Physics 5403: Computational Physics – Project 5

due date: October 19, 2022

Geometric structure of multi-charge clusters

The goal of this project is to find the stable geometric structure of clusters of Na^+ ions and Cl^- ions by minimizing the total energy. The energy of a cluster is the sum over all pair interaction energies,

$$E = \sum_{i<j} V(r_{ij})$$

where r_{ij} is the distance between ions i and j. The pair interaction energy $V(r)$ can be modeled by (see Kittel: Solid State Physics):

$$V(r) = \pm k\frac{e^2}{r} + \alpha e^{-r/r_0} + \beta\left(\frac{r_1}{r}\right)^{12} \quad .$$

The first term represents the Coulomb interaction between ions of equal or opposite charges $\pm e$, the second term represents a short-range repulsion of the electron shells, and the third term has been added to prevent a collapse at distance $r = 0$ for opposite charges. The parameters are: $\alpha = 1090\text{eV}$, $r_0 = 0.321\text{Å}$, $\beta = 1\text{eV}$, $r_1 = 0.1\text{Å}$. The Coulomb term ke^2 is 14.4eV Å.

a) Consider the simplest cluster, NaCl, consisting of one sodium and one chlorine ions. Find the optimal distance between the ions. To do so, write a program that minimizes $V(r)$ w.r.t. r. You are not expected to write your own optimization code. Use the praxis package provided on the course web site or scipy.optimize.minimize (Python) or fminsearch (MatLab) or similar. Plot $V(r)$ and verify the minimum position in the plot.

b) Now consider the general case of N_+ sodium and N_- chlorine ions. The total number of degrees of freedom for a cluster of $N_p = N_+ + N_-$ particles is $3N_p$. How many of these d.o.f. describe the geometry of the cluster? You will want to discard the translational and rotational motion of the cluster as a whole. How can you achieve this in your program?

c) Using the insight gained in part b), write a program which minimizes the total energy of a cluster of N_+ sodium and N_- chlorine ions. Print out the positions of all particles and the total energy in the minimum configuration.

d) Consider the clusters NaCl, Na_2Cl^+, Na_2Cl_2, $Na_3Cl_2^+$, and Na_3Cl_3. What structure do you expect for these clusters? The higher clusters may have several configurations of similar energy. Perform the simulation for the above clusters. Record energy and structure of all metastable configurations (you may have to start from several different guesses for each of the higher clusters). Plot the resulting structures, e.g. as a 3D plot or via projections on the xy and xz planes.