MATRL 218: Assignment 5

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1. The Lennard-Jones potential for a monoatomic system is:

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

   Where ϵ is the well depth and σ is the atomic (or particle) diameter. (i) Sketch the distance-dependence of this potential using scaled units, *ie.* set $\sigma = 1$ and $\epsilon = 1$. Approximately how many atomic diameters does one need to be separated by before there is effectively no interaction. (ii) Determine by setting $\partial U(r)/\partial r = 0$, the value of r/σ for which the potential is minimum.

2. Why do you expect the dispersion (van der Waals) attraction between larger noble gas atoms to be larger than for smaller ones.

3. Sketch two interpenetrating square lattices, whose origins are separated by $(0.5, 0.5)$, and assign atoms at the corners of the two lattices with opposite charges (a "2D CsCl", actually a rock-salt). Can you write out the first few terms of the geometric Madelung constant for the above lattice. Does it look like you can sum it up to ∞.

4. Sketch the E *vs.* k dispersion relation for a square lattice of p_x and p_y orbitals, and pay attention to σ and π interactions. The points defining the Brillouin zone boundaries are $\Gamma(0,0)$, $X(\pi/a, 0)$, $Y(0, \pi/a)$, and $M(\pi/a, \pi/a)$. Sketch the densities of state alongside. Note that a single band could be σ or σ^*-like in some parts of the Brillouin zone, and π or π^*-like in others, and label these.

5. Now stretch the above the lattice in the y direction so that it is rectangular, with $a < b$. This is a little akin to a Peierls distortion. How does this modify the band structure. Remember that the BZ boundaries are $\Gamma(0,0)$, $X(\pi/a, 0)$, $Y(0, \pi/b)$, and $M(\pi/a, \pi/b)$. Does such a distortion can result in a gap between filled and unfilled states?

6. Collaborations are fine on this: Write a code in a language of your choice to calculate the geometric Madelung constant for the CsCl structure, using finite chunks of the structure, *ie.* I need to see how the Madelung potential grows with increasing numbers of Cs–Cl pairs, and when it asymptotes. No rush on this.