Homework 4
PHZ 5156
Due Tuesday, October 3

1. Consider a periodic charge density \( \rho(\vec{r}) \) defined such that

\[
\rho(\vec{r} + \vec{R}_{n_1n_2n_3}) = \rho(\vec{r}).
\]  

(1)

We define the vector \( \vec{R}_{n_1n_2n_3} \) to be

\[
\vec{R}_{n_1n_2n_3} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3
\]  

(2)

where \( n_1, n_2, \) and \( n_3 \) are integers and the primitive lattice vectors are defined in terms of a Cartesian system by \( \vec{a}_1 = L\hat{x}, \vec{a}_2 = L\hat{y}, \) and \( \vec{a}_3 = L\hat{z}. \)

a) Determine the appropriate reciprocal lattice vectors \( \vec{G} \) such that we can write the periodic charge density \( \rho(\vec{r}) \) as a summation

\[
\rho(\vec{r}) = \sum_{\vec{G}} \rho_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})
\]  

(3)

where the summation is over all possible vectors \( \vec{G}. \)

b) Show that the Coulomb potential due to this charge density is also periodic and given by (up to a constant),

\[
V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})
\]  

(4)

which can be written in terms of the \( \rho_{\vec{G}} \) as,

\[
V(\vec{r}) = \sum_{\vec{G}} \frac{\rho_{\vec{G}}}{G^2} \exp(i\vec{G} \cdot \vec{r})
\]  

(5)

with \( G^2 = \vec{G} \cdot \vec{G}. \) Hint: Consider the Poisson equation.

c) Show that for a point charge at \( \vec{r}' \) and its periodic images, that \( \rho_{\vec{G}} = \frac{1}{\Omega} \exp(-i\vec{G}\vec{r}') \) with \( \Omega = L^3. \)

d) Determine an expression for the total electrostatic energy density. Explain why \( \rho_{\vec{G}=0} \) must be zero in order for the answer to be sensible. What does this imply for \( \rho(\vec{r})? \)