TRANSPORT THEORY REVISITED

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OUTLINE:

1. Transport in Quasicrystals (QC)
2. Anomalous Transport
3. Quantum Jumps Models
4. Prospects and Problems

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TRANSPORT in QUASICRYSTALS (QC)

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

[2] S. Roche, D. Mayou and G. Trambly de Laissardière, *Electronic transport properties of quasicrystals*, 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**

GaMgZn

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

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

AlPdRe

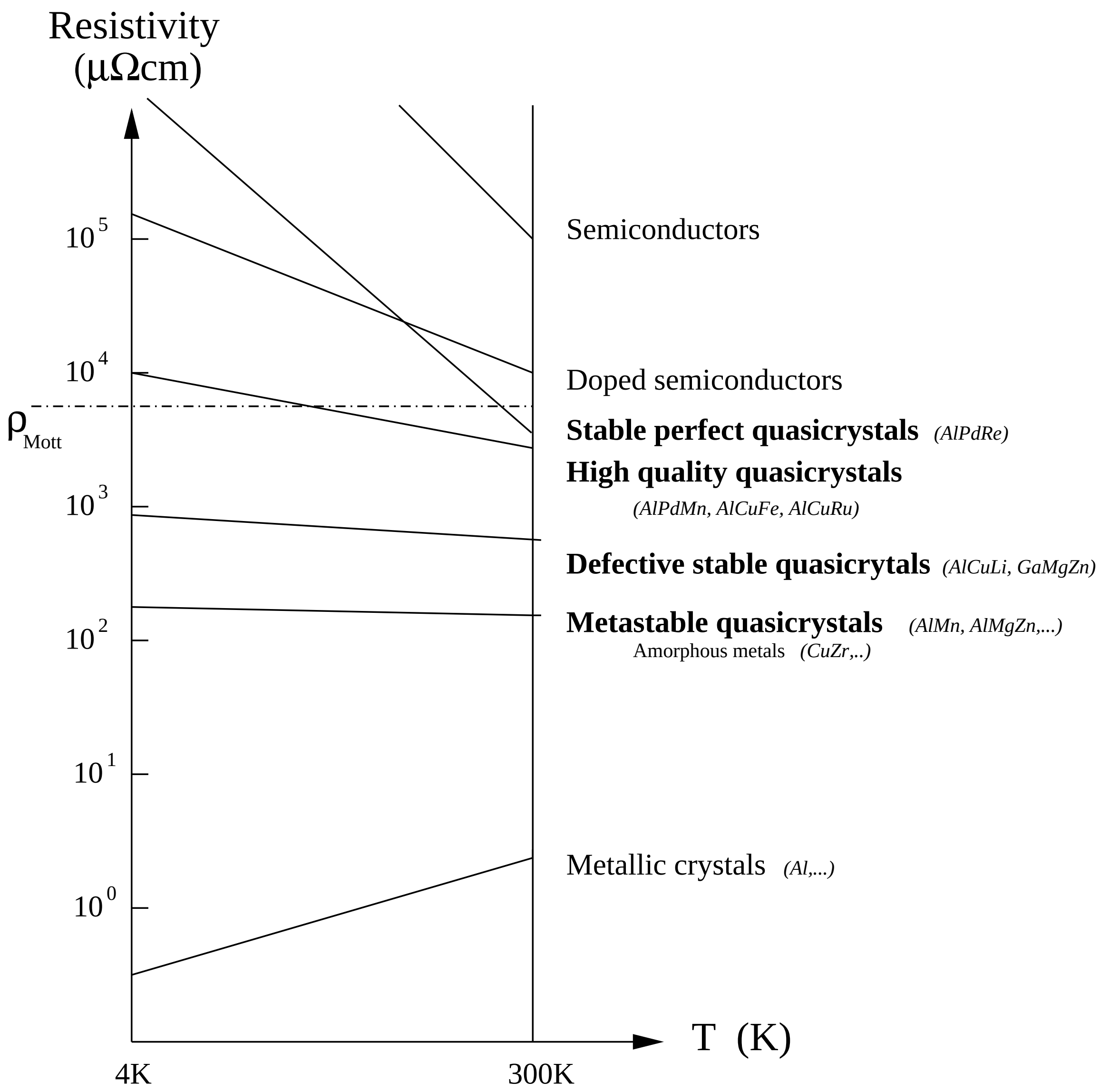
Known Mechanisms of Transport

1. For metals, $\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{T}^{-\mathbf{2}}$,
   $\sigma(\mathbf{T})$ increases as temperature decreases
   (*Fermi liquid theory*).

2. For thermally activated process
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e}^{-\mathbf{\Delta}/\mathbf{T}} \ \left(\textit{If a gap holds at Fermi level}\right).$$

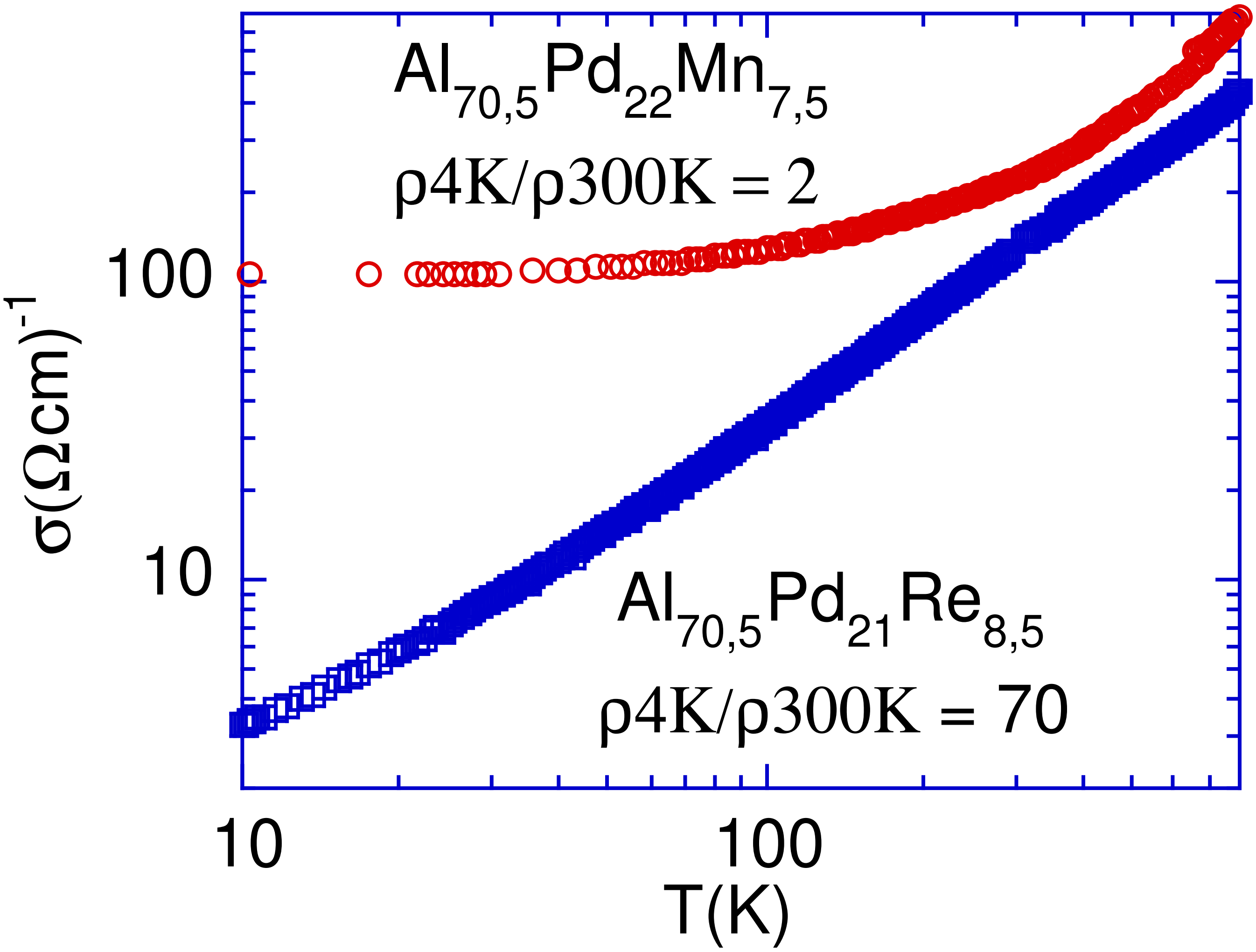
3. For weakly disordered systems:
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\to} \sigma(\mathbf{0}) > \mathbf{0} \quad \left(\textit{residual conductivity}\right).$$

4. For strongly disordered systems in $3D$:
   $$\sigma(\mathbf{T}) \overset{T\downarrow 0}{\sim} \mathbf{e}^{-(\mathbf{T_0}/\mathbf{T})^{\mathbf{1/4}}} \quad \left(\textit{variable range hopping}\right).$$



Typical values of the resistivity

(Taken from *C. Berger* in ref. [1])



Conductivity of two QC's

For QC's

1. Al, Fe, Cu, Pd are very good metals : why is the conductivity of quasicrystalline alloys so low ?

   Why is it decreasing ?

2. At high enough temperature

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

   There is a new mechanism here!

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 $\mathbf{Al_{70.5}Pd_{21}Re_{8.5}}$,

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

   C. Berger et al. (1998)

Some disorder takes place in both alloys and dominates at very low temperature.

ANOMALOUS TRANSPORT

The Kubo Formula

The conductivity at frequency ω

$$\sigma_{i,j}(\omega) \;=\; \frac{q}{\hbar}\mathcal{T}\left\{\partial_i(\rho_{T,\,\mu})\,(\mathcal{C} - \mathcal{L}_H - \imath\,\omega)^{-1}\,(J_j)\right\}$$

1. $\mathcal{T}$ is the **trace per unit volume**.
2. q is the charge of the carriers
3. $\rho_{T,\,\mu} = (\mathbf{1} + \exp\{\beta(H-\mu)\})^{-1}$ is the Fermi-Dirac state at inverse temperature $\beta = 1/k_B T$ and chemical potential μ.
4. $\mathcal{C}$ is an operator containing dissipation. For our purpose, we will take it as $C = 1/\tau$ where τ is the *relaxation time*
5. $\mathcal{L}_H = \imath/\hbar[H, .]$ is the Liouville operator attached to the Hamiltonian H describing the charge carrier motion.
6. J_j is the j-th component of the current operator.

Interpretation

The conductivity can be seen as the **Green function** of the Liouville operator near the spectrum.

- Hilbert space is made of operators with inner product $< A|B >= \mathcal{T}\{A^*B\}$,

- $K = \imath\mathcal{L}_H$ is selfadjoint,

- thus the conductivity can be written as

$$\sigma =< A|\frac{-\imath}{K - (\omega + \frac{\imath}{\tau})} B >$$

  for suitable A and B.

- As the temperature $T \downarrow 0$ then $\tau \uparrow \infty$. Thus we get closer and closer to the real axis.

Transport Exponents

- Set $\vec{X}(t) = e^{\imath tH}\vec{X}e^{-\imath tH}$, $\vec{X}$= position operator.

- The mean square displacement for energies in $\Delta = [E - \epsilon, E + \epsilon]$ is

$$L^2(t) = \overline{< x|\Pi_\Delta \left(X(t) - X(0)\right)^2 \Pi_\Delta|x >} \ ,$$

  where Π_Δ projects on energies in Δ.

- The overline means **space average**.

- Then defines the diffusion exponent by

$$L(t) \overset{t\uparrow\infty}{\sim} t^{\sigma_{\text{diff}}(\Delta)}$$

Quantum Diffusion

- $\sigma_{\rm diff}(\Delta)) = 1$ ballistic motion
  ex. : *free motion in a perfect crystal.*

- $\sigma_{\rm diff}(\Delta)) = 0$ absence of diffusion
  ex. : *localization.*

- $\sigma_{\rm diff}(\Delta)) = 1/2$ quantum diffusion
  ex. : *weak localization.*

- $0 < \sigma_{\rm diff}(\Delta)) < 1/2$ subdiffusion
  ex. : *3D quasicrystals at Fermi level.*

- $1/2 < \sigma_{\rm diff}(\Delta)) < 0$ overdiffusion
  ex. : *2D quasilattices.*

Anomalous Drude Formula

[3] *Lectures on Quasicrystals*, F. Hippert, D. Gratias Eds., Ed. de Physique, Les Ulis, (1994); (a) D. Mayou pp. 417-462, (b) C. Sire pp. 505-533.

[4] J. Bellissard & H. Schulz-Baldes, in *Proceedings of the 5th International Conference on Quasicrystals*, C. Janot, R. Mosseri Eds., World Scientific, Singapore, (1995).

Theorem 1 *Assume that $\tau \uparrow \infty$ as the temperature $T \downarrow 0$ and let $\sigma_F = \lim_{\epsilon\downarrow 0} \sigma_{\rm diff}([\mu-\epsilon, \mu+\epsilon])$, where $\mu = \mu(T)$ is the chemical potential fixed by the charge carrier density n. Then the DC-conductivity (i.e. $\omega = 0$) satisfies*

$$\sigma_{i,i} \quad \stackrel{T\downarrow 0}{\sim} \quad \tau^{(2\sigma_F - 1)}$$

$\square$

Comments:

1. if $\sigma_F = 1$ (ballistic) then $\sigma_{i,i} \stackrel{T\downarrow 0}{\sim} \tau$ (Drude);
2. if $\sigma_F = 0$ (localization) then $\sigma_{i,i} \stackrel{T\downarrow 0}{\sim} 1/\tau$ (anti-Drude);
3. if $\sigma_F = 1/2$ (diffusion) then $\sigma_{i,i} \stackrel{T\downarrow 0}{\sim}$ *const.* (residual conductivity);
4. if $0 < \sigma_F < 1/2$ (subdiffusion) then $\sigma_{i,i} \stackrel{T\downarrow 0}{\sim} 1/\tau^{\alpha}$ (insulator) (**ex.:** quasicrystals !!);
5. if $1/2 < \sigma_F < 1$ (overdiffusion) then $\sigma_{i,i} \stackrel{T\downarrow 0}{\sim} \tau^{\alpha}$ (conductor).

Conductivity in QC's

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

1. *ab initio* calculations using LMTO for $i - AlCuCo$ and taking orbitals hybridization gives

$$\sigma_F = .375$$

2. If only collisions with phonons occur, Bloch's law implies

$$\tau \overset{T\downarrow 0}{\sim} T^{-5}$$

3. Thus we get

$$\sigma_{i,i}(T) \overset{T\downarrow 0}{\sim} T^{1.25}$$

compatible with experiments !

4. At low temperature ($T \leq T_{\mathrm{dis}}$), disorder dominates.

QUANTUM JUMP MODELS

[6] D. Spehner & J. Bellissard, *Kinetic-like Quantum Jump Model*,
in preparation (1999),

[7] J. Bellissard, A. van Elst, H. Schulz-Baldes, J. Math. Phys., **35**, 5373 (1994),

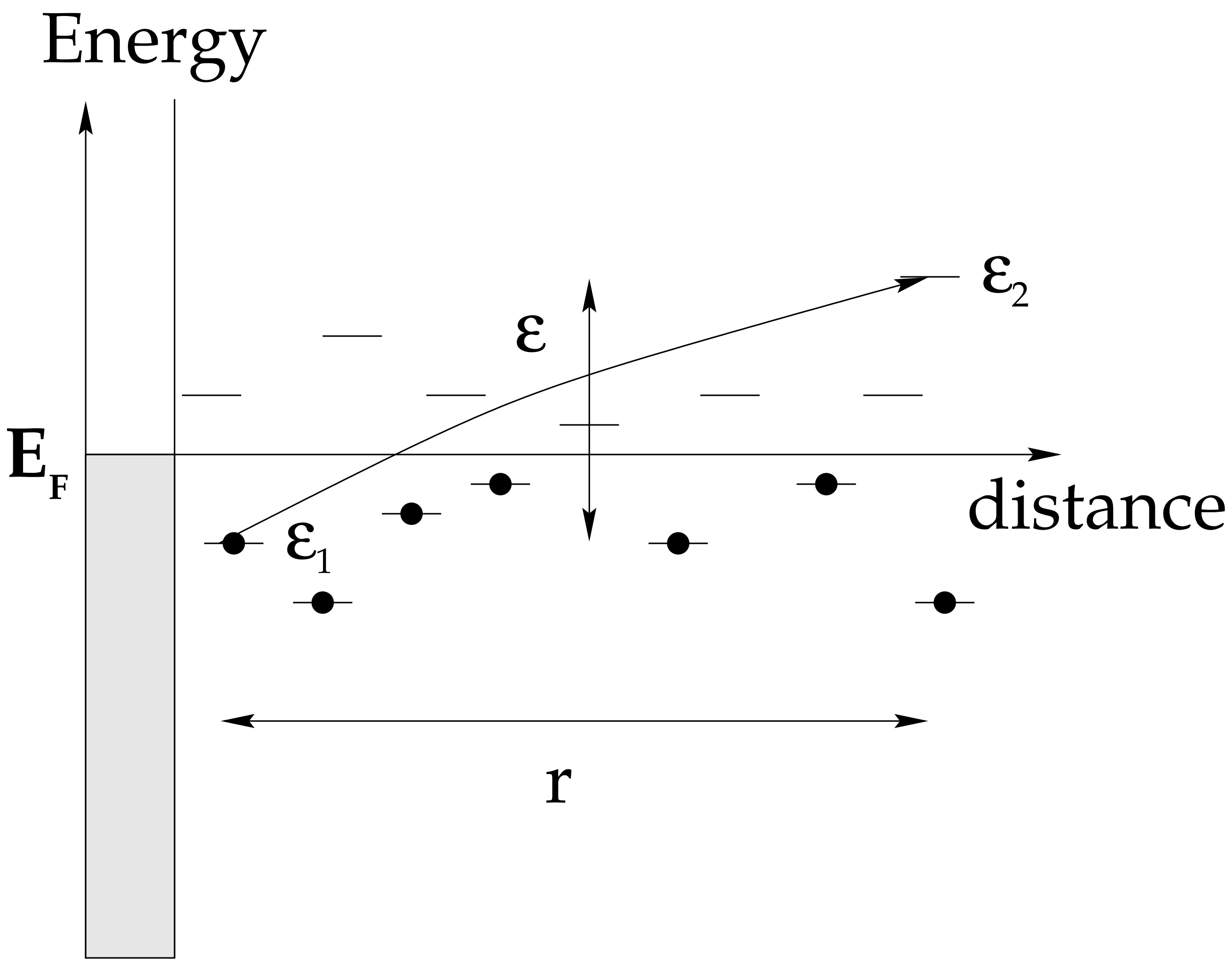
[8] H. Schulz-Baldes, J. Bellissard, J. Stat. Phys., **91**, 991-1026 (1998),

Mott's Variable Range Hopping :

[9] N. Mott, (1968),

see B. Shklovskii, A. L. Effros, *Electronic Properties of Doped Semiconductors*, (Springer-Verlag, Berlin, (1984).

- Strongly localized regime, dimension d,
- Low electronic DOS,
- Low temperature.



Mott's Variable Range Hopping

- Absorption-emission of a phonon of energy ε

$$\mathbf{Prob} \propto \mathbf{e}^{-\varepsilon/\mathbf{k_B T}}$$

- Tunnelling probability at distance $\mathbf{r}$

$$\mathbf{Prob} \propto \mathbf{e}^{-\mathbf{r}/\xi}$$

- Density of state at Fermi level n_F,

$$\varepsilon\, \mathbf{n_F}\, \mathbf{r^d} \approx \mathbf{1}$$

Optimizing, the conductivity satisfies

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

Optimal energy $\varepsilon_{\mathbf{opt}} \sim \mathbf{T}^{\mathbf{d}/(\mathbf{d}+\mathbf{1})} \gg \mathbf{T}$

Optimal distance $\mathbf{r_{opt}} \sim \mathbf{1}/\mathbf{T}^{\mathbf{1}/(\mathbf{d}+\mathbf{1})} \gg \xi$

Random Jump Model

In the strong localization regime

1. Particles live on an infinite (random) subset Λ_∞ in $\mathbf{Z}^d$
2. H_0 is diagonal self adjoint on Λ_∞.

   (H_0 contains the local parts of the energy: random potential, external electric field, etc.)
3. K is a bounded operator with short range matrix elements.

   (K includes both the hopping terms and the energy renormalization due to phonon-electrons interaction)
4. Jumps form site i to site j are described by an operator $W_{i\to j}$ such that $W_{i\to j} - \mathbf{1}$ has matrix elements localized around $\{i, j\}$.
5. Jumps $i \to j$ occur at poissonian independant random times $\{t^n_{i\to j}\}_{n\in\mathbf{Z}}$ with $\cdots t^n_{i\to j} < t^{n+1}_{i\to j} \cdots$.
6. The averaged relaxation times are given by $\Gamma^{-1}_{i\to j}$.

The Instantaneous Random Evolution

The instantaneous evolution is given by $\left(\text{here } \hbar = 1\right)$

$$\begin{aligned} U(t,t') = \; & e^{2\imath\pi(t-t_p)(H_0+K)} \\ & \qquad W_{i_p \to j_p}\, e^{2\imath\pi(t_p-t_{p-1})(H_0+K)} \\ & \cdots\cdots \\ & \qquad\quad W_{i_1 \to j_1}\, e^{2\imath\pi(t_1-t')(H_0+K)} \; . \end{aligned}$$

where

1. $t' < t_1 < \cdots < t_p < t$ are the times at which various kicks occur between t' and t,

2. $(i_r \to j_r)$ are the corresponding jumps.

Averaged Evolution

Averaging over the kick times gives rise to a *Bloch-type equation*

$$\frac{dA}{dt} = \mathcal{L}_H A + \mathcal{C}(A) \ ,$$

where, if $K = K_1 + \imath K_2$, with K_1, K_2 selfadjoints :

$$\mathcal{L}_H A = \imath [H_0 + K_1, A] \ ,$$

and

$$\begin{aligned} \mathcal{C}(A) \ &= \ -\{K_2, A\} + \\ & \quad \cdots \\ & \quad\quad \sum_{i,j \in \Lambda_\infty} \Gamma_{i \to j} \left(W_{i \to j}^{\dagger} A W_{i \to j} - A \right) \ , \end{aligned}$$

This $\mathcal{C}$ is the one occuring in Kubo's formula.

PROSPECTS and PROBLEMS

Mott hopping

The zero frequency conductivity is given by Kubo's formula

$$\sigma_{i,j} \;=\; \frac{q}{\hbar}\mathcal{T}\left\{\partial_i(\rho_{T,\,\mu})\,(\mathcal{C}-\mathcal{L}_H)^{-1}\,(J_j)\right\}$$

In the **strong localization regime**, $\sigma_{i,j} \to 0$ as $\mathcal{C} \to 0$. So

$$\sigma_{i,j} \;\approx\; \frac{q}{\hbar}\mathcal{T}\left\{\partial_i(\rho_{T,\,\mu})\,(\mathcal{L}_H)^{-1}\;\mathcal{C}\;(\mathcal{L}_H)^{-1}\;(J_j)\right\}$$

Problems: Simple models for jumps, based upon the *Fermi golden rule*, and non rigorous arguments show that this formula leads to the Mott estimate.

- Elaborate a realistic model for the $\Gamma_{i\to j}$'s based upon N-body perturbation theory.
- Prove a Mott-like estimate for the conductivity.

Transport Exponents

[10] I. Guarneri, Europhys. Lett., **10**, 95-100, (1989); **21**, 729-733, (1993).

[11] I. Guarneri & H. Schulz-Baldes, *Upper bounds for quantum dynamics governed by Jacobi matrices with self-similar spectra*, mp_arc 98-382, mp_arc 98-457, submitted (1998).

[12] J. Vidal, R. Mosseri & J. Bellissard, *Spectrum and diffusion for a class of tight-binding models on hypercubes*, to appear in J. Math. Phys. A, (1999).

[13] H. Schulz-Baldes & J. Bellissard, in preparation (1999).

1. *Guarneri's bound:* $\sigma_{\text{diff}}(\Delta)) \geq \alpha(\Delta)/d$, where d is the space dimension and $\alpha(\Delta)$ is the scaling exponent for the local density of states (LDOS) at energies in Δ. (see [10])
   (It indicates whether the spectrum is absolutely continuous ($\alpha = 1$), pure-point ($\alpha = 0$) or singular continuous ($0 < \alpha < 1$).)
2. $\exists$ a class of $1D$ models for which $0 < \sigma_{\text{diff}} < 1$ [11].
3. $\exists$ a class of models on an infinite hypercube ($d = \infty$) whith smooth LDOS and any $0 < \sigma_{\text{diff}} < 1$ [12].
4. $\exists$ direct sums of $1D$ models, in $d \geq 3$ with absolutely continuous spectrum and $\sigma_{\text{diff}} < .5$ [13].

Problems:

- Elaborate a predictive theory for transport exponents.

- Can one justify the numerical value $\sigma_{\mathrm{diff}} = .375$ found by Fujiwara & Roche ?

- Prove or disprove that in $d \geq 3$ at low coupling, the Schödinger Hamiltonian has absolutely continuous spectrum for any *generic* homogeneous potentials.

- Found the microscopic origin of the disorder occuring in QC's. Why is the difference between $AlPdMn$ and $AlPdRe$ so striking ?