac{n_c e^2}{i\omega m^*}\ \frac{\omega}{\omega_0^2 - \omega^2 - i\omega/\tau}$$

$\omega = 0 \quad \mathrm{Re}\,\sigma_{dc} = 0$

$$\varepsilon = \mathrm{Im}\,\sigma(0)/\omega = 1 + \frac{4\pi n_c e^2}{m^*\omega_0^2} + \frac{4\pi n e^2 \xi^2}{m\Delta^2}$$

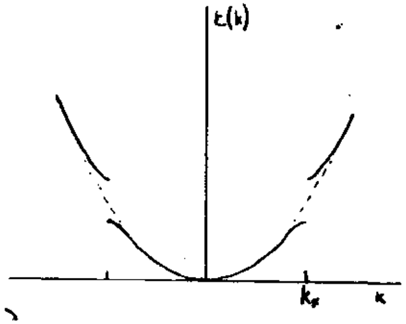
↑ single particle



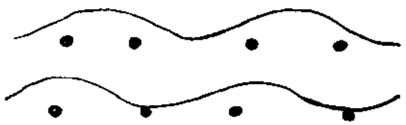
$m^*/m \approx 300$

$\omega_0/2\pi = 10^{11}\ Hz$

G. Mihály, T.W. Kim, G. Grüner (1985)



$$\rho = \rho_0 + \rho_1 \cos(2k_F r + \varphi)$$



commensurate

energy depends on φ

incommensurate

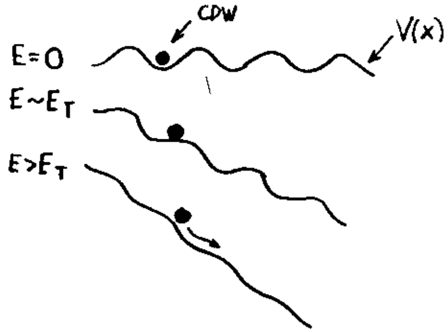
energy independent of φ

CDW slides : electrons move

ions oscillate

2 electrons $/\lambda$

Classical model



Grüner, Zawadowski
Chaikin (1981)

$$\frac{d^2x}{dt^2} + \frac{1}{\tau}\frac{dx}{dt} + \frac{\omega_0^2}{Q} G = \frac{eE}{M_F}$$

M_F : effective mass

$\tau = M_F/\Gamma$ damping constant

G = periodic potential . Sinusoidal

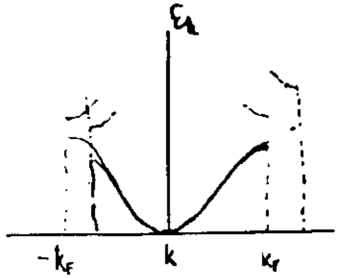
or quadratic

good qualitative picture for

electric field dependent conductivity

frequency dependent conductivity

current oscillations



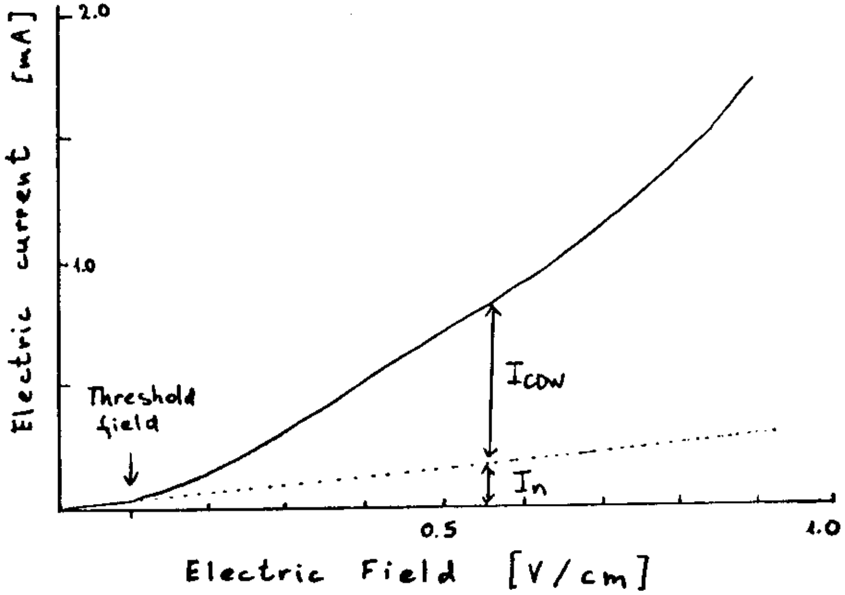
$$j_{CDW} = n_c e v_d$$

$$\frac{2\pi}{\lambda} v_d = d\varphi/dt$$

$$\rho = \rho_0 + \rho_1 \cos\left(2k_F x + \varphi(t)\right) = \rho_0 + \rho_1 \cos\left[\frac{2\pi}{\lambda}(x + v_d t)\right]$$

$$v_d = \frac{1}{2\pi}\frac{d\varphi}{dt}$$

$Rb_{0.3}MoO_3$
43K



I_{CDW} : collective motion of CDW coupled to PLD

$$I_{CDW} = n_c e v(E)$$

2/"chain" drift velocity at T=0

I_n : normal excitations current

$$I_n = n e v_n$$

$\sim e^{-\Delta/2kT} \to 0$ at T=0

Sliding CDW conductivity

Early history:

Fröhlich (1954) suggests a collective mode of the coupled electron-phonon system may lead to a special type of superconductivity

Bardeen (1973) suggests this mode may be effective in TTF-TCNQ

Monceau, Ong, Portis, Meerschaut and Rouxel (1976) find an electric field dependent conductivity in $NbSe_3$

Fleming, Moncton and McWhan (1978) find Peierls distortion in $NbSe_3$. The distortion is independent of field

Sliding CDW conducting materials:

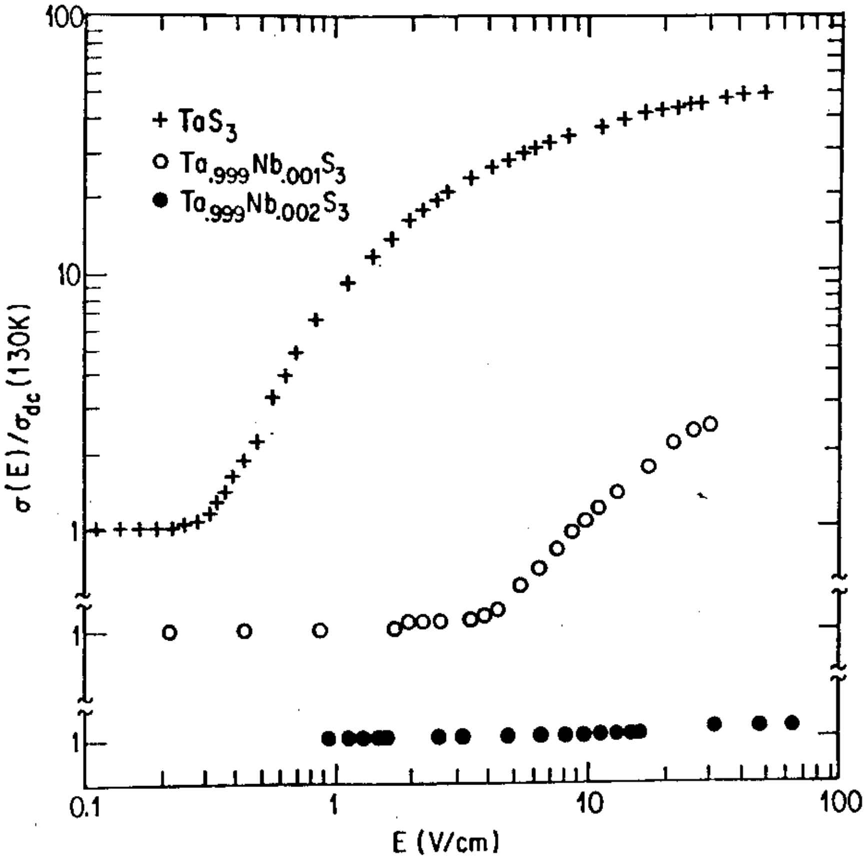
$NbSe_3$ metal at all temperature
(3 inequivalent chains)

NbS_3
TaS_3 orthorhombic and monoclinic
$(TaSe_4)_2I$
$(NbSe_4)_{10}I_3$
$K_{0.3}MoO_3$; $Rb_{0.3}MoO_3$

} Fermi surface fully destroyed in distorted phase

TTF - TCNQ

Morphology: diverse
very different crystal structures but all contain chains
incommensurate superlattice
- metal insulator transition
- electric field dependent conductivity
- frequency " "
- "narrow band" noise
- anomalous thermo- and magnetoelectricity
- sensitivity to impurities at levels 10^{-4}
- metastable states



Methods of measuring v:

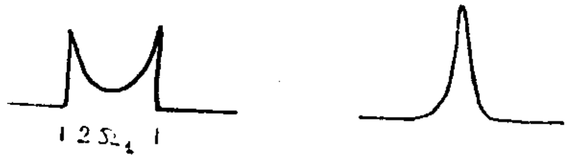
1.) current - voltage charateristics

$$v = j/ne$$

2.) voltage noise frequency

$v = \lambda \nu_{noise}$ (other models: $v = \lambda/2\, \nu$)

3.) NMR lineshape



$v = \lambda\, \nu_{local\ field}$

$v \ll \Omega_1 \lambda$ $v \gg \Omega_1 \lambda$

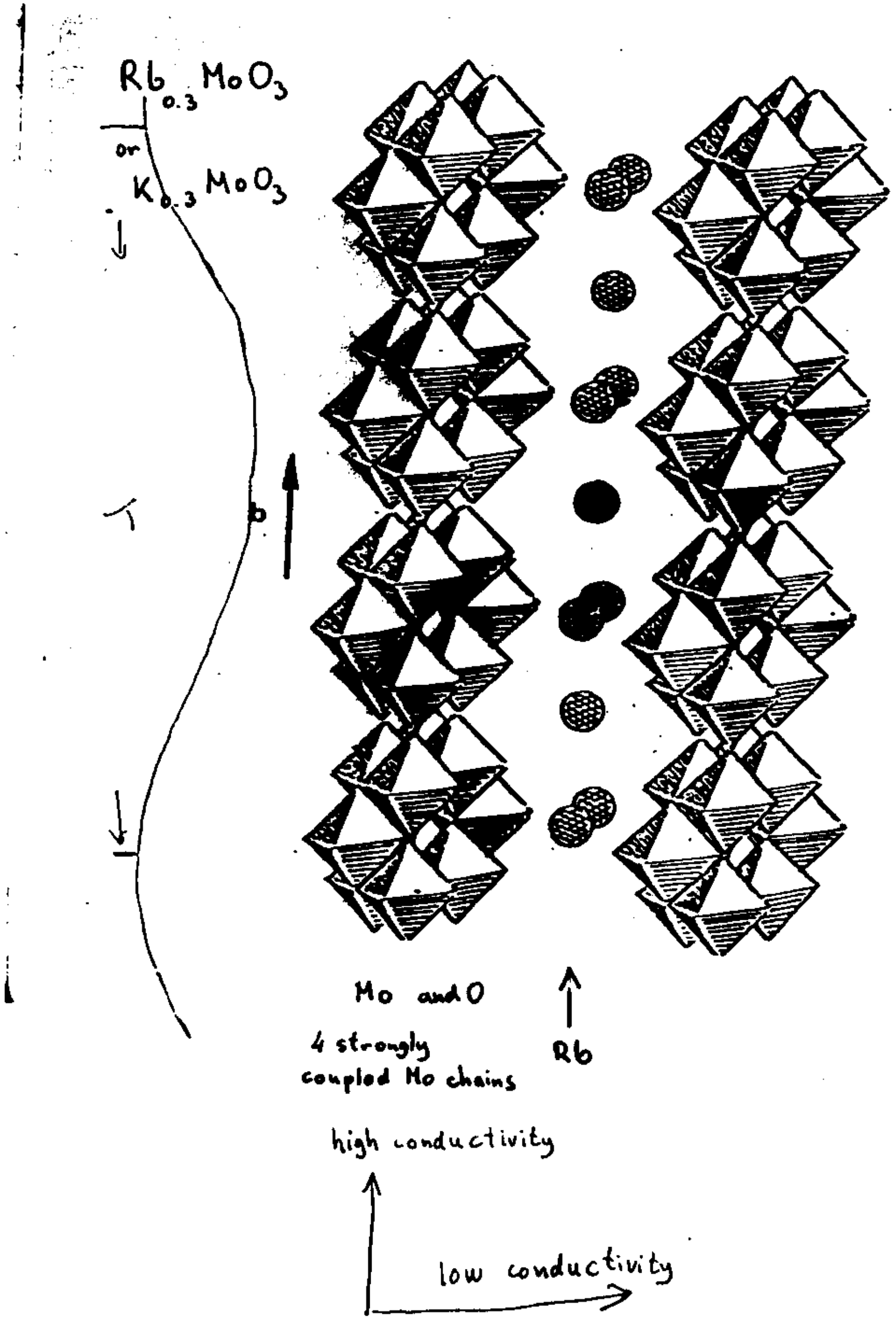
4.) Doppler shift of neutron scattering

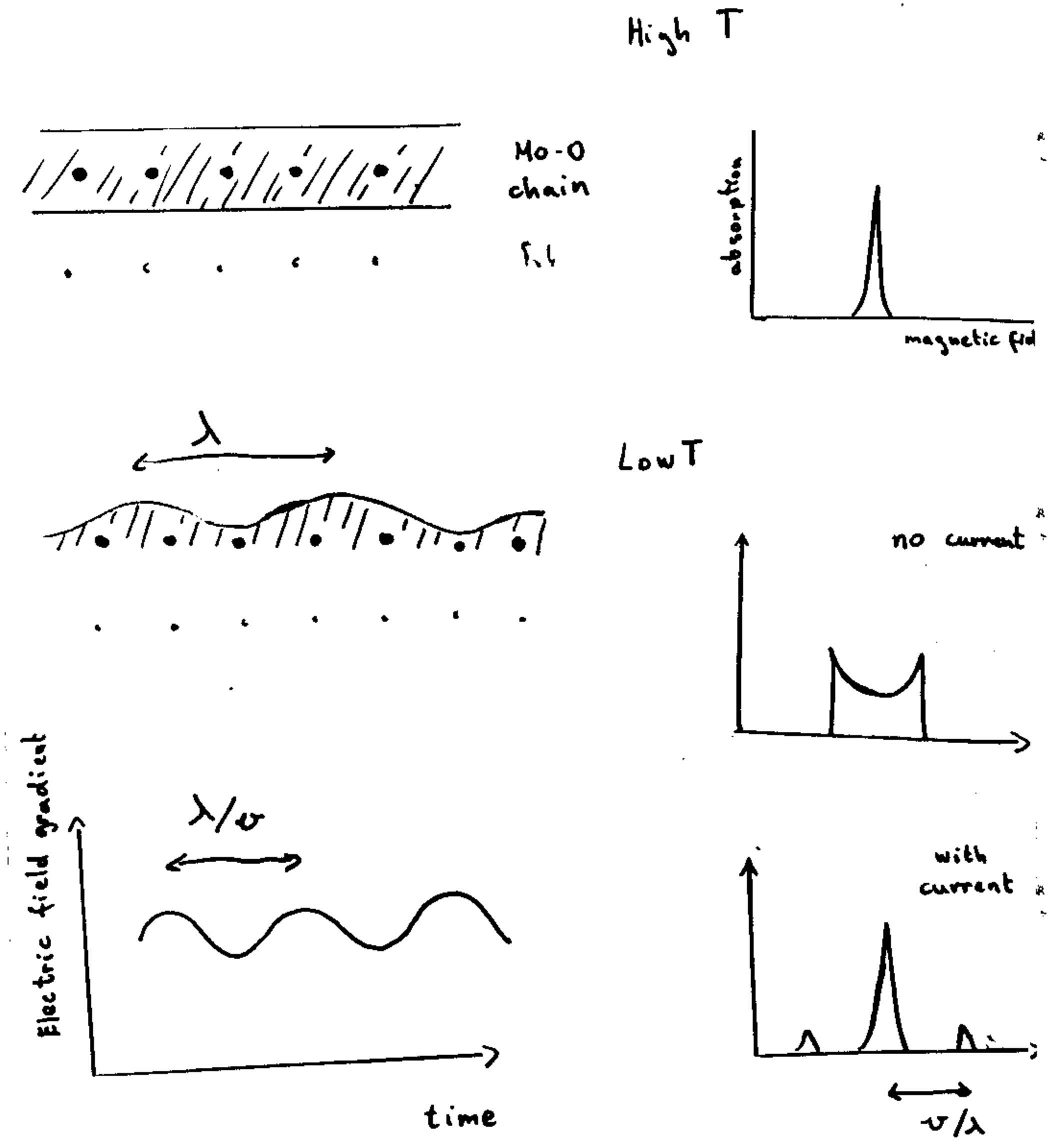
$q = 2k_F$ component of potential drifting with CDW:

$$\rho_q(r_i) = A_q \cos(q r_i + q v t) = A_q \cos\left(q(r_i + v t)\right)$$

This talk:

Measurements 1.) 2.) and 3.) on same sample


$Rb_{0.3}MoO_3$
or
$K_{0.3}MoO_3$
b
Mo and O
4 strongly coupled Mo chains
Rb
high conductivity
low conductivity


High T
Mo-O chain
absorption
magnetic field
λ
Low T
no current
Electric field gradient
λ/v
with current
time
v/λ

NMR lineshape

sliding CDW

nucleus at R_j

$$\Omega_L(t) = \Omega_L^0 + \Omega_1 \cos(2k_F R_j + \phi(t))$$

$$\phi(t) = \Omega t = 2\pi\lambda^{-1} v t \qquad M(t) \sim \frac{1}{N}\sum_j e^{i\int_0^t \omega(R_j,t')\,dt'}$$

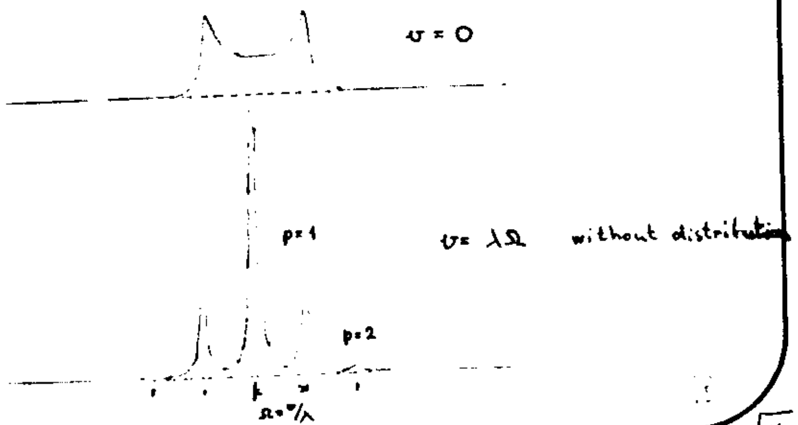
lineshape:

$$g(\omega) = \left\{ \sum_{p=-\infty}^{\infty} \left[J_p(\Omega_1/\Omega)\right]^2 \delta(\omega - p\Omega) \right\} * h(\omega)$$

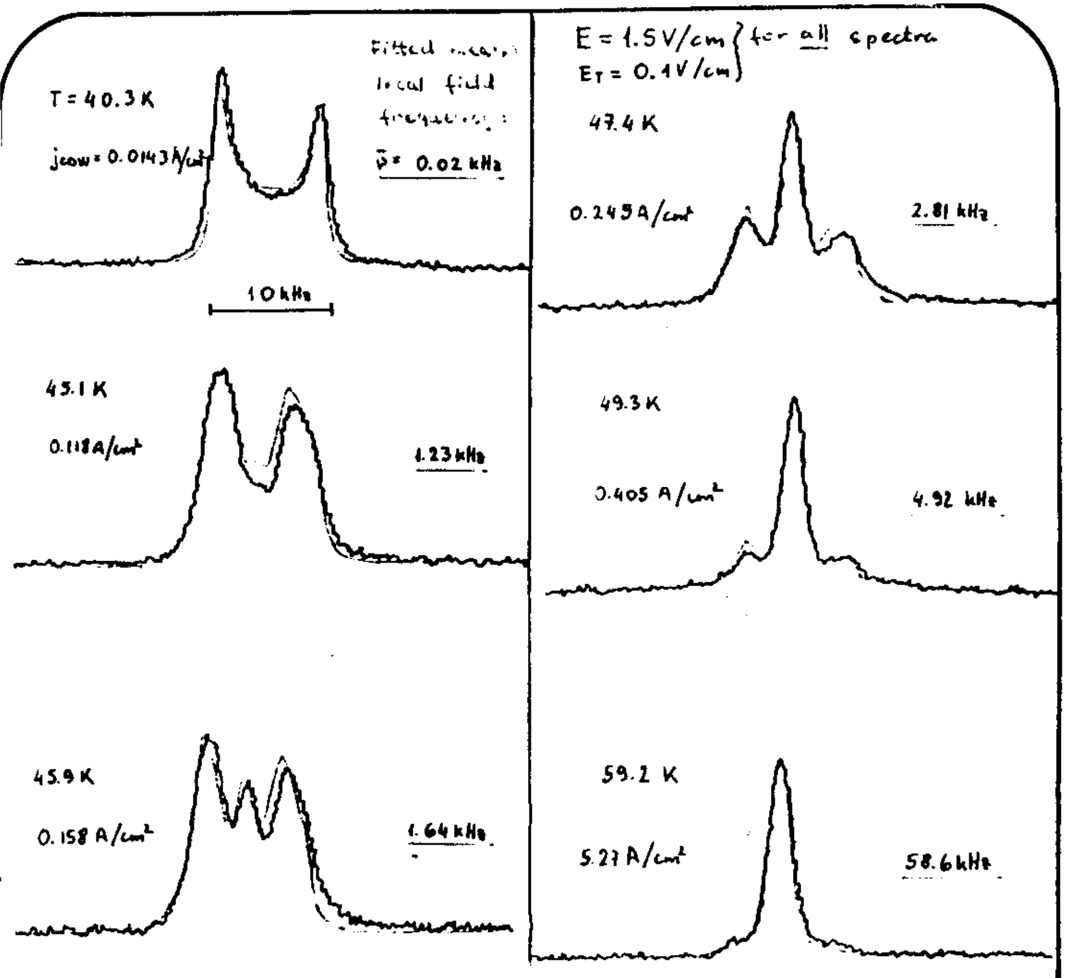
J_p: Bessel function

$h(\omega)$: dipolar broadening, temporal incoherence

J_0 = const central line independent of v for $v/\lambda \gg \Omega_1$



14

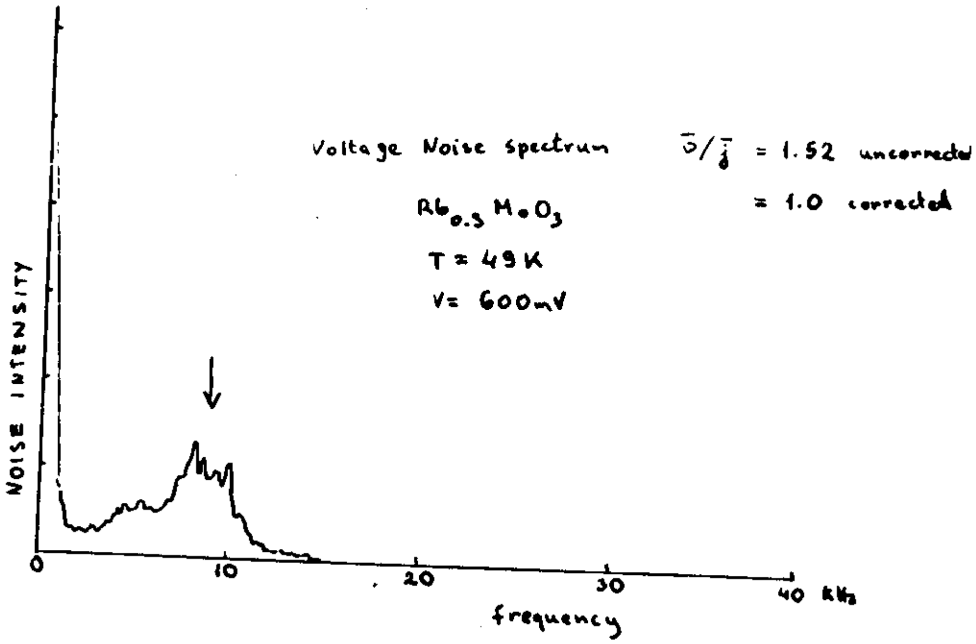


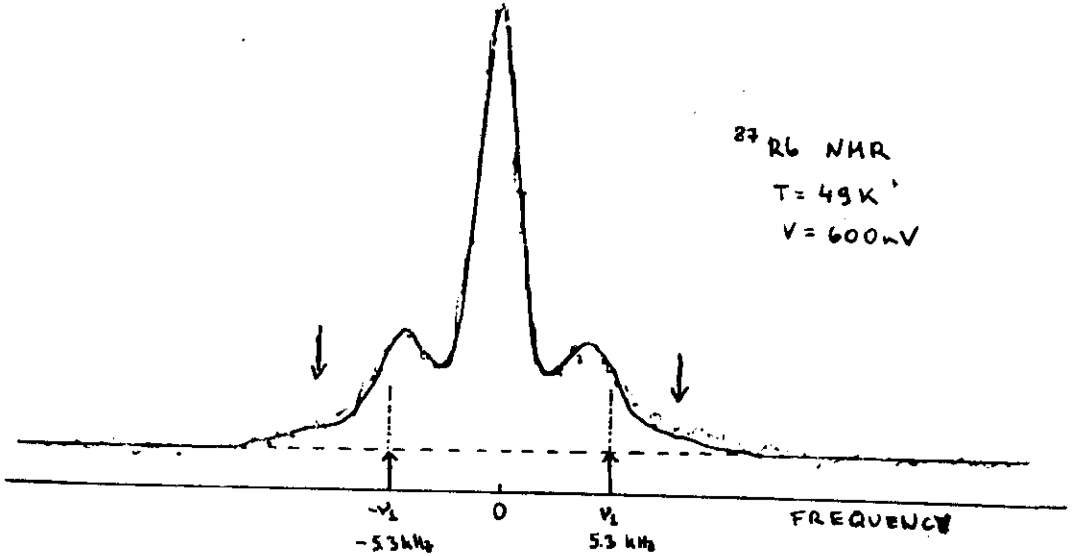
Measured: $\bar{\nu}/j_{CDW} = 11 \pm 1$ kHz / A cm^{-2}

theory: $(ne\lambda)^{-1} = 12.5$ kHz / A cm^{-2}

A. Jánossy, P. Ségransan, C. Berthier, P. Butaud (1987)

15





Effect of impurities

Pinning of the CDW

pinning frequency: $\omega_0^2 = K/m^*$

static dielectric constant: $\varepsilon = 1 + \frac{4\pi n_c e^2}{K}$

threshold field: $E_T = \alpha \frac{\lambda}{2} \frac{K}{e}$

$\varepsilon(T, n_i)$ $\quad E_T(T, n_i)$ but $\varepsilon E_T = \alpha 4\pi c \ldots$

single degree of freedom model too simple: $\varepsilon(E)$ incorrec[t]

Fukuyama, Lee, Rice model

only $\varphi(r)$ deformable, Δ not

$$\mathcal{H} = \frac{n_c \hbar v_F}{4\pi} \int (\nabla\varphi)^2 dr + \int \rho_c V(r) \cos(2k_F r + \varphi(r))$$

$V(r) = V_0 \, \delta(r - r_i)$ $\quad r_i$: random sites

I CDW deformation energy

II impurity - CDW interaction

Strong pinning: II large

weak pinning: I large

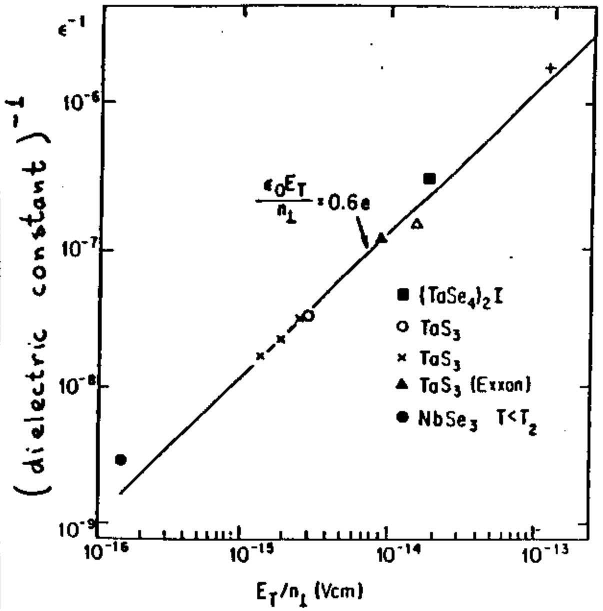
phase coherence $\langle \varphi(r)\varphi(0) \rangle \sim e^{-r/L_0}$

L_0 : Lee Rice domain

$E_T \sim n_i$ Strong pinning

$E_T \sim n_i^2$ weak pinning

24



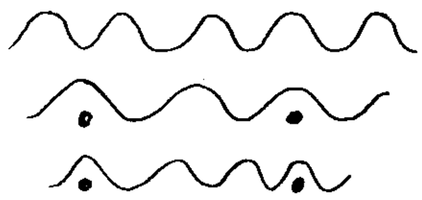
Threshold electric field for nonlinear conduction

Rigid CDW model: $\epsilon_0 E_T = \alpha \frac{2e}{q}$

UCLA (1983)

Metastable states

deformable CDW allows for states with nearly equal pinning energy



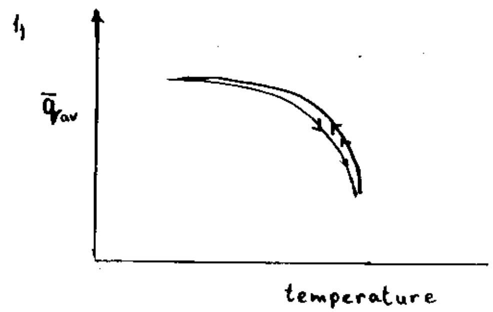
equilibrium
no impurity $q = q_0$

state I $q < q_0$

state II $q > q_0$

(strong pinning model)

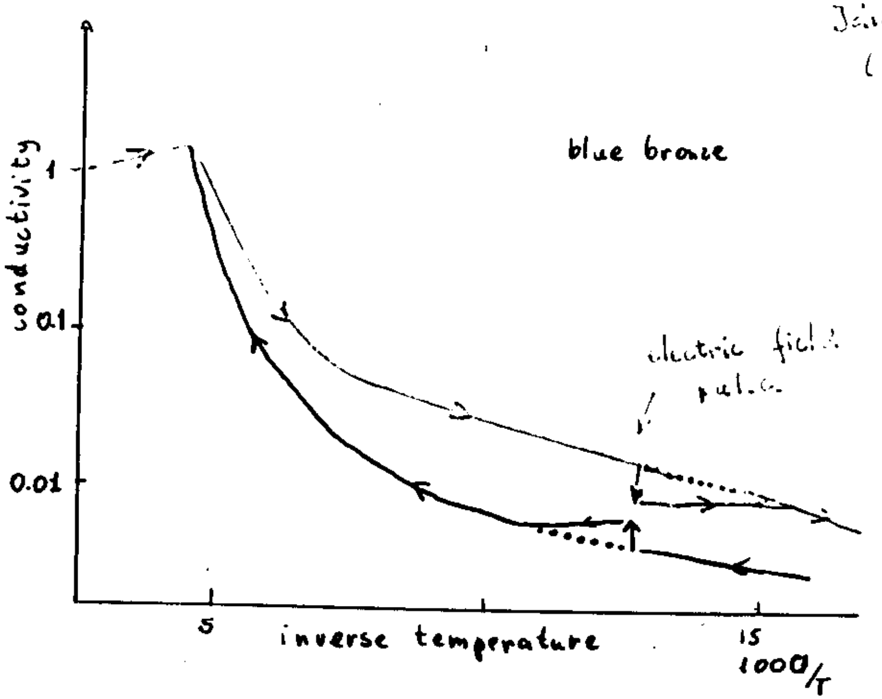
Types: 1) thermally induced
2) electric field induced



idea
not proven

41

Kriza
Jánossy
(1985)

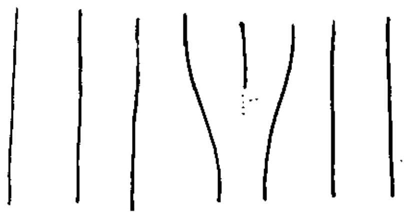


thermal equilibrium?

models: $\lambda = 2q_F(T)$

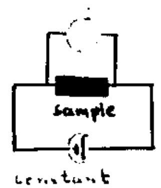
impurities

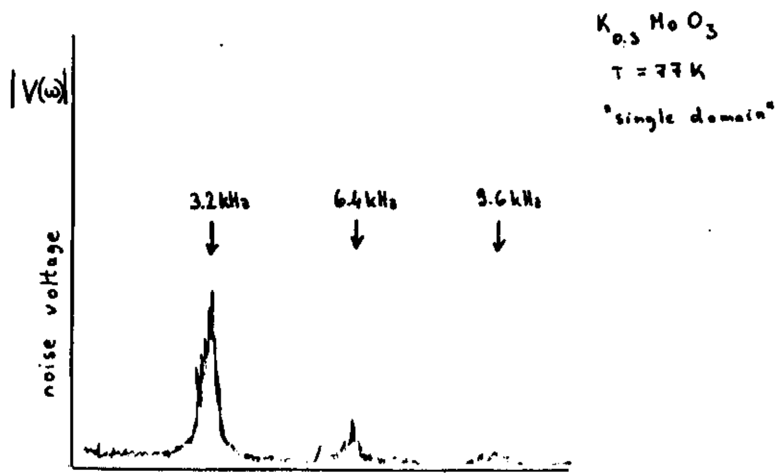
$\Delta(\ast)$: topological defects of CDW:



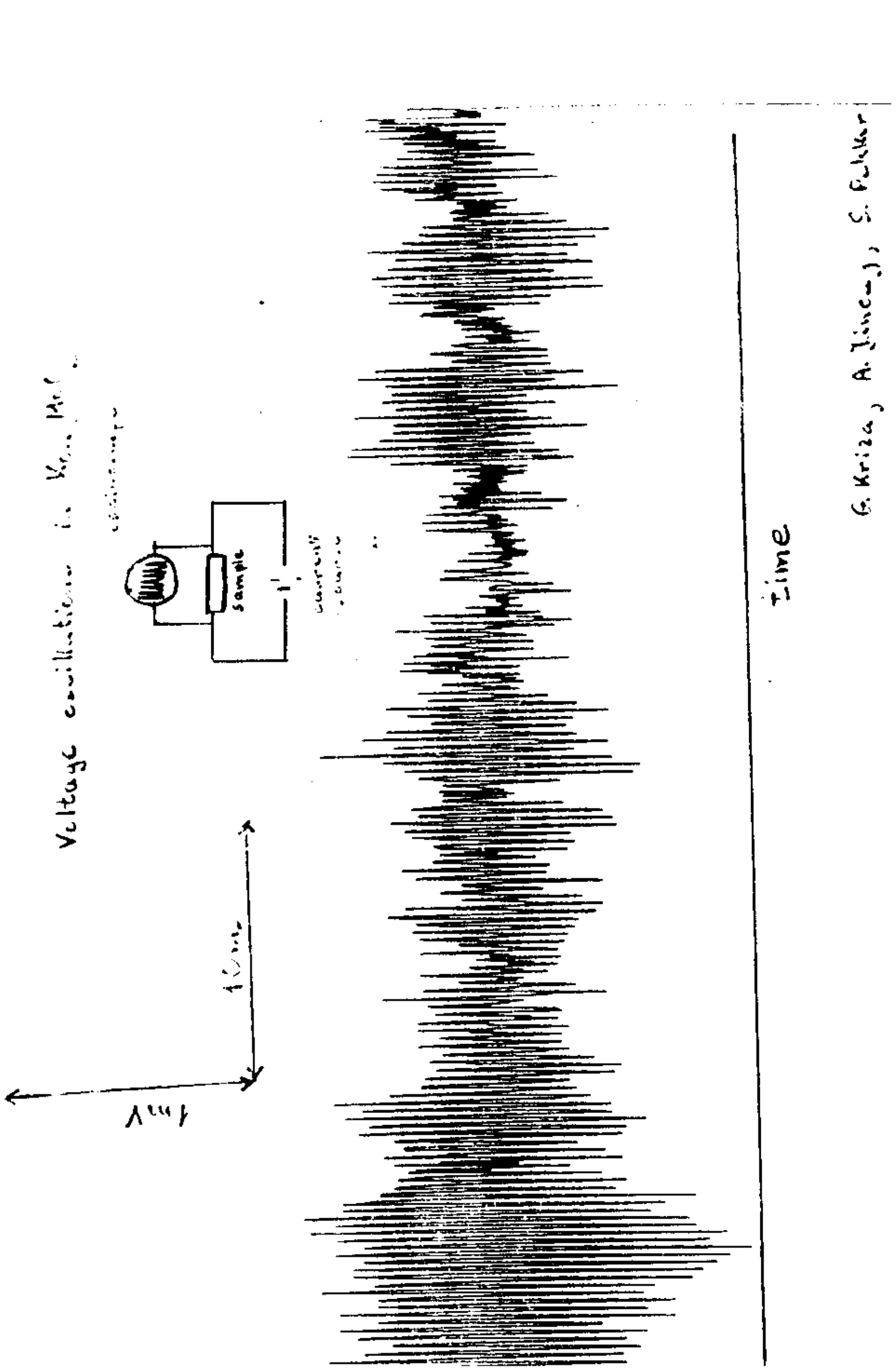
Narrow band voltage noise

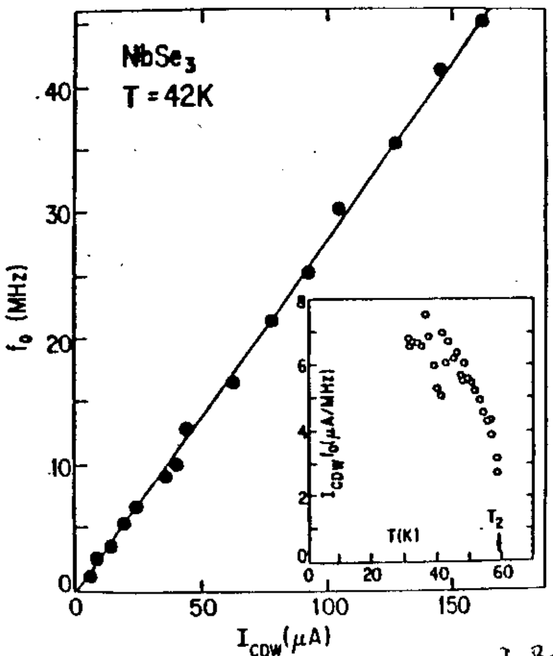
Fleming and Grimes 1979





Kriza and Jánossy (1986)





T = 0

$$I = n_0 e v$$

$$f_0 = v/\lambda$$

$$n_0 = \frac{2}{a^* c^* \lambda}$$

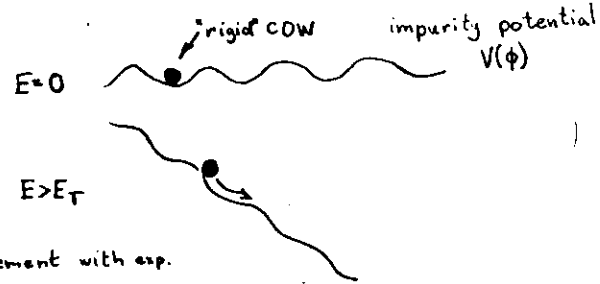
$$I/f_0 = \frac{2e}{a^* c^*}$$

J. Bardeen
E. Ben-Jacob
A. Zettl
G. Grüner
PRL 49 493 (82)

Origin of narrow band noise

a) periodic motion of CDW over finite number of impurities

Grüner, Zawadowski, Chaikin
Monceau, Richard, Renard



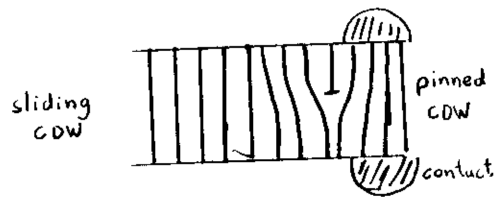
$I = nev$

$f = v/\lambda$

$I/f = ne\lambda$ in agreement with exp.

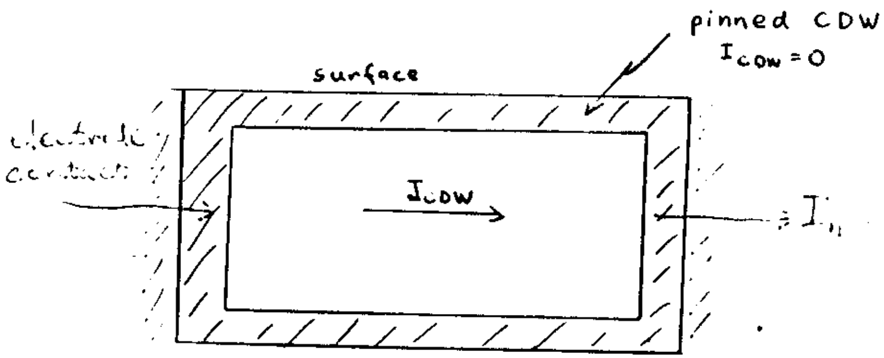
b) periodic instability at boundary between sliding and pinned CDW regions

Ong, Verma, Maki
Gorkov



$I/f = ne\lambda$ like for single impurity

(46)



Boundary problem:

1.) transversely moving vortices

Ong, Verma, Maki (1984)
Gorkov

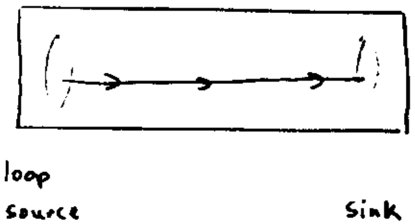
2.) longitudinally moving vortices

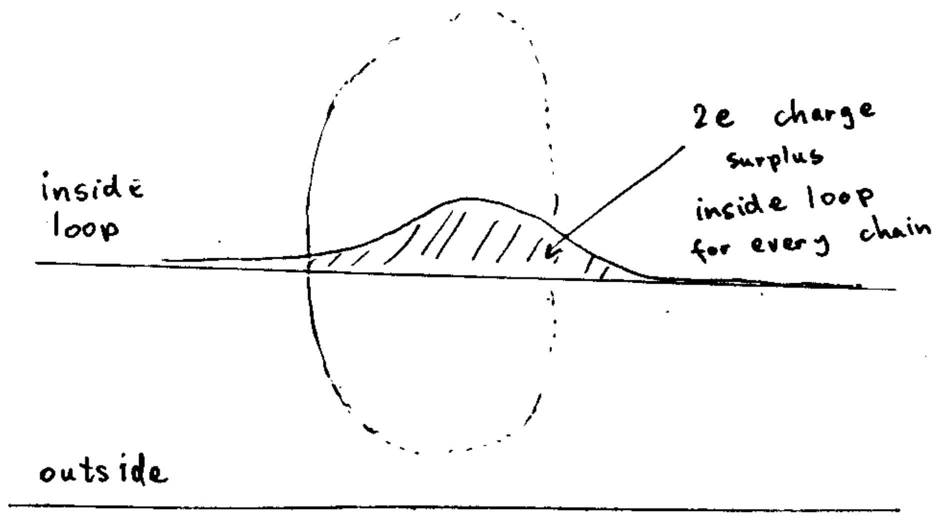
Lee and Rice (1977)

Models for voltage noise

2. b. Loops moving along crystal

Lee and Rice ([illegible])

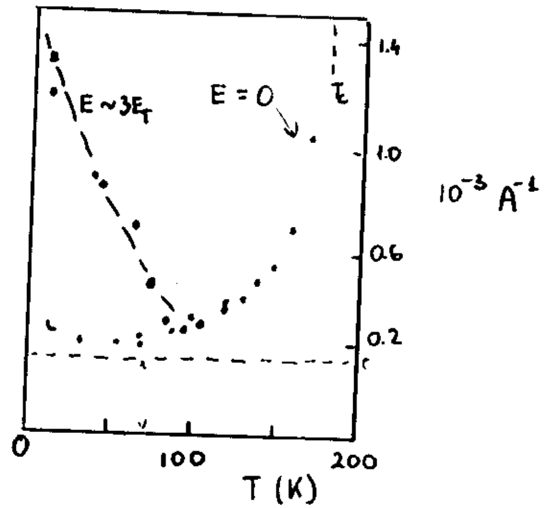




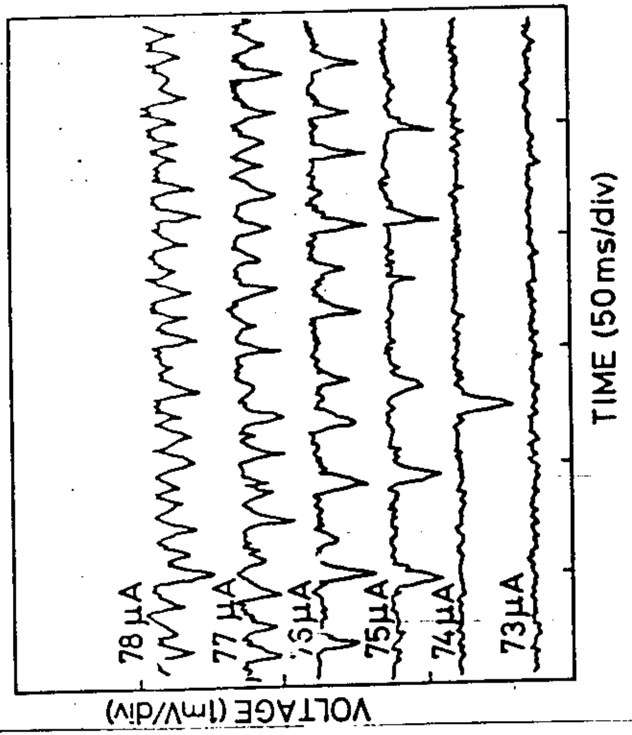
longitudinal coherence length instrumentally limited
~ 1000 Å resolution in blue bronze

transverse coherence length:

Fleming, Dunn
Schneemayer
(1985)



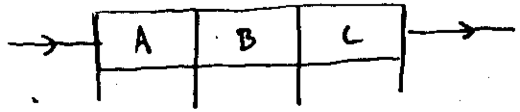
7

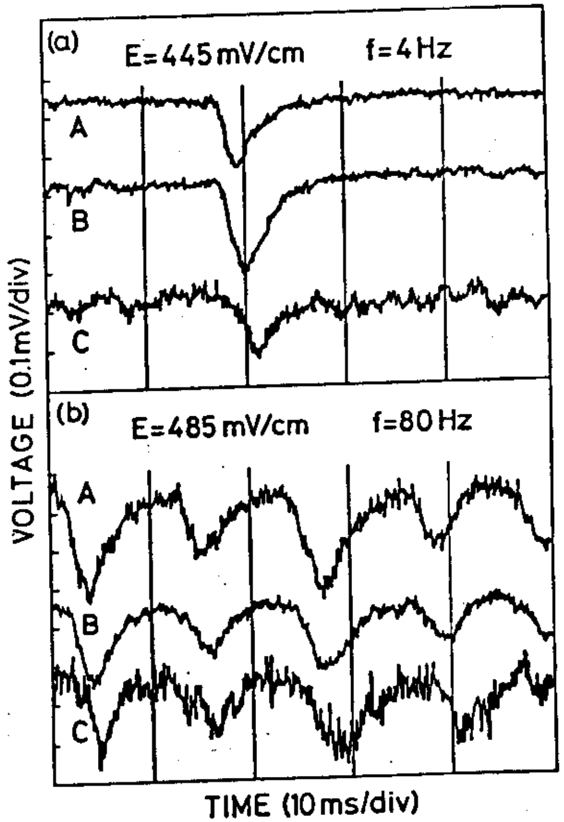


similar pulses:
Gill and Higgs ($NbSe_3$)
Ong, Kalem, Eckert (TaS_3)
Dumas, Schlenker, Marcus, Buder } ($K_{0.3}MoO_3$)

Csiba T., Jánossy A., K. Gy., 1989.

54





charge: positive but
may be negative under
other conditions

velocity ~ 1m/s
if homogeneous

$Rb_{0.3}MoO_3$

T. Csiba
G. Kriza
A. Jánossy

sample: RBL

Reviews

General

G. Grüner — Reviews of Modern Physics **60** 1129 (1988)

Comments on Solid State Physics **10** 173 (1983)

J.C. Gill — Contemp. Phys. **27** 37 (1986)

A. Jánossy, C. Berthier, P. Ségransan
Physica Scripta **T 19** 578 (1987)

P. Monceau in "Electronic properties of inorganic quasi one dimensional metals" Part II. p139
Reidel Publ. Co. Holland (1985)

Structure and excitations

J. Pouget and R. Comes in "Charge density waves in solids" (L.P. Gor'kov and G. Grüner Eds)
Volume of the "Modern Problems in Condensed Matter Series" (Elsevier) 1989 (?)

NMR

P. Butaud, P. Segransan, A. Jánossy, C. Berthier
J. de Physique 1990 January

Voltage noise propagation

T. Csiba, G. Kriza and A. Jánossy
Phys. Rev. **B40** 10088 (1989)