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

Class notes for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

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

PHY 712 Electrodynamics

MWF 10-10:50 AM	Olin 103	Webpage: http://www.wfu.edu/~natalie/s24phy712/

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

---

Course schedule for Spring 2024

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Wed: 01/17/2024	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/19/2024
2	Fri: 01/19/2024	Chap. 1	Electrostatic energy calculations	#2	01/29/2024
3	Mon: 01/22/2024	Chap. 1	Electrostatic energy calculations	#3	01/29/2024
4	Wed: 01/24/2024	Chap. 1 & 2	Electrostatic potentials and fields	#4	01/29/2024

PHY 712 -- Assignment #2

Assigned: 1/19/2024 Due: 1/29/2024

Continue reading Chapter 1 in **Jackson**.

1. Jackson Problem #1.5. Be careful to take into account the behavior of $\Phi(\mathbf{r})$ for r-->0.

Example in HW2

The electrostatic potential of a neutral H atom is given by:

$$\Phi(r) = \frac{q}{4\pi\epsilon_0}\frac{e^{-\alpha r}}{r}\left(1+\frac{\alpha r}{2}\right).$$

Find the charge density (both continuous and discrete) for this potential.

Hint #1: For continuous contribution you can use the identity:

$$\nabla^2\Phi(r) = \frac{1}{r}\frac{\partial^2(r\Phi(r))}{\partial r^2} = -\frac{1}{\epsilon_0}\rho(r)$$

Hint #2: Don't forget to consider possible discrete contributions, recalling that: $\nabla^2\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right) = -4\pi\delta^3(\mathbf{r}-\mathbf{r}')$

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

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

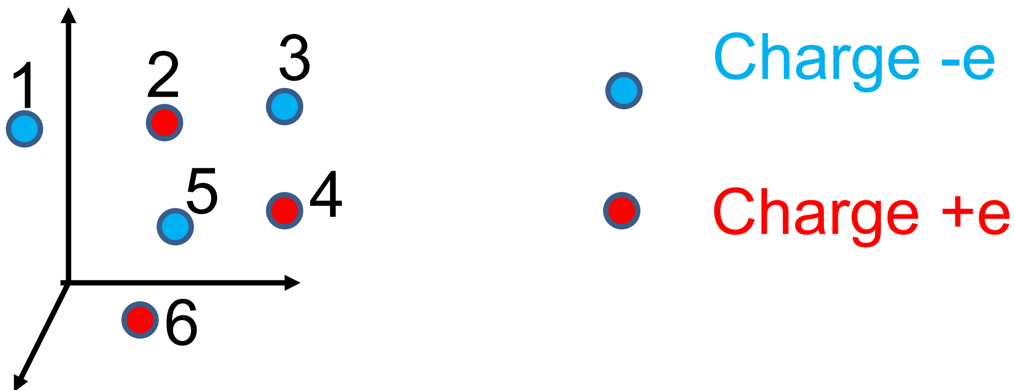
Here the summation is over all pairs of (i, j), excluding $i = j$.

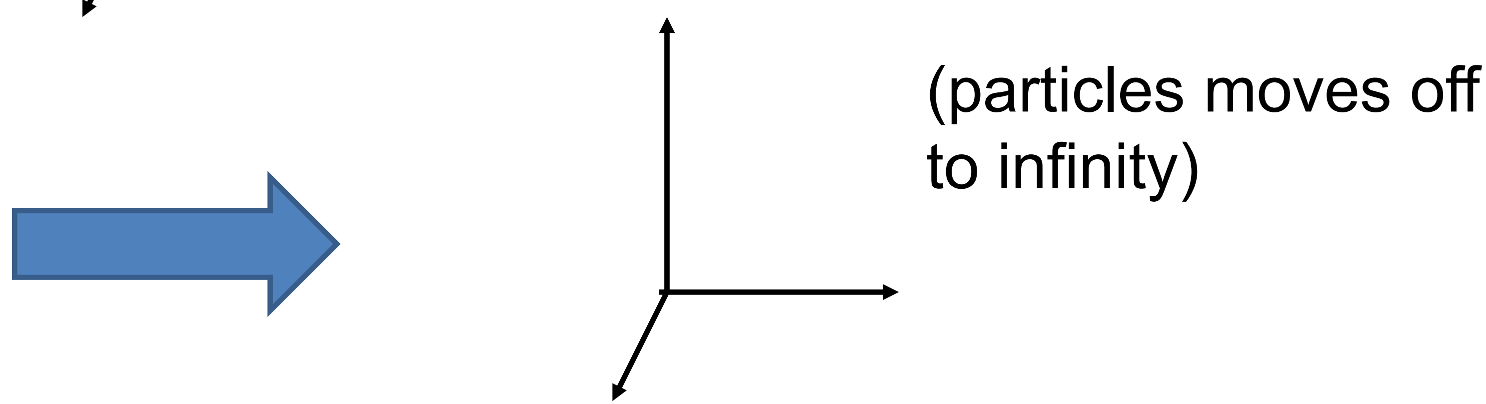
Define $W_{ij} \equiv \frac{q_i q_j}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$.

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

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





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

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

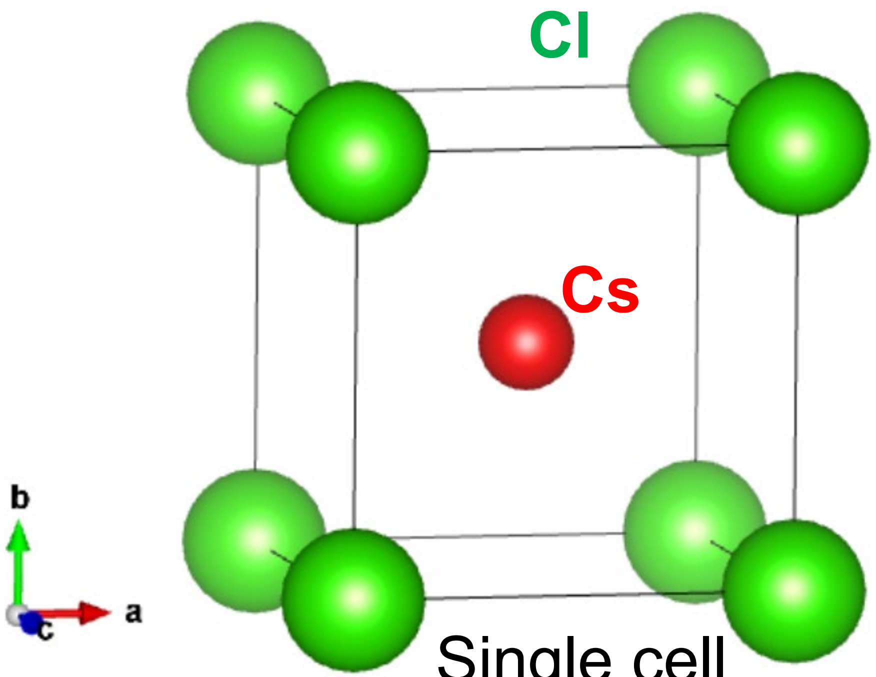
$$W = \frac{1}{2}\int d^3r\; \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2}\int d^3r\left(\nabla^2\Phi(\mathbf{r})\right)\Phi(\mathbf{r}).$$

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

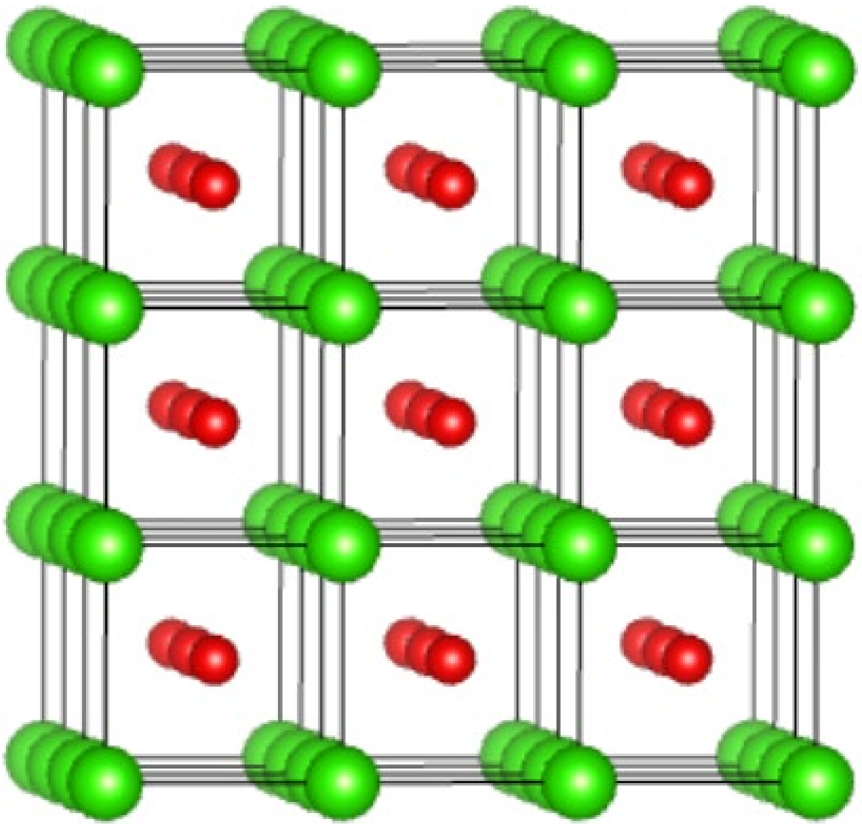
Note that, because of the inclusion of the self-interaction energies, there *may* be mathematical divergences involved in evaluating these quantities.

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:

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

➔See Ewaldnotes.pdf