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

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Lecture 2 – Ewald summation methods – Motivation

Consider a collection of point charges $\{q_i\}$ located at points $\{\mathbf{r}_i\}$. The energy to separate these charges to infinity ($\{\mathbf{r}_i \to \infty\}$ is

$$W = \frac{1}{4\pi\epsilon_0} \sum_{(i,j;i>j)} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1}$$

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:

$$W = \frac{1}{8\pi\epsilon_0} \sum_{i,j;i\neq j} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{2}$$

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.

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Lecture 2 – Ewald summation methods – slight digression

When the discrete charge distribution becomes a continuous charge density: $q_i \to \rho(\mathbf{r})$, the electrostatic energy becomes

$$W = \frac{1}{8\pi\epsilon_0} \int d^3r \; d^3r' \; \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \tag{3}$$

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

$$W = \frac{1}{2} \int d^3r \; \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2} \int d^3r \left(\nabla^2\Phi(\mathbf{r})\right) \Phi(\mathbf{r}). \tag{4}$$

$$W = \frac{\epsilon_0}{2} \int d^3r \, |\nabla\Phi(\mathbf{r})|^2 = \frac{\epsilon_0}{2} \int d^3r \, |\mathbf{E}(\mathbf{r})|^2 . \tag{5}$$

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

$$\frac{W}{N} = \sum_{\alpha\beta} \frac{q_\alpha q_\beta}{8\pi\varepsilon_0} \left(\frac{4\pi}{\Omega} \sum_{\mathbf{G}\neq\mathbf{0}} \frac{e^{-i\mathbf{G}\cdot\tau_{\alpha\beta}}\ e^{-G^2/\eta}}{G^2} - \sqrt{\frac{\eta}{\pi}}\delta_{\alpha\beta} + \sum_{\mathbf{T}}{}' \frac{\mathrm{erfc}(\frac{1}{2}\sqrt{\eta}|\tau_{\alpha\beta} + \mathbf{T}|)}{|\tau_{\alpha\beta} + \mathbf{T}|} \right) - \frac{4\pi Q^2}{8\pi\varepsilon_0\Omega\eta}. \tag{6}$$