Earlier in the class we solved S. Eqn for independent electrons placed in this repeating potential. Approximate solutions are LCAO states built from s-orbitals, p-orbitals etc.

a) If there was one infinitely deep square muffin tin centered at the origin, what would be the ground state wave function \( \psi(x,y) \)?

If there was one square muffin tin at the origin with finite depth, \( V_0 \), the ground state wavefunction would be similar to the infinite case (the main difference is that the wave function would penetrate the walls of a finite potential). Call this wavefunction \( \psi_0(x,y) \).

b) Use the LCAO approximation to find the ground state wave function of the infinite array of finite square muffin tins shown in the Figure. Write your answer in terms of \( \psi_0(x,y) \).
Effective Lattice Potential, $V_{\text{eff}}(r)$

In silicon, the highest energy electrons see something like this (after accounting for presence of all other electrons)

Most materials lie somewhere between these two extremes

In aluminum, the highest energy electrons see something like this (after accounting for the presence of all other electrons)
The “simple” metals fit the free electron model

Sodium

Magnesium

Aluminum
(see hw#6)
Comparing the approximation methods

Free electron bands, Na

s-orbital LCAO states, Na

DFT calculation, Na