From hopping to balistic transport in topologically disordered quantum systems

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Heat Control and Thermoelectric Efficiency

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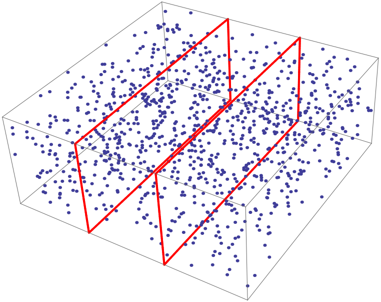
Contents

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)

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

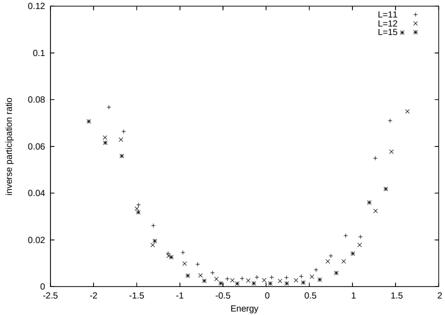
- May the quantum motion of a particle in such a system be described as diffusive, localized, ballistic, etc.?
- If so what are diffusion coefficients, mobilities, mean free paths, etc?

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

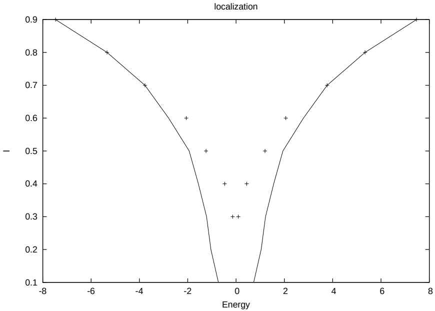
Cheap check of localization

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" $\hat{n}(X)$

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

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

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

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

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

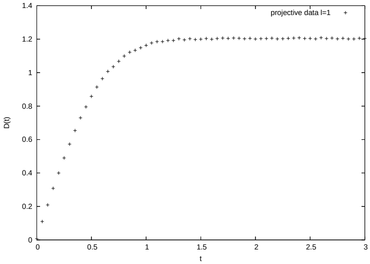
$$\Rightarrow \dot{m}_q = -\sum_{n,q'} \lambda^n K_{n,q,q'}(t) m'_q \quad (n : \mathrm{even})$$

"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

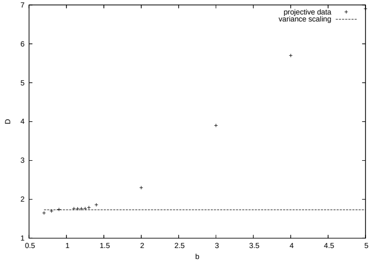


looks nice but....

Projection onto density waves

...is that correct in the sense that the second order contains the relevant physics?
⇒ vary projector by varying slab thickness:

diff. coeff. vs. slab thickness

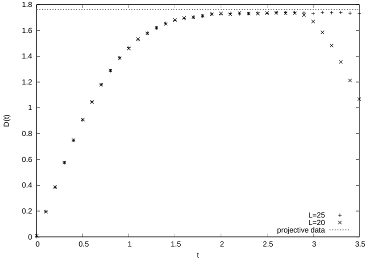


Better countercheck by another method!

$n(x)$ diffusive implies linear increase of spatial variance $\delta_n^2(t) = 2Dt$

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

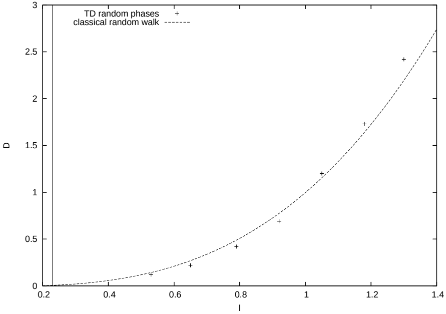
increase of variance vs. time



Everything seems to fit nicely ⇒ use projective approach for longer hopping lenghts ⇒

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 sintes wiht rates given by the absolute squares of the hopping amplitues, i.e., $|R(x,y)|^2$

Failure of projection onto density waves for "constant phase model"

Second model class: again

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

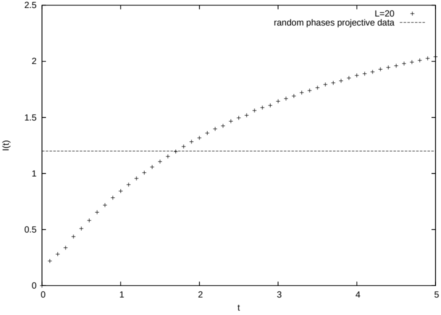
$$R(x,y) = \exp(-|x-y|/l - i\Phi(x,y))$$

but now, no phases of hopping amplitues, i.e., $\Phi(x,y) = 0$.
The above second order projective approach essentially yields unaltered results. But countercheck now via the relation between the temporal integral of the current-autocorrelation function and the diffusion coefficient:

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

Calculate $D(t)$ from a finite cube via exact diagonalization:

$D(t)$ vs. time



- no agreement with second order projection onto density waves
- no conclusive result from exact diagonalization due to finite size effects
- what to do now?
- decay of current looks exponential

Mapping onto impurity model

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

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

this set is:

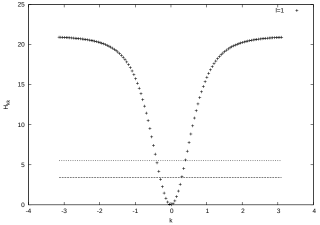
- normalized
- slightly non-orthogonal
- slightly under or overcomplete

Display nevertheless the Hamiltonian in this basis, i.e., calculate

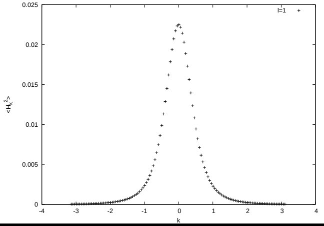
$$\langle k|\hat{H}|k'\rangle := H_{kk'}$$

Mapping onto impurity model

diagonal elements vs. momentum



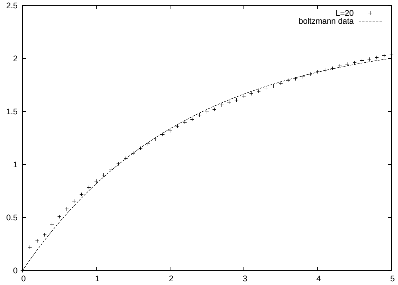
mean squared off-diag. elemets vs. momentum



- Diagonal elements are large and systematic, $\Rightarrow$ interprete as Bloch-waves with corresponding dispersion relation.
- Off-diagonal elements are small and "non-systematic", except for an overall dependence on $|k|$, $\Rightarrow$ interprete as impurity scattering amplitudes
- Employ a TCL-projection onto occupation numbers of "grains" in momentum space to map the corresponding dynamics on a linear Boltzmnann equation with time dependent rates (C. Bartsch et. al PRB 2010)
- Identify the sector on which there is time-scale separation: relaxation time $>>$ time on which rates become constant
- Calculate integral over current correlation function based on Boltzmann equation on that sector

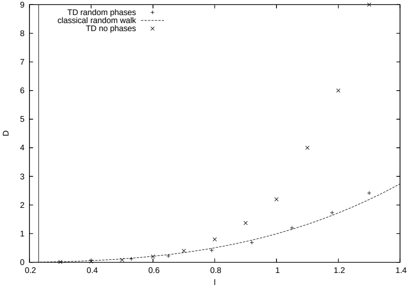
Mapping onto impurity model

$D(t)$ vs. time



This seems to fit reasonably, thus diffusion coefficients may be calculated for all hopping lengths based on the above Boltzmann equation.

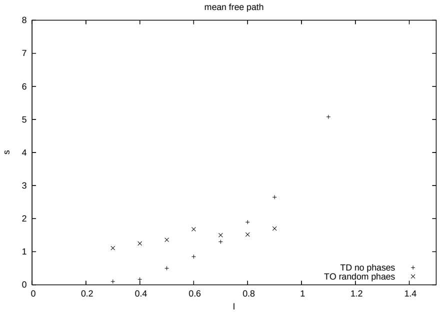
diffusion coefficients vs. hopping lengths



It looks like the constant phase model undergoes some kind of transition around $l \approx 0.8$. Probably it undergoes a similar transition with energy.

Mean free paths / Conclusions / Acknowledgements

mean free paths vs. hopping lengths



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 or changing the energy
- The "mobility edge" in, e.g., amorphous silicon may rather be a "hopping edge"

Thanks to Christian Bartsch, Robin Steinigeweg and you the audience!