PHY 712 Electrodynamics
9-9:50 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**

1

Colloquium: "First-Principles Investigation on Quantum Materials Using Beyond-DFT Methods"

Dr. Subhasish Mandal,
Department of Physics and Astronomy
Rutgers University
Piscataway, NJ
George P. Williams, Jr. Lecture Hall, (Olin 101)
Wednesday, January 15, 2020 at 3:00 PM

There will be a reception in the Olin Lounge at approximately 4 PM following the colloquium. All interested persons are cordially invited to attend.

2

PHY 712 Electrodynamics

MWF 9-9:50 AM	OPL 103	http://www.wfu.edu/~natalie/s20phy712/

Instructor: Natalie Holzwarth	Phone:758-5510	Office:300 OPL	e-mail:natalie@wfu.edu

Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/17/2020
2	Wed: 01/15/2020	Chap. 1	Electrostatic energy calculations	#2	01/22/2020
3	Fri: 01/17/2020	Chap. 1	Electrostatic potentials and fields		
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020	Chap. 1 - 3	Poisson's equation in 2 and 3 dimensions		
5	Fri: 01/24/2020	Chap. 1 - 3	Brief introduction to numerical methods		
6	Mon: 01/27/2020	Chap. 2 & 3	Image charge constructions		
7	Wed: 01/29/2020	Chap. 2 & 3	Cylindrical and spherical geometries		
8	Fri: 01/31/2020	Chap. 3 & 4	Spherical geometry and multipole moments		
9	Mon: 02/03/2020	Chap. 4	Dipoles and Dielectrics		

3

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.

1/15/2020 PHY 712 Spring 2020 -- Lecture 2 4

4

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

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

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.

1/15/2020 PHY 712 Spring 2020 -- Lecture 2 5

5

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:

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

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

1/15/2020 PHY 712 Spring 2020 -- Lecture 2 6

6