Anomalously localized electronic states in three-dimensional disordered samples

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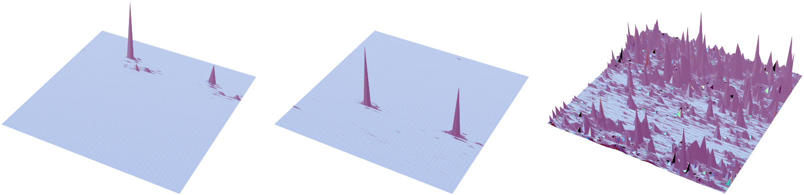
Anomalously localized states (ALS)



- ALS originate from statistical fluctuations of the disorder potential.
- Even for weak average disorder specific local disorder configurations lead to states that are localized in a finite region.
- ALS in the metallic regime can be neglected for infinite system because of their point-like spectra. [V. Uski et al., PRB **62**, R7699 (2000)]
- ALS at the transition regime can lead to deviations in the critical properties even for infinite system size [H. Obuse and K. Yakubo, PRB **69**, 125301 (2004)]
- Quantitative definition of ALS required.

Anderson Model of Localization

- Non-interacting electrons in a disordered energy landscape

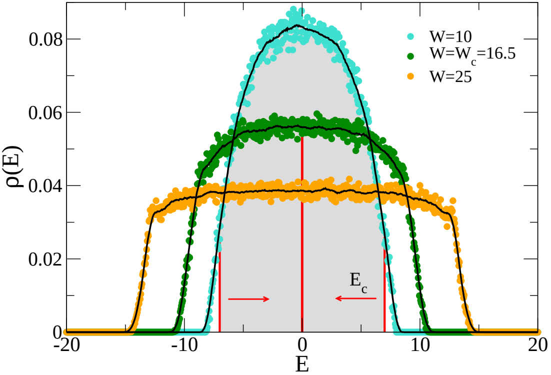
  [P. W. Anderson, Phys. Rev. **109**, 1492 (1958)]

$$\mathcal{H} = \sum_{i=1}^{N} \epsilon_i |i\rangle\langle i| + \sum_{<i,j>} t_{i,j} |i\rangle\langle j|.$$

- Random onsite energies $\epsilon_i \in \left[-\frac{W}{2}, \frac{W}{2}\right]$ describe potential disorder.
- Nearest-neighbor hopping integrals $t_{i,j} = 1$ set energy scale and boundary conditions (here *periodic*).
- Disorder induced transition from metal (delocalization) to insulator (localization) at disorder strength $W_c = 16.5$.

Density of States

- Mobility edge E_c separates extended states in the band center from localized states in the tails.
- When approaching the transition ($W \longrightarrow W_c$) all states become localized ($E_c \longrightarrow 0$).

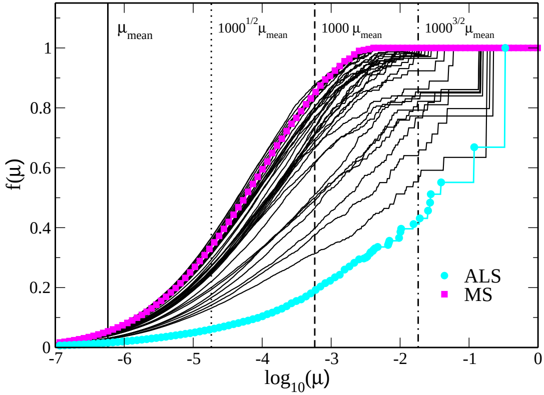


Numerical methods

- Efficient diagonalization of large sparse matrices.
  - Full spectrum very expensive (time,memory).
  - Therefore only selected Eigenvalues and Eigenfunctions.
  - For a long time Cullum/Willoughby implementation of the **Lanczos** algorithm state of the art (2000: 14 critical wave functions for $N = 111^3$ took 27 days on a XP1000 667 Mhz).
  - Only recently more efficient Jacobi-Davidson method with multilevel incomplete LU preconditioning **[JADAMILU]** (2007: 20 critical wave functions for $N = 120^3$ take 1 hour on a Opteron 8216 2.4 Ghz).
- Huge memory requirements.

system size N	40^3	80^3	120^3
memory in byte	$500K$	$3.9M$	$13.2M$
# of wave functions	1600	1000	1040

Distribution of wave function amplitudes

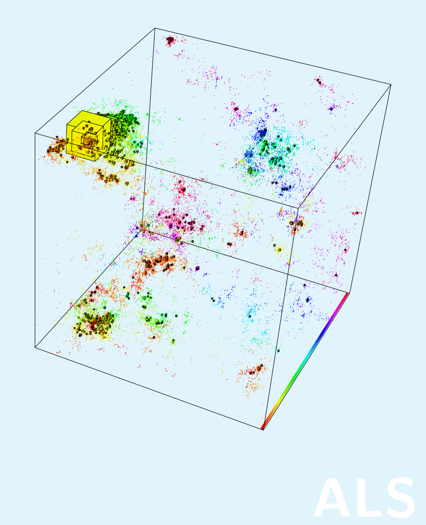


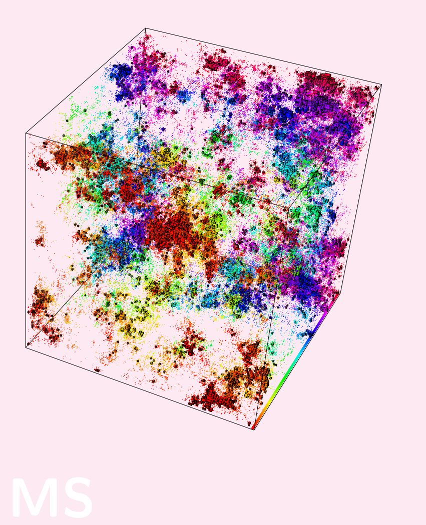
$$f(\mu) = \sum_{\mu_j < \mu} \mu_j$$

with $\mu_j = |\Psi_j|^2$.

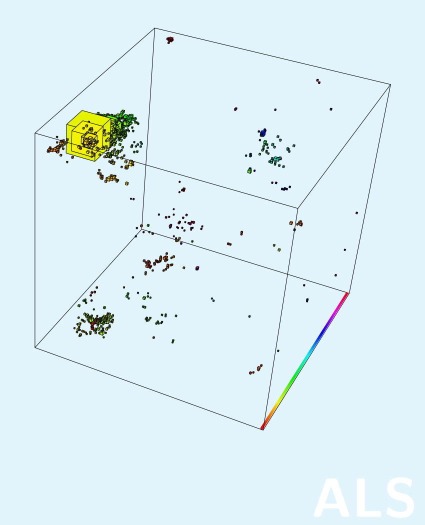
54 from the 1040 critical states for $N = 120^3$.

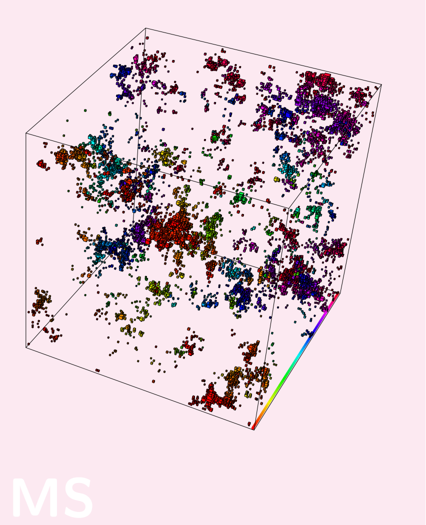
ALS vs. MS $\mu_j > \mu_{\text{mean}}$



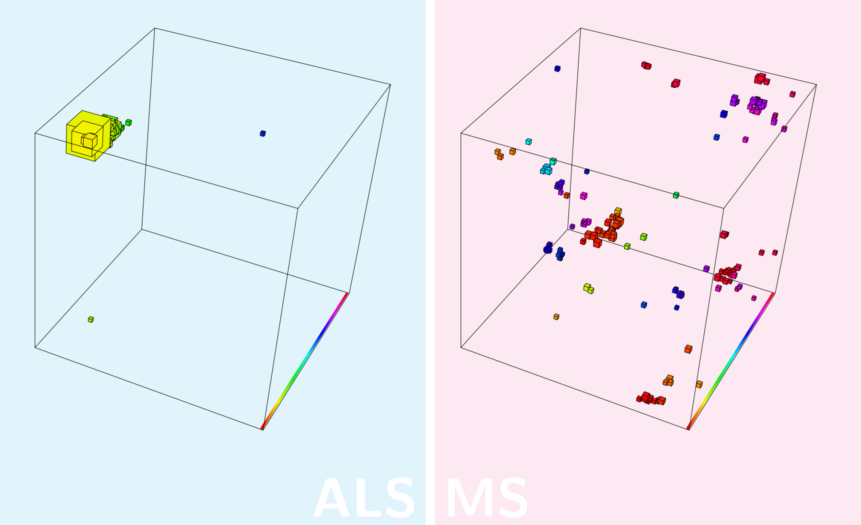


ALS vs. MS $\mu_j > \sqrt{1000}\mu_{\text{mean}}$

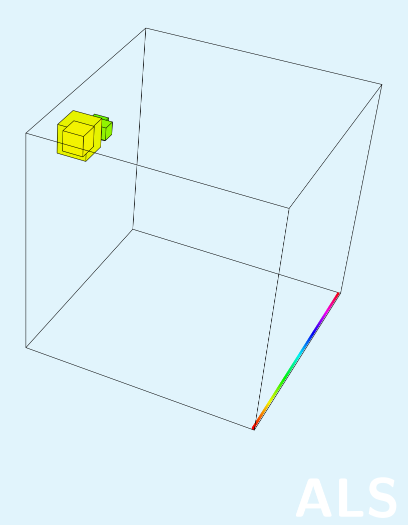




ALS vs. MS $\mu_j > 1000\mu_{\text{mean}}$



ALS vs. MS $\mu_j > \sqrt{1000}^3 \mu_{\mathrm{mean}}$



# of $\mu_i >$	ALS	MS
μ_{mean}	17103	96622
$\sqrt{1000} \times \mu_{\mathrm{mean}}$	1442	7810
$1000 \times \mu_{\mathrm{mean}}$	111	142
$\sqrt{1000}^3 \times \mu_{\mathrm{mean}}$	7	0

Multifractality

- Divergence of the correlation length at the transition implies scale invariant critical wave function → **multifractal (MF) properties**.
- Consider a local box measure for box width L_b

$$\mu_i(L_b) = \sum_{j \in box(i)} |\Psi_j|^2$$

and define

$$Z_q(L_b) = \sum_i \mu_i^q(L_b)$$

- For a MF wave function (MS) one observes a power law

$$Z_q(L_b) \propto L_b^{\tau(q)}$$

with mass exponent $\tau(q)$.

MF correlations I

- Study general MF correlation function

$$\mathrm{M}_q(L_b, r, L) \equiv \left\langle \mu_i^q(L_b)\mu_{i+r}^q(L_b)\right\rangle_L$$

where $\langle . \rangle_L$ is the average over all pairs of boxes with fixed distance r within system of width L.

- Employing scaling behavior it follows

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

$$\mathrm{M}_q(L_b, r, L) \propto L_b^{x(q)} L^{-y(q)} r^{-z(q)}.$$

MF correlations II

- Restrict choice to special cases for fixed system width L where:

  [H. Obuse and K. Yakubo, PRB **69**, 125301 (2004)]

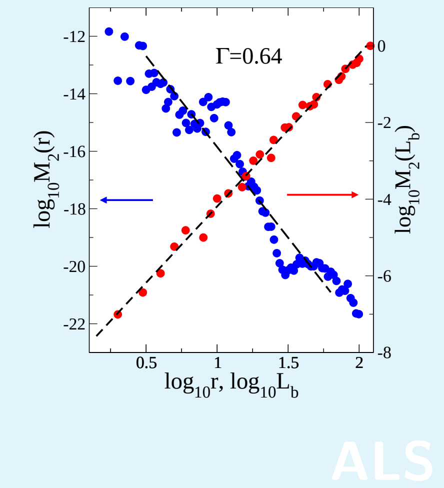
  - $r = 0$: $M_q(L_b) \equiv M_q(L_b, r = 0, L) \propto L_b^{x(q)} \propto L_b^{d+\tau(2q)}$
  - $L_b = 1$: $M_q(r) \equiv M_q(L_b = 1, r, L) \propto r^{-z(q)}$

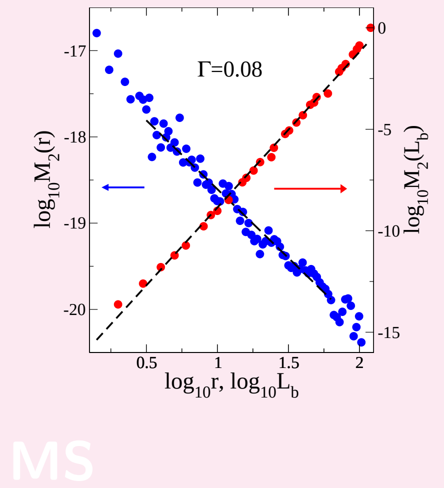
- Influence of ALS should result in observable deviations from scaling.
- Variances Γ of the correlation exponents obtained from the power-law fit gives quantitative measure for each wave function

  $$\Gamma = \Gamma_z + \alpha\Gamma_\tau$$

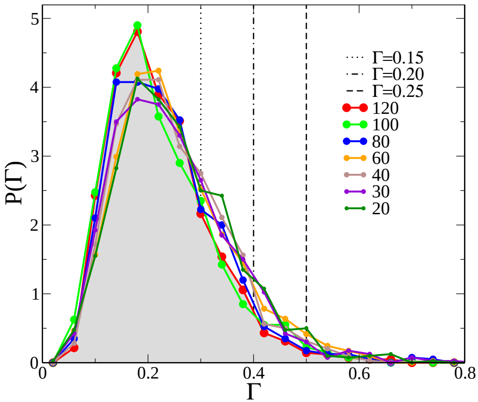
  where the α compensates the different mean values of Γ_z and Γ_τ.
- Suitable limit Γ^* separates ALS ($\Gamma > \Gamma^*$) from MS ($\Gamma \leq \Gamma^*$).

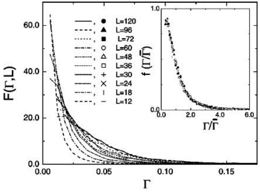
Multifractal correlation functions $M_2(L_b)$ and $M_2(r)$





Distribution of the variance Γ





[H. Obuse and K. Yakubo, PRB **69**, 125301 (2004)]

Computation of $z(q)$

- Investigate scaling relation

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

$$\mathrm{z(q)=d+2}\tau(q) - \tau(2q)$$

derived from asymptotic behavior (vanishing $r = L_b$ vs. large $r = L$) of

$$M_q(r, L_b, L) \equiv \left\langle \mu_i^q(L_b)\mu_{i+r}^q(L_b)\right\rangle_L \propto L_b^{x(q)} L^{-y(q)} r^{-z(q)}.$$

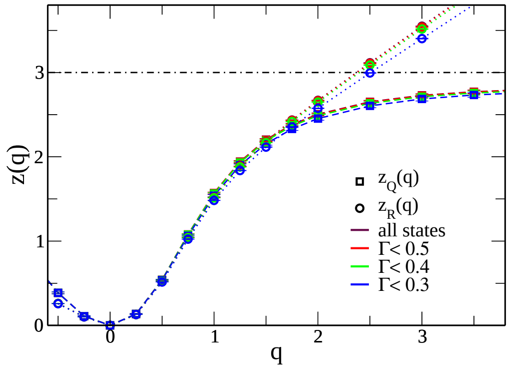
- Compare correlation exponent $z(q)$ calculated from

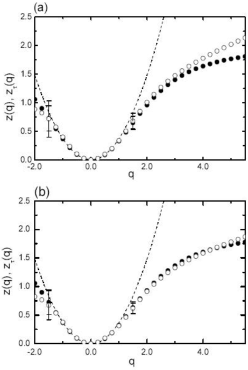
$$M_q(r) \propto r^{-z(q)}$$

with $z(q)$ obtained from the mass exponent $\tau(q)$ as computed from

$$M_q(L_b) \propto L_b^{2\tau(q)}.$$

Comparison of z(q)





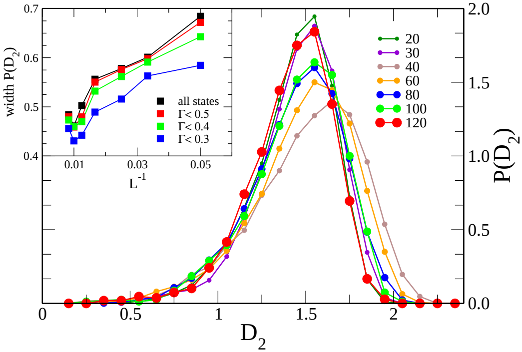
[H. Obuse and K. Yakubo,

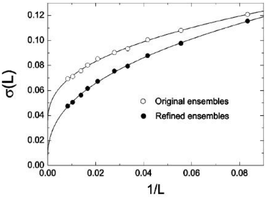
J. Phys. Soc. Japan, **73**, 2164 (2004)]

- Significant deviations between different methods for $q > 2$.
- For $q > 2.5$ value exceeds theoretical upper limit $z(q) < 3$ even for smallest Γ^*.

Fluctuation of the Correlation Dimension D_2

Definition: $Z_2(L_b) \propto L_b^{D_2}$ thus $D_2 = \tau(2)$





[H. Obuse and K. Yakubo, PRB **69**, 125301 (2004)]

ALS lead to finite width for $L \to \infty$

Conclusion

- ALS affect critical properties at the delocalization-localization transition in the 3D Anderson model of localization.
- Influence of ALS less pronounced as for the 2D SU(2) model.
- For better statistics are more critical states and more disorder realizations required.
  $\rightarrow$ higher numerical effort for 3D in comparison to 2D.