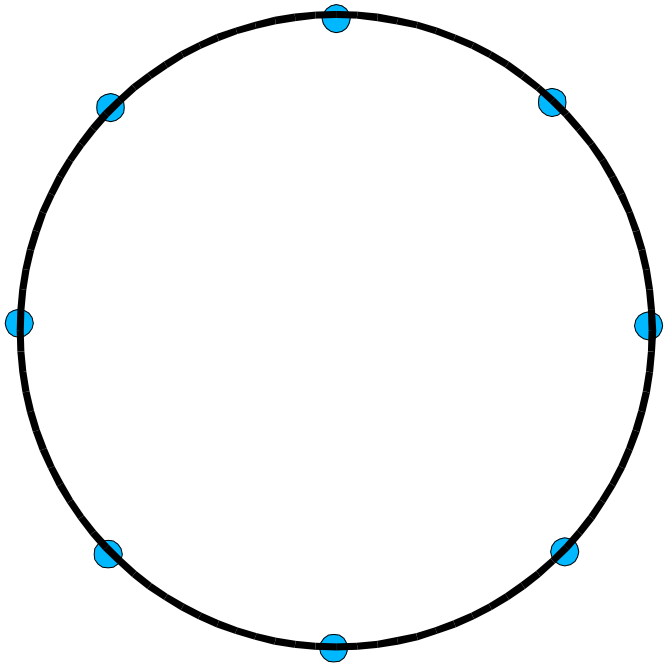
Cluster vs. Periodic Boundary Conditions − Approximating an Infinite Crystal by a Finite one

For a calculation of a finite piece of a crystal (N atoms or basis elements), what boundary conditions on the Schrödinger equation give the most information about the band structure?

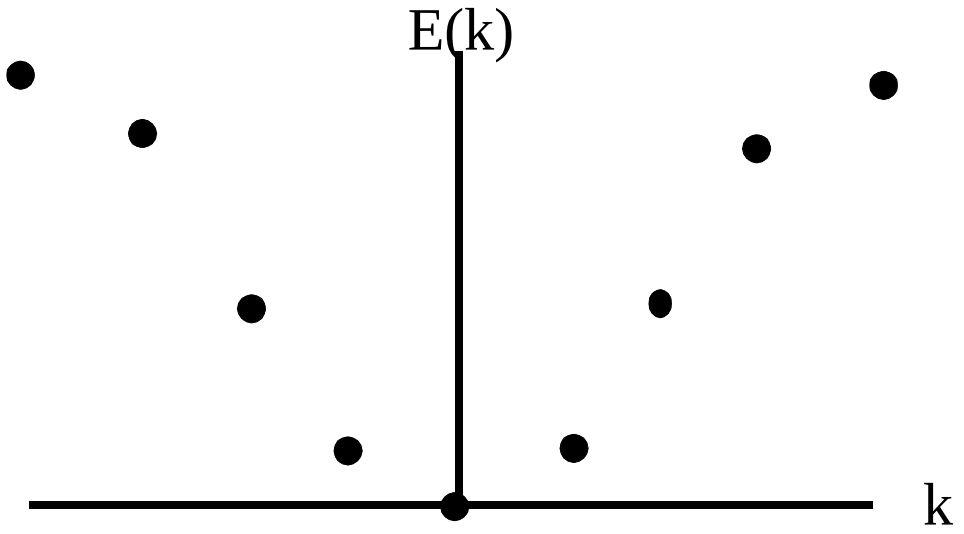
A surface is a defect of the crystal, so you might think that a cluster with no surfaces, that is a cluster with periodic boundary conditions, would give a better band structure.

This is not true in the sense that you get the most distinct points of the band structure by requiring the wave functions to be zero outside a cluster whose shape maximally breaks the symmetries of the crystal.

A One−Dimensional Tight−binding Example

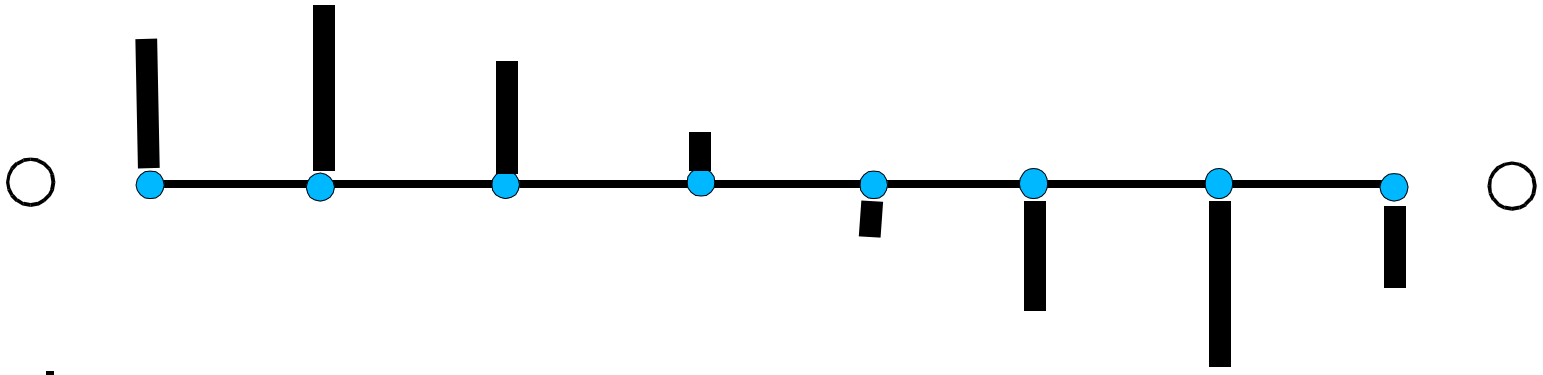


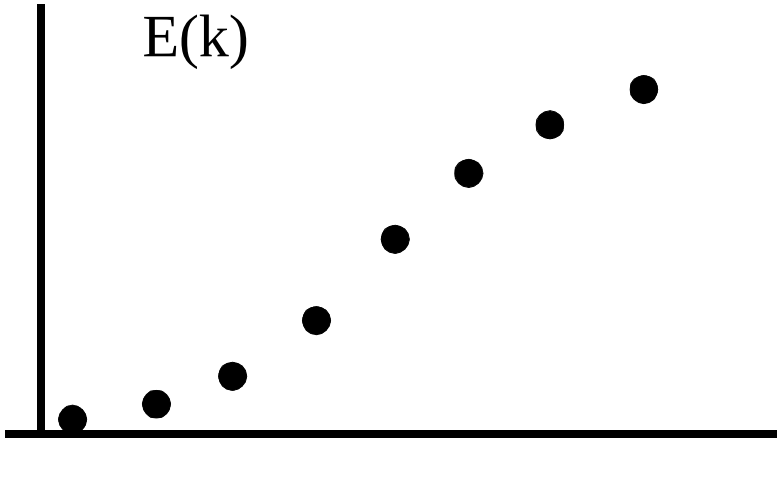
8 atoms with periodic boundary conditions



3 time−reversal doublets and two time−reversal singlets − 5 band energies.

8 atoms with cluster boundary conditions





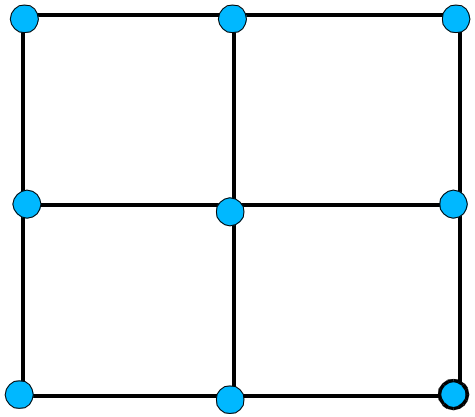
8 time−reversal singlets −
8 band energies

Speculations on the general relation between cluster shape and distinct band energies

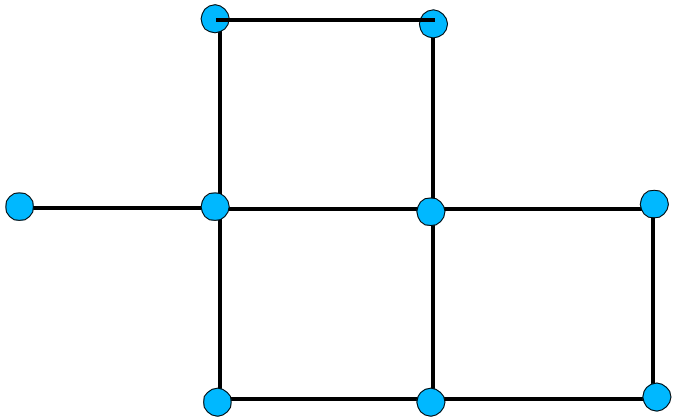
Degeneracies occur in the spectrum of the cluster due to the presence of multi−dimensional irreducible representations of the crystal symmetry, or multiple copies of the same one−dimensional irreducible representation.

The best cluster has no multi−dimensional irreducible representations, or multiple copies of the same one−dimensional irreducible representation.

In most cases this is the same as there being no rotational symmetries present in a connected cluster.



Bad Cluster



Good Cluster