**SELF-CONSISTENT CALCULATIONS OF EFFECTIVE POTENTIALS**

Wien2k and other DFT programs go through many computational iterations attempting to find "self-consistent solutions"

\[ V_{\text{eff}}(\rho), \text{ EFFECTIVE POTENTIAL FROM NUCLEI \& ELECTRONS} \]

\[ \rho(\vec{r}), \text{ ELECTRON DENSITY} \]

\[ \text{SOLVE S. EQUATION} \]

An early method of performing this computational loop is the "Hartree-Fock Method" (see wikipedia). Modern DFT methods have replaced the Hartree-Fock Method.
Caption: This figure shows a crude approach using single-electron wavefns $\psi_1(x)$ & $\psi_2(x)$ rather than a multiparticle wavefn $\psi(x_1, x_2)$. 2 electrons in 1 square well potential. Input, the starting point. Modify $V_1(x)$ to account for presence of electron 2. Modify $V_2(x)$ to account for presence of electron 1.
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).