Exercises

Computational Materials Science

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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).

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, (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. An other alternative (vi) is to treat the Hubabrd model with local interaction U using the dynamical mean field theory (DMFT) and the ED program from the 2nd exercise or (vii) to solve the Anderson disorder model on a finite cluster exactly.