Towards solids: an exercise in band structure

Introduction

This problem illustrates what happens to a system as you introduce periodicity, e.g. by connecting a number of finite square wells together. This helps to provide some intuition for the emergence of band structure in solid-state physics.

The flowfile

This flowfile looks deceptively simple, but there is a lot going on inside the *Scopes* that have been built for the exercise. However, you only have to be concerned with the three things: the spatial dimension, the separation between the wells, and the number of wells. Note that to change the number of wells, you have to connect the appropriate output (labelled with the number of wells you want) to both *Potential* inputs on the *Hamiltonian* and *Energy Plot* nodes.

You have to pay attention to the *Spatial Dimension* node, because if the parameter determining the separation between the wells is too high, all of the wells will not fit within the defined *Spatial Dimension*. Remember that Composer assumes infinite walls at the boundary!

Exercise

- How many bound states are there for a single well? How does this change as you increase the number of wells? Note that you can change the number of eigenstates shown on the *Energy Plot*.
- How do the energy levels of the system change as you add wells? How do they change as you change the separation of the wells?
- Now, instead of looking at the energy levels, change the view on the plot in order to look at different eigenstates of the system.(That is, change the plot do that the box labelled E_n is unchecked and the ψ_n box is checked.) How do the bound eigenstates change as you change the number of wells and their spacing?
- What do you think happens as the number of wells goes to infinity? How will the energy levels arrange themselves? How would you expect an eigenstate to look in position space? How would you expect it to look in momentum space?
- What is the connection between this and the energy bands and bandgaps that arise in solids? Which bands are the valence bands? Which bands are the conduction bands?