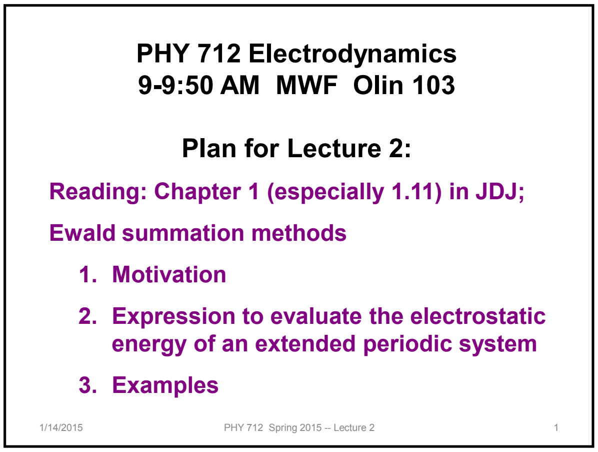


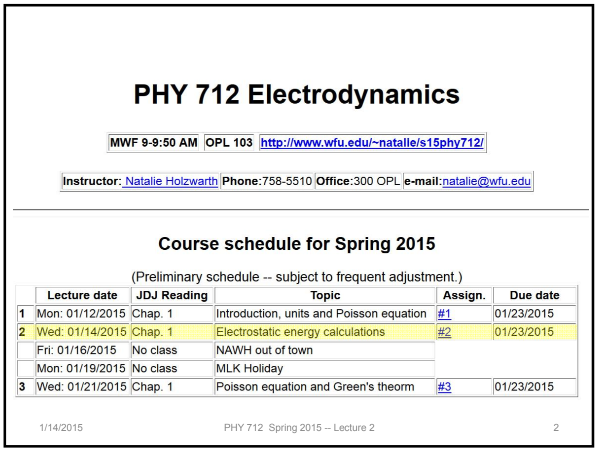
PHY 712 Electrodynamics
9-9:50 AM MWF Olin 103

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**



PHY 712 Electrodynamics

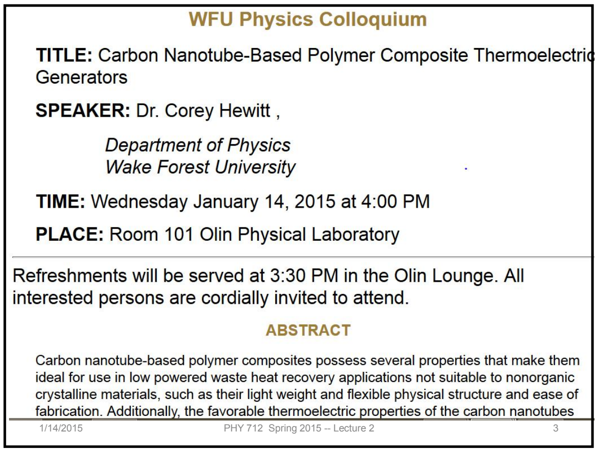
MWF 9-9:50 AM **OPL 103** http://www.wfu.edu/~natalie/s15phy712/

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

Course schedule for Spring 2015

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1	Introduction, units and Poisson equation	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1	Electrostatic energy calculations	#2	01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1	Poisson equation and Green's theorm	#3	01/23/2015



WFU Physics Colloquium

TITLE: Carbon Nanotube-Based Polymer Composite Thermoelectric Generators

SPEAKER: Dr. Corey Hewitt ,

Department of Physics
Wake Forest University

TIME: Wednesday January 14, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Carbon nanotube-based polymer composites possess several properties that make them ideal for use in low powered waste heat recovery applications not suitable to nonorganic crystalline materials, such as their light weight and flexible physical structure and ease of fabrication. Additionally, the favorable thermoelectric properties of the carbon nanotubes

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($\mathbf{r}_i \to \infty\}$ 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 to compensate for the double counting:

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

Here the summation is over all pairs of i, 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.

Ewald summation methods – slight digression

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''. This expression can be written in terms of the electrostatic potential $\Phi(\mathbf{r})$ and field $\mathbf{E}(\mathbf{r})$:

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

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

Ewald summation methods – exact results for periodic systems

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

See lecture notes for details.