The STRANGE PROPERTIES of QUASICRYSTALS

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SUMMARY

1. Quasicrystalline Compound
2. Quasiperiodic Structures
3. Electronic Properties
4. Spectral Properties
5. Transport Properties
6. Anomalous Transport
7. Why are $AlPdMn$ and $AlPdRe$ so different ?
8. Conclusion

References :

1. *Lectures on Quasicrystals*, F. Hippert & D. Gratias Eds., Editions de Physique, Les Ulis, (1994),

2. *Quasicrystals*, S. Takeuchi & T. Fujiwara Eds., World Scientific, (1998),

3. *Electronic transport properties of quasicrystals*, S. Roche, D. Mayou and G. Trambly de Laissardière, J. Math. Phys., **38**, 1794-1822 (1997),

Quasicrystalline alloys :

Metastable QC's: **AlMn**

(*Shechtman D., Blech I., Gratias D. & Cahn J., PRL* **53**, *1951 (1984)*)

AlMnSi

AlMgT $(T = Ag, Cu, Zn)$

Defective stable QC's: **AlLiCu**

(*Sainfort-Dubost, (1986)*)

GaMgZn

(*Holzen et al., (1989)*)

High quality QC's: **AlCuT** $(T = Fe, Ru, Os)$

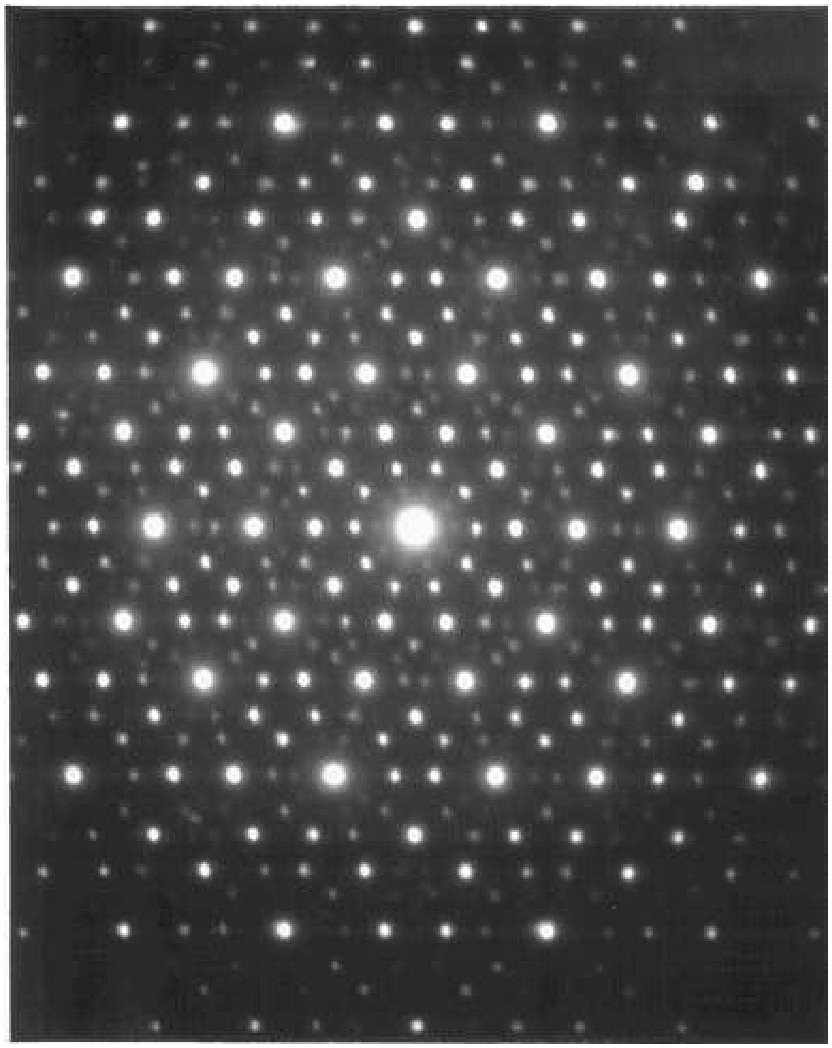
(*Hiraga, Zhang, Hirakoyashi, Inoue, (1988)*)

(*Gurnan et al., Inoue et al., (1989)*)

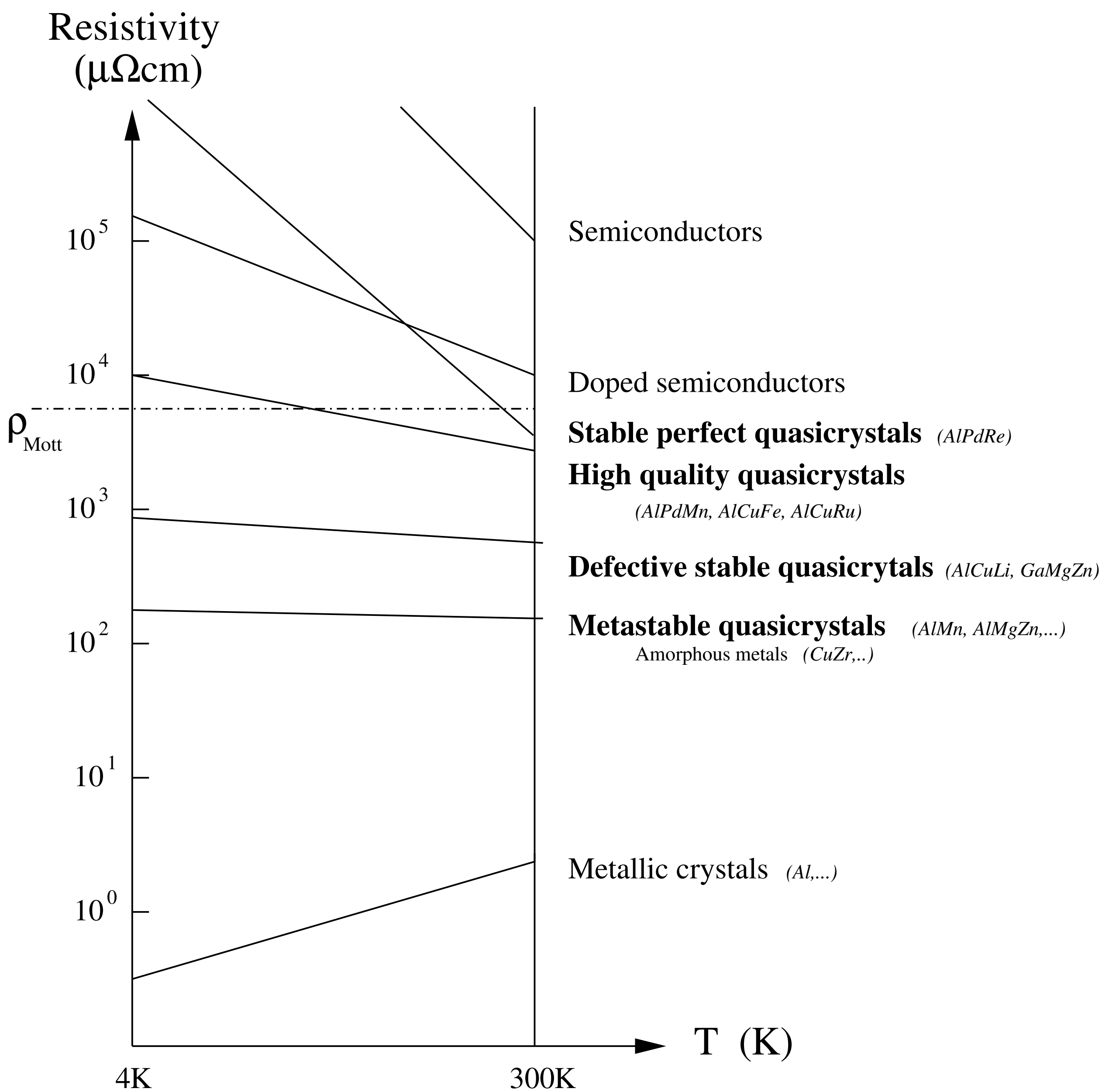
(*Y. Calvayrac et al., (1990)*)

"Perfect" QC's: **AlPdMn**

AlPdRe



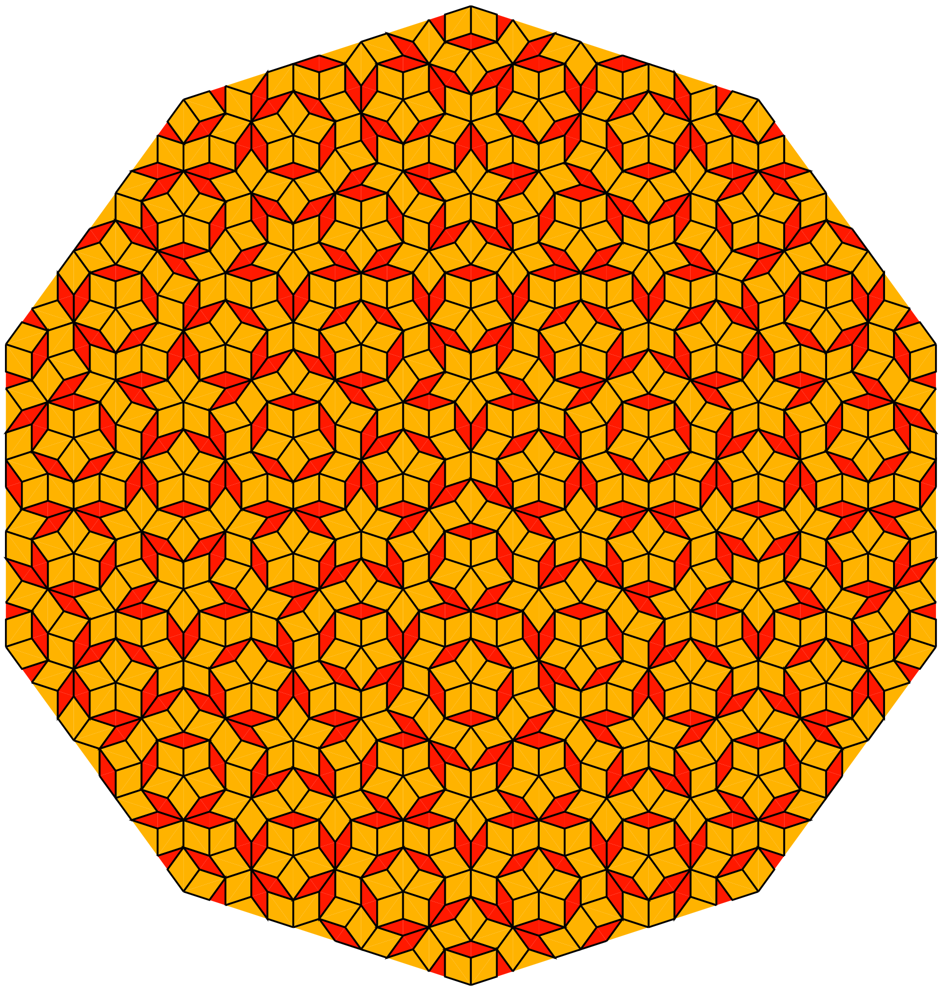
- Typical TEM diffraction pattern -
- with 5-fold symmetry -



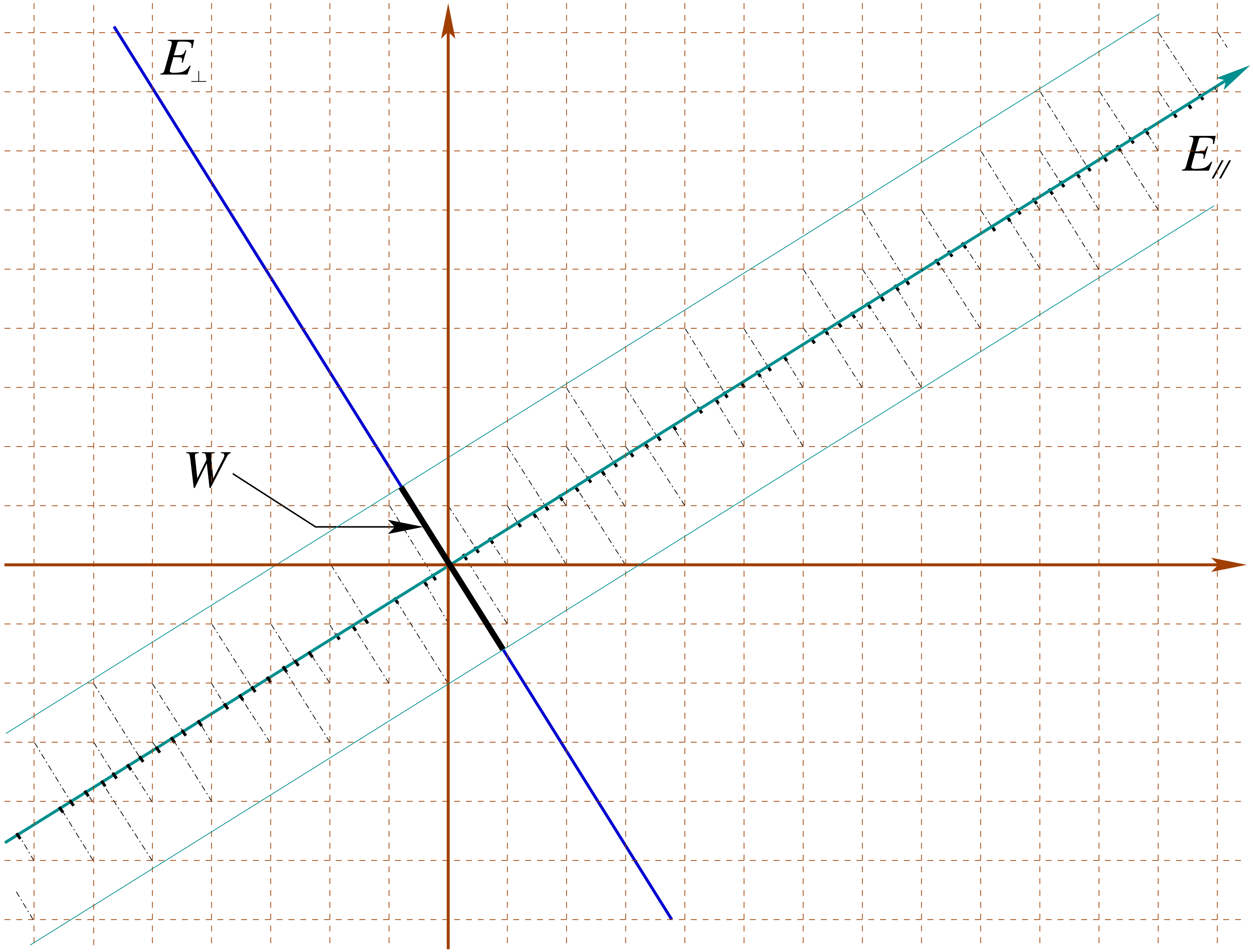
Typical values of the resistivity

(Taken from *C. Berger* in ref. [2])

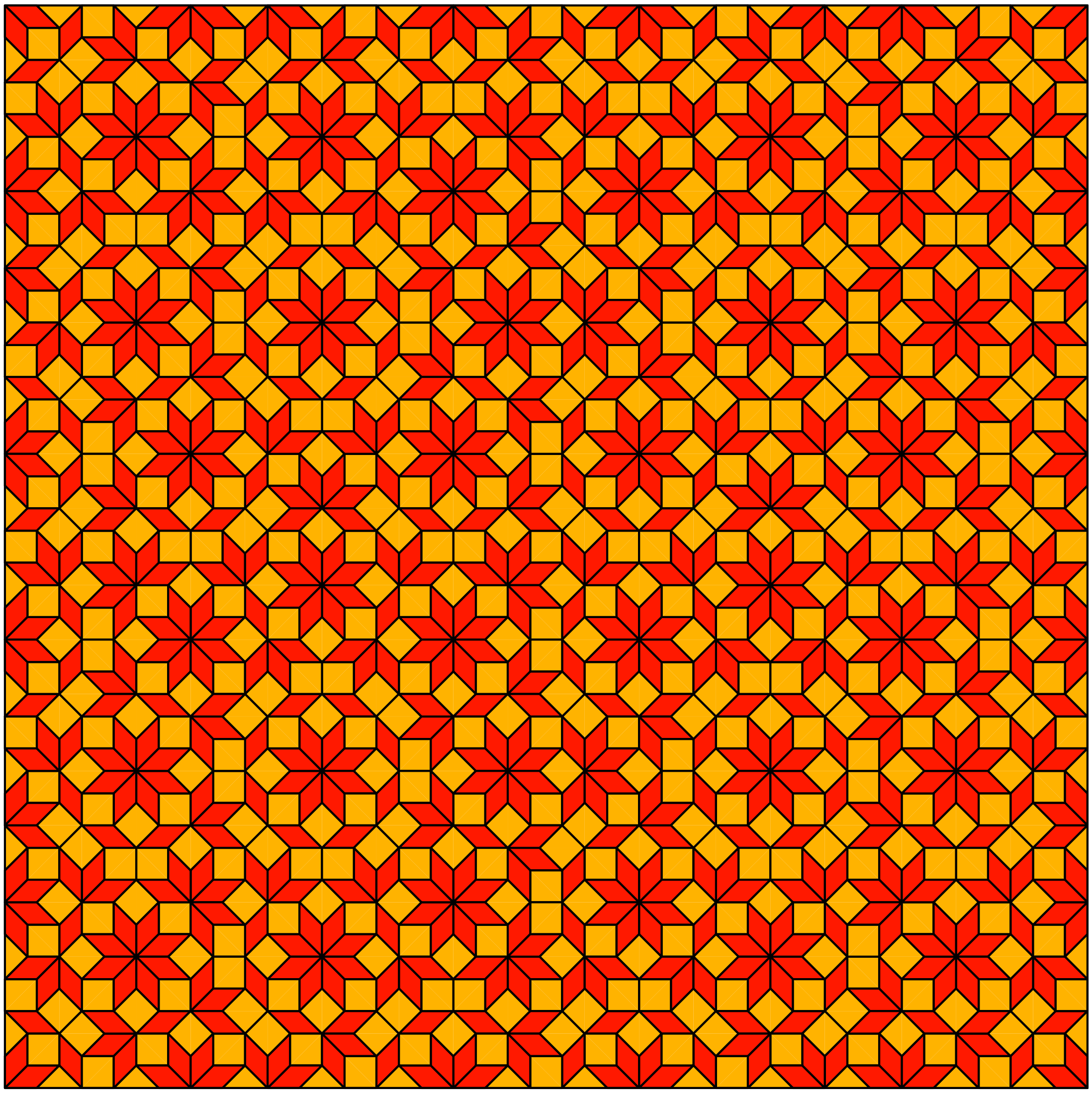
QUASIPERIODIC STRUCTURES :



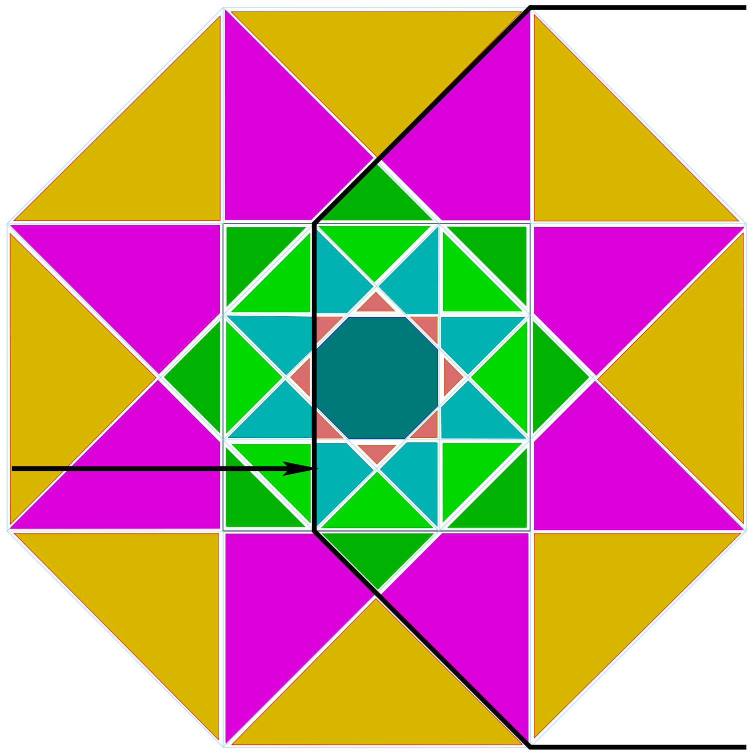
- The Penrose Tiling -

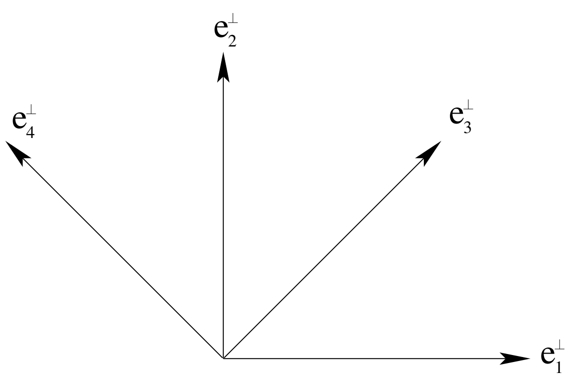


– The cut–and–project construction –



- The Octagonal Tiling -





- The Window of the Octagonal Tiling -

ELECTRONIC PROPERTIES :

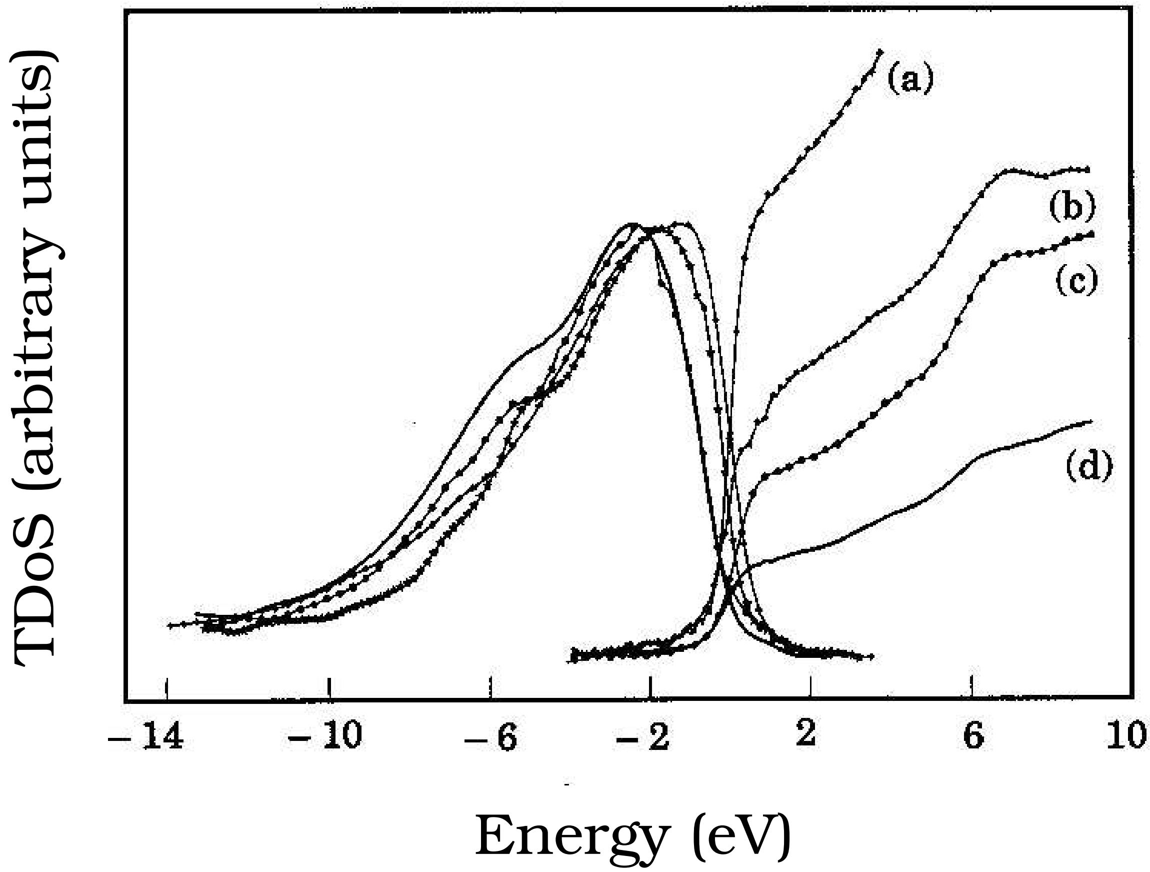
Measure or Computation of the Density of States (DOS) near the Fermi level.

Experimental Methods

1. Soft X-ray Emission Spectroscopy (SXES)
2. Soft X-ray Photoabsorption Spectroscopy (SXAS)
3. Electron Photoemission Spectroscopy (XPS)
4. Electron Energy Loss Spectroscopy (EELS)
5. Tunneling Effect Junction.

Numerical Methods

LMTO-ASA computations
(Linear Muffin-Tin Orbital Method in the Atomic Sphere Approximation)



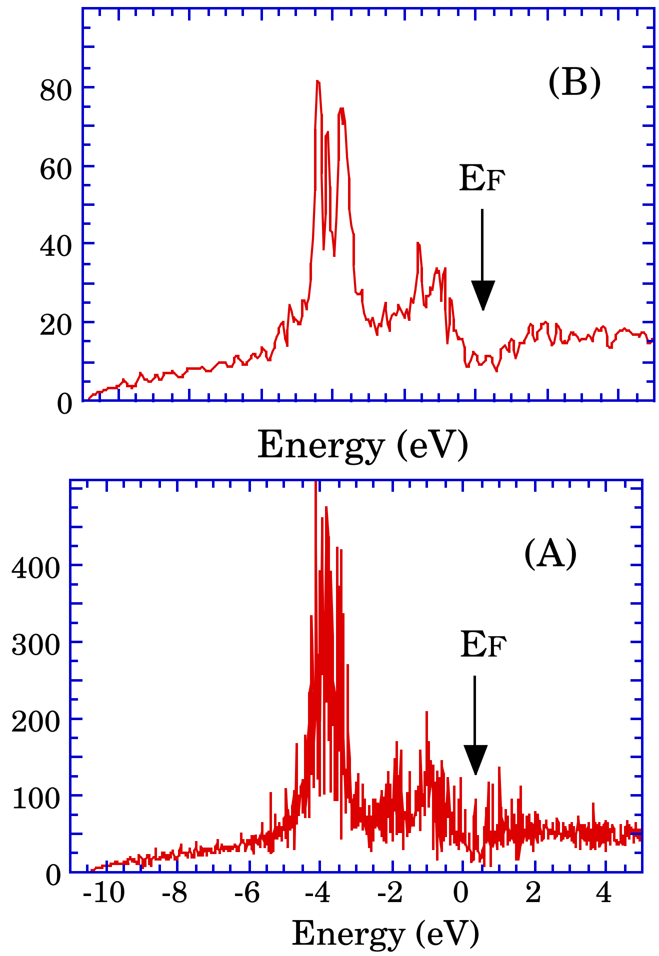
Partial DOS measured by SXES or SXAS:

(a) pure Al,

(b) $\omega - Al_7Cu_2Fe$,

(c) rhombohedral approximant $Al_{62.5}Cu_{26.5}Fe_{11}$,

(d) icosahedral phase $Al_{62}Cu_{25.5}Fe_{12.5}$ (*E. Belin et al. (1992)*)

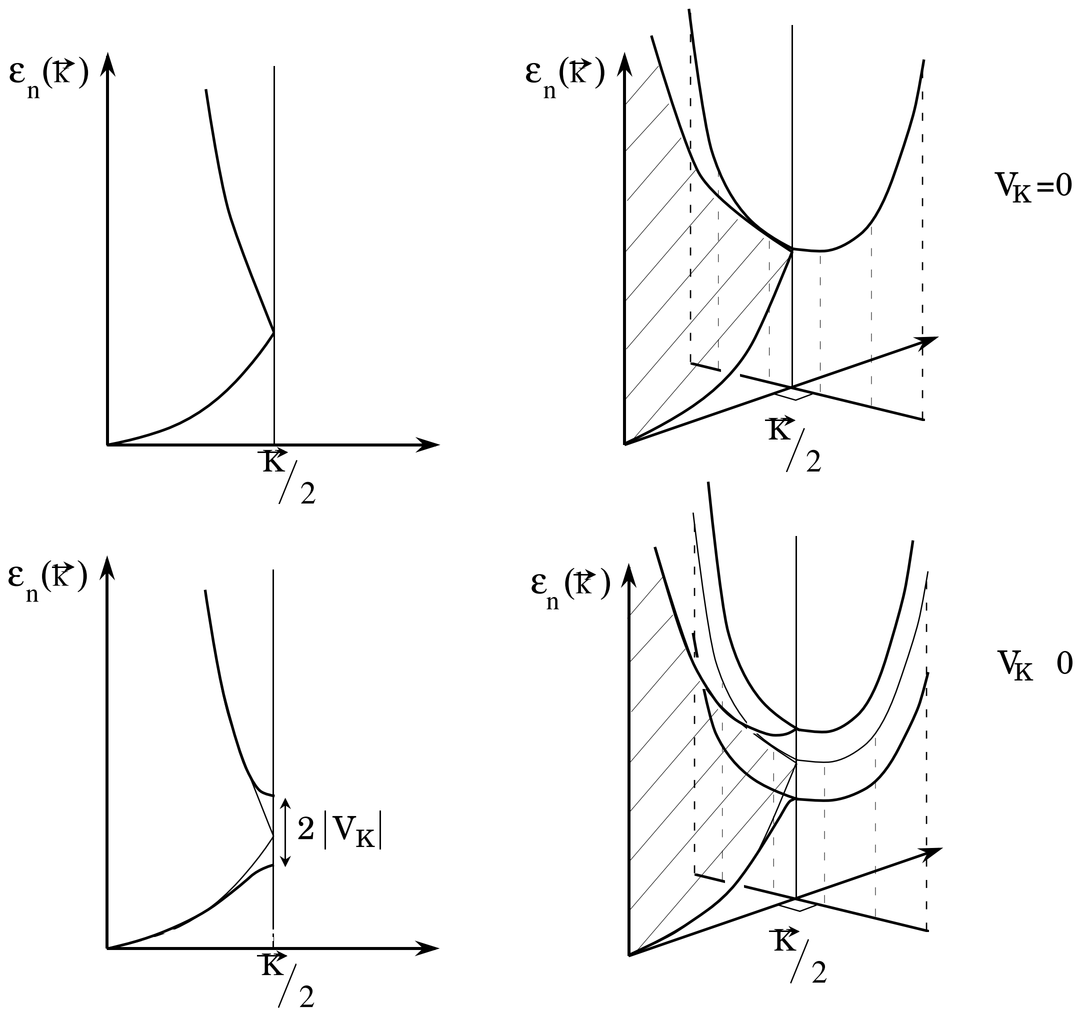


Total DOS of alloys with close composition:

(A) approximant 1/1 $i - Al_{62.5}Cu_{25}Fe_{12.5}$ 128 atoms/unit cell,

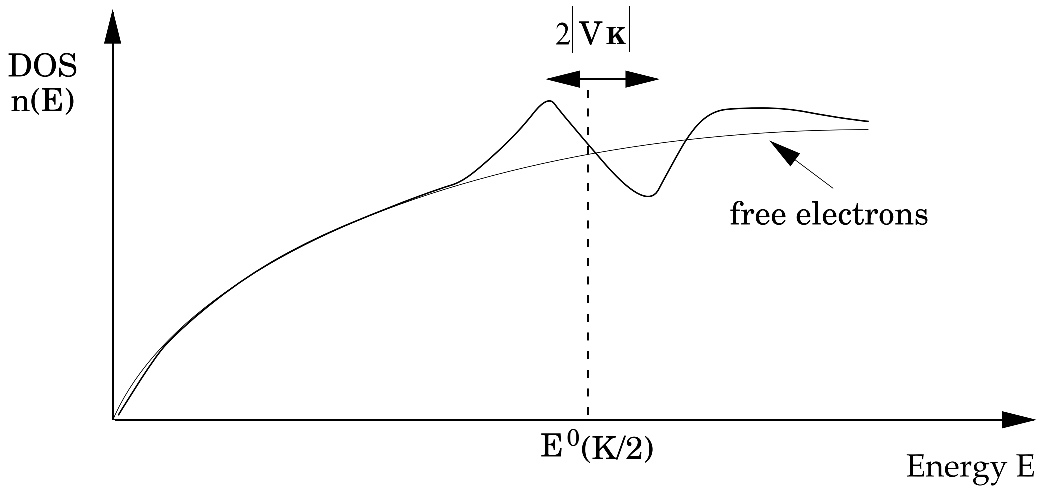
(B) non-approximant $\omega - Al_7Cu_2Fe$, 40 atoms/unit cell.

(*Roche et al. (1997)*)



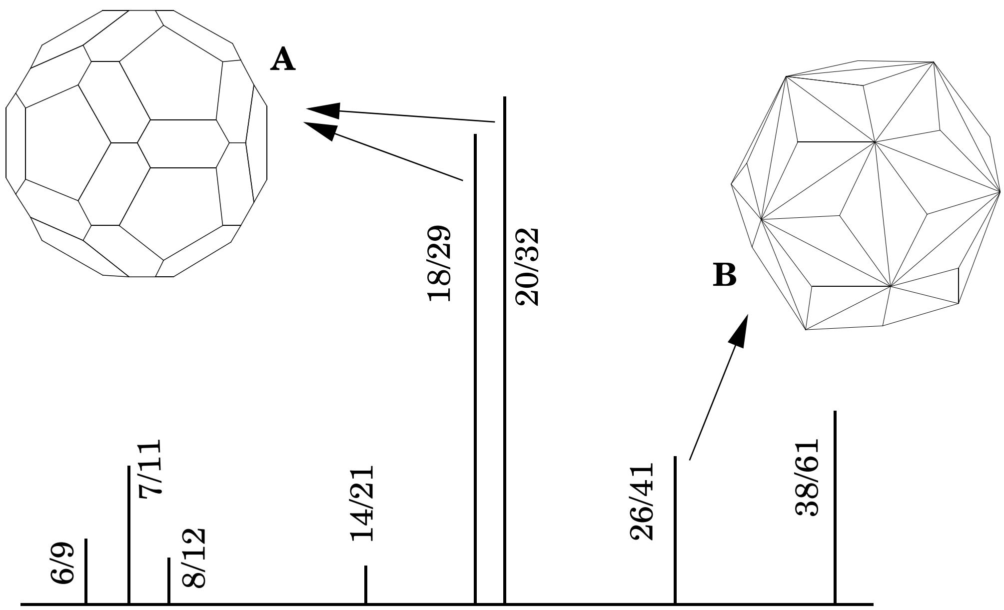
Effect of Bragg diffraction on electronic bands

(*S. Roche et al. (1997)*)



Representation of a Pseudo-gap

(*S. Roche et al. (1997)*)



Examples of pseudo-Brillouin-zones of the icosahedral phase.

A: 42 (30+12) facets (main pseudo-zone for $AlCuFe, ALPdMn$;
B: 60 facets (main pseudo-zone for $AlCuLi$).
The arrows are issued from the peaks which together with all equivalent peaks (by the icosahedral symmetry) define the facets of the pseudo-zone.
(*S. Roche et al. (1997)*)

Similarity with Hume-Rothery metals

SPECTRAL PROPERTIES :

Density of States (DoS) :

If H = 1-particle Hamiltonian

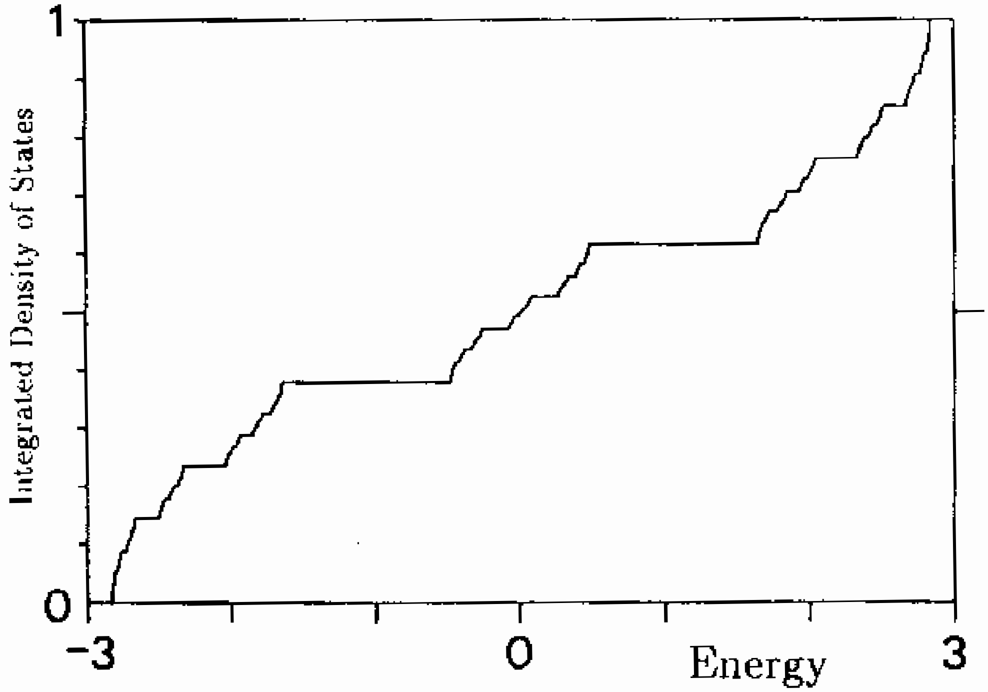
- Then

$$\mathcal{N}(E) = \lim_{\Lambda \uparrow \mathbf{R}^d} \frac{1}{|\Lambda|} \# \{\text{eigenvalues of } H|_\Lambda \leq E\}$$

is called the **Integrated Density of States** or **IDoS**.

- $\mathcal{N}$ is non negative, non decreasing and constant on spectral gaps. $\mathcal{N}(E) = 0$ for $E < \inf(SpH)$.
For $E \to \infty$ then $\mathcal{N}(E) \sim \mathcal{N}_0(E)$
where $\mathcal{N}_0$ is the free particle IDoS.

- $d\mathcal{N}/dE = n_{\text{DOS}}$ defines a measure (according to Stieljes) called the **Density of States** or **DOS**.



IDoS for Fibonacci's chain.

(*S. Roche et al. (1997)*)

Local Density of states (LDoS) :

If $|\psi>$ is an initial state :

$$<\psi|(H-E)^{-1}|\psi> = \int dE' \; \frac{n_{\text{LDOS}}(E')}{E'-E}$$

g is called the **Local Density of States** or **LDoS**

Spectral Exponents :

Spectral Exponents are defined by

$$\int_{E-\varepsilon}^{E+\varepsilon} dE' \, n(E') \quad \overset{\varepsilon\downarrow 0}{\sim} \quad \varepsilon^{\alpha(E)}$$

One associates $\alpha_{\text{DOS}}(E)$ and $\alpha_{\text{LDOS}}(E)$ to the DoS and LDoS.

Lebesgue's Theorem :

Every "measure" can be decomposed as a sum of
(i) an *absolutely continuous* measure ($\alpha(E) = 1$),
(ii) a *pure point* one (sum of Dirac peaks) and
(iii) a *singular continuous* one ($0 < \alpha(E) < 1$)

Some Results :

- **Rigorous**
  For quasiperiodic chains (QC $1D$):
  both the LDoS and DoS are singular continuous,
  the spectrum is a Cantor set of zero Lebesgue measure.
  The exponent is model dependent.

- **Exacts**
  For $D \geq 2$, the Labyrinth model (*Sire et al.*):
  there is a transition between a Cantor spectrum
  of zero Lebesgue measure and
  a gapless continuous spectrum,
  as the hopping parameters increases.

- **Numerical**
  Tight-binding models behave like the labyrinth one
  But there is level repulsion (Quantum Chaos).

Interactions Effects :

Coulomb's interaction between electrons in a disordered system is responsible for a pseudo-gap at Fermi level :

- In the strong localized regime (Anderson insulator) :

$$n_{\text{DOS}}(E) \;\sim\; |E - E_F|^{D-1} \quad \big(\textit{Efros \& Schklovsky}\big)$$

- In the weak localisation regime (Anderson metals) :

$$n_{\text{DOS}}(E) \;\sim\; \sqrt{|E - E_F|} \quad \big(\textit{Altshuler \& Aronov}\big)$$

TRANSPORT PROPERTIES :

1. Al, Fe, Cu, Pd are good metals :
   why is the conductivity of QC's so low ?
   Why is it decreasing with temperature ?
2. At high enough temperature

$$\sigma \propto \mathbf{T}^{\gamma} \qquad \mathbf{1} < \gamma < \mathbf{1.5}$$

   this is a new mechanism !
3. At low temperature for $\mathbf{Al_{70.5}Pd_{22}Mn_{7.5}}$,

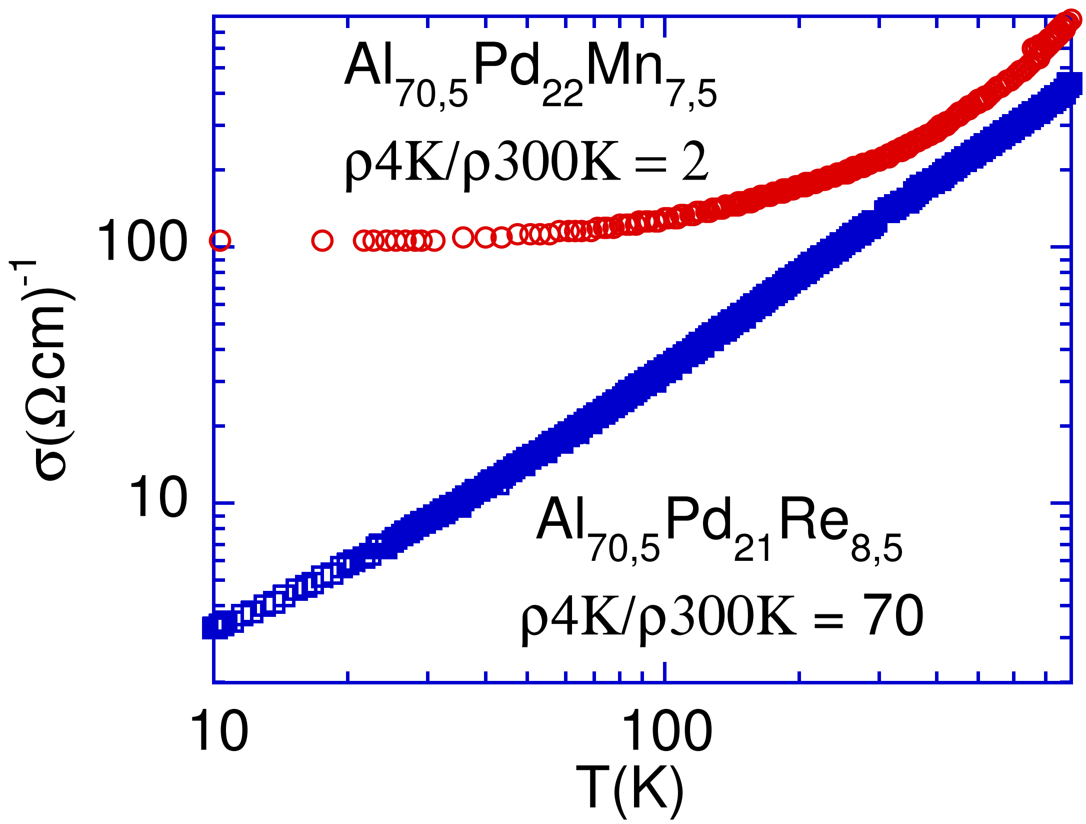
$$\sigma \approx \sigma(\mathbf{0}) > \mathbf{0}$$

4. At low temperature for $\mathbf{Al_{70.5}Pd_{21}Re_{8.5}}$,

$$\sigma \propto \mathbf{e}^{-(\mathbf{T_0}/\mathbf{T})^{\mathbf{1/4}}}$$

C. R. Wang et al. (1997); C. Berger et al. (1998)

Disorder seems to dominate at low temperature.



Comparison between conductivities of the two QC's

ANOMALOUS TRANSPORT :

J. Bellissard & H. Schulz-Baldes, Rev. Math. Phys., **10***, 1-46 (1998).*

Transport Exponents

The diffusion exponents $\sigma_{\text{diff}}(E)$ are defined by

$$\overline{< \psi_E|(\vec{X}(t) - \vec{X})^2 > |\psi_E >}^{\,disorder} \quad \overset{t\uparrow\infty}{\sim} \quad t^{2\beta(E)} \ ,$$

where ψ_E is a typical eigenvector with energy E.

Guarneri's Inequality

$$\alpha^{+}_{\text{LDOS}}(\mathbf{E}) \ \leq \ \mathbf{D} \cdot \beta(\mathbf{E}) \ ,$$

where D is the space dimension.

Anomalous Drude formula

At low temperature, the conductivity σ behaves like :

$$\sigma \ \sim \ \tau^{(\mathbf{2}\beta_{\mathbf{F}} - \mathbf{1})}$$

Here, τ is the *inelastic relaxation time*,
E_F is the Fermi level and $\beta_F = \beta(E_F)$.

Interpretation

The inelastic relaxation time τ diverges at low temperature.

- $\beta(E) = 1$ ballistic motion
  ex. : *free particles in a perfect crystal.*
  $\sigma \ \sim \tau$ (Drude's law).

- $\beta(E) = 0$ absence of diffusion
  ex. : *localisation.*
  $\sigma \ \sim 1/\tau$ (anti-Drude).

- $\beta(E) = 1/2$ quantum diffusion
  ex. : *weak localisation.*
  $\sigma \ \sim 1$ (residual conductivity).

- $0 < \beta(E) < 1/2$ subdiffusion
  ex. : *most quasicrystals 3D at Fermi level.*
  $\sigma \ \sim 1/\tau^{(1-2\beta)} \downarrow 0$ (insulating behaviour).

- $1/2 < \beta(E) < 0$ overdiffusion
  ex. : *quasiperiodic 2D lattices.*
  $\sigma \ \sim \tau^{(2\beta-1)} \uparrow \infty$ (metallic behaviour).

Conductivity in QC's

S. Roche & Fujiwara, Phys. Rev., **B58**, *11338-11396, (1998).*

1. LMTO *ab initio* computations for $i-AlCuCo$ give $\beta_F = 0,375$
2. If only electron-phonon collisions are considered, *Bloch's law* leads to : $\tau \overset{T\uparrow\infty}{\sim} T^{-5}$.
3. Hence

$$\sigma(\mathbf{T}) \overset{\mathbf{T}\uparrow\infty}{\sim} \mathbf{T^{1.25}}$$

   compatible with experimental results !

4. At low temperature ($T \leq T_{\rm dis}$), if disorder dominates then :
   (a) for $AlPdMn$, $T_{\rm dis} \approx 300K$. There should then be a *high density of defects or impurities*, implying *weak localisation* and a *residual conductivity*.
   (b) fr $AlPdRe$, $T_{\rm dis} \approx 10K$. There should be a *low density of defects or impurities* implying *strong localisation* and *une Mott's variable range hopping conductivity*.

Variable range hopping conductivity

(*Mott (1968)*)

In the strong localized regime and with a small DoS, the low temperature conductivity behaves like :

$$\sigma \propto \mathbf{e}^{-(\mathbf{T_0}/\mathbf{T})^{\mathbf{1}/\mathbf{D}+\mathbf{1}}} \qquad \textit{Mott's law}$$

Competing mechanism: quantum chaos

JB speculations

1. Numerical simulations performed for the octagonal lattice exhibit level repulsion and Wigner-Dyson's distribution (*Zhong et al. 1998*).

2. For a sample of size L :
   Mean level spacing $\Delta \sim L^{-D}$.
   Thus Heisenberg time $\tau_H \sim L^D$.

3. Thouless time for anomalous diffusion $L \sim t_{Th}^{\beta}$.
   Heisenberg's length $L_H \sim L^{D\beta}$.

4. Thus :

   (a) if $\beta > 1/D$ level repulsion dominates implying
   - quantum diffusion $\langle x^2 \rangle \sim t$
   - *residual conductivity*
   - absolutely continuous spectrum at Fermi level;

   (b) if $\beta < 1/D$ level repulsion can be ignored and
   - anomalous diffusion dominates $\langle x^2 \rangle \sim t^{2\beta}$
   - insulating behaviour with scaling law
   - singular continuous spectrum near Fermi level.

CONCLUSIONS

1. Forbiden symetries imply quasiperiodic lattices of atomic positions.
2. The Fermi sea stabilizes the structure thanks to the Hume-Rothery mechanism.
   Thus appearance of a *pseudo-gap* at Fermi level.
3. Coulomb's interaction create a vanishing of the DOS at Fermi level with $n_{\text{DOS}} \sim \sqrt{|E - E_F|}$.
4. This pseudo-gap is partially filled probably due to impurities or defects.
5. At large enough temperature, the quasiperiodic structure leads to anomalous transport with $\beta < 1/2$. Hence an *insulating behaviour*.
6. At low temperature two mechanisms compete:
   - the effect of disorder, like in semiconductors, may produce a metallic or insulating behaviour, with either a residual conductivity or
   a Mott variable range hopping.
   - the effect of level repulsion may produce a residual conductivity if $\beta > 1/D$ whereas anomalous transport dominates if $\beta < 1/D$.