Physics 431 - Homework 5

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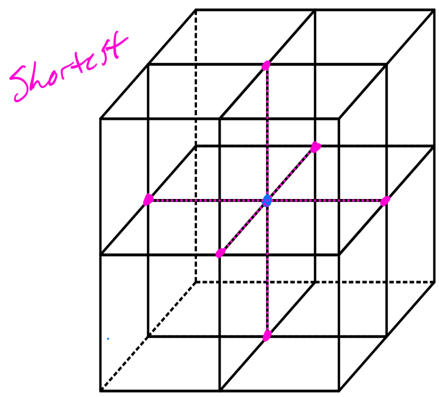
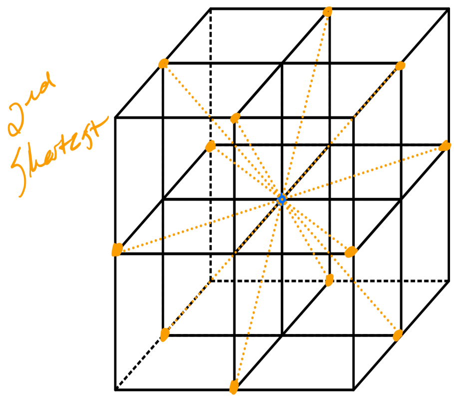
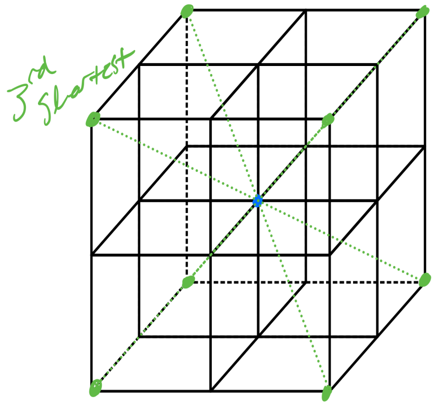
Problem 1

Part A







Part B

$$\begin{aligned}\textbf{Shortest} &= 6_{neighbors}\hat{a} \\ \textbf{2nd Shortest} &= 12_{neighbors}\sqrt{2}\hat{a} \\ \textbf{3rd Shortest} &= 8_{neighbors}\sqrt{3}\hat{a}\end{aligned} \tag{1}$$

Part C

$$p_{ij} \text{ has no dimension}$$

For: $\sum(\frac{1}{p_{ij}})^{12}$

$$\begin{aligned}\sum(\frac{1}{p_{ij}})^{12} &= 6(\frac{1}{1})^{12} + 12(\frac{1}{\sqrt{2}})^{12} + 8(\frac{1}{\sqrt{3}})^{12} \\ &= 6 + 12(\frac{1}{\sqrt{2}})^{12} + 8(\frac{1}{\sqrt{3}})^{12} \\ &= 6.1985\end{aligned} \tag{2}$$

For: $\sum(\frac{1}{p_{ij}})^6$

$$\begin{aligned}\sum(\frac{1}{p_{ij}})^6 &= 6(\frac{1}{1})^6 + 12(\frac{1}{\sqrt{2}})^6 + 8(\frac{1}{\sqrt{3}})^6 \\ &= 6(\frac{1}{1})^6 + 12(\frac{1}{\sqrt{2}})^6 + 8(\frac{1}{\sqrt{3}})^6 \\ &= 7.7962\end{aligned} \tag{3}$$

Part D

F or $\sum(\frac{1}{p_{ij}})^{12}$, the number agrees pretty well. Since we estimated just using the nearest neighbors from 8 unit cells, this tells us that the repulsion potential is almost entirely from the atoms closest to it. This makes sense since since the Pauli exclusion principle states two electrons cannot be in the same state at the same time, there for the repulsion an atom experiences should be greater as it gets closer to another atom.

F or $\sum(\frac{1}{p_{ij}})^6$, the number is pretty off. Again, since this is an estimation just using the closest unit cells, this tells us there is a contribution coming from the next closest unit cells that is not negligible and therefore makes our approximation off. In the context of both numbers, we can expect that at the same p_{ij}, the repulsive term will be more accurate the closer we are, while as we move further away, the attractive term will become more accurate as an approximation.

Problem 2

Part A

BCC Lattice sums

$$\sum_j(\frac{1}{p_{ij}})^{12} = 9.11418,\ \sum_j(\frac{1}{p_{ij}})^6 = 12.2533$$

FCC Lattice sums: Found in lecture 10 page 3

$$\sum_j(\frac{1}{p_{ij}})^{12} = 12.131,\ \sum_j(\frac{1}{p_{ij}})^6 = 14.45$$

I tried to calculate the FCC sums but could not get it.

$$U(R) = 2\epsilon N[\alpha_{12}(\frac{\sigma}{R})^{12} - \alpha_6(\frac{\sigma}{R})^6] \tag{4}$$

$$\begin{aligned}\frac{\partial}{\partial R}U(R) &= 2\epsilon N\frac{\partial}{\partial R}[\alpha_{12}(\frac{\sigma}{R})^{12} - \alpha_6(\frac{\sigma}{R})^6] \\ &= 2\epsilon N[\alpha_{12}\sigma^{12}\frac{\partial}{\partial R}R^{-12} - \alpha_6\sigma^6\frac{\partial}{\partial R}R^{-6}] \\ &= 2\epsilon N[-12\alpha_{12}(\frac{\sigma^{12}}{R^{13}}) + 6\alpha_6(\frac{\sigma^6}{R^7})]\end{aligned} \tag{5}$$

Solve for R_o

$$
\begin{aligned}
\frac{\partial}{\partial R}U(R) &= 0 \\
0 &= 2\epsilon N[-12\alpha_{12}(\frac{\sigma^{12}}{R^{13}}) + 6\alpha_6(\frac{\sigma^6}{R^7})] \\
&= [-12\alpha_{12}(\frac{\sigma^{12}}{R^{13}}) + 6\alpha_6(\frac{\sigma^6}{R^7})] \\
12\alpha_{12}(\frac{\sigma^{12}}{R^{13}}) &= [6\alpha_6(\frac{\sigma^6}{R^7})] \\
(\frac{\sigma^6}{R_o^6}) &= [\frac{\alpha_6}{2\alpha_{12}}] \\
\frac{2\alpha_{12}\sigma^6}{\alpha_6} &= R_o^6
\end{aligned} \tag{6}
$$

$$
\begin{aligned}
(BCC)R_o^6 &= 1.488\sigma^6 \\
(BCC)R_o^{12} &= 2.213\sigma^{12} \\
(FCC)R_o^6 &= 1.679\sigma^6 \\
(FCC)R_o^{12} &= 2.819\sigma^{12}
\end{aligned}
$$

Now take ratio

$$
\begin{aligned}
(BCC)U(R_o) &= 2N\epsilon[\frac{9.11418}{2.213} - \frac{12.2533}{1.488}] \\
&= 2N\epsilon[-4.116]
\end{aligned} \tag{7}
$$

$$
\begin{aligned}
(FCC)U(R_o) &= 2N\epsilon[\frac{12.131}{2.819} - \frac{14.45}{1.679}] \\
&= 2N\epsilon[-4.211]
\end{aligned} \tag{8}
$$

$$
\frac{(BCC)U(R_o)}{(FCC)U(R_o)} = 0.956 \tag{9}
$$

Part B: R_o for BCC

Please see the derivative above for the full calculation of the derivative

$$
\begin{aligned}
\frac{2 * 9.11418\sigma^6}{12.2533} &= R_o^6 \\
1.488 * \sigma &= R_o \\
1.488 * (2.74) &= R_o \\
4.076 &= R_o \\
&\textit{For neon}
\end{aligned} \tag{10}
$$