PHY 712 Electrodynamics
12-12:50 AM MWF Olin 103

Class notes 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

Comment on HW #1

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

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

Your questions –

From Nick –

1) When you say the results should not depend on /eta., is it that /eta doesn't matter or that there's something intrinsic about the energy that shouldn't matter what eta is? Will you walk through the calculations to show why they are slightly different?
2) On the last slide, is this 2 triple integrals? Why do we have d^3r and d^3r' ?

From Gao –

How can the expression of electrostatic energy show its justification in the continuous case as it can not exclude the "self-interaction"?

From Tim –

In the extra notes section on page six you say "there are two kinds of sites...." What do you mean by sites?

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		

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$(\mathbf{r}_i \rightarrow \infty\}$ 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 $i = j$.

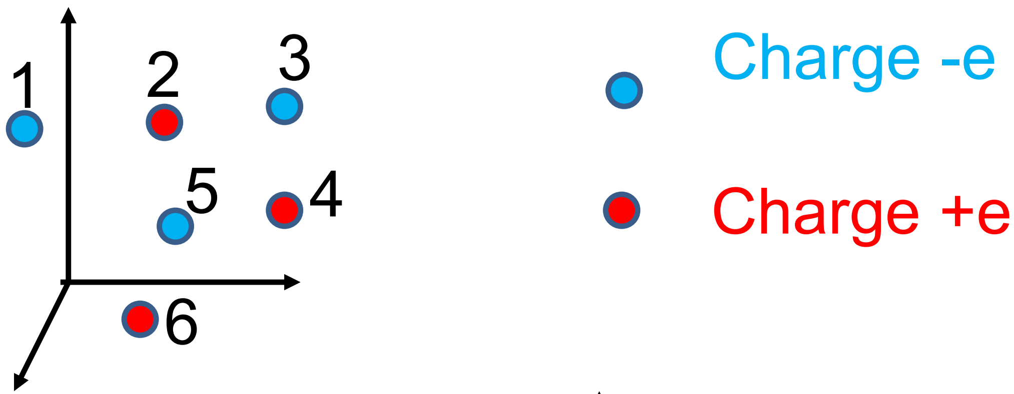
It is convenient to sum over all particles and divide by 2 in order to compensate for the double counting:

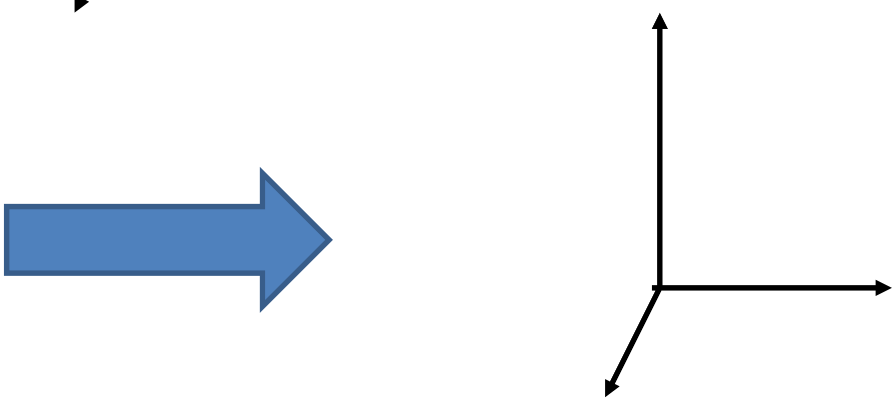
$$W = \frac{1}{8\pi\epsilon_0} \sum_{i,j;i\neq j} \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

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

The energy W scales as the number of particles N. As N $\rightarrow \infty$, 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





(particles moves off to infinity)

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

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.

Your question – How is it that the Ewald summation does not depend upon η?

Comment – This is because of the genius of Ewald (assuming that the summation terms are well converged).

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:

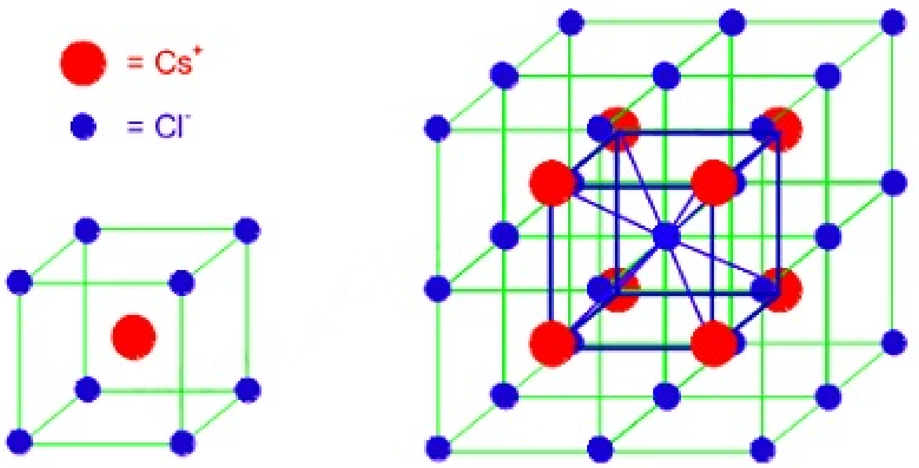
$$W = \frac{1}{2}\int d^3r\ \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2}\int d^3r \left(\nabla^2\Phi(\mathbf{r})\right)\Phi(\mathbf{r}).$$

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

Your question – What happens to the electrostatic case for continuous charge densities with respect to the self energy contribution.

Comment – It sometimes causes trouble.

Now 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