EXERCISES

Computational Materials Science

Prof. K. Held

SHEET 4

Exercise 4: Coherent potential approximation

In this exercise a tight-binding model shall be supplemented by a bipartitie disorder potential $\{0, \epsilon\}$ of equal probability $x = 50\%$. Note that the low energy phsics of some materials such as $PbVO_3$ or many cuprates can be described by a single band around the Fermi level. We use here a simple tight-binding energy-momentum relation

$$\epsilon_{\mathbf{k}} = -2t\left(\cos(k_x a) + \cos(k_y a)\right) \tag{1}$$

with $t \equiv 1$ ($a \equiv 1$) setting our unit of energy (momentum).

Task 1)

Write a program to solve this disorder problem using the coherent potential approximation (CPA).

Task 2)

Study the spectral function (density of states) as a function of ϵ for (a) $\mu = 0$ and (b) $\mu = -\epsilon/2$. (c) Show that your program reproduces the Fermi's golden rule result at weak coupling. (d) At which disorder strength ϵ does a metal-insualtor transition occur? Please also report which $\mathbf{k}$-, ω-grid, δ you have chooses.

For going beyond, i.e. for the (exam) talk

For example you may (i) study convergence w.r.t. to the $\mathbf{k}$-, ω-grid and δ; (ii) consider other disorder distributions or other lattices; (iii) study a doped model and/or adjust μ to a fixed number of particles; or (iv) determine the self energy in the limit of strong disorder strength and compare with the exact solution. Further alternatives are to (v) compare CPA to the exact solution or (vi) to treat the Hubbard model with local interaction U using the dynamical mean field theory (DMFT) where the impurity problem becomes an Anderson impurity model.