1 Infinite, One-Dimensional Chain of Atoms

1. Together, in class, we developed a code to solve the infinite, one-d chain of evenly-spaced atom using plane waves and Bloch functions. Ensure that your code can perform/answer the following questions/tasks.

1. Write a member function that produces a band structure diagram. Ensure that the density of the points is sufficient to see the trend.

2. Look at a few of the low energy eigenfunctions and verify that they seem reasonable. (i.e. What wavefunction would you expect for large atomic separation, small separation)

3. Investigate what physical properties of the situation affect the width of an energy band.

4. We know that the only unique values for k lie between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$. Verify that this is true by looking at the wavefunction for $k = \frac{\pi}{2a}$ and again for $k = \frac{\pi}{2a} + \frac{2\pi}{a}$

5. Does the size of the first Brillioun zone (unit cell in k-space) increase or decrease with the atomic spacing (i.e. the size of the unit cell)?

6. Replace the square wells that we have been using with something more Coulombic. (Warning, the coulomb potential diverges at $x = 0$. That won't be a good thing for the numerics. Instead, make the potential well flat for very small x.)

7. Make a band-structure diagram for the coulombic potential and notice any differences from the square-well potential.