

Analysis of localisation-delocalisation transitions in corner-sharing tetrahedral lattices

Short Introduction

Analysis of localisation-delocalisation transitions in corner-sharing tetrahedral lattices



Martin Puschmann, Philipp Cain and Michael Schreiber
Chemnitz University of Technology, Institute of Physics, Chemnitz, Germany
matthias.puschmann@physik.tu-chemnitz.de

- Abstract**
 - a corner-sharing tetrahedral (CST) lattice emerges as natural model for the electronic properties of various materials, e.g. diamond, graphite, silicon, spinels and perovskites.
 - we analyse the critical behavior of localisation-delocalisation (LD) transitions in the CST lattice by using the Density Matrix Renormalization Group (DMRG) method.
 - similar critical behavior is observed by scaling experiments
 - compare to a recent study from F. Faalka et al.
- 1. Introduction**
 - CST is appropriate to reason energy and have it changing diagonally $\Delta = \pm 3\epsilon$.
 - effusive electrons are apparently with highest critical disorder
 - the critical disorder $\epsilon_c = 0.137\epsilon$
 - critical exponent $\nu = 1.57$
 - all numerical results are in accordance with the scaling behavior in the vicinity of the critical point
 - most results are more precise, accurate and detailed than the literature

- Corner-sharing tetrahedral lattice**
- Part of a CST lattice (left). The yellow highlighted hexagon has two red shaded faces, which are the generic corner-sharing hexagons and red and green shaded faces, which are the generic edge-sharing hexagons. Every lattice has four red shaded neighbors.
 - all planar states are presented in shaded units along diagonal lines.

- Anderson model of localisation**
 - three dimensional Anderson-Hamiltonian for non-interacting electrons [2]
$$H = -\frac{1}{2} \sum_{\langle i,j \rangle} \delta_{ij} + \epsilon_i \delta_{ii}$$

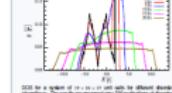
- in the limit of small site disorder ϵ and large lattice size N , the pairs of eigenstates are localized (green shaded regions).

- with the increasing potential ϵ delocalized states (blue shaded regions) appear.

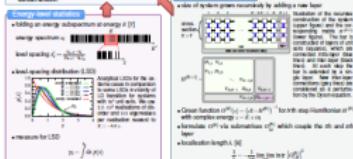
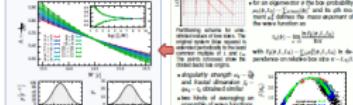
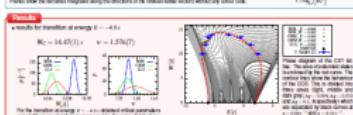
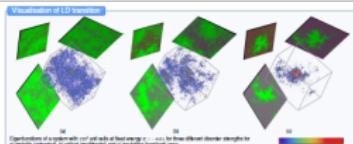
- the hopping integral t is used as an energy unit.

- localisation-delocalisation transitions can be studied with DMRG based on Lanczos Method [2]

- numerical results are obtained by DMRG and DMRG based on direct diagonalisation and DMRG



- 2009 for a regular ($N=1000$) and a disordered ($N=1000$) CST lattice. The figure shows the distribution of level spacings on a logarithmic scale for different energy ranges.



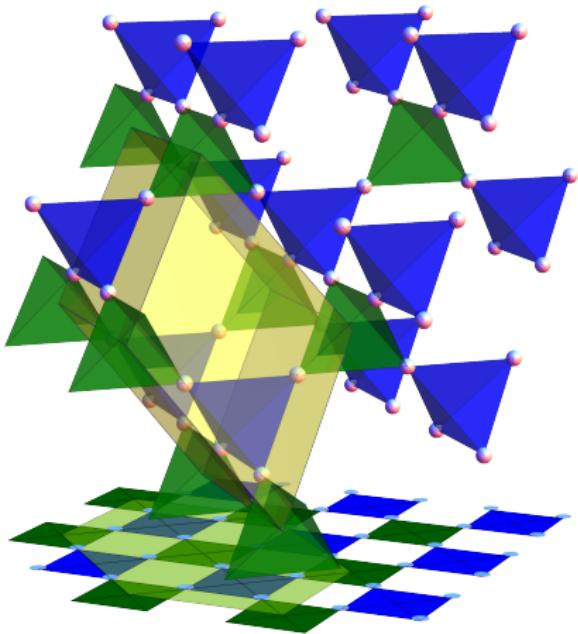
Martin Puschmann

(Philipp Cain and Michael Schreiber)



TECHNISCHE UNIVERSITÄT
CHEMNITZ

Corner-sharing tetrahedral lattice



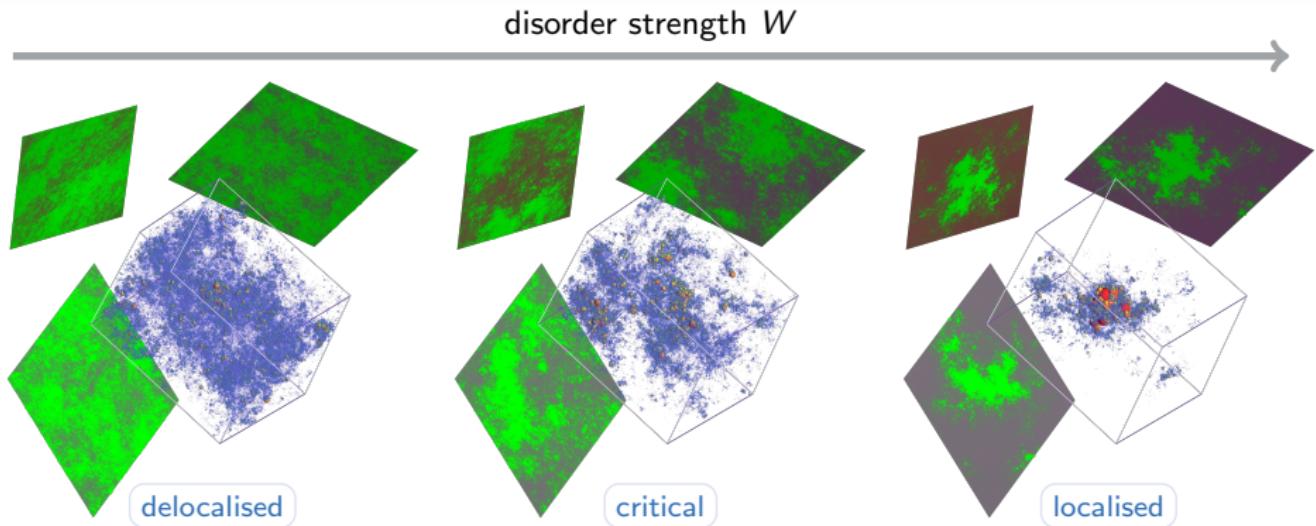
- Anderson Hamiltonian

$$H = \sum_i v_i |i\rangle \langle i| - t \sum_{\langle i,j \rangle} |i\rangle \langle j|$$

- random on-site potentials

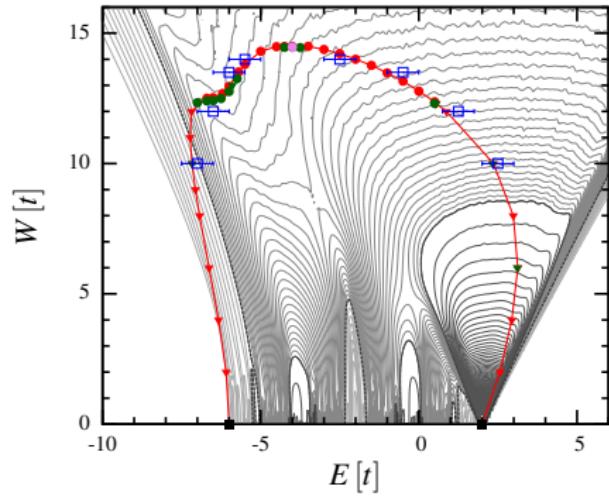
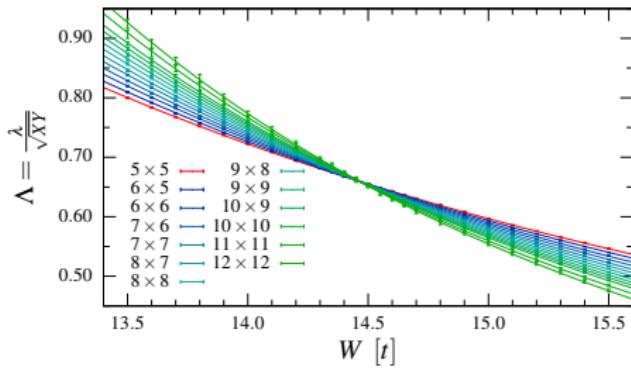
$$v_i \in \left[-\frac{W}{2}, \frac{W}{2} \right]$$

localisation-delocalisation transition



Calculation

- use measures of three different methods
 - multifractal analysis
 - Green resolvent method
 - energy-level spacing
- finite-size scaling in vicinity of critical point



phase diagram