PHY 712 Electrodynamics
9-9:50 AM MWF Olin 103

Plan for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

Ewald summation methods

1. **Motivation**
2. **Expression to evaluate the electrostatic energy of an extended periodic system**
3. **Examples**

PHY 712 Electrodynamics

MWF 9-9:50 AM	OPL 103	http://www.wfu.edu/~natalie/s17phy712/

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Course schedule for Spring 2017

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Wed: 01/11/2017	Chap. 1	Introduction, units and Poisson equation	#1	01/18/2017
2	Fri: 01/13/2017	Chap. 1	Electrostatic energy calculations	#2	01/18/2017
	Mon: 01/16/2017		*MLK Holiday - no class*		
3	Wed: 01/18/2017				
4	Fri: 01/20/2017				
5	Mon: 01/23/2017				

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

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

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 in order to compensate for the double counting:

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

Now the summation is over all i and 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.

Ewald summation methods – slight digression

When the discrete charge distribution becomes a continuous charge density: $q_i \rightarrow \rho(\mathbf{r})$, the electrostatic energy becomes $W = \frac{1}{8\pi\epsilon_0}\int d^3r\, d^3r' \,\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}.$

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 $\mathbf{E}(\mathbf{r})$:

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

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

Evaluation of the electrostatic energy for *N* point charges:

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

Ewald summation methods – exact results for periodic systems

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

Note that the results should not depend upon η (assuming that all summations are carried to convergence). In the example of CsCl having a lattice constant a, we show two calculations produce the result:

$$\frac{W}{N} = -\frac{e^2}{8\pi\epsilon_0}\frac{4.070722970}{a} \quad \text{or} \quad \frac{W}{N} = -\frac{e^2}{8\pi\epsilon_0}\frac{4.070723039}{a}$$

See lecture notes for details.