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

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Abstract

We study the (Anderson) metal-insulator transition (MIT) in tight binding models (TBM) of disordered systems using the scaling behavior of the typical density of states (GDOS) as localization criterion. The GDOS is obtained as the geometrical mean value of the local density of states (LDOS) averaged over many different lattice sites and disorder realizations. The LDOS can efficiently be obtained within the kernel polynomial method (KPM). To check the validity and accuracy of our approach, we first apply it to the "standard" Anderson model of disordered systems, for which well-known results (for instance for the critical disorder strength of the Anderson transition) already exist thanks to other methods.

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: "sample size" 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]
$\rho_{\mathrm{tot}}(E) = \frac{1}{S}\sum_{i=1}^{S} \rho_i(E)$	$\rho_{\mathrm{typ}}(E) = e^{\frac{1}{S}\sum_{i=1}^{S} \log \rho_i(E)}$
(non-critical)	*(critical at MIT)*

→ use convergence criterion for the (iterative) averaging process, depending on the required relative accuracy ("smoothness") of the densities

This usually results in sample sizes of about $S \approx 10^5 \ldots 10^6$.

→ 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

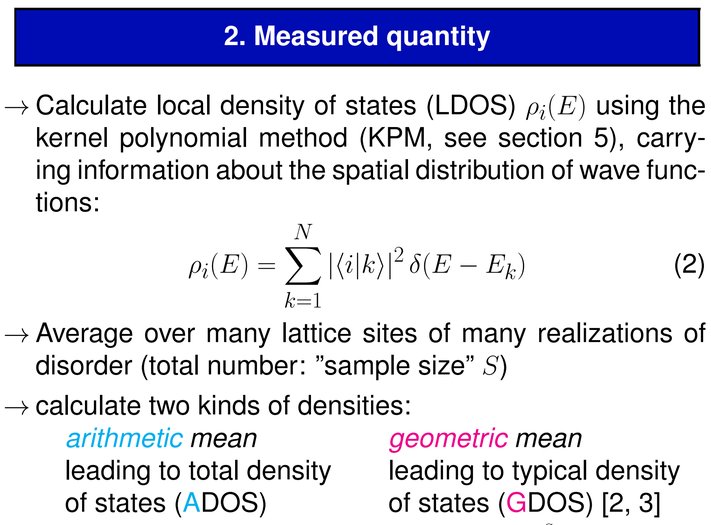

Figure 2: *The total (ADOS) and the typical (GDOS) density of states for different disorder parameters $W/t \in \{0, 1, 2, \ldots, 17\}$ (from top to bottom). System size is $N = L^d = 40^3 = 64000$ and truncation limit is $M = 140$.*

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)

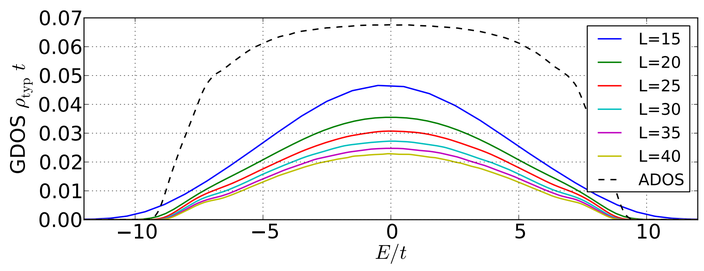

Figure 3: *Typical density of states (GDOS) for different system sizes $N = L^d$ (disorder: $W/t = 13.2$).*

→ do curve fitting at various energies, assume a simple power-law (for now):

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

→ Due to our choice to keep the ratio M/L^d constant, extended states show a $1/L$ behavior ($b \geq 0$), whereas localized states behave like $1/L^p$ with $p > 1$ ($b = 0$).

For convenience, we have fixed $b = 0$. It is clear that the data belonging to metallic states now cannot be fitted very well anymore. However, in this way the fit algorithm produces curves with $p < 1$ in the metallic regime. This can be turned into an advantage, because then the MEs can easily be determined as those energies at which the function $p(E)$ crosses the cutoff $p(E_{\mathrm{M}}) = 1$.

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 metallic and insulating regions within the band for every disorder strength

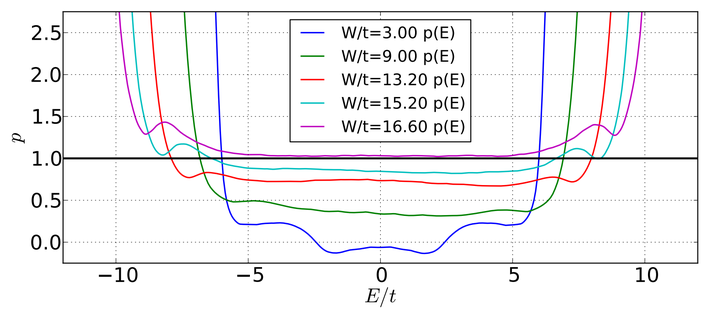

Figure 5: *Scaling exponent p as a function of energy E for different disorder parameters W. The thick black line indicates the cutoff $c = 1t$ that is used to read off the mobility edges.*

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 $c = 1$ 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

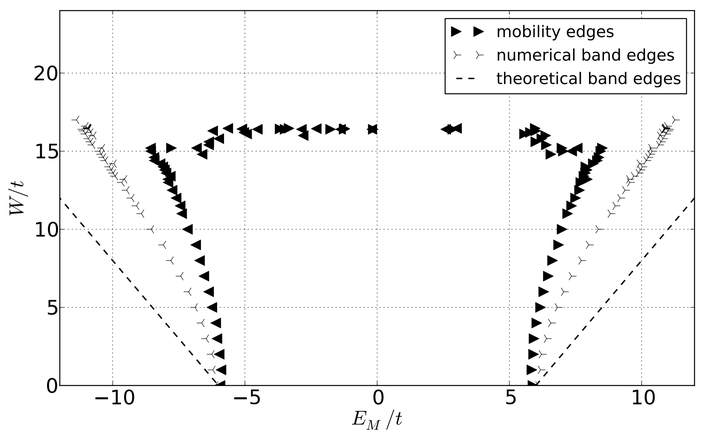

Figure 6: *Phase diagram of disorder as obtained by our method with the accuracy of our current data.*

→ 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 $W_{\mathrm{c}} = 16.5t$

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

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 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

→ push relative accuracy further up (especially near the phase transition/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, study more interesting systems like binary alloys and magnetic semiconductors (Anderson-Hubbard model)

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