Anderson transitions and multifractal finite-size scaling

Ph.D. thesis booklet

László Ujfalusi
Supervisor: Dr. Imre Varga

Budapest University of Technology and Economics
Department of Theoretical Physics

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1 Introduction

Disordered-induced metal-insulator transition -also called Anderson-localization- is in the forefront of condensed matter physics since the middle of the XX. century. The Anderson transition - apart from few exceptions - happens in three-dimensional systems, in one- or two-dimensional systems arbitrarily small disorder causes localization. Disorder can be introduced in various forms, e.g. crystal defects, randomly placed impurities or a random potential which shifts atomic energy levels. Because of the universality principle many physical quantities behave independently of the specific form of disorder. A perfect crystal is a perfect conductor, electrons propagate ballistically. Adding some disorder to the system electrons scatter a few times, electrons propagate diffusively and the overall behavior is still metallic. Increasing disorder further multiple scattering can trap (Anderson-localize) electrons, and the system turns into an insulator.

Investigating the wave-functions of the electrons in the metallic regime one can see that they extend over the whole lattice, they are effectively three-dimensional. In the insulating phase effectively zero-dimensional, exponentially localized wave-functions are present. Since the metal-insulator transition is a second order phase transition, approaching the transition point -which is a true critical point- from the metallic (insulating) side the correlation (localization) length diverges, the system is scale-free. This induces the self-similarity of the system, which is a property of fractals, therefore one would expect similar behavior to fractals. As it turns out, the wave-functions of the electrons show multifractal properties. Multifractals are generalizations of fractals. They have very strong fluctuations, therefore - instead of one fractal dimension - they can be described through infinitely many fractal dimensions, D_q or α_q, depending on the continuous parameter, q. Beside D_q or α_q other generalized fractal dimensions - in other words multifractal exponents - can be defined.

2 Objectives

The main goal of my research was to show that multifractals are present in various disordered systems, and to extract critical parameters of these models using multifractals. Disordered systems belong to different universality classes depending on the presence or absence of time-reversal and spin-rotational symmetry. I investigated that how the presence or absence of these symmetries affect the critical point, critical exponent (which describes the divergence of the correlation/localization length) and the multifractal exponents in an Anderson-model which introduces disorder through a random potential. Disorder can be introduced through defects in the crystal for which percolation is a basic model. Considering nearest-neighbor hopping on a percolated lattice leads to the quantum percolation model. Examining the wave-functions of this model I experienced very similar behavior to the Anderson model, therefore my goal was to show the presence of multifractals at the transition point, p_c^Q, and to extract the critical parameters for this model also. The previously used methods assumed that the lattice is regular three-dimensional crystal, therefore my further goal was to improve the methods to be applicable for irregular lattices with missing sites. Anderson localization of the quark wave-functions in a Quantum chromodynamics model at large temperature was also observed. With increasing energy the quark wave-functions turns from localized into extended states, which was investigated through spectral statistics. Our goal with the group who discovered the transition was to examine the transition through wave-functions and to show their multifractality at the transition point.

3 Methods

I investigated the disordered systems described above numerically. I considered only nearest neighbor hopping for the Anderson model and for the quantum percolation model, therefore the corresponding Hamiltonian is very sparse. The mathematical task was to find an eigenvector inside the spectrum which describes the wave-function of an electron. To this end I used Jacobi-Davidson iteration (PRIMME library) with ILU preconditioning (ILUPACK library). Since the Hamiltonian is very sparse, I could investigate systems containing up to a million sites, which led to very accurate results. To the computations I used the cluster of the Department of Theoretical Physics of BUTE and the supercomputer of BUTE. To simulate the quark-gluon system we used an already existing GPU code. From the eigenvectors I computed the finite-size version of the multifractal exponents near the transition point, called generalized multifractal exponents. Since on the metallic side of the transition $D_q \equiv 3$, and on the insulating side $D_q \equiv 0$ holds for $q > 0$ and $D_q \equiv \infty$ holds for $q < 0$, one can use the generalized multifractal exponents as order parameter. I measured these quantities at different system sizes and at different values of disorder, then I performed finite-size scaling: I fitted a scaling function to the raw data of the generalized multifractal exponents. Before computing the generalized multifractal exponents one can coarse grain the wave-function, by adding the wave-function values in a box much smaller than the system size. After that one can use two methods: fixing λ, which is the ratio of the box size and the system size, results in a single-varable scaling function, while allowing various values of λ leads to a two-variable scaling function. The finite-size scaling procedure resulted the critical point, the critical exponent and other physically interesting quantities.

4 New scientific results

In this Section I list the thesis statements.

1. I examined the three-dimensional Anderson models belonging to the conventional Wigner-Dyson symmetry classes with the help of multifractal finite-size scaling. With the fixed λ and varying λ methods I confirmed the presence of multifractality in all three Wigner-Dyson symmetry classes. I obtained the critical point, critical exponent and irrelevant exponent for each symmetry class. These parameters were in agreement with each other for the different methods, and with previous results known from the literature. The varying λ method provided significantly different critical exponents for the different symmetry classes. I computed the multifractal exponents also for every symmetry class. Multifractal exponents of different symmetry classes were very close to each other for fixed q, but significantly different for most of the values of q.
   Publication **[a]** is related to this thesis point.

2. I investigated numerically the quantum percolation model in 3D. In order to describe the localization transition I used multifractal finite-size scaling. I determined the mobility edge of the system, confirming previous calculations. For the critical exponent I obtained energy-independent values within 95% confidence level. The average of these values is the same as the critical exponent of the orthogonal Anderson model, implying that quantum percolation belongs to the chiral orthogonal Anderson universality class. I also determined the multifractal exponents D_q and α_q along the mobility edge, and for larger values of p_c^Q I found no significant difference from the Anderson model confirming the statement of the universality class further.
   Publication **[b]** is related to this thesis point.

3. I have shown that the Anderson model at strong localization shows non-trivial behavior especially approaching the band-edge. I showed that only a 2-site or a 3-site model can describe qualitatively well the system.
   Publication **[c]** is related to this thesis point.

4. I investigated the Anderson transition in the spectrum of the Dirac operator of Quantum chromodynamics at high temperature. I found similar correlations between the eigenvectors of the Dirac operator of QCD and the Hamiltonian of the unitary Anderson model. Multifractal finite-size scaling with the fixed λ method resulted matching results with previous works for the critical point, and with my results for the critical exponent for the unitary Anderson model. The approximate values of the multifractal exponents were compatible with the multifractal exponents of the unitary Anderson model. My work confirms that there is a metal-insulator phase transition in the spectrum of the Dirac operator of QCD, and it belongs to the chiral-unitary Anderson class.
   Publication **[d]** and **[e]** are related to this thesis point.

5 Publications

Publications related to this thesis:

1. L. Ujfalusi and I. Varga : Finite size scaling and multifractality at the Anderson transition for the three Wigner-Dyson symmetry classes in three dimensions, *Physical Review B* **91**, 184206 (2015).

2. L. Ujfalusi and I. Varga: Quantum percolation transition in three dimensions: Density of states, finite-size scaling, and multifractality, *Physical Review B* **90**, 174203 (2014).

3. L. Ujfalusi and I. Varga: Anderson localization at large disorder, *Physical Review B* **86**, 125143 (2012).

4. M. Giordano, T. G. Kovács, F. Pittler, L. Ujfalusi and I. Varga : Dirac eigenmodes at the QCD Anderson transition, PoS LATTICE2014 (2015) 212.

5. L. Ujfalusi, M. Giordano, F. Pittler, T. G. Kovács and I. Varga: Anderson transition and multifractals in the spectrum of the Dirac operator of Quantum Chromodynamics at high temperature, submitted to PRB

Other publication:

6. L. Ujfalusi, D. Schumayer and I. Varga: Quantum chaos in one dimension?, *Physical Review E* **84**, 016230 (2011).