

EXERCISES  
**Computational Materials Science**

Prof. K. Held

SHEET 4

Exercise 4: Coherent potential approximation

Write a program to solve the half-filled Bethe lattice with binary disorder using the coherent potential approximation (CPA) or, alternatively, with local interaction  $U$  using the dynamical mean field theory (DMFT). For the latter you can use the ED program from the 2nd exercise.

Calculate the Green function and self energy for different disorder/interaction strengths and determine at which disorder/interaction strength a metal-insulator transition occurs.

You can explore your own paths beyond:

For example, (i) consider other disorder distributions, (ii) other lattices, or (iii) a doped model; determine the self energy in the limit of (iv) weak or (v) strong disorder strength and compare with the exact solution.