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

D. Jung[1] **G. Czycholl**[2] **S. Kettemann**[1,3]

[1] School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany
[2] Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany
[3] Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), San 31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea

d.jung@jacobs-university.de s.kettemann@jacobs-university.de

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 geometrical mean of the local density of states (LDOS) of many different lattice sites and realizations of disorder. The LDOS can be performantly 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]:

$$\mathrm{H} = \sum_i \epsilon_i |i\rangle\langle i| + t \sum_{i,j} |j\rangle\langle i| \qquad (1)$$

$\epsilon_\mathbf{i}$	uncorrelated random site potentials, box distribution (width W)
$\mathbf{t}$	constant isotropic next-neighbor hopping parameter
$\|\mathbf{i}\rangle, \|\mathbf{j}\rangle$	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) $\rho_i(E)$ using the kernel polynomial method (KPM, see section 5), carrying information about the spatial distribution of wave functions:

$$\rho_i(E) = \sum_{k=1}^{N} |\langle i|k\rangle|^2 \, \delta(E - E_k) \qquad (2)$$

→ Average over many lattice sites of many realizations of disorder (total number: S)

→ calculate two kinds of densities:

arithmetic mean	*geometric mean*
leading to total density of states (ADOS)	leading to typical density of states (GDOS) [2, 3]
$\rho_{\text{tot}}(E) = \frac{1}{S}\sum_{i=1}^{S} \rho_i(E)$	$\rho_{\text{typ}}(E) = e^{\frac{1}{S}\sum_{i=1}^{S} \log \rho_i(E)}$
(non-critical)	*(critical at MIT)*

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

This usually results in $10^5 \ldots 10^7$ sites of several hundreds of realizations of disorder.

→ GDOS:

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

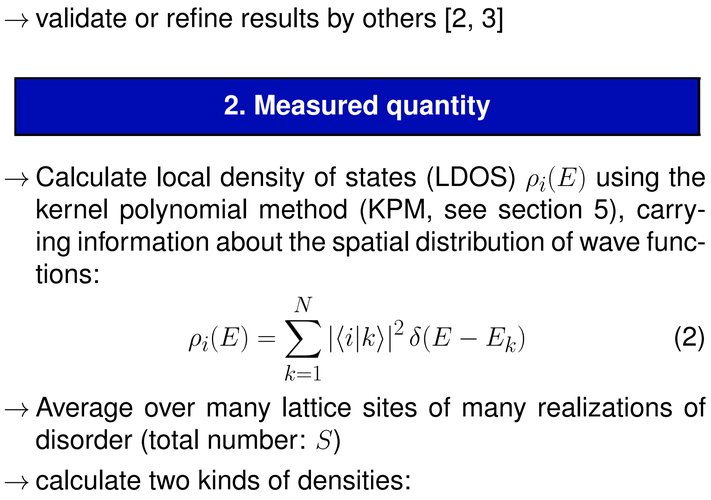

Figure 2: *The total (ADOS) and the typical (GDOS) density of states for different disorder parameters $W/t \in \{0, 1, 2, \ldots, 17\}$ (from top to bottom). System size is $N = L^d = 40^3 = 64000$ and truncation limit is $M = 140$.*

3. Distinction between localized and extended states

→ do finite size scaling analysis with GDOS data

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

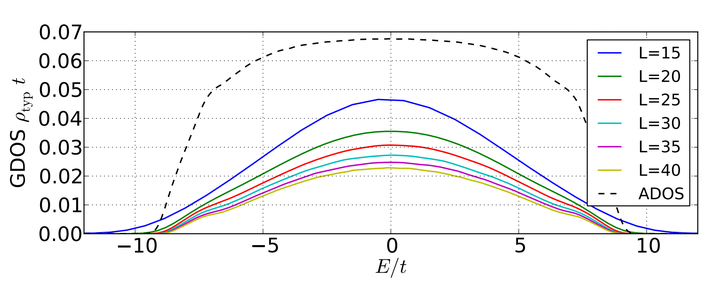

Figure 3: *Typical density of states (GDOS) for different system sizes $N = L^d$ (disorder: $W/t = 13.2$).*

→ do curve fitting for every energy interval, assume a simple power-law:

$$\rho_{\text{typ}}(L) = \frac{a}{L^p} \qquad (3)$$

→ Due to our choice to keep the ratio M/L^d constant, extended states seem to show a $1/L$ behavior, whereas localized states behave like $1/L^p$ with $p > 1$.

An additional constant term would surely better fit GDOS data belonging to extended states which remain finite in the limit of infinite system size. But this can even be turned into an advantage because it only means that the (poor) fits in those regions will lead to exponents $p < 1$. This is nice, because now the cutoff to read off the mobility edges can be chosen exactly to $c = 1t$.

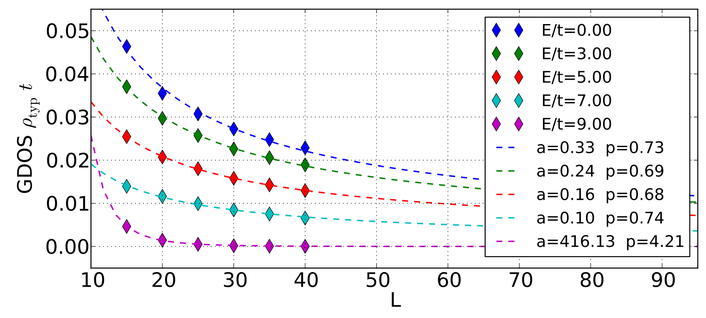

Figure 4: *Examples for the scaling behavior of the GDOS with increasing system edge length L for different band energies E (disorder: $W/t = 13.2$). Resulting fit parameters from fit model (3) in the legend.*

→ distinguish different regions within the band by looking at the energy dependency of the fitting parameters of the model function (3)

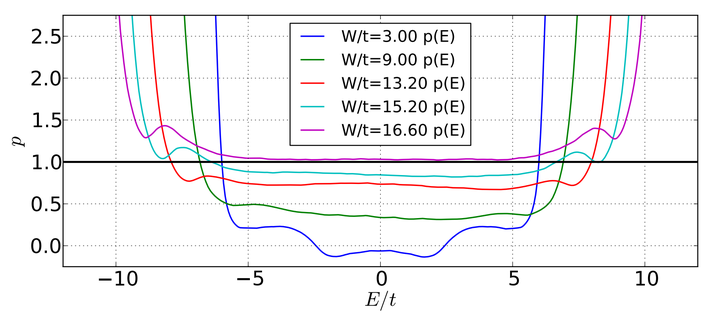

Figure 5: *Scaling exponent p as a function of energy E for different disorder parameters W. The thick black line indicates the cutoff $c = 1t$ that is used to read off the mobility edges.*

References

[1] P. W. Anderson. Absence of diffusion in certain random lattices. *Phys. Rev.*, 109(5):1492–1505, Mar 1958. doi: 10.1103/PhysRev.109.1492.

[2] G. Schubert and H. Fehske. Quantum percolation in disordered structures. In Bikas K. Chakrabarti, Kamal K. Bardhan, and Asok K. Sen, editors, *Quantum and Semiclassical Percolation and Breakdown in Disordered Solids*, volume 762 of *Lecture Notes in Physics*, pages 1–28. Springer Berlin / Heidelberg, 2009. URL http://dx.doi.org/10.1007/978-3-540-85428-9_5.

[3] Alexander Weiße, Gerhard Wellein, Andreas Alvermann, and Holger Fehske. The kernel polynomial method. *Rev. Mod. Phys.*, 78(1):275–306, Mar 2006. doi: 10.1103/RevModPhys.78.275.

4. Phase diagram of disorder

→ use cutoff $c = 1t$ to read off the mobility edges (ME) E_M from the function $p(E)$ for every disorder parameter W

→ plot mobility edges E_M against disorder parameter W

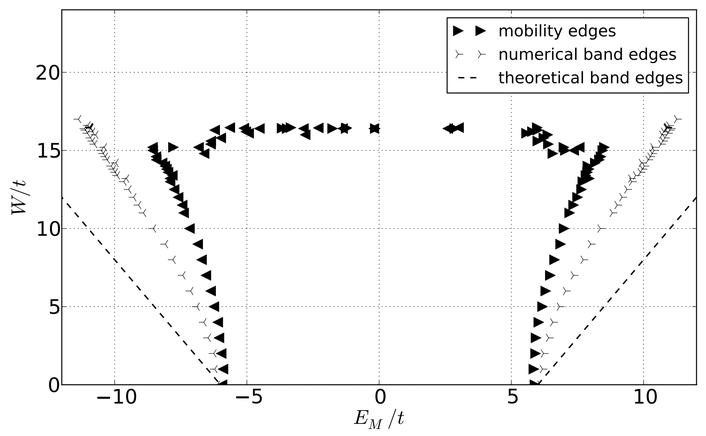

Figure 6: *Phase diagram of disorder as obtained by our method with the accuracy of our current data.*

→ resulting phase diagram agrees mostly with other findings [2, 3]:

- for zero disorder, the mobility edges coincide with the band edges
- upcoming localized states in the band tails for increasing disorder
- reentrance behavior, but turning points slightly different ($E \approx 8.3t$ instead of $E \approx 7.6t$ [2])
- critical disorder of about $W_\text{c} = 16.5t$ (probably slightly below)

→ fluctuations in the function $p(E)$ still lead to poor results when approaching the critical disorder ($W_\text{c}/t = 16.5$)

5. The kernel polynomial method

→ polynomial series expansion based on Chebychev polynomials [3]:

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}} \left(\mu_0 + 2\sum_{n=1}^{\infty} \mu_n T_n(x) \right) \qquad (4)$$

→ Chebychev polynomials:

$$T_n(x) = \cos(n \arccos(x)) \qquad (5)$$

→ coefficients ("Chebychev moments") in the case of LDOS ($f(x) \equiv \rho_i(E)$):

$$\mu_n = \int_{-1}^{1} f(x)\, T_n(x)\, \mathrm{d}x = \langle i|T_n(\underline{\underline{H}})|i\rangle \qquad (6)$$

→ there exist recursive formulas to calculate the moments μ_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 M (truncation limit)

→ no need for diagonalization of $\underline{\underline{H}}$

Outlook

→ accuracy still has to be improved (especially near the critical disorder)

→ maybe extend implementation to VMKPM (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_c)

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