EXERCISES

Computational Materials Science

Prof. K. Held

SHEET 4

Exercise 4: Coherent potential approximation

In this exercise the tight-binding model for $PbVO_3$ shall be supplemented by a bipartitie disorder potential $\pm\epsilon/2$ of equal probability. Remind that, within DFT, $PbVO_3$ has a single band near the Fermi level that is well described by the tight-binding energy-momentum relation

$$\epsilon_{\mathbf{k}} = \epsilon_0 + 2t_1 \left(\cos(k_x a) + \cos(k_y a)\right) + 4t_2 \cos(k_x a)\cos(k_y a) \tag{1}$$

with $a = 3.8\mathring{A}$, $\epsilon_0 = 0.03$eV, $t_1 = -0.154$eV and $t_2 = -0.05$eV.

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) $\epsilon_0 = 0$, $t_2 = 0$, $\mu = 0$ and b) the values for $PbVO_3$. At which disorder strength ϵ does a metal-insualtor transition occur? Which **k**-, ω-grid, δ did you choose?

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

For example you may (i) study convergence w.r.t. to the **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; determine the self energy in the limit of (iv) weak or (v) strong disorder strength and compare with the exact solution. An other alternative (vi) is 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 (we would provide an impurity solver).