PHY 712 Electrodynamics
12-12:50 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**

This lecture details some special properties of the electrostatic energy of an extended system. It illustrates some special properties of the long range nature of the Coulomb interaction. Ewald summation methods may or may not be important for your particular field of study. However, it is at least important to be aware of the ideas.

PHY 712 Electrodynamics

MWF 10-10:50 PM	Online	http://www.wfu.edu/~natalie/s21phy712/

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Course schedule for Spring 2021

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Wed: 01/27/2021	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/29/2021
2	Fri: 01/29/2021	Chap. 1	Electrostatic energy calculations	#2	02/01/2021
3	Mon: 02/01/2021	Chap. 1	Electrostatic potentials and fields		
4	Wed: 02/03/2021	Chap. 1 - 3	Poisson's equation in 2 and 3 dimensions		
5	Fri: 02/05/2021	Chap. 1 - 3	Brief introduction to numerical methods		
6	Mon: 02/08/2021	Chap. 2 & 3	Image charge constructions		

The homework problem assigned this time exercises the ideas presented in this lecture.

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

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

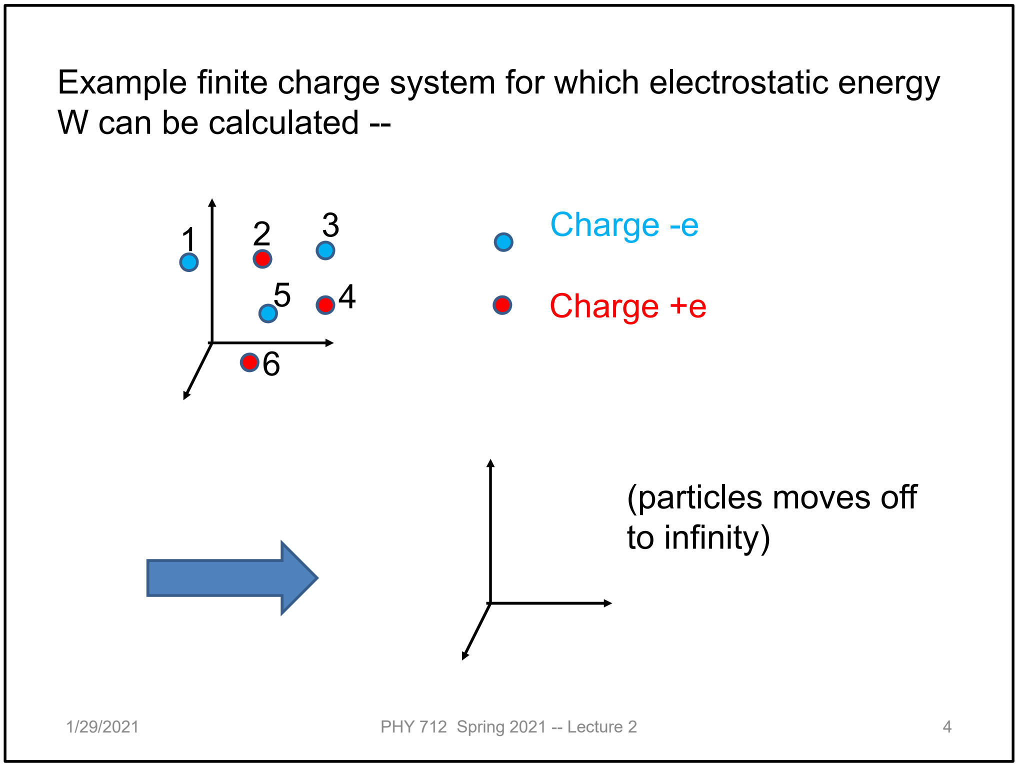
Here the summation is over all pairs of (i, j), excluding $i = j$.

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.



Summation for a finite number of particles is straightforward, but extension to an infinite system runs into difficulty.

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.

In the Extra lecture notes this expression will be derived and illustrated.

Slight digression:

Comment on electrostatic energy evaluation --

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

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

Notice, in this case, it is not possible to exclude the ``self-interaction".

Electrostatic energy in terms of $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

Previous expression can be rewritten in terms of the electrostatic potential or field:

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

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

We will see and used these expressions. However, the so-called self energy often leads to difficulties….