PHY 712 Electrodynamics
10-10:50 AM MWF Olin 103

Class notes for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

1. Calculation of the electrostatic energy for a finite system
2. Electrostatic energy in terms of electrostatic fields
3. Electrostatic energy of extended systems -- introduction to Ewald summation methods

Physics Colloquium
Thursday, January 12, 2023
4 PM in Olin 101

Professor John Weisel,
U. Pennsylvania,
Perelman School of Medicine

"Blood clot contraction: Mechanisms, pathophysiology, and disease"

(hosts: M. Guthold and S. Baker)

https://physics.wfu.edu/wfu-phy-news/colloquium/seminar-2023-spring/

PHY 712 Electrodynamics

MWF 10-10:50 AM	Olin 103	Webpage: http://www.wfu.edu/~natalie/s23phy712/

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

Course schedule for Spring 2023

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/9/2023	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/13/2023
2	Wed: 01/11/2023	Chap. 1	Electrostatic energy calculations	#2	01/18/2023
3	Fri: 01/13/2023	Chap. 1	Electrostatic energy calculations thanks to Ewald	#3	01/18/2023
	Mon: 01/16/2023		MLK Holiday -- no class		

Note: Please turn in your worksheets, pdf files, or screenshots for Maple, Mathematica, Wolfram, etc. If you use it to work your HW problems.

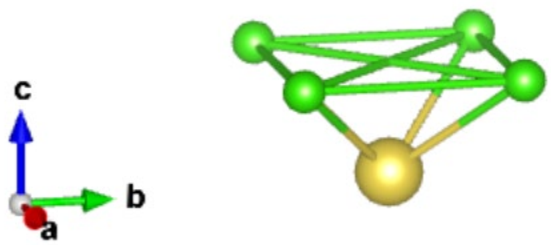
PHY 712 -- Assignment #2

January 11, 2023

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

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

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



Comment on online materials

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Lecture Notes

Typos corrected

- Lecture 1 -- Introduction and electrostatics PP slides PDF Extra PP Extra PDF
- Lecture 2 -- Evaluation of electrostatic energy PP slides PDF Ewald notes PDF

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Last modfied: Monday, 09-Jan-2023 23:05:09 EST

Your questions –
From Sam: What does the electrostatic energy of a system of particles tell us about it's properties? I would Imagine higher energy would simply mean that the lattice is more tightly bound together.

Short answer: Typically, we want to compare the energies of various materials in their various structures. The electrostatic energy is an important component of the "total energy". All energies must be compared to a standard. In this case, the standard is that all of particles are separated far away from eachother.

More questions:

From David: Slide 8: How do we use the Dirac-delta function to obtain a continuous charge distribution from the discrete charge distribution?

Slide 9:Could you talk about why we use an elliptic as the foundation for Poisson's equation?

Slide 11: What are the forces acting in the limit of a periodic crystal?

Some answers --

"Continuous" representation of discrete charges using Dirac delta function:

$$\rho(\mathbf{r}) = \sum_i q_i \ \delta(\mathbf{r} - \mathbf{r}_i) \equiv \sum_i q_i \ \delta(x - x_i)\delta(y - y_i)\delta(z - z_i)$$

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($\mathbf{r}_i \rightarrow \infty\}$ is

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

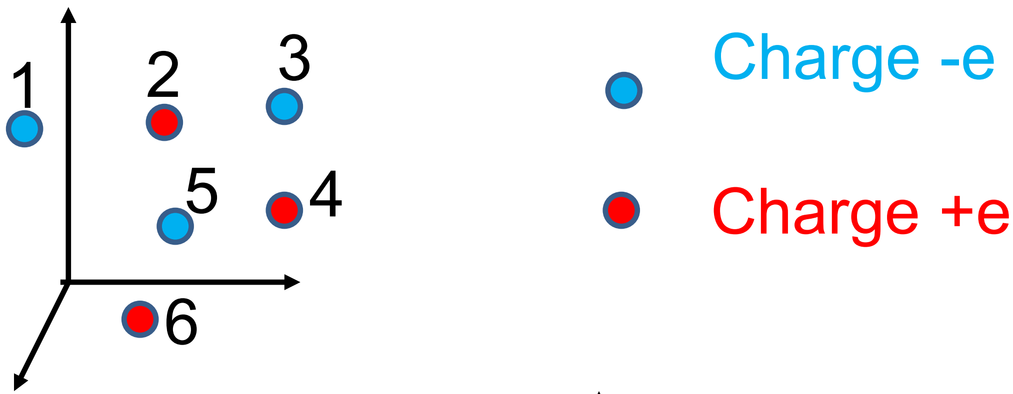
Here the summation is over all pairs of (i, j), excluding $i = j$.

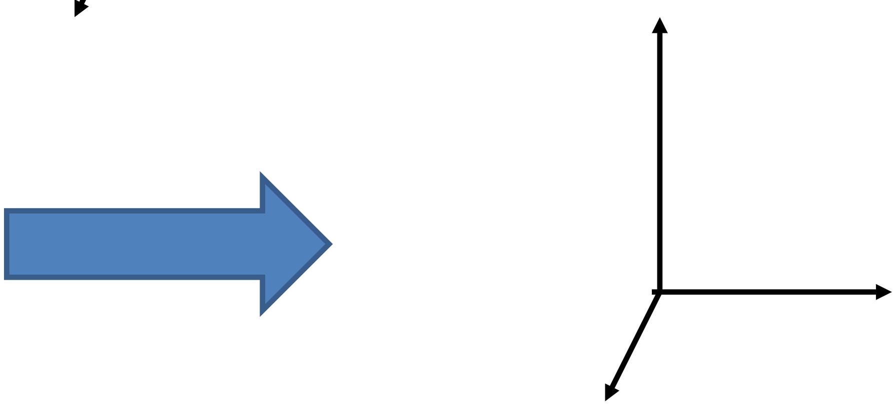
Define $$W_{ij} \equiv \frac{q_i q_j}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} .$$

$$W = \sum_{(i,j;i>j)} W_{ij}$$

Note that this result is likely to grow in magnitude with increasing numbers of charged particles.

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





(particles moves off to infinity)

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

Summary --

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 sometimes 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.

Slight digression:

Comment on electrostatic energy evaluation --

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".

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:

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

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

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 for continuum --
Electrostatic energy

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

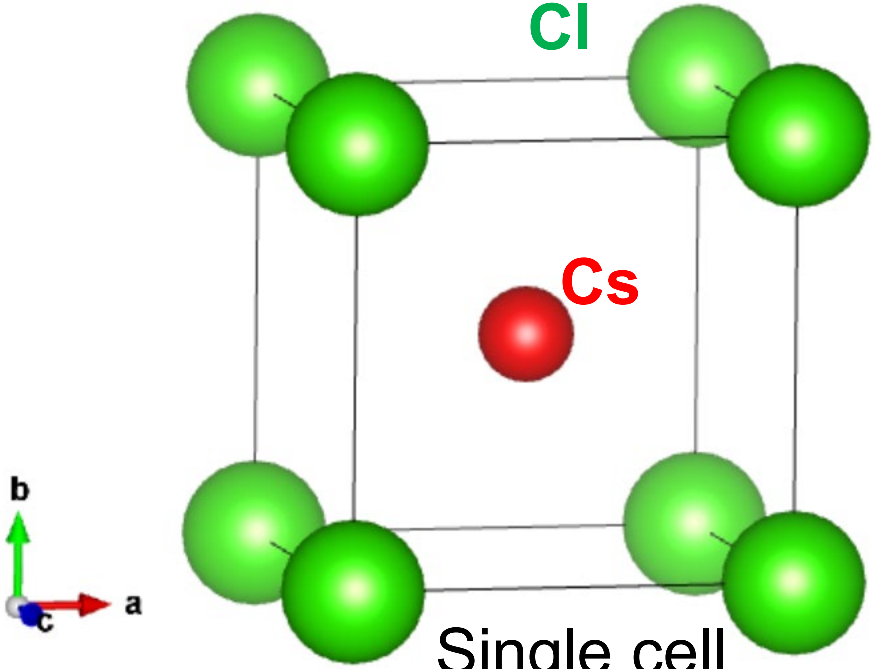
Evaluation of electrostatic energy in terms of potential $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

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

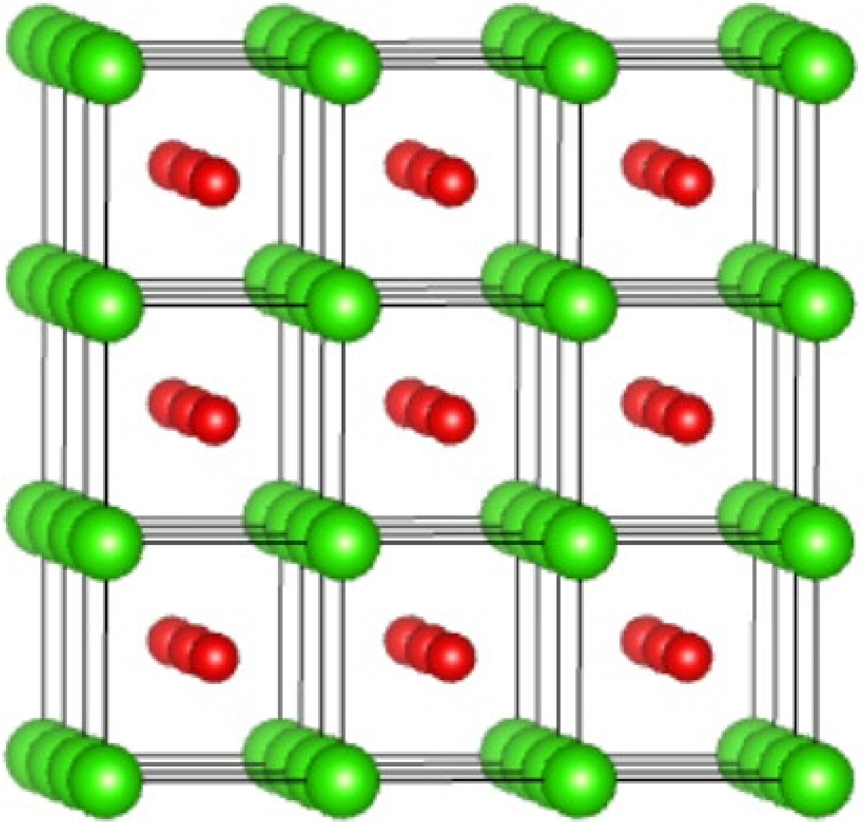
$$W = \frac{\epsilon_0}{2}\int d^3r\left|\nabla\Phi(\mathbf{r})\right|^2 = \frac{\epsilon_0}{2}\int d^3r\left|\mathbf{E}(\mathbf{r})\right|^2.$$

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



Single cell



Multiple cells

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 direct summation of the electrostatic terms of an infinite ionic system diverges, however using Ewald's ideas the single divergent summation can be represented by two converging summations (plus a few corrections).

The formula that we will derive and use for a lattice with periodic real space translations T and reciprocal space translations G is:

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