PHY 712 Electrodynamics
11-11:50 AM MWF Olin 103

Class notes for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

1. **Calculation of the electrostatic energy**
2. **Evaluation of the electrostatic energy of an extended periodic system using Ewald summation methods**

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.

PHYSICS AND CHEMISTRY JOINT COLLOQUIUM

4 PM Olin 101

THURSDAY

•

JANUARY 13, 2022

"Human Caused Earthquakes: How Bad Can They Be?"

The rate of seismicity in parts of the Central U.S has increased dramatically in the past decade—increasing from an average historical rate of three earthquakes of greater than magnitude 3 per year, to approximately 12 per year since 2008. Numerous studies have linked the increase in seismicity to wastewater injection and other activities associated with oil and gas production, hence they are referred to as human-induced earthquakes. Damage from these events, particularly larger magnitude events such as the 2011 Magnitude 5.7 Prague, OK and 2016 Magnitude 5.8 Pawnee, OK earthquakes, have resulted in millions of dollars of insurance claims and class action lawsuits against oil and gas companies. This presentation will discuss research investigating the vulnerability of infrastructure to induced earthquakes, including an overview of the geophysics associated with human-induced earthquakes and the mechanics-based approach to determining their potential to cause damage.

Patricia Clayton, Ph.D.
Associate Professor
Department of Engineering
Wake Forest University
Winston-Salem, NC

4:00 pm - Olin 101*

*Link provided for those unable to attend in person.

Note: For additional information on the seminar or to obtain the video conference link, contact

PHY 712 Electrodynamics

MWF 11-11:50 AM	**Olin 103**	Webpage: **http://www.wfu.edu/~natalie/s22phy712/**

Instructor: Natalie Holzwarth	**Office:**300 OPL	**e-mail:**natalie@wfu.edu

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 1	Electrostatic energy calculations	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 1	Electrostatic energy calculations	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		

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

Comment on HW #1

For Prob. 1.5, what if the potential function had the form:

$$\Phi(r) = \frac{q}{4\pi\epsilon_0}\left[\frac{e^{-2r/a_0}}{r}\left(1+\frac{r}{a_0}\right)-\frac{1}{r}\right]?$$

Contribution from only the electron in its ground state

PHY 712 -- Assignment #2

January 12, 2022

Continue reading Chap. 1 in **Jackson**.

Calculate the electrostatic energy of the following 5 ion molecule scaled by the factor $(1/(4\pi\varepsilon_0))\ (q^2 / a)$. Note that **x**, **y**, and **z** denote unit vectors in the three Cartesian directions.

1. Charge = 4q Position = 0
2. Charge = -q Position = (a/2)(**x+y+z**)
3. Charge = -q Position = (a/2)(**-x-y+z**)
4. Charge = -q Position = (a/2)(**x-y-z**)
5. Charge = -q Position = (a/2)(**-x+y-z**)

Calculation of the electrostatic energy of a system of charges --

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 $i = j$.

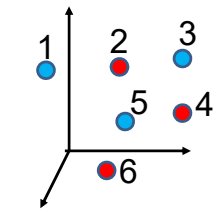
It is convenient to sum over all particles and divide by 2 in order to compensate for the double counting:

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

Now the summation is over all i and j, excluding $i = j$.

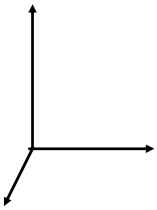
The energy W scales as the number of particles N. As N $\to \infty$, the ratio W / N remains well-defined in principle, but difficult to calculate in practice.

Example finite charge system for which electrostatic energy W can be calculated in a straightforward way



Charge -e

Charge +e



(particles moves off to infinity)

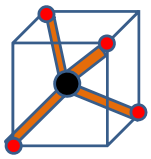
$$W = W_{12} + W_{13} + W_{14} + W_{15} + W_{16} + W_{23} + W_{24} + W_{25} + W_{26} + W_{34} + W_{35} + W_{36} + W_{45} + W_{46} + W_{56}$$

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

Homework problem #2

Calculate the electrostatic energy of the following 5 ion molecule scaled by the factor $(1/(4\pi\varepsilon_0))\ (q^2 / a)$. Note that **x**, **y**, and **z** denote unit vectors in the three Cartesian directions.

1. Charge = 4q Position = 0
2. Charge = -q Position = (a/2)(**x**+**y**+**z**)
3. Charge = -q Position = (a/2)(-**x**-**y**+**z**)
4. Charge = -q Position = (a/2)(**x**-**y**-**z**)
5. Charge = -q Position = (a/2)(-**x**+**y**-**z**)



Now consider the case of an infinite periodic system --

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.

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:

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

Details to follow --

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 use these expressions throughout the course. However, the so-called self energy often leads to difficulties….

Some details --

Electrostatic potential

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

Electrostatic field

$$\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$$

Poisson equation

$$\nabla^2\Phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}$$

Summary --
Electrostatic energy

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

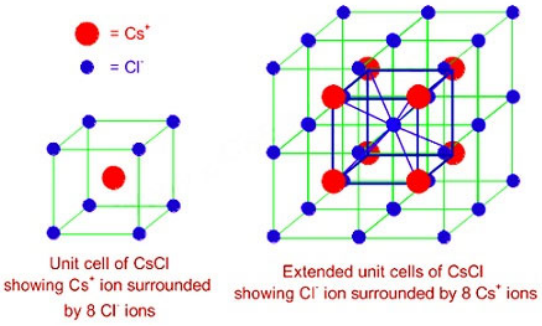
Evaluation of electrostatic energy in terms of potential $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

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

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

In general, the evaluation of the electrostatic energy of an extended system can be numerically tricky because of the long range nature of the Coulombic forces.

Now consider the electrostatic energy of a periodic crystal of CsCl



In general, the evaluation of the electrostatic energy of an extended system can be numerically tricky because of the long range nature of the Coulombic forces.

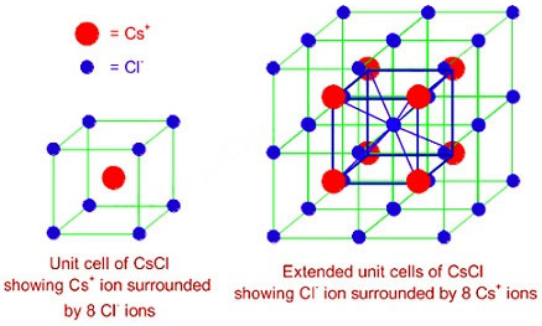
However, thanks to very clever mathematicians, it is possible to perform this sort of calculation for periodic systems.

Ewald, Paul Peter, 1888-1985

American crystallographer, emigrated from Germany

The Ewald summation algorithm is used to evaluate the poorly convergent summations needed to evaluate the electrostatic energy of a periodic ionic solid.

As an example, we will consider the electrostatic energy of a periodic crystal of CsCl



Unit cell of CsCl showing Cs^+ ion surrounded by 8 Cl^- ions

Extended unit cells of CsCl showing Cl^- ion surrounded by 8 Cs^+ ions