Homework 4

1. [20 pt] Derive the density of states for a

   a. 1D tight-binding model, $\epsilon(k) = \epsilon_0 - 2t\cos(ka_0)$, with lattice constant a_0.
   b. 3D free-electron system, $\epsilon(k) = \frac{1}{2}k^2$.

2. [15 pt] Consider a 1D tight-binding model above, at half-filling ($E_\mathrm{F} = \epsilon_0$, or $k_\mathrm{F} = \pi/(2a_0)$). Analytically determine the total energy by integrating the electronic state energies up to the Fermi energy.

3. [20 pt] For the same 1D tight-binding model at half-filling

   a. Numerically integrate using a discrete set of k-points,

   $$k_n = \frac{\pi}{a_0}\frac{2n - N_k}{N_k}$$

   for $n = 0 \ldots N_k - 1$ without any smearing. Plot your energy as a function of N_k, and fit your energy as a function of N_k.
   b. Repeat your integration, but this time use a smearing method of your choice. How does the convergence change? Try with different smearing parameters.

4. [20 pt] Use the Kerker construction to make a pseudopotential for the $2s$ and $2p$ states of hydrogen. What differences do you notice compared with the pseudopotential for $1s$?

5. [15 pt] Would a pseudopotential be useful for a Gaussian basis? Why or why not?

6. [10 pt] For a simple cubic cell with lattice constant $a_0 = 3$Å, how many planewaves are there for an energy cutoff of 250eV? 400eV? How many for a $3 \times 3 \times 3$ supercell with lattice constant 9Å?