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:
Quasicrystalline alloys:

Metastable QC’s: \textbf{AlMn}  

\textbf{AlMnSi} \\
\textbf{AlMgT} \ (T = Ag, Cu, Zn)

Defective stable QC’s: \textbf{AlLiCu}  
(Sainfort-Dubost, (1986))

\textbf{GaMgZn}  
(Holzen et al., (1989))

High quality QC’s: \textbf{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: \textbf{AlPdMn} \\
\textbf{AlPdRe}
- Typical TEM diffraction pattern -
  - with 5-fold symmetry -
Resistivity (µΩcm)

\[ T \text{ (K)} \]

- Semiconductors
- Doped semiconductors
- Stable perfect quasicrystals \((\text{AlPdRe})\)
- High quality quasicrystals \((\text{AlPdMn, AlCuFe, AlCuRu})\)
- Defective stable quasicrystals \((\text{AlCuLi, GaMgZn})\)
- Metastable quasicrystals \((\text{AlMn, AlMgZn, ...})\)
- Amorphous metals \((\text{CuZr, ...})\)
- Metallic crystals \((\text{Al, ...})\)

**Typical values of the resistivity**

\((\text{Taken from C. Berger in ref. [2]})\)
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

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

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 $E < \inf (\text{Sp } H)$. 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

$$\int_{E-\varepsilon}^{E+\varepsilon} dE' \ n(E') \ \varepsilon \uparrow 0 \ \varepsilon^{\alpha(E)}$$

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):

  \[ n_{\text{DOS}}(E) \sim |E - E_F|^{D-1} \quad (\text{Efros} & \text{ Schklovsky}) \]

- In the weak localisation regime (Anderson metals):

  \[ n_{\text{DOS}}(E) \sim \sqrt{|E - E_F|} \quad (\text{Altshuler} & \text{ Aronov}) \]
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

   \[ \sigma \propto T^\gamma \quad 1 < \gamma < 1.5 \]

   this is a new mechanism!

3. At low temperature for \( \text{Al}_{70.5}\text{Pd}_{22}\text{Mn}_{7.5} \),

   \[ \sigma \approx \sigma(0) > 0 \]

4. At low temperature for \( \text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5} \),

   \[ \sigma \propto e^{-\left(\frac{T_0}{T}\right)^{1/4}} \]

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

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{conductivity_plot.png}
\caption{Comparison of conductivities for two quasicrystals: Al\textsubscript{70.5}Pd\textsubscript{22}Mn\textsubscript{7.5} and Al\textsubscript{70.5}Pd\textsubscript{21}Re\textsubscript{8.5}.}
\end{figure}
ANOMALOUS TRANSPORT:


Transport Exponents

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

$$< \psi_E | (\vec{X}(t) - \vec{X})^2 | \psi_E > \tuparrow \infty \sim t^{2\beta(E)},$$

where $\psi_E$ is a typical eigenvector with energy $E$.

Guarnieri’s Inequality

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

where $D$ is the space dimension.

Anomalous Drude formula

At low temperature, the conductivity $\sigma$ behaves like:

$$\sigma \sim \tau^{(2\beta_F - 1)}$$

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

The inelastic relaxation time $\tau$ 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

1. LMTO \textit{ab initio} computations for \textit{i-AlCuCo} give $\beta_F = 0.375$

2. If only electron-phonon collisions are considered, \textit{Bloch’s law} leads to: $\tau \sim T^{-5}$.

3. Hence

$$\sigma(T) \xrightarrow{T \uparrow \infty} T^{1.25}$$

compative with experimental results!

4. At low temperature ($T \leq T_{\text{dis}}$), if disorder dominates then:

(a) for \textit{AlPdMn}, $T_{\text{dis}} \approx 300K$. There should then be a \textit{high density of defects or impurities}, implying \textit{weak localisation} and a \textit{residual conductivity}.

(b) for \textit{AlPdRe}, $T_{\text{dis}} \approx 10K$. There should be a \textit{low density of defects or impurities} implying \textit{strong localisation} and \textit{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:

\[ \sigma \propto e^{-\left(\frac{T_0}{T}\right)^{1/D+1}} \quad \text{Mott's law} \]
Competing mechanism: quantum chaos

JB speculations

1. Numerical simulations performed for the octagonal lattice exhibit level repulsion and Wigner-Dyson’s distribution \( (\text{Zhong et al. 1998}) \).

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. Forbidden symmetries 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 $\beta < 1/D$. 