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

Class notes for Lecture 2:

Reading: Chapter 1 (especially 1.11) in JDJ;

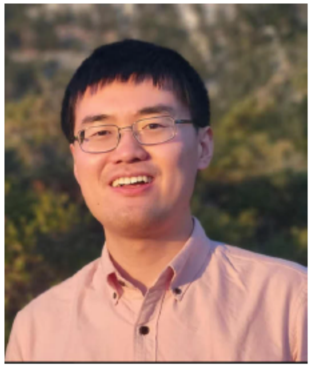
1. More comments on the electrostatic potential energy
2. Calculation of the electrostatic energy for a finite system
3. Electrostatic energy in terms of electrostatic fields
4. Electrostatic energy of extended systems -- introduction to Ewald summation methods

Reminder:

Physics Colloquium

- Thursday -

January 16, 2025



Dr. Tong Wang
Brigham and Women's Hospital
Harvard Medical School

Quantitative methods for microbiome research and precision nutrition

Due to highly personalized biological and lifestyle characteristics, individuals may have different metabolic responses to specific foods and nutrients. In particular, the gut microbiota, a collection of trillions of microorganisms living in our gastrointestinal tract, is highly personalized and plays a key role in our metabolic responses to foods and nutrients. Characterizing the metabolic profile of a microbial community and accurately predicting metabolic responses to dietary interventions based on individuals' gut microbial compositions are crucial for understanding its impact on the host and hold great promise for precision nutrition. Here, I will present my past research that investigates the complex microbiome and precision nutrition using different computational methods, such as mathematical models, multi-omics data analysis, and deep learning methods. After that, I will include my vision for future research that solves ecological and biomedical problems through computational approaches.

4 PM Olin 101

Reception 3:30
Olin Lobby

Colloquium 4:00

Your questions –

From Edoardo – "When computing the electrostatic energy of a discrete distribution of point-like charged particles we take into account only the electrostatic interactions. Thus, for some configurations, the value can be < 0. In the case of a continuous distribution, we also include the self-interaction energies, and the total electrostatic energy is always > 0 (it is proportional to the square of the electric field). Can we think about the self-interaction terms as the energy to generate the sources of the electric field?"

From Pablo – "Why shouldn't there be a self interaction considered in the energy of a discrete system? How is the energy density defined in this case?"

Course schedule for Spring 2025

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/13/2025	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/15/2025
2	Wed: 01/15/2025	Chap. 1	Electrostatic energy calculations	#2	01/17/2025
3	Fri: 01/17/2025	Chap. 1	Electrostatic energy calculations	#3	01/22/2025
	Mon: 01/20/2025	No Class	Martin Luther King Jr. Holiday		

PHY 712 -- Assignment #2

Assigned: 1/15/2025 Due: 1/17/2025

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

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

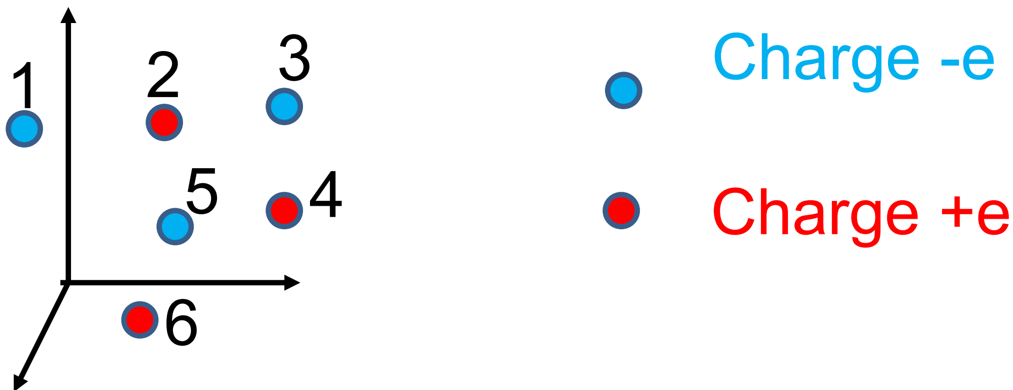
Here the summation is over all pairs of (i, j), excluding $i = j$.

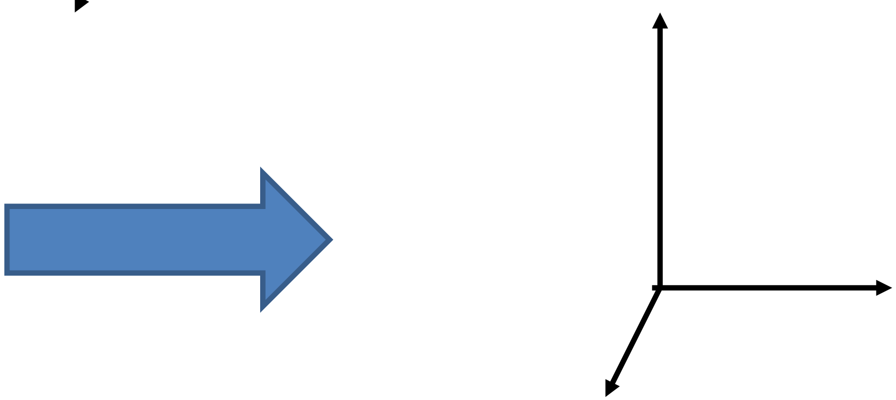
Define $$W_{ij} \equiv \frac{q_i q_j}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} .$$

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

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





(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$(\mathbf{r}_i \rightarrow \infty\}$ 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 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 $\rightarrow \infty$, 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 $\mathbf{E}(\mathbf{r})$:

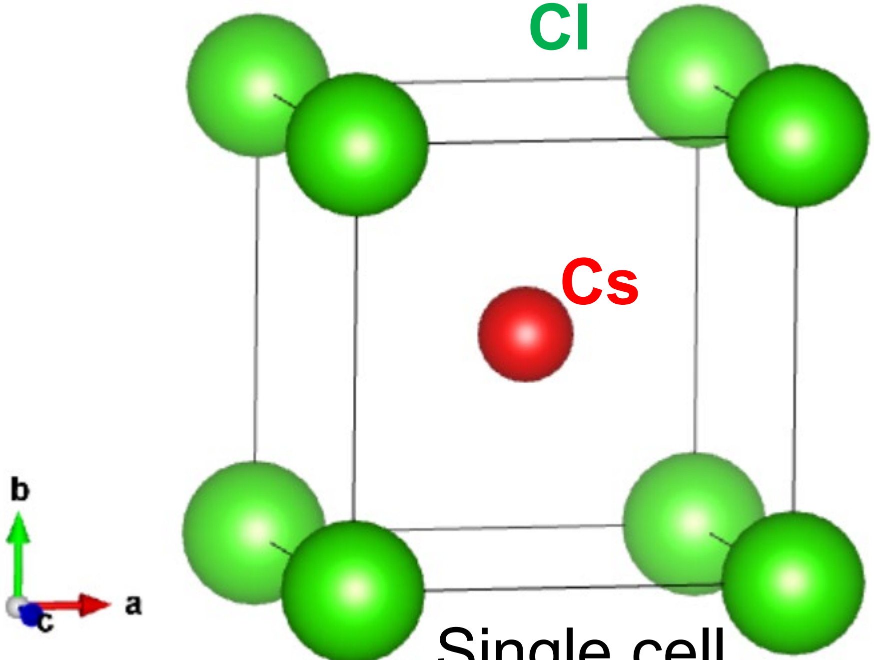
$$W = \frac{1}{2}\int d^3r\; \rho(\mathbf{r})\Phi(\mathbf{r}) = -\frac{\epsilon_0}{2}\int d^3r\left(\nabla^2\Phi(\mathbf{r})\right)\Phi(\mathbf{r}).$$

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

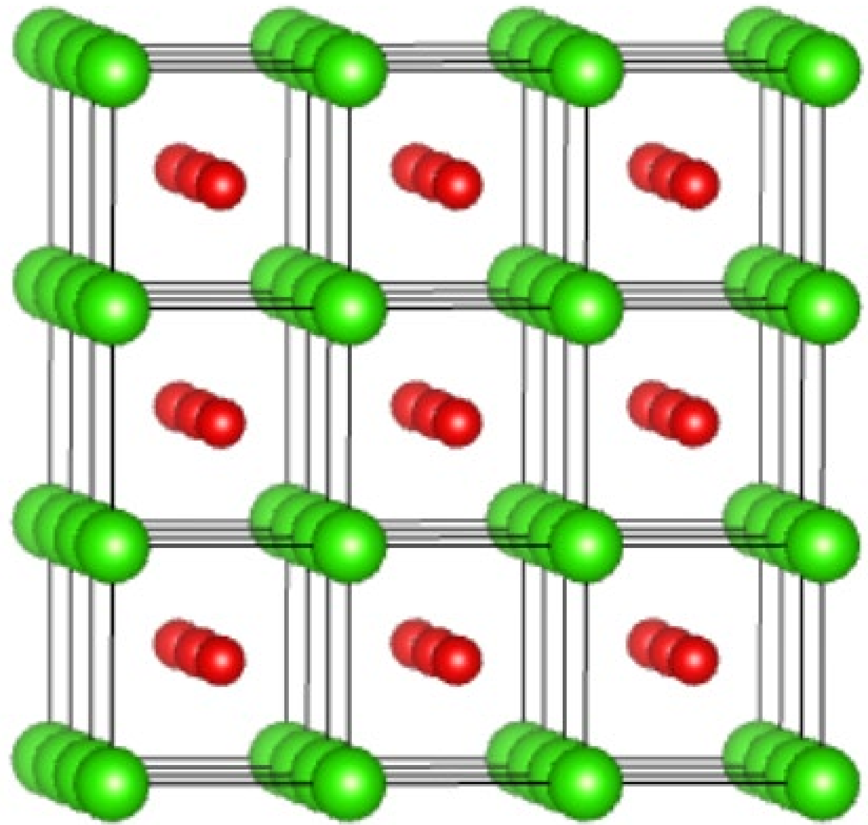
Note that, because of the inclusion of the self-interaction energies, there *may* be mathematical divergences involved in evaluating these quantities.

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