Transport in topologically disordered condensed mater quantum models

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Contents

Hamiltonians:

Anderson: ordered lattice, disordered onsite potentials

$$\hat{H} = \sum_i \epsilon_i \, \hat{a}_i^\dagger \hat{a}_i + \sum_{i,j:\mathbf{NN}} \hat{a}_i^\dagger \hat{a}_i + \text{h.c.}$$

ϵ_i: random numbers, $\bar{\epsilon_i} = 0$, $\sigma^2 = \langle \epsilon^2 \rangle$

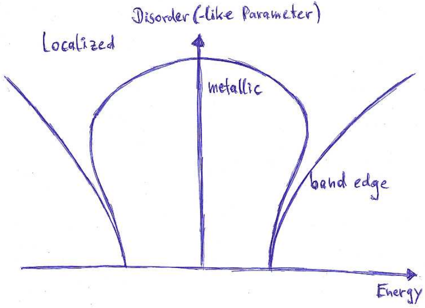
Lifshitz: disordered lattice, distance dependent hopping amplitudes

$$\hat{H} = \sum_{i \neq j} R(|\mathbf{x}_i - \mathbf{x}_j|) \hat{a}_i^\dagger \hat{a}_j + h.c.$$

hopping amplitudes (overlap integrals): we choose

$$R(|\mathbf{x}_i - \mathbf{x}_j|) = \exp\left(\frac{-4(\mathbf{x}_i - \mathbf{x}_j)^2}{\pi \tilde{l}^2} + i\Phi_{ij}\right)$$

$\tilde{l}$: mean overlap length, Φ_{ij}: (random) hopping phases



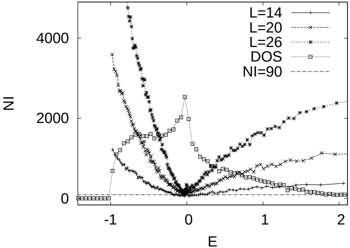
- localized $\hat{=}$ isolator
- metallic $\hat{=}$ delocalized

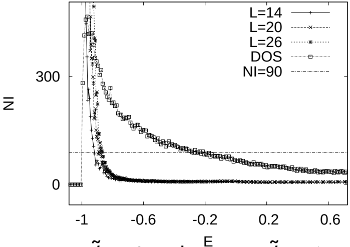
We intend to address disorder parameters at which almost all states are delocalized $\Rightarrow$ must find them!

Cheap check of localization

inverse participation ratio: $I(E) = \sum_i |\langle E|\hat{a}_i^+ \hat{a}_i|E\rangle|^4$, $\quad I \leq 90/N$: delocalized

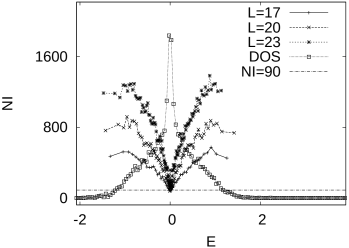
$\Phi = 0$

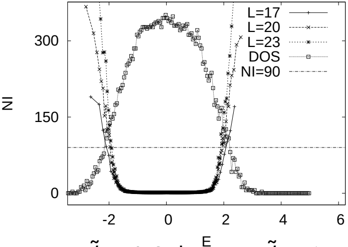




top: $\tilde{I} = 0.7$, bottom: $\tilde{I} = 1$

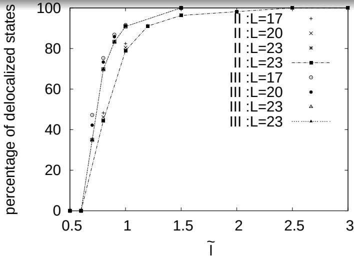
$\Phi \hat{=} \text{random}$





top: $\tilde{I} = 0.6$, bottom: $\tilde{I} = 1$

Current dynamics and transport types



obviously for $\tilde{l} > 1.3$ almost all states are delocalized

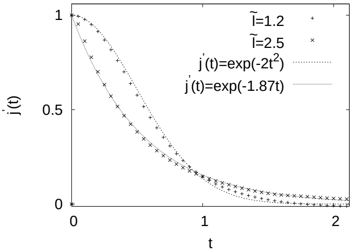
current operator $\hat{j} = \mathrm{i}[\hat{H}, \hat{x}]$

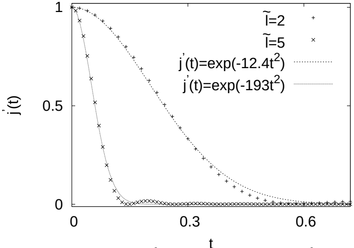
position operator $\hat{x} = \sum_{i=1}^{N} x_i \hat{a}_i^\dagger \hat{a}_i$

scaled current correlation function

$$j'(t) := \mathrm{Tr}\{\hat{J}(t)\hat{J}(0)\}/\mathrm{Tr}\{\hat{J}^2(0)\}$$

Drude model: $j'(t) = e^{-\gamma t}$





top: $\Phi = 0$, bottom: Φ random

$\Phi = 0$: transition from hopping- to Boltzmann or Drude transport

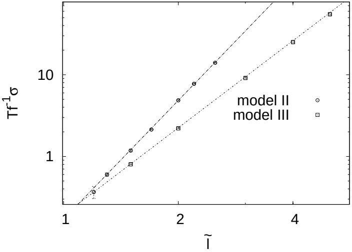
Conductivity and Einstein relation

conductivity from linear response (Kubo) at low fillings f and high temperature:

$$\sigma(t) = \frac{f}{T}\int_0^t \frac{1}{N}\mathrm{Tr}\{\hat{J}(t')\hat{J}(0)\}dt'$$

$$\sigma_{dc} = \sigma(t \to \infty)$$

scaled conductivities:



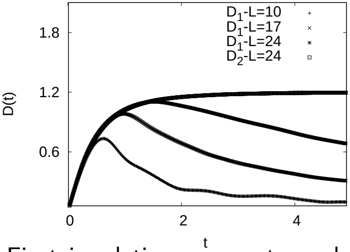
conductivities scale like power laws

Einstein relation: $D_2(t) = \frac{T}{\epsilon^2}\sigma(t)$

direct calculation of diffusion constant

$$D_1(t) = \frac{1}{2}\frac{d}{dt}\mathrm{Tr}\{\hat{x}^2(t)\rho(0)\}$$

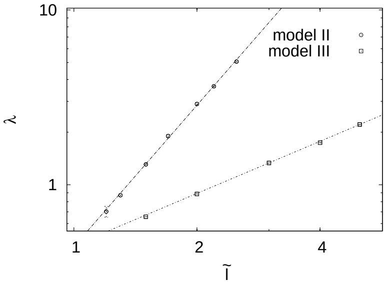
$$\rho(0) \propto e^{-\frac{\hat{x}^2}{4}},$$



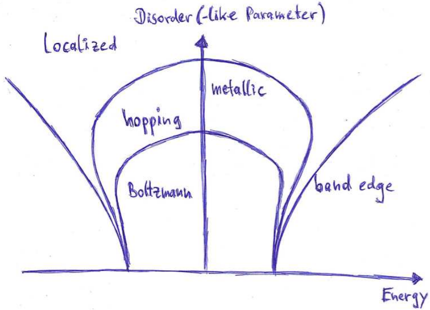
Einstein relation appears to apply

Note that the dynamics of the system is initially ballisitic.

mean free path λ: spreading of the initial distribution during the first, ballisitic period.



modified overall picture:



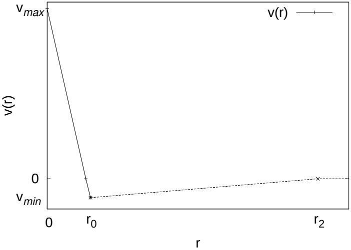
There indeed seems to be a (smooth) transition from hopping to Boltzmann transport, even in structurally completely disordered systems

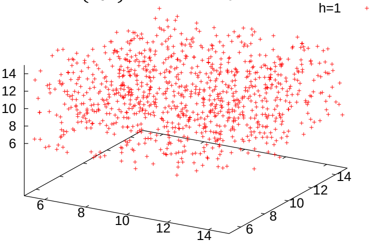
What about a bit of order?

Short range ordered systems

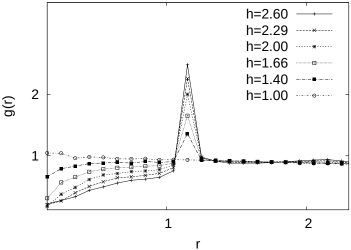
gradient descent method: $x_{\mathrm{i}}^{n+1} = x_{\mathrm{i}}^{n} - \lambda \left.\frac{\partial V}{\partial x_{\mathrm{i}}}\right|_{\{x_{\mathrm{j}}^{n}\}}$ $\qquad V := \sum_{ij} v(r_{ij})$

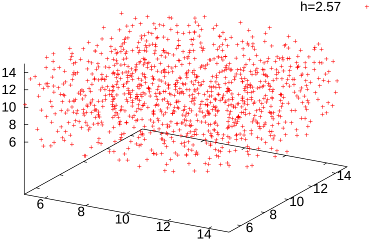
"interatomic potential"



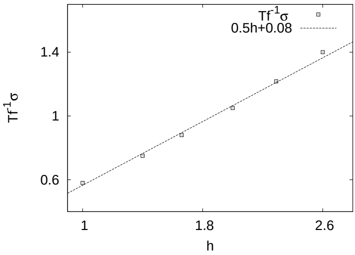


site-pair correlation function

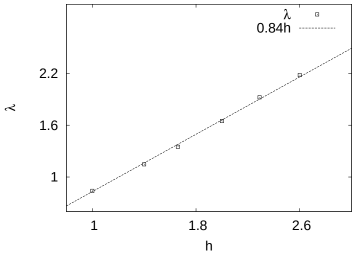




scaled conductivity



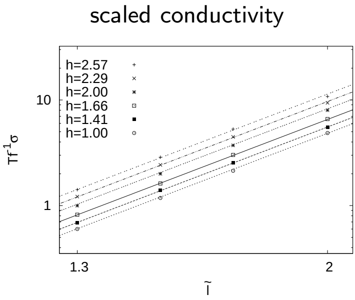
mean free path

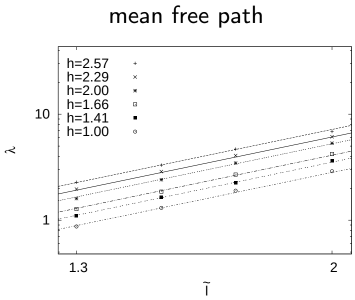


Both, conductivity and mean free path appear to depend linearly on the height of the first maximum of the site pair correlation function

This is at $\tilde{l} = 1.3$. What about other $\tilde{l}$?

Universality of transport behavior?





$$\sigma_{dc}(\tilde{l}, h) = \frac{f}{T} 0.37\,(0.5h + 0.08)\,\tilde{l}^{4.83}$$

$$\lambda(\tilde{l}, h) = 0.42h\tilde{l}^{2.68}$$

More about this:
A. Khodja, H. Niemeyer, J. Gemmer, Phys. Rev. E, **87**, 052133 (2013)

Thank you for your attention!