Electrodynamics – PHY712

Lecture 2 – Ewald summation methods

Reference: Chap. 1.11 in J. D. Jackson’s textbook.

1. Motivation

2. Expression to calculate electrostatic energy of an extended periodic system and its derivation

3. Examples
Consider a collection of point charges $\{q_i\}$ located at points $\{r_i\}$. The energy to separate these charges to infinity ($\{r_i \to \infty\}$) is

$$ W = \frac{1}{4\pi \epsilon_0} \sum_{(i,j; i>j)} \frac{q_i q_j}{|r_i - r_j|}. $$

(1)

Here the summation is over all pairs of $(i, j)$, excluding $i = j$. It is convenient to sum over all particles and divide by 2 to compensate for the double counting:

$$ W = \frac{1}{8\pi \epsilon_0} \sum_{i,j; i \neq j} \frac{q_i q_j}{|r_i - r_j|}. $$

(2)

Here the summation is over all pairs of $i, j$, excluding $i = j$. The energy $W$ scales as the number of particles $N$. As $N \to \infty$, the ratio $W/N$ remains well-defined in principle, but difficult to calculate in practice.
When the discrete charge distribution becomes a continuous charge density: $q_i \to \rho(r)$, the electrostatic energy becomes

$$W = \frac{1}{8\pi\varepsilon_0} \int d^3r \int d^3r' \frac{\rho(r)\rho(r')}{|r - r'|}. \quad (3)$$

Notice, in this case, it is not possible to exclude the “self-interaction”. This expression can be written in terms of the electrostatic potential $\Phi(r)$ and field $E(r)$:

$$W = \frac{1}{2} \int d^3r \rho(r)\Phi(r) = -\frac{\varepsilon_0}{2} \int d^3r (\nabla^2\Phi(r)) \Phi(r). \quad (4)$$

$$W = \frac{\varepsilon_0}{2} \int d^3r |\nabla\Phi(r)|^2 = \frac{\varepsilon_0}{2} \int d^3r |E(r)|^2. \quad (5)$$
Electrodynamics – PHY712

Lecture 2 – Ewald summation methods – exact result for periodic system

\[
\frac{W}{N} = \sum_{\alpha\beta} \frac{q_\alpha q_\beta}{8\pi \varepsilon_0} \left( \frac{4\pi}{\Omega} \sum_{G \neq 0} \frac{e^{i G \cdot \tau_{\alpha\beta}} e^{-G^2/\eta}}{G^2} - \sqrt{\frac{\eta}{\pi}} \delta_{\alpha\beta} + \sum_{T} \text{erfc} \left( \frac{1}{2} \sqrt{\eta} |\tau_{\alpha\beta} + T| \right) \right) \right) - \frac{4\pi Q^2}{8\pi \varepsilon_0 \Omega \eta}.
\]