Finite size scaling of the typical density of states using the kernel polynomial method

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Abstract

We study the metal-insulator transition (MIT) in effective tight binding models (ETBM) by looking at the scaling behaviour of the typical density of states (GDOS) which we obtain by taking the geographical mean of the local density of states (LDOS) of many different lattice sites and realisations of disorder. The LDOS can be efficiently calculated by means of the kernel polynomial method (KPM). Right now we focus on applying this method on the 'standard' Anderson model of disorder to check our own implementation and methodical approach and to validate preceding results by others.

1. Considered model

Anderson model of disorder [1]:

\[ h = \sum_{\{i,j\}} \left( \delta_{ij} + t \right) |j| \left( \delta_{ij} - \delta_{ij} \right) \]  
(1)

- \( \delta \) uncorrelated random site potentials, box distribution (width \( W/t \))
- \( t \) constant isotropic next-neighbour hopping parameter
- \( \{i,j\} \) states of the site-occupation basis (i, j site indices)
- lattice
- 3D simple cubic supercell, \( N = L \times L \times L \) sites

boundaries
- periodic boundary conditions
- used as a starting point to test our method and implementation
- validate or refine results by others [2, 3]

2. Measured quantity

- Calculate local density of states (LDOS) \( \rho(E) \) using the kernel polynomial method (KPM, see section 6)
- calculating information about the spatial distribution of wave functions:

\[ \rho(E) = \sum_{E} \left( \delta_{E} - \delta_{E} \right) \]  
(2)

- Average over many lattice sites of many realisations of disorder (total number: \( S \))

- calculate two kinds of densities:

  - arithmetic mean
  - geometric mean

leading to total density of states (ADOS) \( \rho(E) \) leading to typical density of states (GDOS) \( \rho_{typ}(E) \)

\[ \rho(E) = \frac{1}{S} \sum_{S} \rho_{S}(E) \]  
(3)

- use flexible abort criterion for the (iterative) averaging process, depending on the desired accuracy (smoothness) of the curve

This usually results in 10^5 - 10^7 sites of several hundreds of realisations of disorder.

- GDOs:

  - equals ADOS for zero disorder, is smaller otherwise (not normalised), pronounces small values
  - is suppressed by increasing disorder strength \( W/t \)
  - is suppressed by increasing system size \( N \)

3. Distinction between localised and extended states

- do finite size scaling analysis with GDOs data

- expect change of scaling behavior at the mobility edges (ME)

4. Phase diagram of disorder

- use cutoff \( c = 1 \) to read off the mobility edges (ME) \( \lambda_{ME} \) from the function \( \rho(E) \) for every disorder \( W/t \), plot mobility edges \( \lambda_{ME} \) against disorder parameter \( W/t \)

5. The kernel polynomial method

- polynomial series expansion based on Chebyshev polynomials [3]:

\[ f(x) = \frac{1}{2} \sum_{n=0}^{N} \left[ \mu_{n} + \sum_{k=1}^{n} \mu_{k} \right] \cos(n \pi x) \]  
(4)

- Chebyshev polynomials:

\[ T_{n}(x) = \cos(n \arccos(x)) \]  
(5)

- coefficients ("Chebyshev moments") in the case of LDOS \( f(x) = \rho(E) \):

\[ \rho_{n} = \int_{-1}^{1} f(x) T_{n}(x) \, dx = \left( \rho \frac{1}{\sqrt{n}} \right) \]  
(6)

- there exist recursive formulas to calculate the moments \( \rho_{n} \) iteratively, allowing for efficient algorithms

- core of main iteration loop consists mainly of a sparse matrix-vector multiplication, hence low memory consumption

- order of \( N \) method (given a \( N \times N \) sparse matrix)

- approximation: truncate the series after a finite number of moments \( \rho \) (truncation limit)

- no need for diagonalization of \( T \)

References


Outlook

- accuracy still has to be improved (especially near the critical disorder)
- maybe extend implementation to VMKPIM (variable moment KPM) [2]
- goal: develop a method which does not rely on external parameters for calibration (e.g. by prior knowledge of the critical disorder \( W \))

- After successful application to the Anderson model, we plan to study more interesting systems like binary alloys and magnetic semiconductors.