IWDS08, Benasque, August 2012

Multifractal scaling and universality at the 3-D Anderson transition

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Outline

1. Localization Phenomena — some experimental results —
2. Localization-Delocalization transition: critical (multifractal) states
3. 3-D Anderson Model
4. What's a Multifractal?
   - Multifractal Analysis (MFA) and Distribution Function (PDF) of $|\psi|^2$
5. Multifractal Finite Size Scaling (MFSS)
   - Obtaining critical parameters and multifractal exponents
6. Conclusions

Localization Phenomena

Quantum dynamics of a particle in a 1-D atomic chain

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PERIODIC **DISORDERED**

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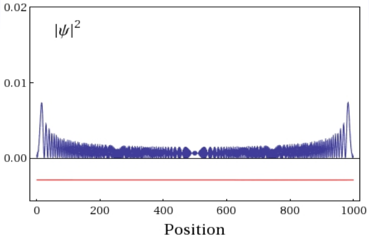

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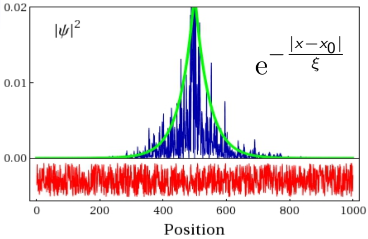

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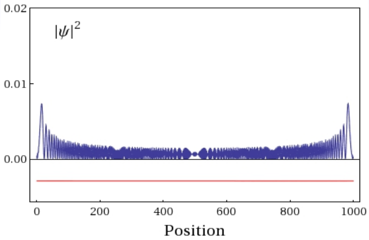

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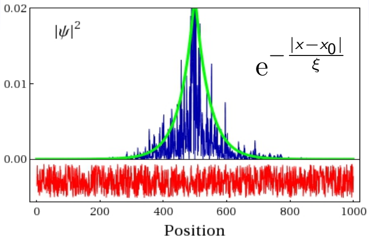


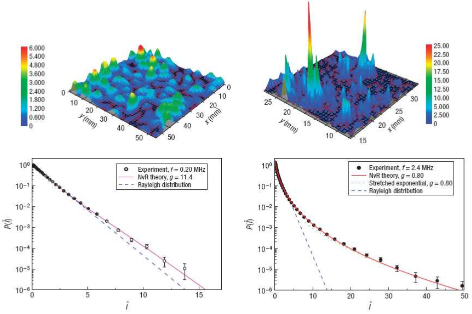
ANDERSON LOCALIZATION [P. W. Anderson, 1958]

- **exponential decay** of wavefunctions and **suppression of transport** due to disorder
- consequence of **destructive interference**. Relevant in **quantum** and **classical** systems

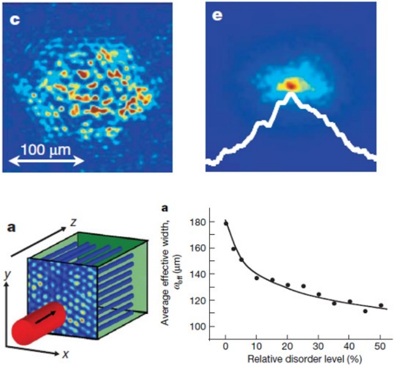
Localization Phenomena

Experimental observations of Anderson localization

Localization of ultrasound in a three-dimensional elastic network
H. Hu *et al.*, Nat. Phys. 4, 945 (2008)



Transport and Anderson localization in disordered 2-D photonic lattices
T. Schwartz *et al.*, Nature 446, 52 (2007)

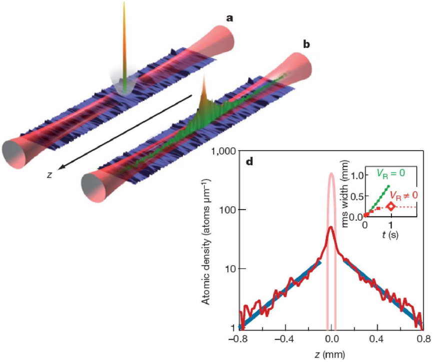


Localization Phenomena

Experimental observations of Anderson localization

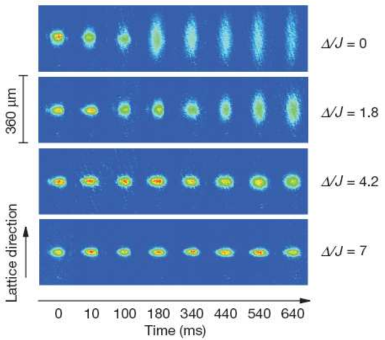
Direct observation of Anderson localization of matter waves in a controlled disorder

J. Billy *et al.*, Nature 453, 891 (2008)



Anderson localization of a non-interacting Bose-Einstein condensate

G. Roati *et al.*, Nature 453, 895 (2008)



Localization Phenomena

Understanding localization phenomena and the localization-delocalization transition is of fundamental importance

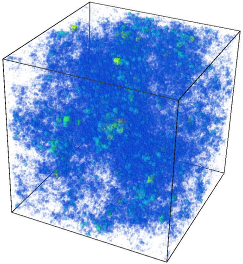
- Classical transport processes
  Propagation of electromagnetic and acustic waves
- Condensed matter systems
  Electronic and phonon localization, metal-insulator transitions, Quantum Hall physics
- Classically chaotic quantum systems
  Dynamical localization in momentum space
- Transport processes in biological and molecular systems
  Charge transport in DNA strands

The Anderson Transition: critical states

Electronic states in a solid with a **disordered potential** energy

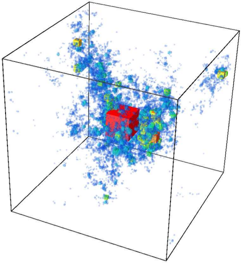
Phase Transition from **metallic** to **insulating** behaviour

EXTENDED
(metal)



$$|\psi(\mathbf{r})|^2 \underset{L\to\infty}{\sim} L^{-d}$$

LOCALISED
(insulator)



$$|\psi(\mathbf{r})|^2 \sim \mathrm{e}^{-\frac{|\mathbf{r}-\mathbf{r}_0|}{\xi}}$$

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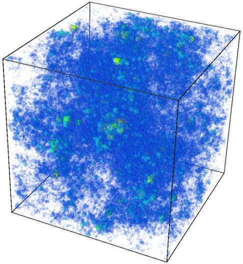

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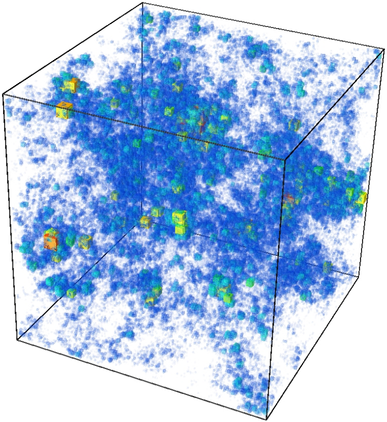

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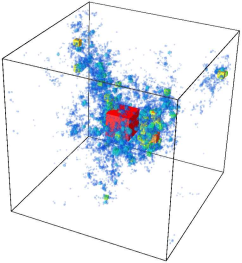

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CRITICAL STATE: Large fluctuations of $|\psi|^2$ at all length scales

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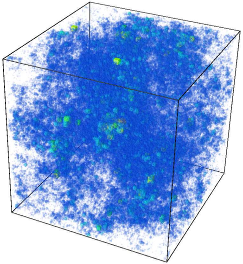

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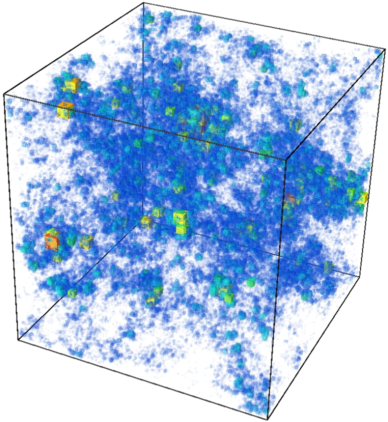

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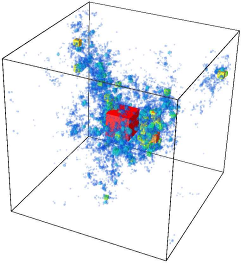

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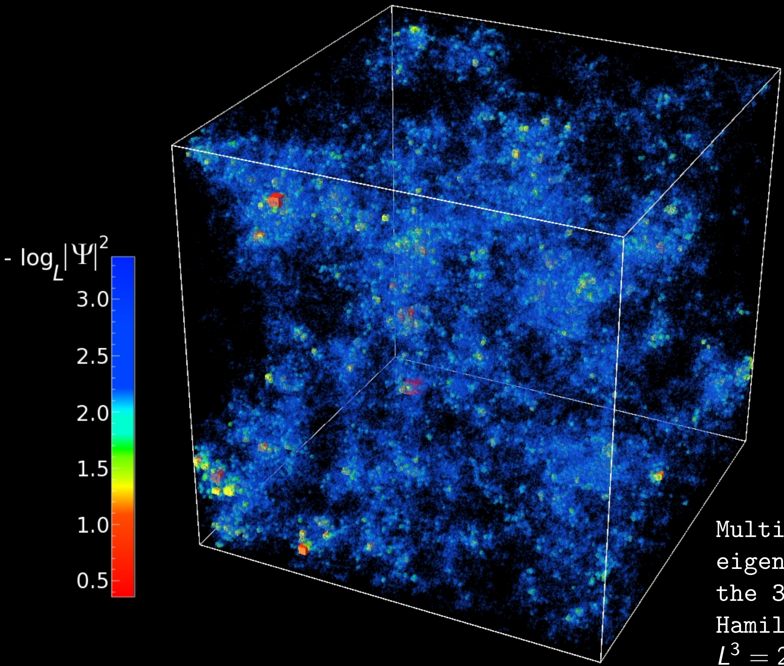
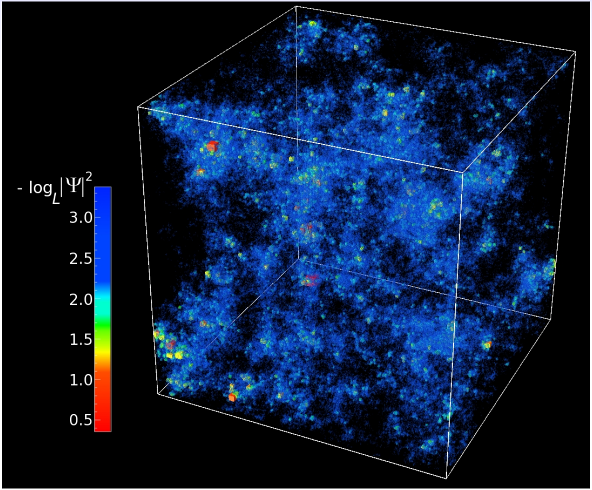


Multifractal eigenstate of the 3-D Anderson Hamiltonian for $L^3 = 240^3$

The Anderson Transition: critical states

- Visualization of 3-D multifractality



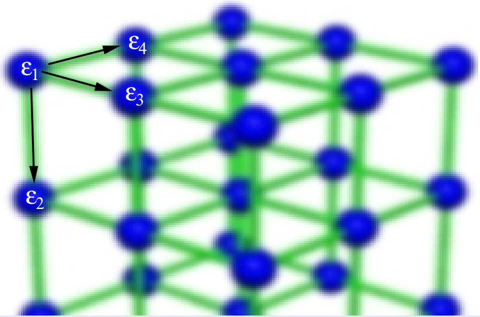
Critical eigenstate of the 3-D Anderson Hamiltonian for $L^3 = 240^3$

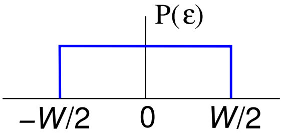
3-D Anderson Model

$$\mathcal{H} = \sum_k \varepsilon_k \left|k\right\rangle\left\langle k\right| + \ t \left|k\right\rangle\left\langle k-1\right| + t \left|k\right\rangle\left\langle k+1\right|$$

$k \equiv (x, y, z) \longrightarrow$ 3-D spatial coordinate of the L^3 system

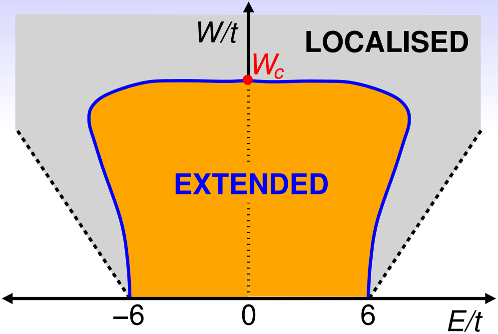
Random onsite energies: $\varepsilon_k \in \left[-\frac{W}{2}, \frac{W}{2}\right]$, $W \equiv$ degree of disorder

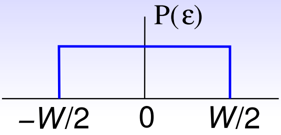




3-D Anderson Model

Phase Diagram

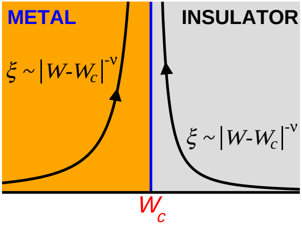




$W_c \equiv$ critical disorder

$W_c \sim 16.5$

- **Transition at fixed energy E = 0**
  The localization (correlation) length ξ diverges as $\xi \sim |W - W_c|^{-\nu}$, as we approach the transition from the insulating (metallic) side
  K. Slevin and T. Ohtsuki, Phys. Rev. Lett. 82, 382 (1999): $\nu = \mathbf{1.57(55, 59)}$ **via TMM**



Meaning of 'multifractal': the spectrum $f(\alpha)$

Wavefunction intensity: $|\psi(\mathbf{r})|^2 \equiv L^{-\alpha}$, $\quad \alpha \equiv -\ln|\psi(\mathbf{r})|^2/\ln L$
The volume of the set of points with the same α scales as $\mathcal{N}_\alpha \sim L^{f(\alpha)}$.

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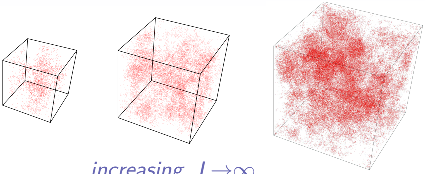
$\alpha \in [\alpha_1, \alpha_1 + \Delta\alpha]$



$\mathcal{N}_{\alpha_1} \sim L^{f(\alpha_1)}$

increasing $L \to \infty$

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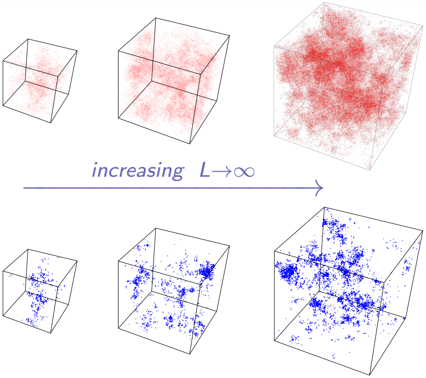

$\alpha \in [\alpha_2, \alpha_2 + \Delta\alpha]$ $\quad \mathcal{N}_{\alpha_2} \sim L^{f(\alpha_2)}$

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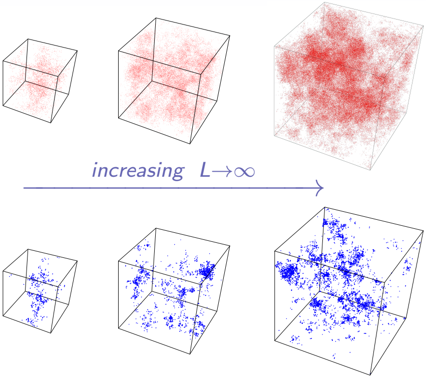


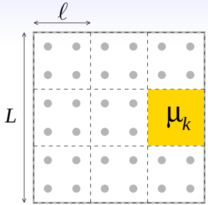
$\alpha \in [\alpha_2, \alpha_2 + \Delta\alpha]$ $\qquad \mathcal{N}_{\alpha_2} \sim L^{f(\alpha_2)}$

f(α) is the set of fractal dimensions of the different α-sets

Standard Multifractal Analysis (MFA) at criticality

- **Obtaining $f(\alpha)$: Scaling of the Inverse Participation Ratios (IPR)**

M. Janssen, Int. J. Mod. Phys. B 8, 943 (1994)



$$\mu_k = \sum_{j \in \text{box } k} |\psi_j|^2 \rightarrow \boxed{R_q \equiv \sum_k \mu_k^q}$$

q-moments of wavefunction

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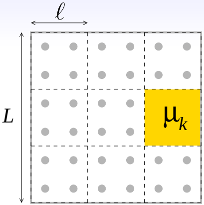

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q-moments of wavefunction

$$\boxed{\langle \mathbf{R_q} \rangle \underset{\lambda \to 0}{\propto} \left(\frac{\ell}{\mathbf{L}} \right)^{\tau_q}}$$

Scale invariance at criticality

$\lambda \equiv \ell / \mathbf{L}$

only relevant scale

$\langle \cdots \rangle$ = average over realizations of disorder

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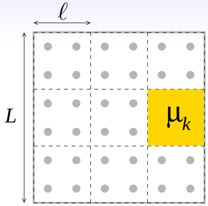

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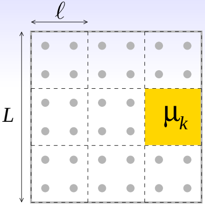
$\langle \cdots \rangle$ = average over realizations of disorder

- **τ_q and $f(\alpha)$ are related by a Legendre transformation**

$$\tau_q = \lim_{\lambda \to 0} \frac{\ln \langle R_q \rangle}{\ln \lambda} \longrightarrow \begin{cases} \alpha_q = \mathrm{d}\tau_q / \mathrm{d}q \\ f(\alpha_q) = q\, \alpha_q - \tau_q \end{cases}$$

'q' parametrizes the values of α and $f(\alpha)$

Standard Multifractal Analysis (MFA) at criticality



$$\mu_k(\ell) = \sum_j |\Psi_j|^2 \;\Rightarrow\; \boxed{R_q(\ell) = \sum_k \mu_k^q(\ell)}$$

Generalised Inverse Participation Ratios

Scaling Law for gIPR

$$\langle \mathbf{R_q}(\boldsymbol{\lambda})\rangle \propto \boldsymbol{\lambda}^{\boldsymbol{\tau}(\mathbf{q})}$$

$$\lambda \equiv \ell/L$$

$$\Rightarrow \begin{cases} \alpha_q = \mathrm{d}\tau(q)/\mathrm{d}q \\ f(\alpha_q) = q\,\alpha_q - \tau(q) \end{cases}$$

$$\tau(q) = \lim_{\lambda\to 0} \frac{\ln\langle R_q(\lambda)\rangle}{\ln\lambda} \Rightarrow \begin{cases} \alpha_q = \lim_{\lambda\to 0} \frac{1}{\ln\lambda}\left\langle \sum_k \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \ln \mu_k(\lambda) \right\rangle \\ f(\alpha_q) = \lim_{\lambda\to 0} \frac{1}{\ln\lambda}\left\langle \sum_k \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \ln \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \right\rangle \end{cases}$$

Approaching the Thermodynamic Limit

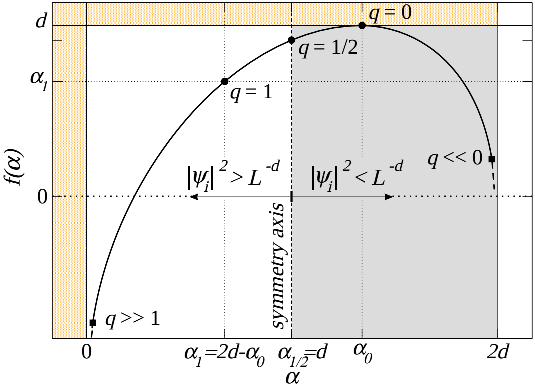
- varying $\ell \to 0$ **BOX-SIZE SCALING**
- varying $L \to \infty$ **SYSTEM-SIZE SCALING**

General features of $f(\alpha)$

- Since $|\Psi_j|^2 \leqslant 1 \;\Rightarrow\; \alpha \geqslant 0$
- $f(\alpha)$ can have negative values!
- Convex function. Maximum at $f(\alpha_0 > d) = d$
- Independent of all length scales, e.g. L

Symmetry Law: $f(2d-\alpha) = f(\alpha)+d-\alpha$

A. D. Mirlin, Y .V Fyodorov, A .Mildenberger, F. Evers, Phys. Rev. Lett. 97, 046803 (2006)



- Changing q in $\langle|\Psi_j|^{2q}\rangle$ we obtain different α_q: we sample different values of $|\Psi_j|^2$
- Parametrization of wavefunction: $|\Psi_j|^2 = L^{-\alpha}$
- Number of points with the same α: $\mathcal{N}_\alpha \sim L^{f(\alpha)}$

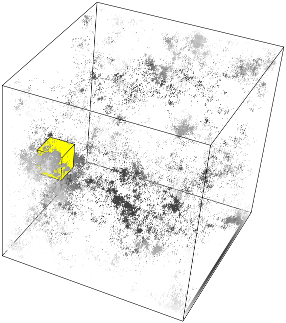
Negative fractal dimensions

Measuring the 'degree of emptiness' of a set

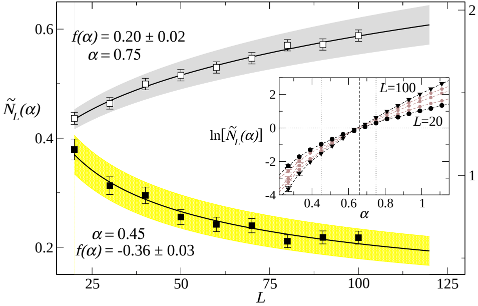
- B.B.Mandelbrot, J. Stat. Phys. 110, 739 (2003)

Scaling of the volume of the α-set: $\widetilde{\mathcal{N}}_L(\alpha) \equiv L^d \frac{\mathcal{P}_L(\alpha)}{\mathcal{P}_L(\alpha_0)} \Rightarrow \widetilde{\mathcal{N}}_L(\alpha) = L^{f(\alpha)}$

- $f(\alpha) < 0$ corresponds to those α-sets whose volume decreases with L.
- **RARE EVENTS**: localized-like regions of anomalously high $|\Psi_i|^2$



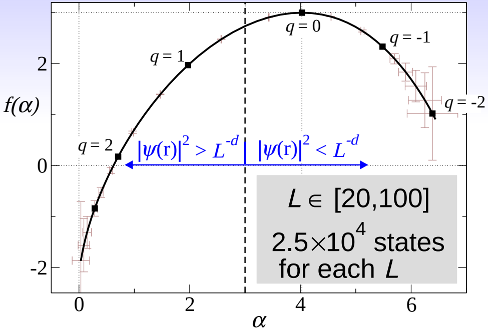
The yellow box encloses a single site with $|\Psi_i|^2 = 0.45$



Numerically calculated $f(\alpha)$

- **$f(\alpha)$ is independent of all length scales, e.g. L, ℓ**
- Changing q we sample different values of $|\psi(\mathbf{r})|^2 \equiv L^{-\alpha}$
- The number of points with the same α scales as $L^{f(\alpha)}$

Vasquez, Rodriguez, Römer, PRB 78, 195106; 195107 (2008)



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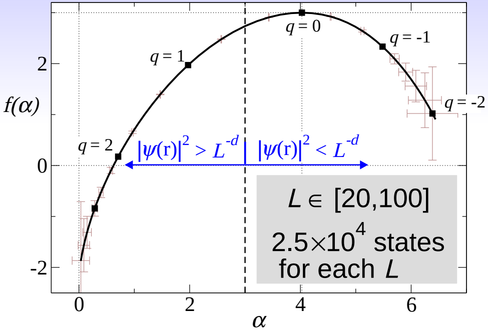


$f(\alpha)$ from the Probability Density Function (PDF) $\mathcal{P}(\alpha)$

Probability that $\alpha \equiv -\frac{\ln|\psi(\mathbf{r})|^2}{\ln L}$ lies in $[\alpha, \alpha + d\alpha] \Rightarrow \boxed{\mathcal{P}(\alpha) \propto L^{f(\alpha)-d}}$

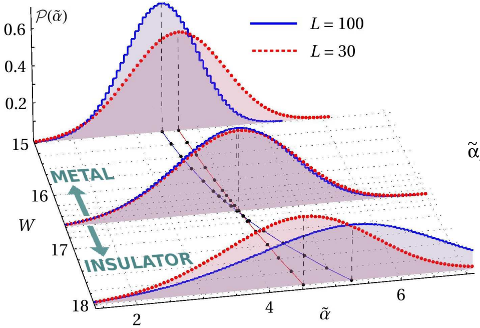
$f(\alpha)$ can be obtained from histograms of wavefunction intensities

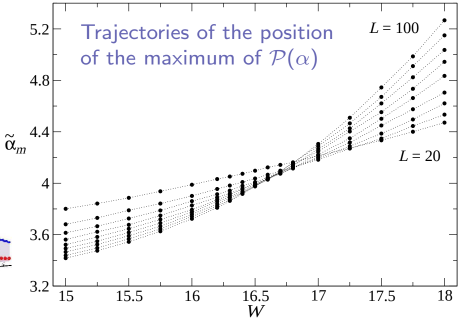
Rodriguez, Vasquez, Römer, PRL 102, 106406 (2009)

Scaling of the Probability Density Function $\mathcal{P}(\alpha)$

$$\mu_k = \sum_{j \in \text{box } k} |\psi_j|^2 \rightarrow \mu \equiv \left(\frac{L}{\ell}\right)^{-\alpha}, \alpha \equiv \frac{\ln \mu}{\ln(\ell/L)} \xrightarrow[\text{at critical point}]{\text{multifractality}} \boxed{\mathcal{P}(\alpha) \propto \left(\frac{L}{\ell}\right)^{f(\alpha)-d}}$$

SCALING AT FIXED $\lambda = \ell/L$

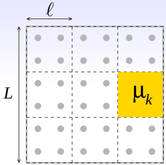




Can we extend the MFA formalism to describe this scaling behaviour and quantitatively characterise the transition?

Extension of the MFA formalism

- **Scaling of the Inverse Participation Ratios at W_c (critical point)**



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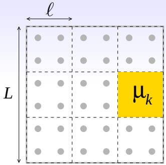
Extension of the MFA formalism

- **Scaling of the Inverse Participation Ratios at W_c (critical point)**



$\mu_k = \sum_j |\psi_j|^2 \quad \rightarrow \quad R_q \equiv \sum_k \mu_k^q$

$$\langle \mathbf{R_q} \rangle \underset{\lambda \to 0}{\propto} \left(\frac{\ell}{\mathbf{L}} \right)^{\tau_q}$$

Scale invariance at criticality

$\boldsymbol{\lambda \equiv \ell / L}$

only relevant scale

- **No scale invariance at** $W \neq W_c \Rightarrow R_q$ will depend on W, L, ℓ

Scaling hypothesis close to the transition:

$$\langle R_q \rangle (W, L, \ell) = \lambda^{\tau_q} \mathcal{R}_q \left(\frac{L}{\xi}, \frac{\ell}{\xi} \right)$$

where $\xi(W) \propto |W - W_c|^{-\nu}$ is the localization $(W > W_c)$ / correlation $(W < W_c)$ length.

Extension of the MFA formalism

Close to the transition:

$$\langle R_q \rangle(W, L, \ell) = \lambda^{\tau_q} \, \mathcal{R}_q \left(\frac{L}{\xi}, \frac{\ell}{\xi} \right), \qquad \lambda \equiv \frac{\ell}{L}, \quad \xi \propto |W - W_c|^{-\nu}$$

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GENERALISED MULTIFRACTAL EXPONENTS

$$\frac{\ln\langle R_q\rangle}{\ln\lambda} \equiv \;\; \boldsymbol{\widetilde{\tau}_q(W,L,\ell) = \tau_q + \frac{q(q-1)}{\ln\lambda}\mathcal{T}_q\left(L/\xi,\ell/\xi\right)}$$

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↓ *Legendre transformation*

$$\frac{\langle\sum_k \mu_k^q \ln\mu_k\rangle}{\langle R_q\rangle\ln\lambda} \equiv \widetilde{\alpha}_q(W,L,\ell) = \alpha_q + \frac{1}{\ln\lambda}\mathcal{A}_q\left(L/\xi,\ell/\xi\right)$$

$$\widetilde{f}(\widetilde{\alpha}_q) = q\,\widetilde{\alpha}_q - \widetilde{\tau}_q$$

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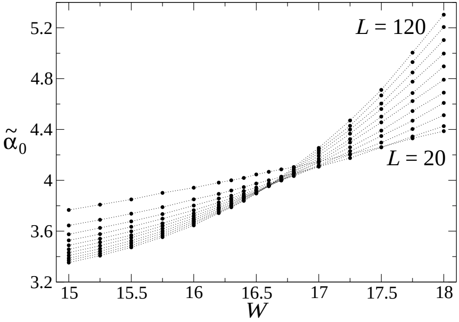
Critical parameters W_c, ν and multifractal exponents can be obtained from finite size scaling studies using $\widetilde{\tau}_q$, $\widetilde{\alpha}_q$, and the probability density function $\mathcal{P}(\alpha)$.

First test: Finite Size Scaling (FSS) at fixed $\lambda \equiv \frac{\ell}{L}$

$$\widetilde{\alpha}_q(W, L, \ell) \xrightarrow{\text{fixed } \lambda} \widetilde{\alpha}_q(W, L) = \mathcal{F}(L/\xi) \longrightarrow \boxed{\widetilde{\boldsymbol{\alpha}}_{\mathbf{q}} = \boldsymbol{\mathcal{F}}\left(\boldsymbol{\rho}\mathbf{L}^{1/\boldsymbol{\nu}}, \boldsymbol{\eta}\mathbf{L}^{-|\mathbf{y}|}\right)}$$

$\rho \equiv \rho(W)$, $\eta \equiv \eta(W)$ are the **relevant** and **irrelevant scaling fields**.



$\mathcal{F}$ is Taylor expanded in their variables $(\rho L^{1/\nu}, \eta L^{-|y|})$ and the fields $\rho(W), \eta(W)$ are subsequently expanded in the degree of disorder W around the critical value W_c.

The localization(correlation) length is obtained via $\xi = |\rho(W)|^{-\nu}$.

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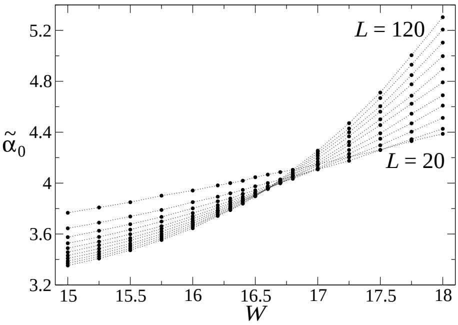

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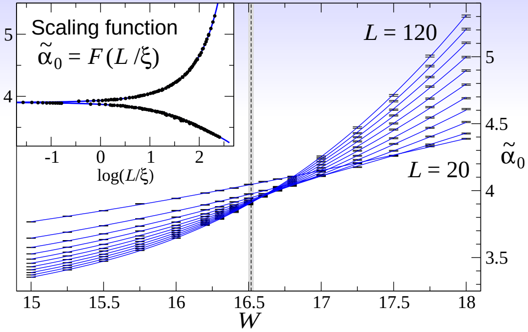
Results from one-parameter FSS at fixed λ

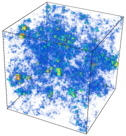


System sizes: $\mathbf{L^3 = 20^3, \ldots, 120^3}$

Disorder values: $\mathbf{W \in [15.0, 18.0]}$

$\sim$ **5 000** states for each pair (W, L)

$\sim \mathbf{10^6}$ wavefunctions



	λ	ν	W_c	N_D	N_P	χ^2	Q
$\widetilde{\alpha}_0$	0.1	1.61(59,63)	16.52(50,53)	187	10	175	0.5
$\widetilde{\alpha}_{-0.5}$	0.1	1.62(60,64)	16.52(50,54)	187	10	184	0.3
$\widetilde{\tau}_{1.5}$	0.1	1.62(57,69)	16.48(43,53)	187	11	175	0.5
$\widetilde{\tau}_{-1}$	0.1	1.62(60,64)	16.52(50,54)	187	10	181	0.4

Multifractal FSS: two-variable scaling

- Multifractal FSS provides a simultaneous estimation of the critical parameters W_c, ν, and the scale invariant multifractal exponents

$$\widetilde{\alpha}_q(L/\xi, \ell/\xi) = \alpha_q + \frac{1}{\ln(\ell/L)} \mathcal{A}_q\left(L/\xi, \ell/\xi\right)$$

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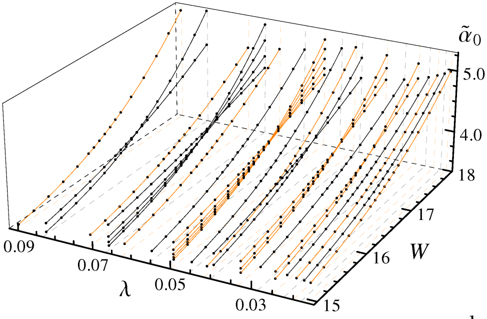

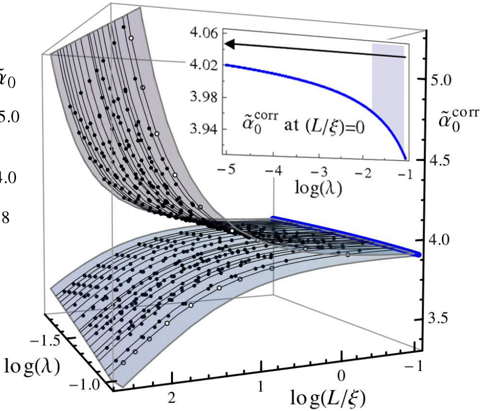

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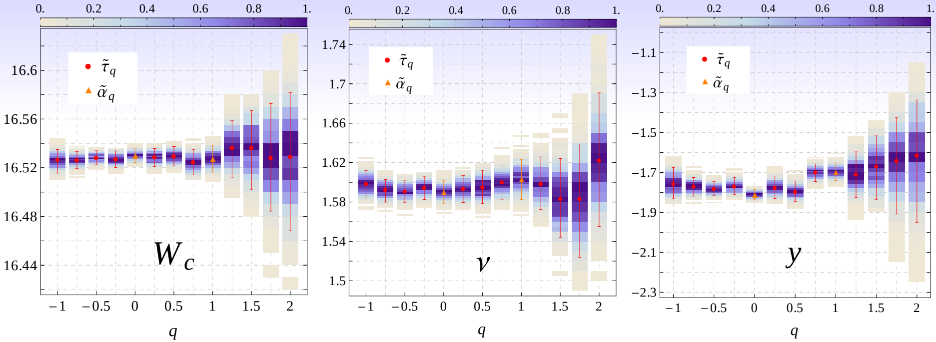


MF exponent	ν	W_c	N_D(prec.%)	N_P	χ^2	Q
$\widetilde{\tau}_{-1}$	−7.844(854, 832)	1.598(584, 612)	16.526(516, 535)	680 (0.27)	25	667	0.4
$\widetilde{\alpha}_0$	4.048(045, 050)	1.590(579, 602)	16.530(524, 536)	493 (0.05)	27	473	0.4
$\widetilde{\alpha}_1$	1.958(953, 963)	1.603(583, 623)	16.528(516, 538)	612 (0.12)	27	597	0.3
$\widetilde{\tau}_2$	1.237(208, 273)	1.622(555, 691)	16.529(468, 582)	544 (0.41)	19	566	0.1

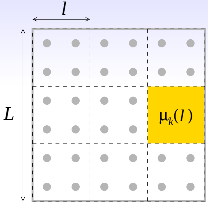
Conclusions

- *Generalisation of multifractal formalism* to study Anderson transitions
  Valuable approach to analyse wavefunction and LDOS experimental data
- The PDF of wavefunction amplitudes can be used to monitor and characterise the Anderson transition
- *Multifractal finite size scaling* allows simultaneous estimation of critical parameters and multifractal exponents
- Universality of the localization-delocalization transition
  most recent estimates for ν in 3-D:
  - 3-D Anderson model (MFSS): $\nu = 1.590(579, 602)$
  - electrons with topological disorder: $\nu = 1.61(55, 68)$
    [Krich and Aspuru-Guzik, PRL 106, 156405 (2011)]
  - disordered Leonard-Jones fluid: $\nu = 1.60(53, 67)$
    [Haung and Wu, PRE 79, 041105 (2009)]
  - self-consistent theory of localization $\nu = 1.5$ does not agree
    [Garcia-Garcia, PRL 100, 076404 (2008)]

Further Reading

- *Multifractal finite-size scaling and universality at the Anderson transition*, A. Rodriguez, L. J. Vasquez, K. Slevin, RAR, Phys. Rev. B 84, 134209 (2011)
- *Critical parameters from generalised multifractal analysis at the Anderson transition*, A. Rodriguez, L. J. Vasquez, K. Slevin, RAR, Phys. Rev. Lett. 105, 046403 (2010)
- *Multifractal analysis with the probability density function at the 3D Anderson transition*, A. Rodriguez, L. J. Vasquez, RAR, Phys. Rev. Lett. 102, 106406 (2009)

Standard Multifractal Analysis (MFA)



$\mu_k(l) = \sum_j |\Psi_j|^2 \;\Rightarrow\; \boxed{R_q(l) = \sum_k \mu_k^q(l)}$ Generalised Inverse Participation Ratios

Scaling Law for gIPR

$$\langle \mathbf{R_q(\lambda)} \rangle \propto \boldsymbol{\lambda}^{\boldsymbol{\tau}(\mathbf{q})}$$

$$\Rightarrow \begin{cases} \alpha_q = \mathrm{d}\tau(q)/\mathrm{d}q \\ f(\alpha_q) = q\,\alpha_q - \tau(q) \end{cases}$$

$$\lambda \equiv l/L$$

$$\tau(q) = \lim_{\lambda\to 0} \frac{\ln\langle R_q(\lambda)\rangle}{\ln\lambda} \Rightarrow \begin{cases} \alpha_q = \lim_{\lambda\to 0} \frac{1}{\ln\lambda} \left\langle \sum_k \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \ln \mu_k(\lambda) \right\rangle \\ f(\alpha_q) = \lim_{\lambda\to 0} \frac{1}{\ln\lambda} \left\langle \sum_k \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \ln \frac{\mu_k^q(\lambda)}{\langle R_q(\lambda)\rangle} \right\rangle \end{cases}$$

Approaching the Thermodynamic Limit $\begin{cases} \text{varying } l \to 0 \\ \text{varying } L \to \infty \end{cases}$

- varying $l \to 0$ **BOX-SIZE SCALING**
- varying $L \to \infty$ **SYSTEM-SIZE SCALING**

MFA with the Probability Density Function (PDF)

- The meaning of $f\left(\alpha \equiv -\frac{\ln|\Psi|^2}{\ln L}\right)$ implies that $\boxed{\mathcal{P}_L(\alpha) \sim L^{f(\alpha)-d}}$

Solving the L-dependence in $\mathcal{P}_L(\alpha)$

Since $f(\alpha_0) = d$ where α_0 is the position of the maximum, then

$$\boldsymbol{\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha_0) L^{f(\alpha)-d}}.$$

It follows that α_0 is also the position of the maximum of the PDF, and so $\mathcal{P}_L(\alpha_0)$ is the maximum value of the distribution.
Moreover, from the normalization condition of the PDF we have

$$\mathcal{P}_L(\alpha_0) = \left(\int_0^\infty L^{f(\alpha)-d} d\alpha\right)^{-1} \sim \sqrt{\ln L}$$

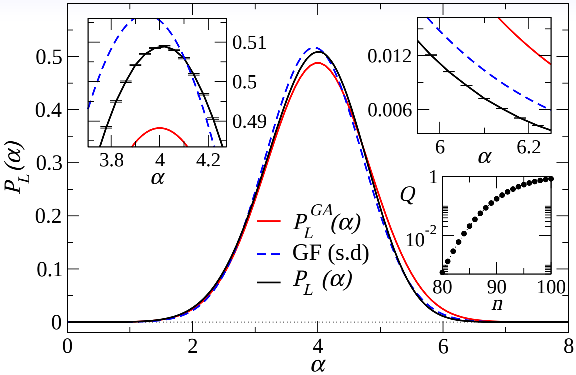
Numerically, the PDF is approximated by the histogram

$$\mathcal{P}_L(\alpha) \underset{\Delta\alpha\to 0}{\equiv} \left\langle \theta\left(\Delta\alpha/2 - \left|\alpha + \ln|\psi_i|^2/\ln L\right|\right)\right\rangle /\Delta\alpha,$$

where θ is the Heaviside step function.

Non-parabolicity of the $f(\alpha)$

Results from perturbation theory [F. Wegner, Nucl. Phys. B316, 663 (1989)] predict a parabolic $f(\alpha)$ and hence a Gaussian PDF: $\mathcal{P}_L^{GA}(\alpha) = \sqrt{\frac{\ln L}{4\pi}} L^{-(\alpha-4)^2/4}$

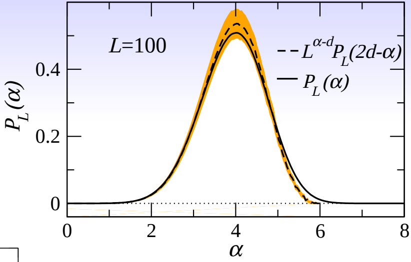


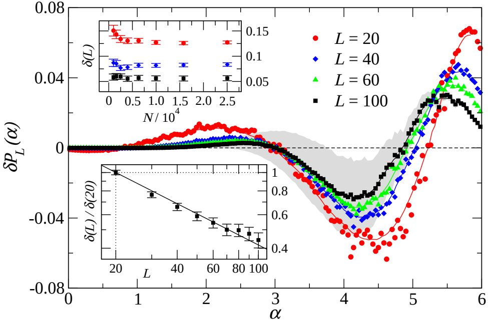
- According to the numerical analysis **the PDF is non-Gaussian** and hence $f(\alpha)$ is not parabolic.

Symmetry Relation for the PDF: $\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha_0) L^{f(\alpha)-d}$

Symmetry relation for $f(\alpha)$

$$f(2d-\alpha) = f(\alpha) + d - \alpha$$
$$\Downarrow$$
$$\mathcal{P}_L(2d-\alpha) = L^{d-\alpha}\mathcal{P}_L(\alpha)$$





Measuring the degree of symmetry

$$\delta\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha) - L^{\alpha-d}\mathcal{P}_L(2d-\alpha)$$

$$\delta(L) = \int_0^{2d} d\alpha |\delta\mathcal{P}_L(\alpha)|$$

$$\delta(L) \sim L^{-0.545\pm0.017}$$

Finite Size Scaling at fixed λ

$$\widetilde{\alpha}_{\mathrm{m}}(W,L) = \mathcal{F}(L/\xi) \quad \longrightarrow \quad \boxed{\widetilde{\boldsymbol{\alpha}}_{\mathbf{m}} = \boldsymbol{\mathcal{F}}\left(\boldsymbol{\rho}\mathbf{L}^{\mathbf{1}/\boldsymbol{\nu}}, \boldsymbol{\eta}\mathbf{L}^{-|\mathbf{y}|}\right)}$$

$\rho \equiv \rho(W)$ and $\eta \equiv \eta(W)$ are the **relevant** and **irrelevant scaling fields**.

- *Expansion of the scaling function:*

$$\mathcal{F}(\rho L^{1/\nu}, \eta L^{-|y|}) = \mathcal{F}_0(\rho L^{1/\nu}) + \eta L^{-|y|}\mathcal{F}_1(\rho L^{1/\nu})$$

and $\mathcal{F}_s(\rho L^{1/\nu}) = \sum_{k=0}^{n_s} a_{sk}(\rho L^{1/\nu})^k$

- *Expansion of the scaling fields around W_c:*

$$\rho = \sum_{m=1}^{m_\rho} b_m (W - W_c)^m, \quad \eta = \sum_{m=0}^{m_\eta} c_m (W - W_c)^m, \quad \text{with } b_1 = c_0 = 1$$

The expansions are truncated at orders $\{\mathbf{n_0}, \mathbf{n_1}, \mathbf{m}_\rho, \mathbf{m}_\eta\}$, which should be kept as low as possible, while giving an acceptable goodness of fit.

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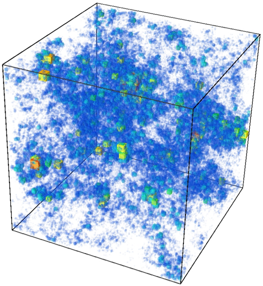
3-D Anderson Model

$$\mathcal{H} = \sum_k \varepsilon_k \left|k\right\rangle\left\langle k\right| + t\left|k\right\rangle\left\langle k-1\right| + t\left|k\right\rangle\left\langle k+1\right|$$

$k \equiv (x, y, z) \longrightarrow$ 3-D spatial coordinate of the L^3 system

Random onsite energies: $\varepsilon_k \in \left[-\frac{W}{2}, \frac{W}{2}\right]$, $W \equiv$ degree of disorder

- Diagonalization of $L^3 \times L^3$ Hamiltonian at $E = 0$ and $W \sim W_c \sim 16.5$
  –JADAMILU library–
  `http://homepages.ulb.ac.be/jadamilu/`
- Largest L considered $L = 240$ ($L^3 = 13\,824\,000$)
  Total amount of data $\sim$ 5 TB

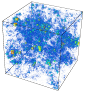


Large Scale Anderson Diagonalization

2 levels of iterations to solve $H\Psi = E_0\Psi$ 100^3

Outer iteration: Jacobi-Davidson (JD)
Inner iteration: ILUPack$^+$ to solve shift-and-invert problem

- iterative methods use $H^n\Psi_0 \to E^n_{\max}\Psi_{\max}$, 1999 30 days
  Krylov sequence $\Psi_{n+1} = H\Psi_n = H^2\Psi_{n-1} = \ldots$ 2006 3 days
- shift-and-invert approach $H \to 1/(H - E_0)$ to target E_0 region
  rewrite as $(H - E_0)\Psi_{n+1} = \Psi_n$, aka sys. lin. equations 6 hrs
- fast *iterative* SLE solver ILUPack and tricks 40 min
- JD is ok with approximate states Ψ_{n+1} 20 min
- tinkering with ILUPack and jdbsym interface 12 min
- use new package JADAMILU 10 min



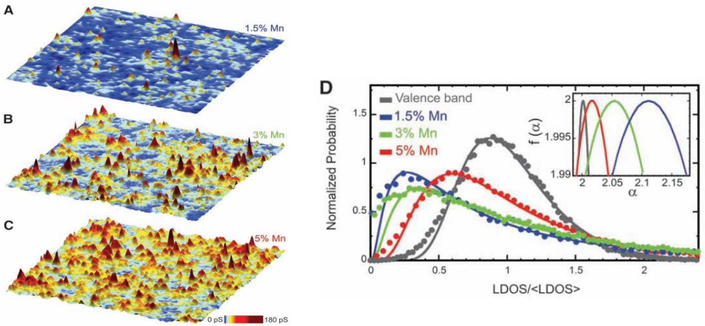
$N = L^3 = 350^3 = 42.875.000$ **in 2006!**

Schenk *et al.*, SIAM Reviews 50, 91–112 (2008)

Relevance of MFA and PDF relation

- LDOS and wavefunction data close to criticality can now be measured

  Visualizing critical correlations near the metal-insulator transition in $Ga_{1-x}Mn_xAs$, A. Richardella *et al.*, Science 327, 665 (2010)



- The PDF-based MFA offers a new way to characterize the metal-insulator transition potentially applicable to this kind of experimental data

$f(\alpha)$ from the Probability Density Function (PDF)

- Probability that $\alpha_j \equiv -\frac{\ln |\Psi_j|^2}{\ln L}$ lies in $[\alpha, \alpha + d\alpha] \Rightarrow \mathcal{P}_L(\alpha) d\alpha \sim L^{f(\alpha)-d}$

Rodriguez, Vasquez, Römer, Phys. Rev. Lett. 102, 106406 (2009)

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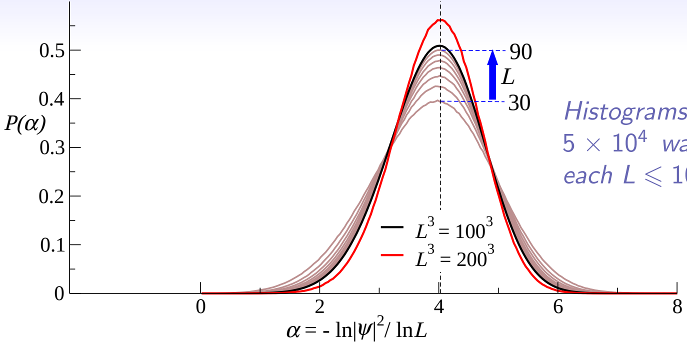

Histograms obtained from 5×10^4 wavefunctions for each $L \leqslant 100$

$$\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha_0)L^{f(\alpha)-d} \longrightarrow f(\alpha) = d + \ln[\mathcal{P}_L(\alpha)/\mathcal{P}_L(\alpha_0)]/\ln L$$

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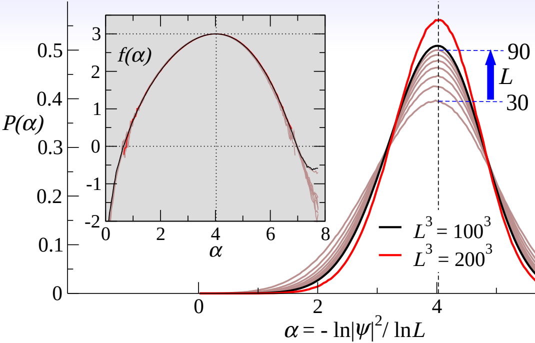

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Rodriguez, Vasquez, Römer, Phys. Rev. Lett. 102, 106406 (2009)

System-size scaling with the PDF: $\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha_0) L^{f(\alpha)-d}$

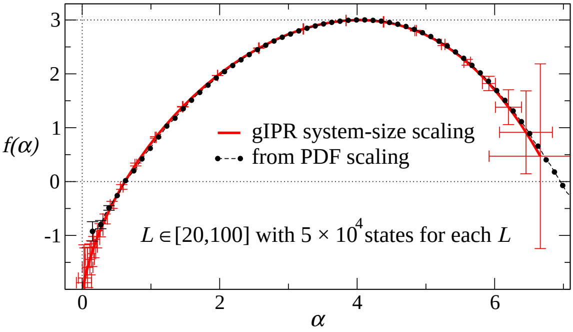
- **Reducing finite size effects**

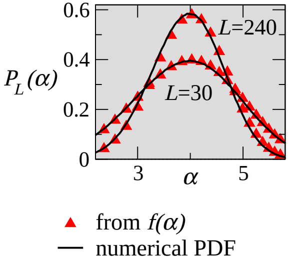
Points per wavefunction with $\alpha \in \left[\alpha - \frac{\Delta\alpha}{2}, \alpha + \frac{\Delta\alpha}{2}\right]$: $\mathcal{N}_L(\alpha) \equiv L^d \mathcal{P}_L(\alpha)\Delta\alpha$

Normalized volume of the α-set: $\widetilde{\mathcal{N}}_L(\alpha) \equiv L^d \frac{\mathcal{P}_L(\alpha)}{\mathcal{P}_L(\alpha_0)} \Rightarrow \widetilde{\mathcal{N}}_L(\alpha) = L^{f(\alpha)}$

$$f(\alpha) = \lim_{L\to\infty} \frac{\ln \widetilde{\mathcal{N}}_L(\alpha)}{\ln L}$$

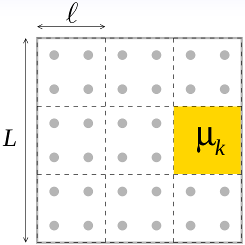
$f(\alpha)$ can be obtained from the slope of the linear fit $\ln \widetilde{\mathcal{N}}_L(\alpha)$ vs $\ln L$ for different values of L





Scaling of the Probability Density Function $\mathcal{P}(\alpha)$

$$\mu_k = \sum_{j \in \text{box } k} |\psi_j|^2 \to \mu \equiv \left(\frac{L}{\ell}\right)^{-\alpha}, \alpha \equiv \frac{\ln \mu}{\ln(\ell/L)} \xrightarrow[\text{at critical point}]{\text{multifractality}} \boxed{\mathcal{P}(\alpha) \propto \left(\frac{L}{\ell}\right)^{f(\alpha)-d}}$$



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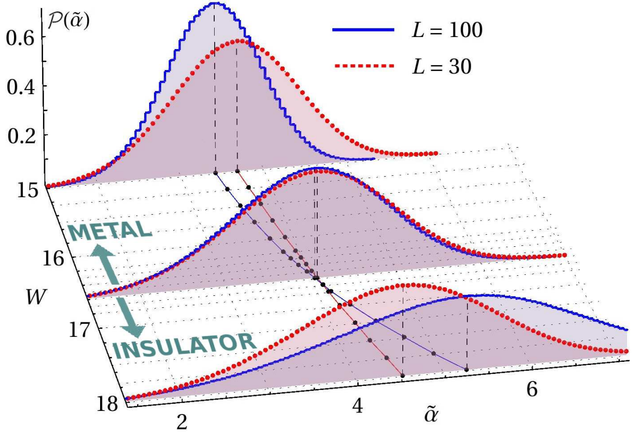
SCALING AT FIXED $\lambda \equiv \ell/L$



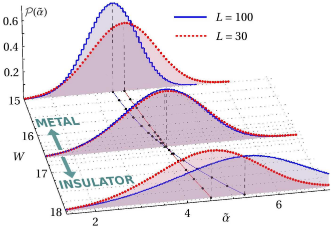
The PDF is scale invariant at the transition

The transition can be monitored by the distribution function of α-values ($|\psi|^2$ intensities)

Scaling of the Probability Density Function $\mathcal{P}(\alpha)$

$W = 15.0$

Scaling at fixed $\lambda = \ell/L$



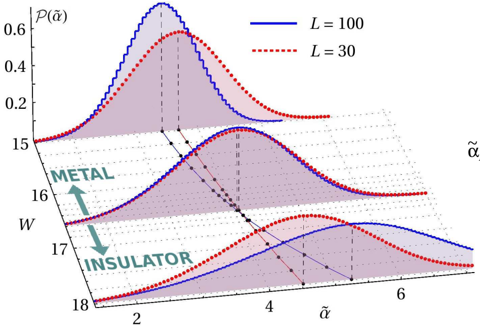
$W = 16.5$

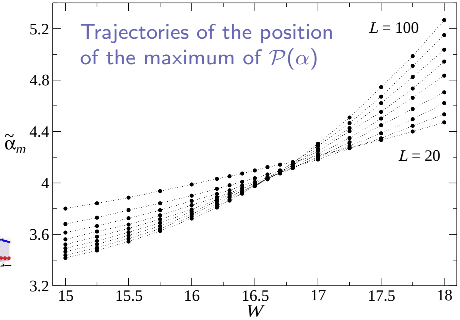
$W = 18.0$

Scaling of the Probability Density Function $\mathcal{P}(\alpha)$

$$\mu_k = \sum_{j \in \text{box } k} |\psi_j|^2 \to \mu \equiv \left(\frac{L}{\ell}\right)^{-\alpha}, \alpha \equiv \frac{\ln \mu}{\ln(\ell/L)} \xrightarrow[\text{at critical point}]{\text{multifractality}} \boxed{\mathcal{P}(\alpha) \propto \left(\frac{L}{\ell}\right)^{f(\alpha)-d}}$$

SCALING AT FIXED $\lambda = \ell/L$





Can we extend the MFA formalism to describe this scaling behaviour and quantitatively characterise the transition?