Impact of Local Magnetic Moments on the Anderson Metal-Insulator Transition

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Table of contents

Table of contents

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- Disorder-induced quantum phase transition
- Nonzero disorder: Localized eigenstates appear
- Critical disorder: Phase transition

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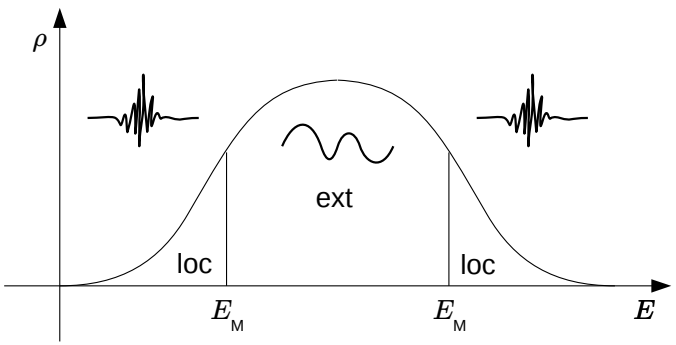
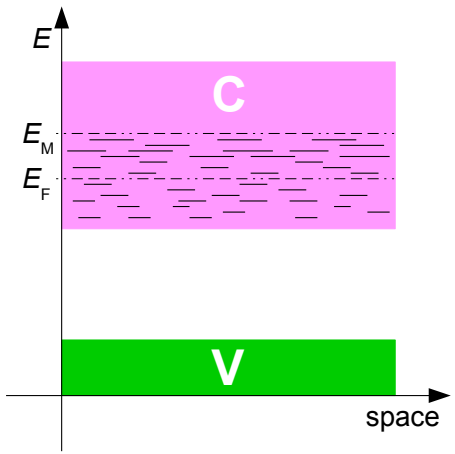
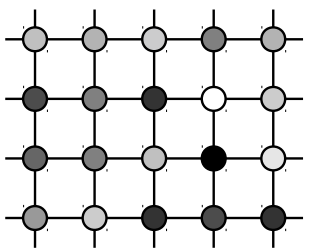


- Mobility edges E_M separate band regions of localized and extended states

Anderson (1958)





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Constant NN hopping, random site-potentials

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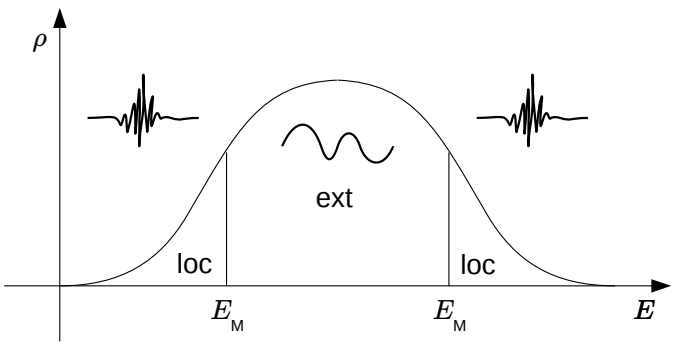

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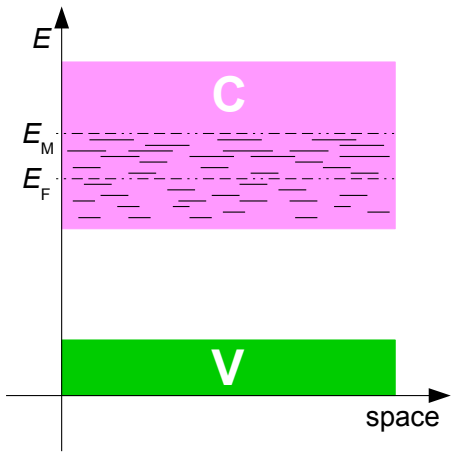

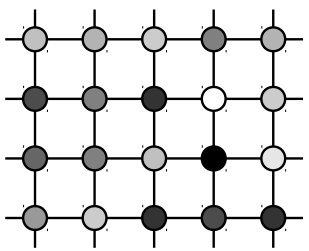

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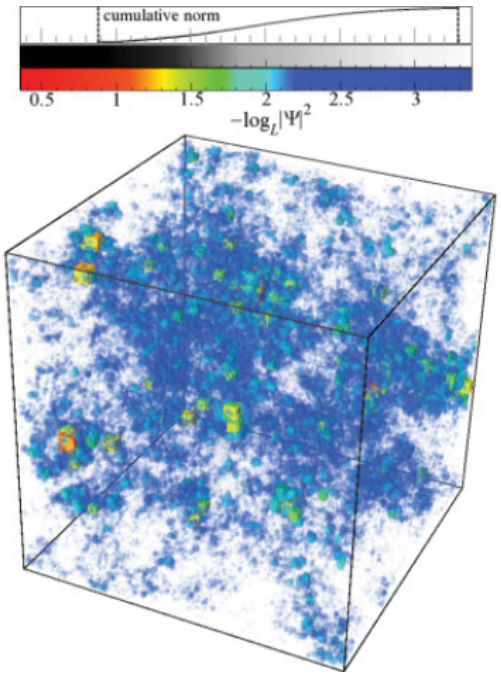
Rodriguez et al. (2011)



Critical eigenstate

$|\psi^2| \sim L^{-\alpha}$

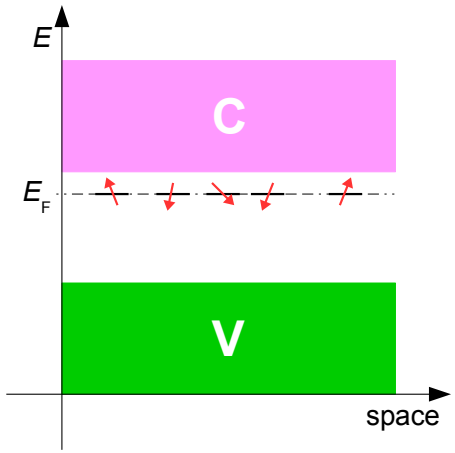
(broad distribution of α, maximum at α_0)

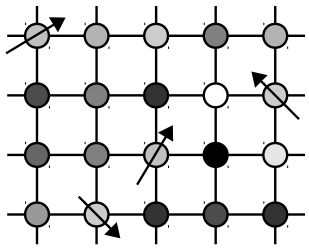
$\rightarrow$ Multifractality

The Anderson-Heisenberg model

- Si:P exhibits a metal-insulator transition, driven by both interaction and disorder
- Further, local magnetic moments have been found

  How do the local magnetic moments influence the transition?





- Start from Anderson model:

$$\mathrm{H}_0 = t \sum_{\langle i,j\rangle,\sigma} |j,\sigma\rangle\langle i,\sigma| + \sum_{i,\sigma} \varepsilon_i \, |i,\sigma\rangle\langle i,\sigma|$$

- Add local exchange coupling to classical magnetic impurities:

$$\mathrm{H} = \mathrm{H}_0 + \mathrm{H}_\mathrm{S} \quad , \quad \mathrm{H}_\mathrm{S} = \sum_\mathrm{i} \mathrm{J}_\mathrm{i}\, \mathbf{s}_\mathrm{i} \cdot \mathbf{S}_\mathrm{i}$$

- Has been introduced as an effective model for the impurity band electrons in Si:P
- Fix concentration of sites carrying a magnetic moment to $n_\mathrm{M} = 5\,\%$
- Compare Heisenberg impurities (random orientation, unitary symmetry) to Ising impurities (only $\uparrow\downarrow$, orthogonal symmetry)

Anderson (1958); Bhatt and Rice (1981); Sachdev (1989); von Löhneysen (2000)

Table of contents

The kernel polynomial method

Use Chebychev expansion to approximate the local density of states:

$$\tilde{\rho}_i(\tilde{E}) = \frac{1}{\pi\sqrt{1-\tilde{E}^2}}\left(\mu_0^{(i)} + 2\sum_{m=1}^{M}\mu_m^{(i)}\, T_m(\tilde{E})\right)$$

Truncation limit: Finite number M of coefficients $\mu_m^{(i)}$

Chebychev polynomials of first kind:

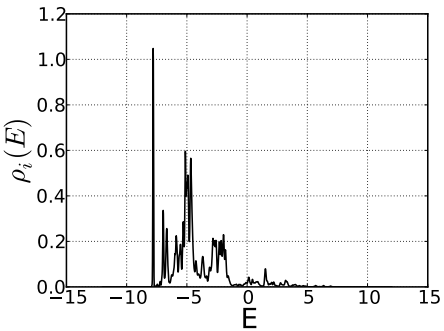
$$T_m(x) = \cos(m \arccos x)$$

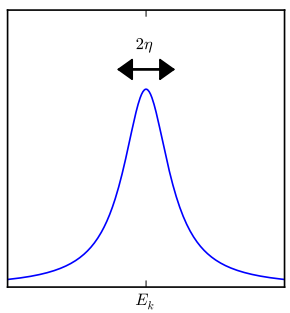
Recursive relations (CP of first kind):

$$T_0(x) = 1 \quad , \quad \mathrm{T}_1(\mathrm{x}) = \mathrm{x}$$
$$T_{m+1}(x) = 2x\, T_m(x) - T_{m-1}(x)$$

Chebychev moments $\mu_m^{(i)}$ for the LDOS:

$$\mu_m^{(i)} = \frac{1}{N}\langle i|\, T_m(\tilde{H})|i\rangle$$





KPM approximation causes an energy broadening η. At $\tilde{E} = 0$:

$$\tilde{\eta} \approx \frac{\pi}{M}$$

Weiße et al. (2006)

The typical density of states

Typical density of states

- Geometric average over the local density of states

$$\rho_{\mathrm{typ}}(E) = \exp\langle \log \rho_i(E) \rangle_{\mathrm{dis}}$$

- Scales with W, L, M
- Thermodynamic limit:

$$\lim_{L\to\infty} \rho_{\mathrm{typ}} = \begin{cases} 0 & \text{localized} \\ \text{const} & \text{extended} \end{cases}$$

$\rightarrow$ Critical at the MIT

Can the typical density of states be used to determine the MIT?

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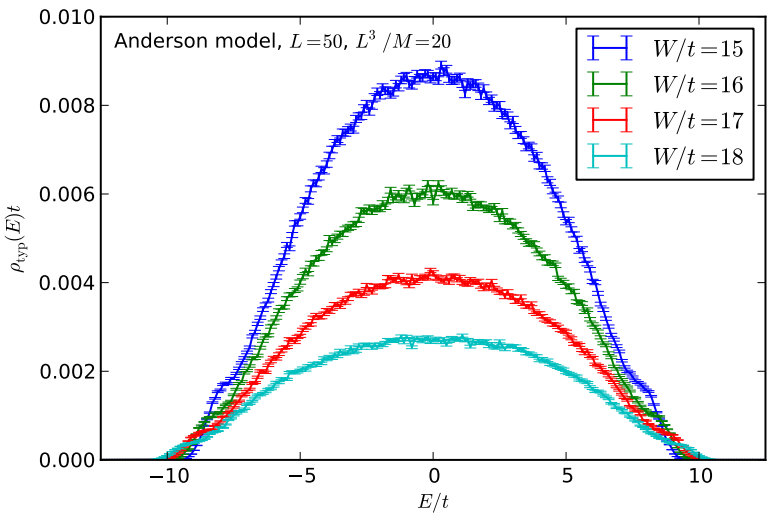
Yes, but: For finite system size, no clear distinction possible.

One would need a cutoff...



How to choose a suitable cutoff?

Adjustment to external calibration parameter necessary...

Schubert and Fehske (2009)

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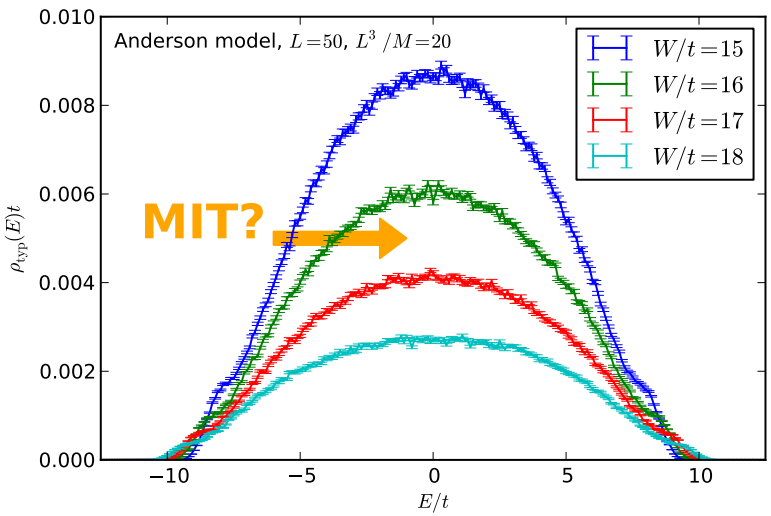

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Finite-size scaling of the typical density of states

Local density of states (with finite broadening η):

$$\rho(E, \mathbf{r}, \eta) = \sum_k \left|\psi_k(\mathbf{r})\right|^2 \delta(E - E_k, \eta)$$

Geometric average of local density of states:

$$\rho_{\mathrm{typ}}(E) = \exp\langle \log \rho_i(E) \rangle$$

At criticality:

$$\rho_{\mathrm{typ}} \sim L^{d-\alpha_0}$$

Janssen (1998)

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Two scales:

- Length scale: L/ξ
  $L/\xi < 1$: State critical
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  $\eta/\Delta \to 0$: High resolution limit
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Scaling ansatz:

$$\Gamma = L^{d-\alpha_0} F(L/\xi, \eta/\Delta)$$

Asada et al. (2006)

Alternative form:

$$\Gamma = L^{d-\alpha_0} F(\varepsilon L^{\frac{1}{\nu}}, \rho_{\mathrm{av}} \eta L^d)$$

$$\Gamma(E) = \frac{\rho_{\mathrm{typ}}(E)}{\rho_{\mathrm{av}}(E)} \quad , \quad \varepsilon = \frac{\mathrm{W_c} - \mathrm{W}}{\mathrm{W_c}}$$

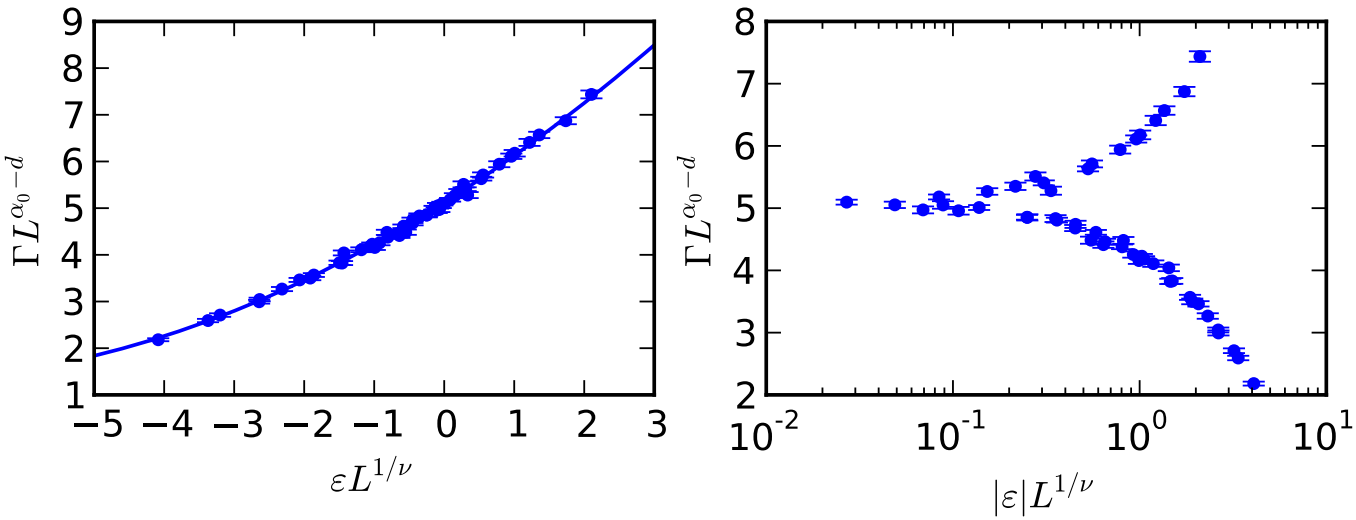
Validity of the scaling ansatz – First argument

→ Keep second argument $\rho_{\mathrm{av}} \eta L^d$ fixed.

Approximation: We fix ηL^d and neglect the disorder dependence of $\rho_{\mathrm{av}}(E)$.

$$\Gamma(W, L) = L^{\alpha_0 - d} \tilde{F}(\varepsilon L^{\frac{1}{\nu}}) \quad , \quad \varepsilon = \frac{\mathrm{W_c} - \mathrm{W}}{\mathrm{W_c}}$$

→ Consider a power law for $\tilde{F}(x)$ (second order)



→ General validity proven for the 3D Anderson model

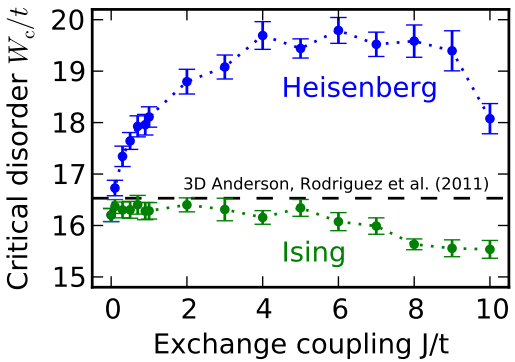
→ Obtain W_c, α_0 and ν as fit parameters

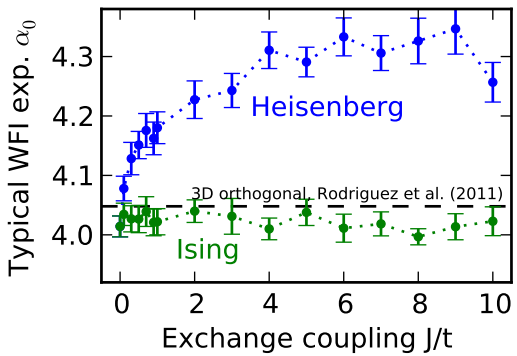
Table of contents

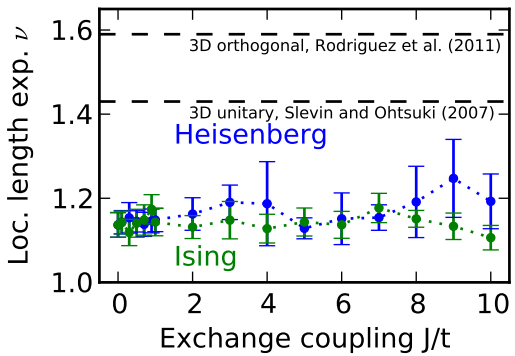
The Anderson-Heisenberg model: Fitting results

Apply scaling ansatz to the Anderson-Heisenberg model, vary exchange coupling J

Fit results:







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Exception: Loc. length exp. ν

Jung, Slevin, and Kettemann (2014), unpublished

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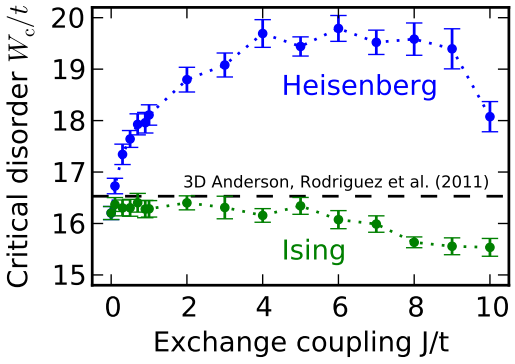

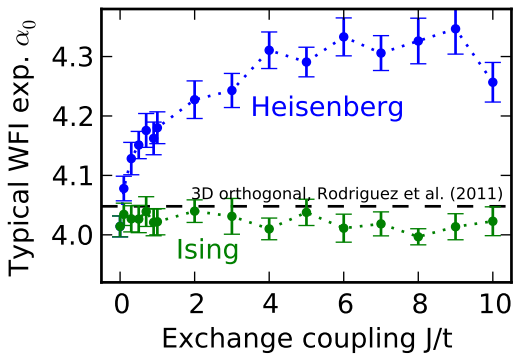

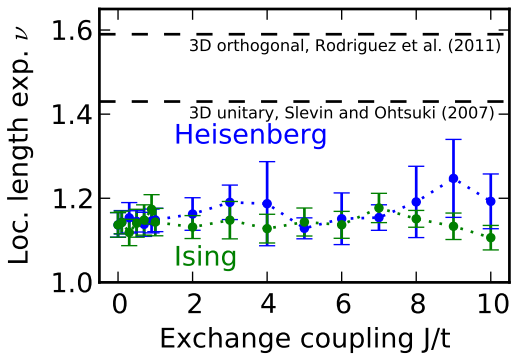

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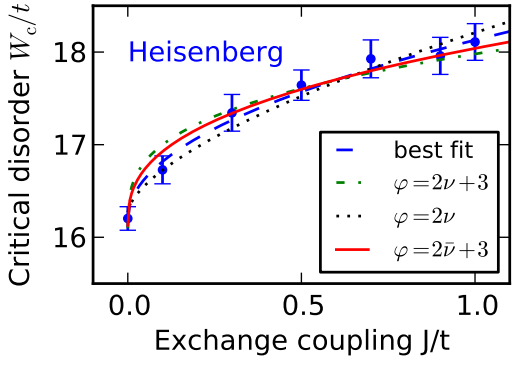
Analytic prediction for $W_c(J)$:

$$W_c(J) \sim J^{2/\varphi}$$

Kettemann et al. (2009, 2012)

Fit $W_c(J)$ for small J:



Predictions for φ:

$\varphi = 2\nu$ Khmel'nitskii and Larkin (1981)

$\varphi = 2\nu + 3$ Wegner (1987)

→ Best fit:

$2/\varphi = 0.49 \pm 0.05$

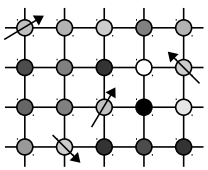
→ No clear distinction possible within the errorbars

Jung, Slevin, and Kettemann (2014), unpublished

Table of contents

Conclusions

- Effective model for the impurity band electrons in materials like Si:P



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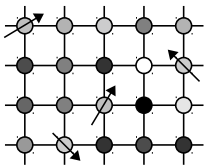

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- Obtain full phase diagrams

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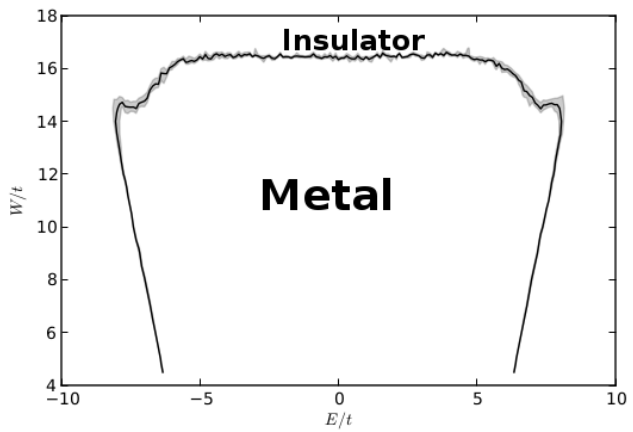

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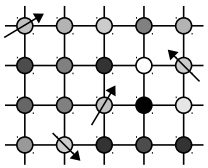

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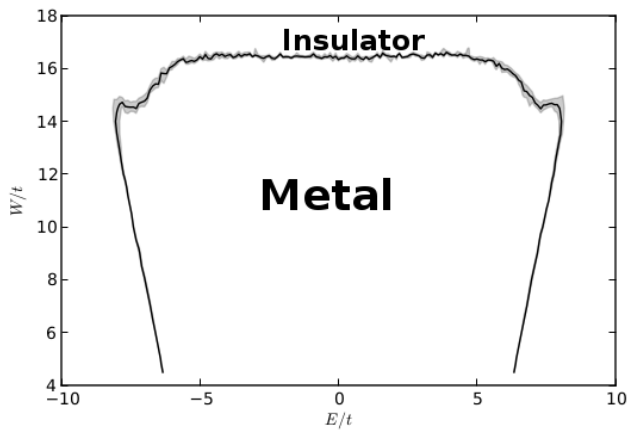


Thank you for your attention!

References I

PW Anderson. Absence of diffusion in certain random lattices. Physical Review, 109:1492–1505, 1958. URL http://prola.aps.org/abstract/PR/v109/i5/p1492_1.

Yoichi Asada, Keith Slevin, and Tomi Ohtsuki. Finite size scaling of the local density of states at the Anderson transition. unpublished, 2006.

RN Bhatt and TM Rice. Single-particle energy levels in doped semiconductors at densities below the metal-nonmetal transition. Physical Review B, 23(4), 1981. URL http://prb.aps.org/abstract/PRB/v23/i4/p1920_1.

B Bulka, M Schreiber, and B Kramer. Localization, quantum interference, and the metal-insulator transition. Zeitschrift für Physik B Condensed Matter, 30:21–30, 1987. URL http://link.springer.com/article/10.1007/BF01312758.

F Evers and AD Mirlin. Anderson transitions. Reviews of Modern Physics, 80(4):63, July 2008. doi: 10.1103/RevModPhys.80.1355. URL http://arxiv.org/abs/0707.4378http://rmp.aps.org/abstract/RMP/v80/i4/p1355_1.

Martin Janssen. Statistics and scaling in disordered mesoscopic electron systems. Physics Reports, 295(1-2):1–91, 1998. ISSN 0370-1573. doi: 10.1016/S0370-1573(97)00050-1. URL http://www.sciencedirect.com/science/article/B6TVP-3SYVR93-5/2/87a41d2897123662b69ed9dbc684da2f.

S Kettemann, E Mucciolo, and I Varga. Critical Metal Phase at the Anderson Metal-Insulator Transition with Kondo Impurities. Physical Review Letters, 103(12):126401, September 2009. ISSN 0031-9007. doi: 10.1103/PhysRevLett.103.126401. URL http://meeting.aps.org/Meeting/MAR10/Session/A38.13http://link.aps.org/doi/10.1103/PhysRevLett.103.126401.

S Kettemann, ER Mucciolo, I Varga, and K Slevin. Kondo-Anderson transitions. Physical Review B, 85(11):115112, 2012. URL http://prb.aps.org/abstract/PRB/v85/i11/e115112.

DE Khmel'nitskii and AI Larkin. Mobility edge shift in external magnetic field. Solid State Communications, 39(10):1069–1070, 1981. URL http://www.sciencedirect.com/science/article/pii/0038109881902106.

N Norris. The standard errors of the geometric and harmonic means and their application to index numbers. The annals of mathematical statistics, 11(4):445–448, 1940. URL http://www.jstor.org/stable/10.2307/2235723.

Alberto Rodriguez, Louella J. Vasquez, Keith Slevin, and Rudolf Römer. Multifractal finite-size scaling and universality at the Anderson transition. Physical Review B, 84(13):134209, October 2011. ISSN 1098-0121. doi: 10.1103/PhysRevB.84.134209. URL http://link.aps.org/doi/10.1103/PhysRevB.84.134209.

Subir Sachdev. Local moments near the metal-insulator transition. Physical Review B, 39(8):5297–5310, 1989. URL http://prb.aps.org/abstract/PRB/v39/i8/p5297_1.

References II

G Schubert and H Fehske. Quantum and Semi-classical Percolation and Breakdown in Disordered Solids, volume 762 of Lecture Notes in Physics. Springer Berlin Heidelberg, Berlin, Heidelberg, 2009. ISBN 978-3-540-85427-2. doi: 10.1007/978-3-540-85428-9. URL http://www.springerlink.com/index/10.1007/978-3-540-85428-9.

H. von Löhneysen. Disorder, electron-electron interactions and the metal-insulator transition in heavily doped Si:P. Advances in Solid State Physics, 40:143–167, 2000. URL http://link.springer.com/chapter/10.1007/BFb0108351.

Franz Wegner. Anomalous dimensions for the nonlinear sigma-model in 2 + ϵ dimensions (II). Nuclear Physics B, 280:210–224, January 1987. ISSN 05503213. doi: 10.1016/0550-3213(87)90145-3. URL http://www.sciencedirect.com/science/article/pii/0550321387901453http://linkinghub.elsevier.com/retrieve/pii/0550321387901453.

Alexander Weiße, Gerhard Wellein, Andreas Alvermann, and Holger Fehske. The kernel polynomial method. Reviews of Modern Physics, 78(1):275–306, March 2006. ISSN 0034-6861. doi: 10.1103/RevModPhys.78.275. URL http://link.aps.org/doi/10.1103/RevModPhys.78.275.

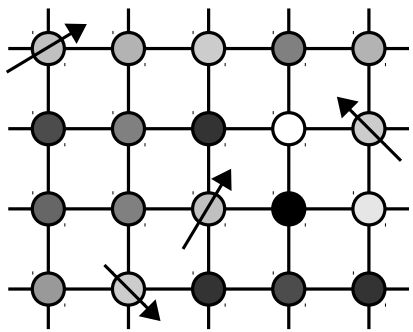
The Anderson-Heisenberg model

Full Hamiltonian:

$$\mathrm{H} = \mathrm{H}_0 + \mathrm{H}_\mathrm{S}$$

Anderson model (with spin):

$$\mathrm{H}_0 = t \sum_{\langle i,j\rangle,\sigma} |j,\sigma\rangle \langle i,\sigma| + \sum_{i,\sigma} \varepsilon_i \, |i,\sigma\rangle \langle i,\sigma|$$



Exchange coupling to classical magnetic impurities:

$$\mathrm{H}_\mathrm{S} = \sum_i J_i \, \mathbf{s}_i \cdot \mathbf{S}_i$$

$$\mathbf{s}_i = \frac{\hbar}{2}\sigma_i$$

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Alternative formulation:

$$\mathrm{H}_\mathrm{S} = S \sum_{i=1}^{N} J_i \left(\cos\theta_i \sum_{\sigma=\pm 1} \sigma \, |i,\sigma\rangle \langle i,\sigma| + \sin\theta_i \sum_{\sigma=\pm 1} \exp(i\sigma\varphi_i) \, |i,\sigma\rangle \langle i,-\sigma| \right)$$

Detailed calculation of Chebychev moments

Chebychev moments for the LDOS:

$$\mu_m^{(i)} = \int_{-1}^{1} \tilde{\rho}_i(\tilde{E})\, T_m(\tilde{E})\, \mathrm{d}\tilde{E}$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \left|\langle i|k\rangle\right|^2 \int_{-1}^{1} T_m(\tilde{E})\, \delta(\tilde{E} - \tilde{E}_k)\, \mathrm{d}\tilde{E}$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \left|\langle i|k\rangle\right|^2 T_m(\tilde{E}_k)$$

$$= \frac{1}{N} \sum_{k,k'=0}^{N-1} \langle i|k\rangle \langle k|\, T_m(\tilde{H})|k'\rangle \langle k'|i\rangle$$

$$= \frac{1}{N} \langle i|\, T_m(\tilde{H})|i\rangle$$

Chebychev moments for the DOS:

$$\mu_m = \int_{-1}^{1} \tilde{\rho}(\tilde{E})\, T_m(\tilde{E})\, \mathrm{d}\tilde{E}$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \int_{-1}^{1} T_m(\tilde{E})\, \delta(\tilde{E} - \tilde{E}_k)\, \mathrm{d}\tilde{E}$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} T_m(\tilde{E}_k)$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \langle k|\, T_m(\tilde{H})|k\rangle$$

$$= \frac{1}{N} \mathrm{Tr}\; T_m(\tilde{H})$$

Weiße et al. (2006)

Sample variance of the geometric mean I

The arithmetic mean $\bar{x}$ of a discrete random variable x is defined as

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \quad , \tag{1}$$

where N is the sample size. It is a good estimator for the population mean. Its (unbiased) sample variance is well known,

$$\sigma_x^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2 = \frac{\overline{x^2}}{N-1} - \frac{\bar{x}^2}{N(N-1)} \quad . \tag{2}$$

We introduce the quantity y, which is defined as the logarithm of the random variable x, $y = \log x$. Its arithmetic mean and variance is calculated according to (1) and (2),

$$\bar{y} = \overline{\log x} = \frac{1}{N}\sum_{i=1}^{N} \log x_i \quad ,$$

$$\sigma_y^2 = \sigma_{\log x}^2 = \frac{1}{N-1}\sum_{i=1}^{N}(\log x_i - \overline{\log x})^2 = \frac{\overline{(\log x)^2}}{N-1} - \frac{\overline{\log x}^2}{N(N-1)} \quad .$$

Sample variance of the geometric mean II

Now, the geometric mean of x is

$$z = \mathrm{e}^{\overline{\log x}} = \mathrm{e}^{y} \quad .$$

We estimate the statistical error of z, given by its standard deviation σ_z, by

$$\sigma_z = z_1 - z_2 = \mathrm{e}^{\bar{y}}(\mathrm{e}^{\sigma_y} - 1) \quad ,$$

with

$$z_1 = \mathrm{e}^{\bar{y}+\sigma_y}$$

$$z_2 = \mathrm{e}^{\bar{y}} \quad .$$

Assuming σ_y to be small, we approximate

$$\sigma_z = \mathrm{e}^{\bar{y}}(\mathrm{e}^{\sigma_y} - 1) \approx \mathrm{e}^{\bar{y}}\sigma_y$$

and hence the estimate of the sample variance of the geometric mean is given by

$$\sigma_z^2 \approx \mathrm{e}^{2\bar{y}}\sigma_y^2 \quad .$$

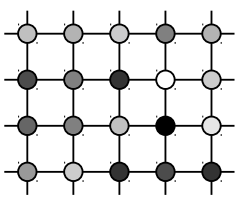
The same result has been obtained by Norris Norris (1940) using more profound mathematical arguments.

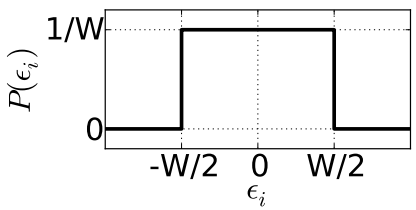
The Anderson model I

Anderson model:

$$\mathrm{H} = t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \varepsilon_i c_i^\dagger c_i$$

Random potentials ε_i:





W: Measure for disorder

The Anderson model I

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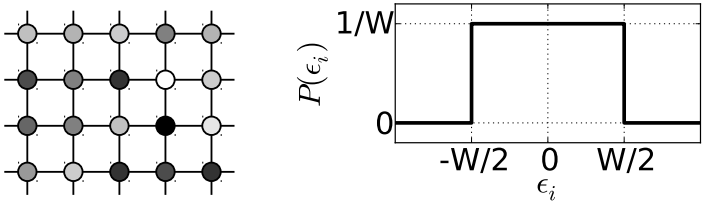
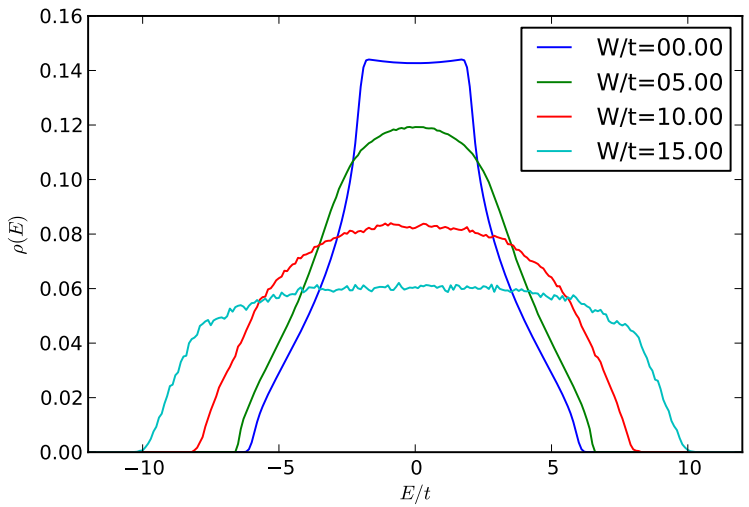


W: Measure for disorder

What happens if translational symmetry gets lost?
→ Bloch theory not applicable anymore

Density of states:

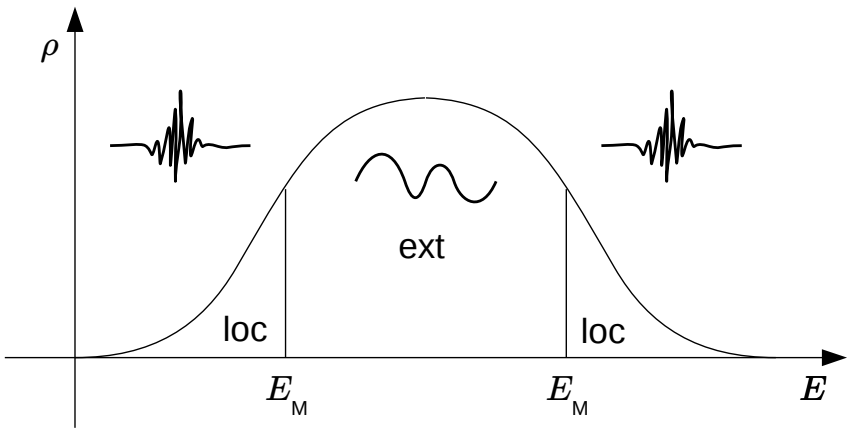


→ Bandwidth increases with W
→ Van-Hove singularities disappear

Anderson (1958)

The Anderson model II

Emergence of localized states in the band tails.
$W > 0$: Localized states emerge

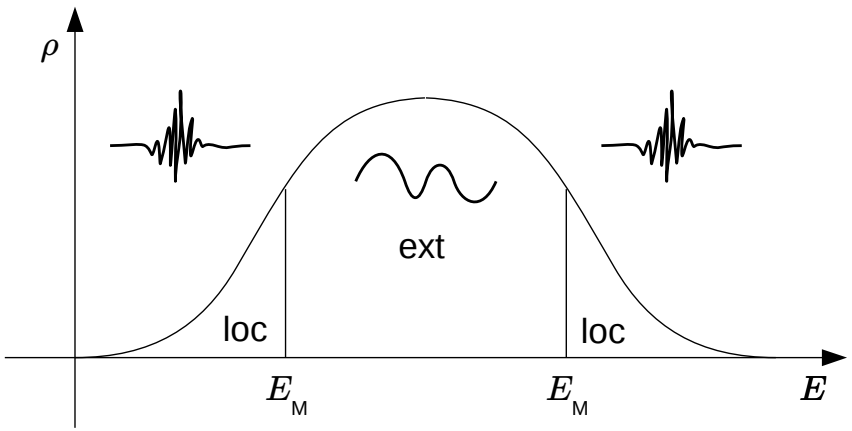


Mobility edges E_M:
Separating energies of localized and extended states

Critical disorder W_c: Mobility edges collapse in the band center
$\rightarrow$ Metal-insulator transition

The Anderson model II

Emergence of localized states in the band tails.
$W > 0$: Localized states emerge



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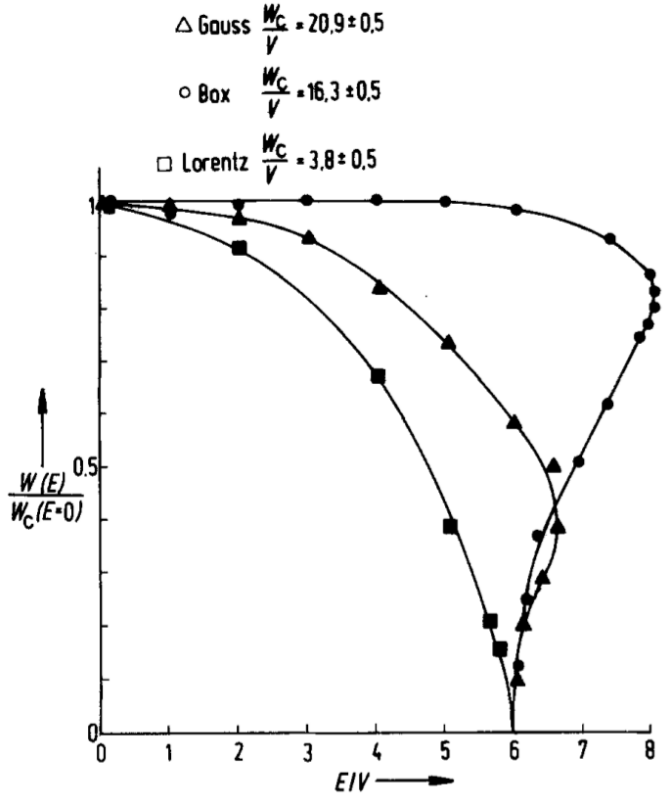
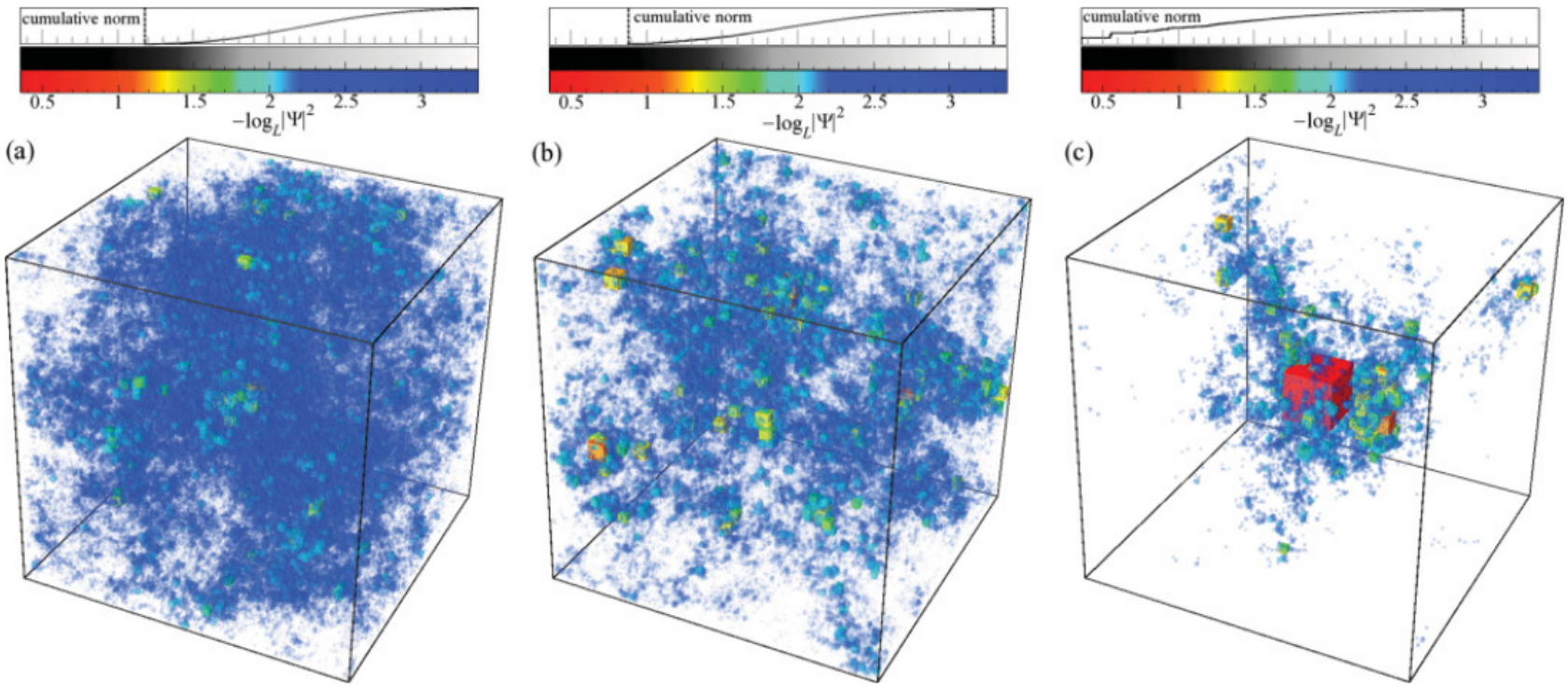
Phase diagram:



→ Mobility edge as function of disorder
Bulka et al. (1987)

3D Anderson model: Visualizing eigenstates

Wave function intensity, $N = 120^3$, $E = 0$



$W/t = 15$
Extended state

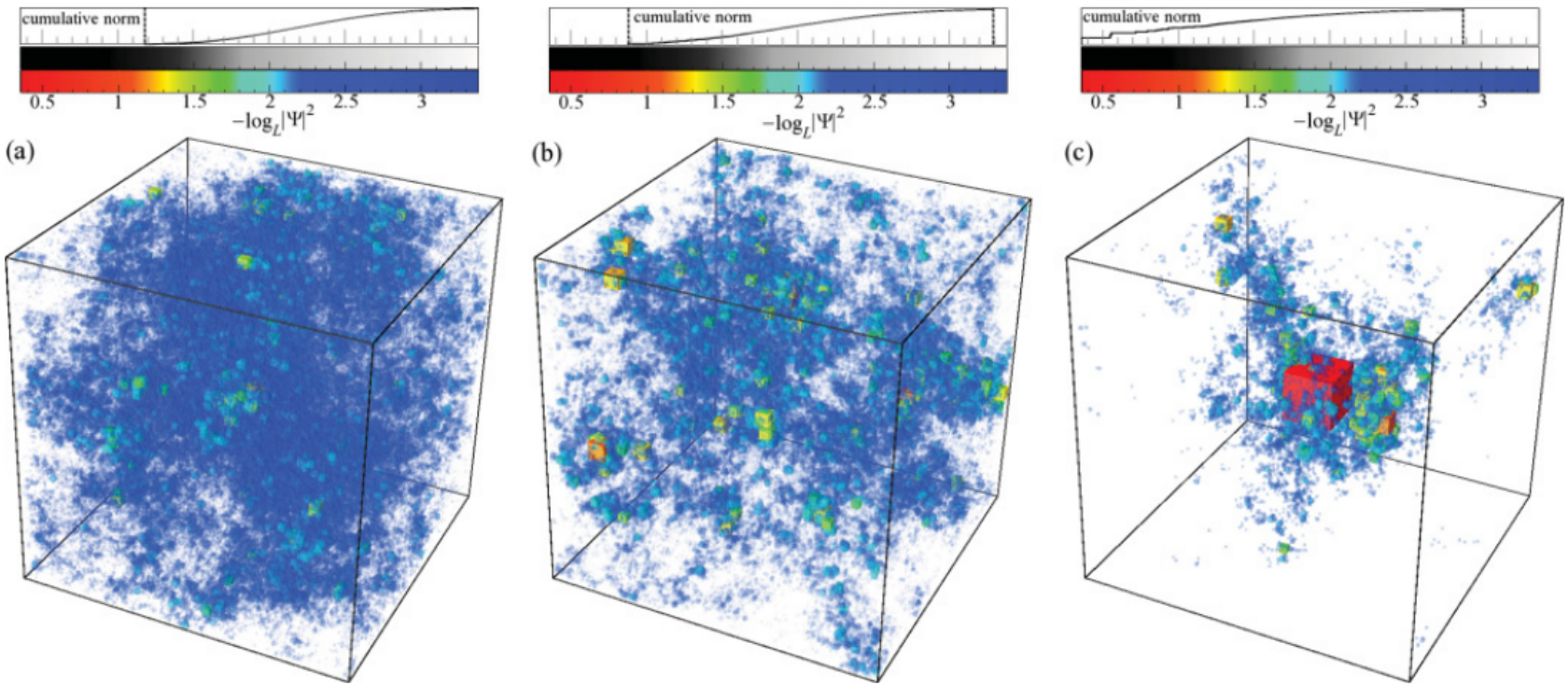
$W/t = 16.5$
Critical state

$W/t = 18$
Localized state

Rodriguez et al. (2011)

3D Anderson model: Visualizing eigenstates

Wave function intensity, $N = 120^3$, $E = 0$



$W/t = 15$
Extended state

$W/t = 16.5$
Critical state
$\rightarrow$ Multifractal

$W/t = 18$
Localized state

Rodriguez et al. (2011)

Multifractality

Electronic wave functions at the MIT are multifractal.

Fractals:

- Self-similarity on all scales
- Fractal dimension D, not necessarily integer

Multifractal objects:

- More than one fractal dimension D

Wave function intensity:

$$\left|\psi(\mathbf{r})\right|^2 \sim L^{-\alpha}$$

Broad distribution of exponents α:

$$P(\alpha) = L^{-\frac{(\alpha-\alpha_0)^2}{4(\alpha_0-d)}}$$

Evers and Mirlin (2008); Kettemann et al. (2009)

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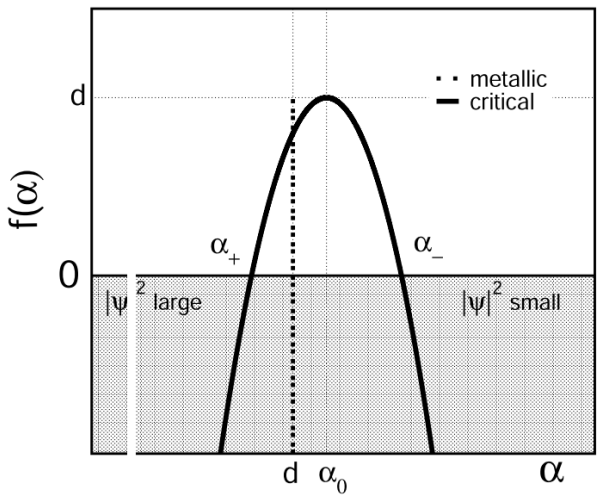
Evers and Mirlin (2008); Kettemann et al. (2009)

Singularity spectrum $f(\alpha)$:



$\rightarrow$ Approximately parabolic, with maximum at α_0

Interpretation of $f(\alpha)$:
Fractal dimension of those points in space where the WFI scales like $L^{-\alpha}$.

Multifractal analysis: Obtain critical parameters of the MIT with high precision

Kernel damping

The Gibbs phenomenon

- Strong oscillations near sharp features (sharp peaks, discontinuities)
- Solution: Multiply Chebychev moments by kernel factors

Dirichlet kernel (trivial case):

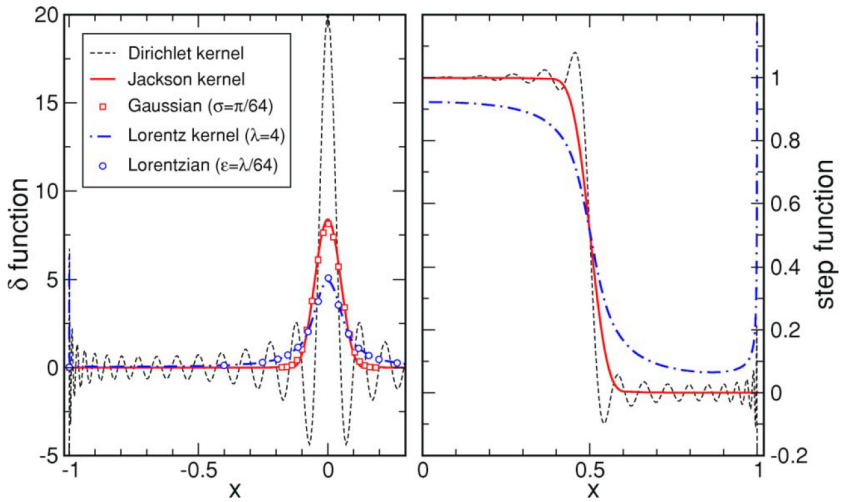
$$g_m^{\mathrm{D}} = 1$$

Jackson kernel (best for DOS and LDOS):

$$g_m^{\mathrm{J}} = \frac{(M-m+1)\cos\frac{\pi m}{M+1} + \sin\frac{\pi m}{M+1}\cot\frac{\pi}{M+1}}{M+1}$$

Weiße et al. (2006)

Comparison of different kernels:



Apply kernel:

$$\mu_m \to g_m \mu_m$$

Spectral dependence of the energy resolution

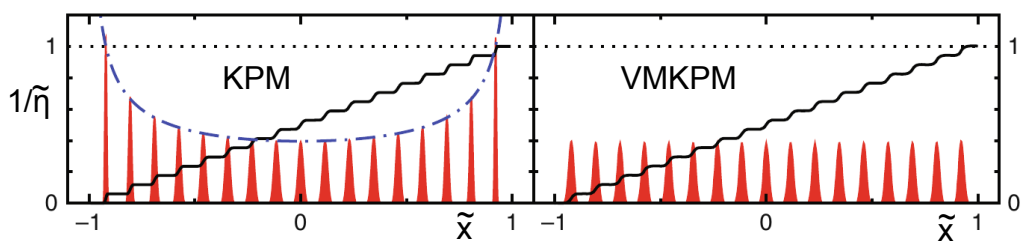
KPM + Jackson kernel

- δ-peak at $\tilde{E} = (E - b)/a$ is well approximated by a Gaussian of width $\tilde{\eta}$ (HWHM)
- $\tilde{\eta}$ depends on the spectral variable $\tilde{x} \in [-1, 1]$

$$\tilde{\eta}(\tilde{E}) = \sqrt{\frac{M - \tilde{x}^2(M-1)}{2(M+1)}(1 - \cos(2\phi))} \approx \frac{\pi}{M}\sqrt{1 - \tilde{x}^2 + \frac{4\tilde{x}^2 - 3}{M}} \quad , \quad \phi = \pi/(\mathrm{M}{+}1)$$

Simple form at $\tilde{x} = 0$:

$$\tilde{\eta} \approx \frac{\pi}{M}$$



Possibility to adjust the truncation limit M to keep η constant
→ Variable-moment KPM (VMKPM)

Schubert and Fehske (2009)