From hopping- to Boltzmann transport in topologically disordered tight-binding models

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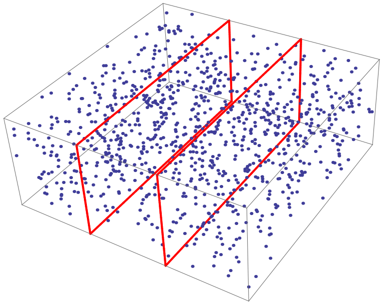
Model class and objectives



- 3-d one-particle tight binding model
- random, uniformly distributed “lattice” sites, unit density
- no interaction or external decohering mechanism

Hamiltonian:

$$\hat{H} = \sum_{x \neq y} R(x,y) \hat{a}_x^+ \hat{a}_y + h.c.$$

hopping amplitudes (integrals)

$$R(x,y) = \exp(-|x-y|/l - i\Phi(x,y))$$

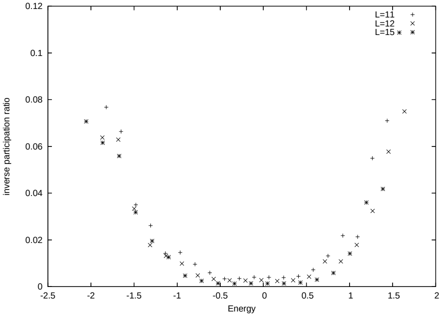
- May the quantum motion of a particle in such a system be described as diffusive, localized, ballistic, etc.?
- If so what are diffusion coefficients, mobilities, mean free paths, etc?

first model class: random phases, i.e., $\Phi(x,y)$ random, uniformly distributed real numbers

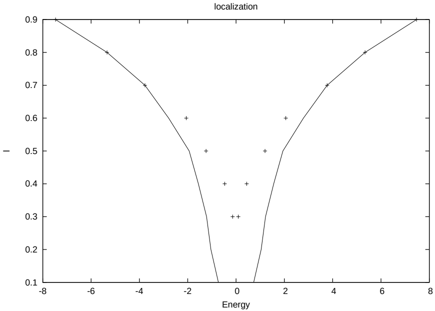
Cheap check of localization

inverse participation ratio: $P^{-1}(E) = \sum_x |\langle E|\hat{a}_x^+ \hat{a}_x|E\rangle|^4$

inverse part. ratio vs. energy



mobility and band edges vs. energy



Seems like above $l \approx 0.3$ there is at least a substantial portion of extended states. Bauer et al. claim an Anderson transition at $l \approx 0.257$ (J. Phys. C. **21** (1988))

Projection onto density waves

Partition "lattice" into "slabs". Define "slab occupation number" $\hat{n}(X)$

$$\hat{n}(X) = \sum_{x \text{from} X} \hat{a}_x^+ \hat{a}_x$$

Define density wave operator $\hat{m}_q$

$$\hat{m}_q = \sum_X \cos(qX)\hat{n}(X)$$

and exp. val. $\mathrm{Tr}\{\hat{m}_q \hat{\rho}(t)\} = m_q(t)$

diffusive implies: $m_q(t) \propto e^{-q^2 Dt}$

Determine $m_q(t)$ with a projection operator method, e.g., "TCL".

projector: $\mathcal{P}\hat{\rho} = \hat{1} + \sum_q \frac{m_q}{\mathrm{Tr}\{\hat{m}_q^2\}} \hat{m}_q$

"perturbative approach" $\hat{H} = \hat{H}_0 + \lambda \hat{V}$, $\hat{H}_0$: intra-slab hopping, $\hat{V}$: inter-slab hopping

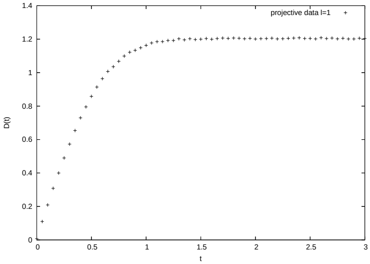
$$\Rightarrow \dot{m}_q = -\sum_{n,q'} \lambda^n K_{n,q,q'}(t) m_{q'} \quad (n : \text{even})$$

"statistical periodicity"

$$K_{2,q,q'}(t) \approx \delta_{qq'} q^2 D(t)$$

diffusive if: $K_{2,q,q}(t)/q^2 \approx \mathrm{D(const.)}$

$K_{2,q,q}(t)/q^2$ vs. time



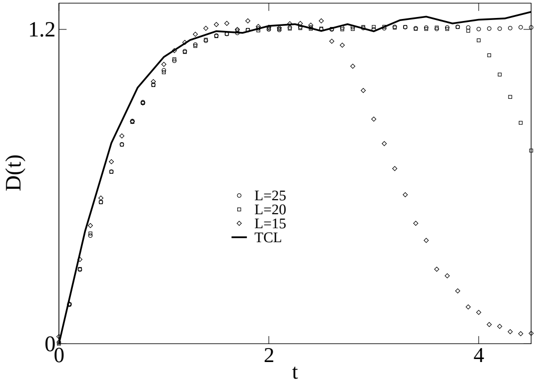
looks nice but....

...is that correct in the sense that the second order contains the relevant physics?
.......better countercheck by another method!

$n(x)$ diffusive implies constant increase of spatial variance $\frac{\partial}{\partial t}\delta_n^2(t) = 2D$

Choose an initial state which has the particle concentrated at the center of a cube. Calculate the increase of the variance by numerical diagonalization $\Rightarrow$ maximum cube size $\approx 25X25X25$.

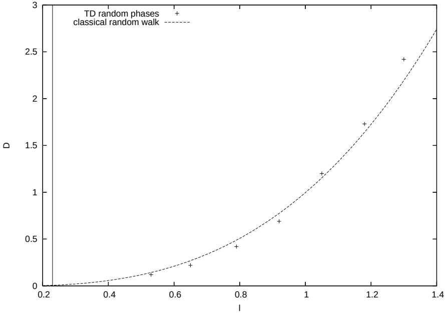
increase of variance vs. time



Everything seems to fit nicely $\Rightarrow$ use projective approach for longer hopping lenghts $\Rightarrow$

Projection onto density waves

diffusion coefficient vs. hopping lengths



quantum and classical

- reasonable suggestions for concrete diffusion coefficients may be obtained for the totally disordered model
- in a wide range the quantum result is in good accord with a classical random walk on the sites with rates given by "Fermis Golden Rule", i.e., $2\pi|R(x,y)|^2$

Failure of projection onto density waves for “constant phase model”

Second model class: again

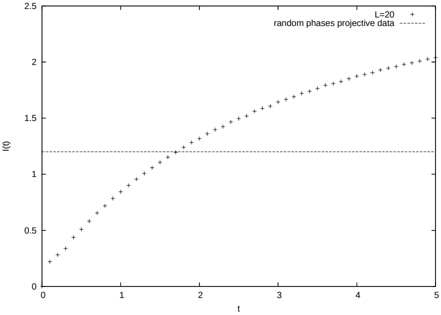
$$\hat{H} = \sum_{x,y} R(x,y)\hat{a}_x^{+}\hat{a}_y + h.c.$$

$$R(x,y) = \exp(-|x-y|/l - \mathrm{i}\Phi(x,y))$$

but now, no phases of hopping amplitues, i.e., $\Phi(x,y) = 0$.
The above second order projective approach essentially yields unaltered results. But counterchecking with increase of variance no longer yields any agreement !

- no agreement with second order projection onto density waves
- no conclusive result from exact diagonalization due to finite size effects

$D(t)$ vs. time



- what to do now?
- Einstein relation implies

$$\int_0^t \mathrm{Tr}\{\hat{j}\hat{j}(t')\}\mathrm{d}t' = D(t)$$

decay of current looks exponential !

Projection onto the current

- current decays exponentially like expected for a periodic model featuring impurities.
- $\Rightarrow$ try to map the model onto an impurity model.
- we try cubic momentum lattice featuring a spacing of $2\pi/L$. This yields a set of "momentum states"

$$|k\rangle := \frac{1}{\sqrt{N}} \sum_x \mathrm{e}^{-ikx} |x\rangle$$

this set is:

- normalized
- slightly non-orthogonal
- slightly under or overcomplete
- transform nevertheless the Hamiltonian into this basis, i.e., calculate $\langle k|\hat{H}|k'\rangle := H_{kk'}$

We find:

- diagonal elements much bigger: $|H_{kk}|^2 >> |H_{kk'}|^2$
- diagonal elements form a "dispersion relation" $H_{kk} =: E(k) \approx (1 + l^2 k^2)^{-2}$
- current operator takes the form $\widehat{J} \approx |k\rangle \partial E / \partial k_x \langle k|$

thus we:

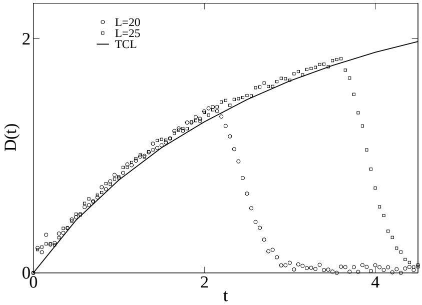
- take the diagonal part in the momentum basis for the unperturbed Hamiltonain $\hat{H}_0$
- project onto the current $\mathcal{P}\rho = \widehat{1} + \widehat{J}\mathrm{Tr}(\widehat{J}\rho)(\mathrm{Tr}(\widehat{J}^2))^{-1}$

this yields:

- a current decay rate R: $\mathrm{Tr}\left(\hat{J}(t)\hat{J}\right) \approx e^{-Rt}$

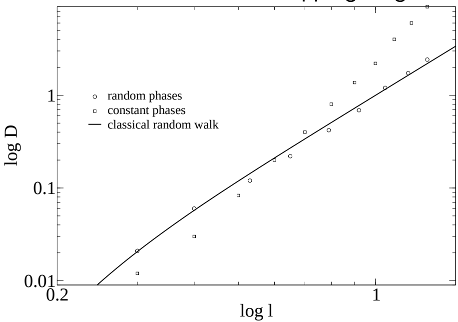
Projection onto the current / Results

$D(t)$ vs. time



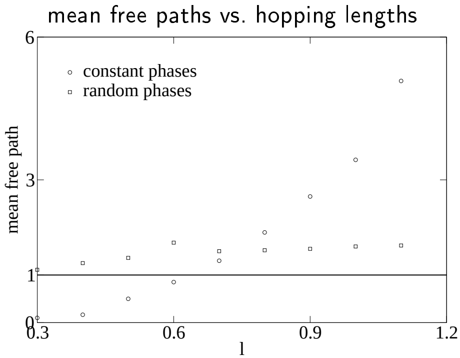
Data from current projection seem to fit reasonably for $l = 1$. Thus we compute diffusion coefficients for larger l only from current projection

diffusion coefficients vs. hopping lengths



Constant phase model and random phase model show clearly different transport properties.

Mean free paths / Conclusions / Acknowledgements



Around $l \approx 0.8$ the constant phase model undergoes a transition from hopping to band-type transport, inspite of its complete topologigal disorder. That does not occur for the random phase model

- Calculation of transport properties of entirely disordered one particle quantum models seems feasible
- Even topologically completely disordered systems may show a transition from hopping to band transport
- The transition may be "induced" by changing the hopping length

If you are interested in Refs. just ask me.

Thanks to Robin Steinigeweg and you the audience!