PHYS 1444 – Section 003
Lecture #7

Wednesday, Sept. 21, 2005

Dr. Jaehoon Yu

- Electric Potential due to Point Charges
- V due to charge distributions
- Equipotential lines and surfaces
- V due to dipoles
- E from V
- Electrostatic Potential Energy

Announcements

- Quiz at the beginning of the class next Monday, Sept. 26
  - Covers: Ch. 21 – 23 (whatever we complete today)
- Reading assignment
  - Ch. 23 – 9

Wang - Microsoft Word

4pm Today!!

Physics Department

The University of Texas at Arlington

COLLOQUIUM

Towards Petaflop Computing in Nanoscience

Dr. Yang Wang

Pittsburgh Supercomputing Center

4:00 pm Wednesday September 21, 2005 Room 103 SH

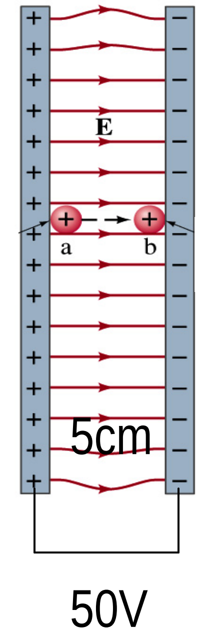
Abstract

Over the last 2-3 decades there has been significant progress in the first principles methods to calculate the properties of materials at the quantum mechanics level. These methods have largely been based on the local density approximation (LDA) to density functional theory (DFT). However, nanoscience places new demands on these first principles methods because of the large numbers of atoms, in the range of thousands to millions of atoms, present in even the simplest of nano-structured materials. Fortunately, recent advances in the locally self-consistent multiple scattering (LSMS) method are making the direct quantum mechicanical simulation of nano-structured materials possible. The LSMS method is an order-N approach to the first principles electronic structure calculation. It is highly scalable on massively parallel processing supercomputers, and is best suited for performing large unit cell simulations to study the electronic and magnetic properties of materials with complex structure. In this presentation, I will give a brief introduction of the LSMS method and the state-of-art high performance computing technology, and will show that this combination effectively accomplishes the first step towards understanding the electronic and magnetic structure of nanoparticles with dimension size as large as 5 nanometers (nm). I will demonstrate, as an example, the electronic and magnetic structure calculated for an iron nanoparticle embedded in iron aluminide crystal matrix. I will also explain to what extent future petaflop computing systems may enable the realistic quantum mechanical simulation of real nano-structured materials.

Refreshments will be served in the Physics Library at 3:30pm

Example 23 – 3

Uniform electric field obtained from voltage: Two parallel plates are charged to a voltage of 50V. If the separation between the plates is 5.0cm, calculate the magnitude of the electric field between them, ignoring any fringing.



What is the relationship between electric field and the potential for a uniform field? $V = -Ed$

Solving for E

$$E = \frac{V}{d} = \frac{50V}{5.0cm} = \frac{50V}{5 \times 10^{-2}m} \equiv 1000V/m$$

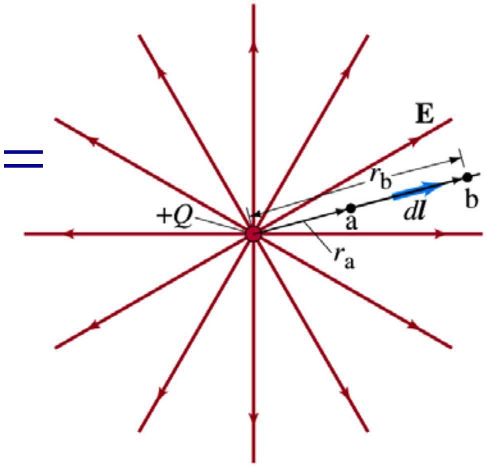
Electric Potential due to Point Charges

- What is the electric field by a single point charge Q at a distance r?

$$E = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r^2} = k\frac{Q}{r^2}$$

- Electric potential due to the field E for moving from point r_a to r_b in radial direction away from the charge Q is

$$V_b - V_a = -\int_{r_a}^{r_b} \vec{E}\cdot d\vec{l} = -\frac{Q}{4\pi\varepsilon_0}\int_{r_a}^{r_b}\frac{\hat{r}}{r^2}\cdot\hat{r}dr =$$

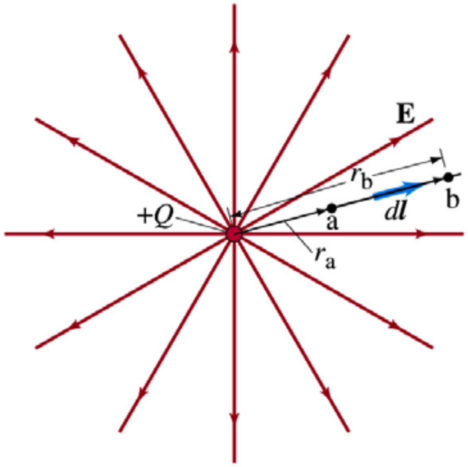


$$= -\frac{Q}{4\pi\varepsilon_0}\int_{r_a}^{r_b}\frac{1}{r^2}dr = \frac{Q}{4\pi\varepsilon_0}\left(\frac{1}{r_b} - \frac{1}{r_a}\right)$$

Electric Potential due to Point Charges

- Since only the differences in potential have physical meaning, we can choose $V_b = 0$ at $r_b = \infty$.
- The electrical potential V at a distance r from a single point charge is

$$V = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r}$$



- So the absolute potential by a single point charge can be thought of as <u>the potential difference by a single point charge between r and infinity</u>

Properties of the Electric Potential

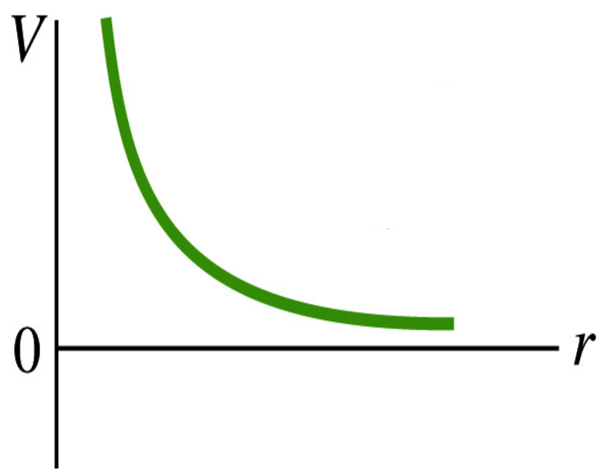
- What is the difference between the electric potential and the electric field?
  - Electric potential
    - Electric potential energy per unit charge
    - Inversely proportional to the distance
    - Simply add the potential by each of the charges to obtain the total potential from multiple charges, since potential is a scalar quantity
  - Electric field
    - Electric force per unit charge
    - Inversely proportional to the square of the distance
    - Need vector sums to obtain the total field from multiple charges
- Potential for the positive charge is large near the charge and decreases towards 0 at a large distance.
- Potential for the negative charge is large negative near the charge and increases towards 0 at a large distance.

Shape of the Electric Potential

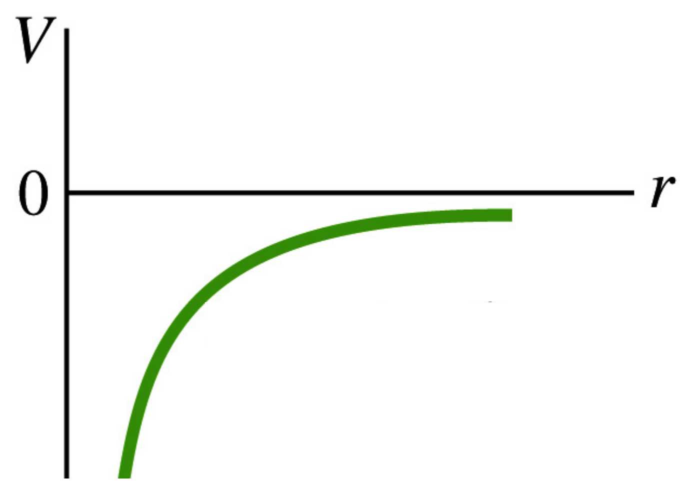
- So, how does the electric potential look like as a function of distance?
  - What is the formula for the potential by a single charge?

$$V = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r}$$

Positive Charge



Negative Charge



Uniformly charged sphere would have the potential the same as a single point charge.

What does this mean? Uniformly charged sphere behaves like all the charge is on the single point in the center.

Example 23 – 6

Work to force two + charges close together: What minimum work is required by an external force to bring a charge q=3.00μC from a great distance away (r=infinity) to a point 0.500m from a charge Q=20.0 μC?

What is the work done by the electric field in terms of potential energy and potential?

$$W = -qV_{ba} = -\frac{q}{4\pi\varepsilon_0}\left(\frac{Q}{r_b} - \frac{Q}{r_a}\right)$$

Since $r_b = 0.500m, r_a = \infty$ we obtain

$$W = -\frac{q}{4\pi\varepsilon_0}\left(\frac{Q}{r_b} - 0\right) = -\frac{q}{4\pi\varepsilon_0}\frac{Q}{r_b} = -\frac{\left(8.99\times10^{9}\, N\cdot m^2/C^2\right)\cdot\left(3.00\times10^{-6}C\right)\left(20.00\times10^{-6}C\right)}{0.500m} = -1.08J$$

Electric force does negative work. In other words, the external force must work +1.08J to bring the charge 3.00μC from infinity to 0.500m to the charge 20.0μC.

Electric Potential by Charge Distributions

- Let's consider that there are n individual point charges in a given space and V=0 at r=infinity.
- Then the potential at a point a, distance r_{ia} from the charge Q_i due to the charge Q_i is

$$V_{ia} = \frac{Q_i}{4\pi\varepsilon_0}\frac{1}{r_{ia}}$$

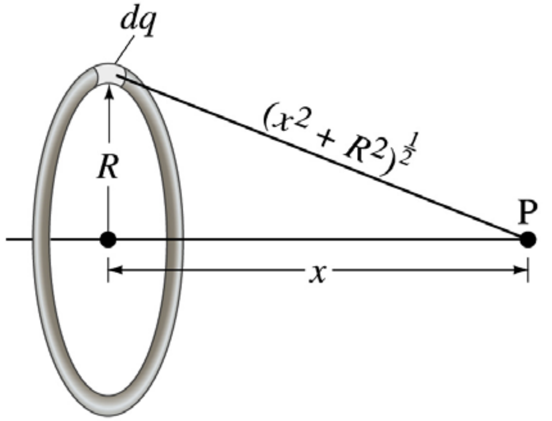
- Thus the total potential V_a by all n point charges is

$$V_a = \sum_{i=1}^{n} V_{ia} = \sum_{i=1}^{n} \frac{Q_i}{4\pi\varepsilon_0}\frac{1}{r_{ia}}$$

- For a continuous charge distribution, we obtain

$$V = \frac{1}{4\pi\varepsilon_0}\int\frac{dq}{r}$$

Example 23 – 8



- **Potential due to a ring of charge**: A thin circular ring of radius R carries a uniformly distributed charge Q. Determine the electric potential at a point P on the axis of the ring a distance x from its center.

- Each point on the ring is at the same distance from the point P. What is the distance?

$$r = \sqrt{R^2 + x^2}$$

- So the potential at P is

$$V = \frac{1}{4\pi\varepsilon_0}\int \frac{dq}{r} = \frac{1}{4\pi\varepsilon_0 r}\int dq =$$

$$\frac{1}{4\pi\varepsilon_0\sqrt{x^2 + R^2}}\int dq = \frac{Q}{4\pi\varepsilon_0\sqrt{x^2 + R^2}}$$

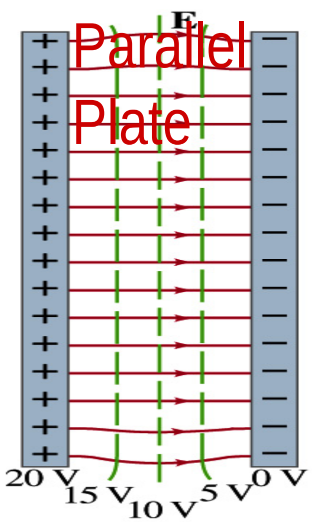
What's this?

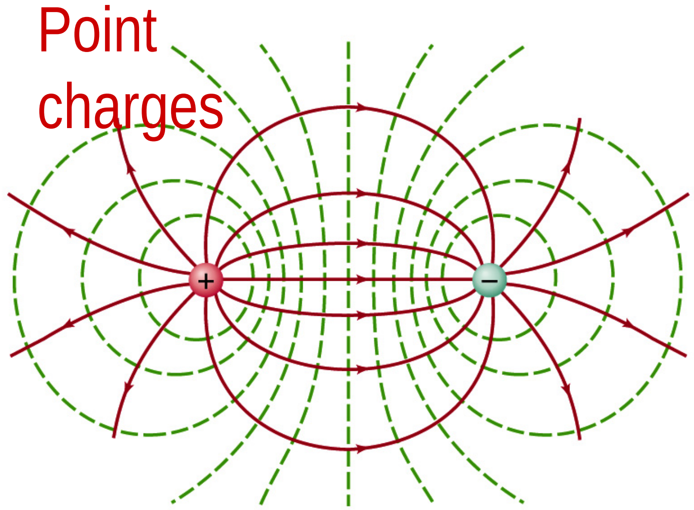
Equi-potential Surfaces

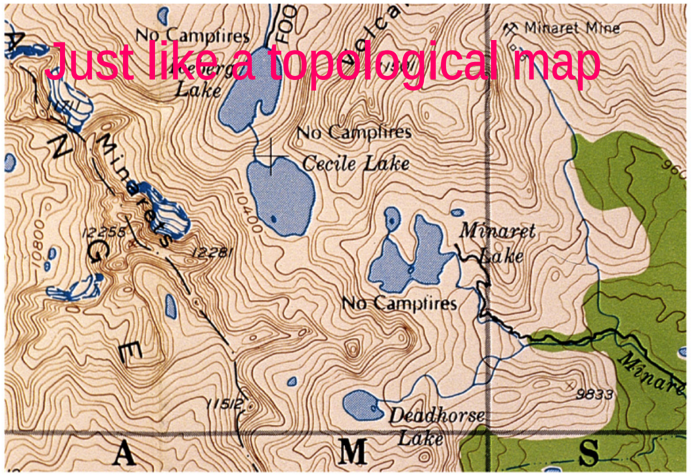
- Electric potential can be graphically shown using the equipotential lines in 2-D or the equipotential surfaces in 3-D
- Any two points on the equipotential surfaces (lines) are on the same potential
- What does this mean in terms of the potential difference?
  - The potential difference between two points on an equipotential surface is 0.
- How about the potential energy difference?
  - Also 0.
- What does this mean in terms of the work to move a charge along the surface between these two points?
  - No work is necessary to move a charge between these two points.

Equi-potential Surfaces

- An equipotential surface (line) must be perpendicular to the electric field. Why?
  - If there are any parallel components to the electric field, it would require work to move a charge along the surface.
- Since the equipotential surface (line) is perpendicular to the electric field, we can draw these surfaces or lines easily.
- There can be no electric field within a conductor in static case, thus the entire volume of a conductor must be at the same potential.
- So the electric field must be perpendicular to the conductor surface.

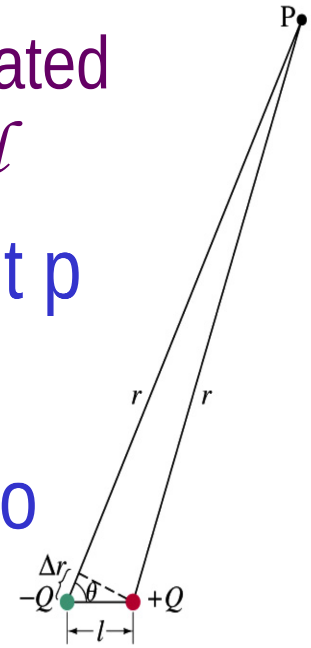






Electric Potential due to Electric Dipoles

- What is an electric dipole?
  - Two equal point charge Q of opposite sign separated by a distance ℓ and behaves like one entity: P=Qℓ
- The electric potential due to a dipole at a point p
  - We take V=0 at r=infinity
- The simple sum of the potential at p by the two charges is



$$V=\sum\frac{Q_i}{4\pi\varepsilon_0}\frac{1}{r_{ia}}=\frac{1}{4\pi\varepsilon_0}\left(\frac{Q}{r}+\frac{(-Q)}{r+\Delta r}\right)=\frac{Q}{4\pi\varepsilon_0}\left(\frac{1}{r}-\frac{1}{r+\Delta r}\right)=\frac{Q}{4\pi\varepsilon_0}\frac{\Delta r}{r+\Delta r}$$

- Since Δr=ℓcosθ and if r>>ℓ, r>>Δr, thus r~r+Δr and

$$V=\frac{Q}{4\pi\varepsilon_0}\frac{l\cos\theta}{r}=\frac{1}{4\pi\varepsilon_0}\frac{p\cos\theta}{r}$$

V by a dipole at a distance r from the dipole

$$V=\frac{1}{4\pi\varepsilon_0}\frac{p\cos\theta}{r}$$

E Determined from V

- Potential difference between two points under the electric field is $V_b - V_a = -\int_a^b \vec{E} \cdot d\vec{l}$
- So in a differential form, we can write

$$dV = -\vec{E} \cdot d\vec{l} = -E_l dl$$

  – What are dV and E_ℓ?
    - dV is the infinitesimal potential difference between two points separated by the distance $d\ell$
    - E_ℓ is the field component along the direction of $d\ell$.
- Thus we can write the field component E_ℓ as

$$E_l = -\frac{dV}{dl}$$

Physical Meaning?

The component of the electric field in any direction is equal to the negative rate of change of the electric potential as a function of distance in that direction.!!

E Determined from V

- The quantity $dV/d\ell$ is called the <u>gradient of V</u> in a particular direction
  - If no direction is specified, the term gradient refers to the direction V changes most rapidly and this would be the direction of the field vector **E** at that point.
  - So if **E** and $d\ell$ are parallel to each other, $E = -\frac{dV}{dl}$
- If E is written as a function x, y and z, ℓ refers to x, y and z $\quad E_x = -\frac{\partial V}{\partial x} \quad E_y = -\frac{\partial V}{\partial y} \quad E_z = -\frac{\partial V}{\partial z}$
- $\frac{\partial V}{\partial x}$ is the "partial derivative" of V with respect to x, with y and z held constant
- In vector form, $\vec{E} = -gradV = -\vec{\nabla} V = -\left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z} \right) V$

$\vec{\nabla} = -\left(\vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z} \right)$ is called the *del* or the *gradient operator* and is a <u>*vector operator*</u>.

Electrostatic Potential Energy; the electron Volt (eV)

- Consider a point charge q is moved between points *a* and *b* where the electrostatic potential due to other charges is V_a and V_b
- The change in electrostatic potential energy of q in the field by other charges is

$$\Delta U = U_b - U_a = q\left(V_b - V_a\right) = qV_{ba}$$

- Now what is the electrostatic potential energy of a system of charges?
  - Let's choose V=0 at r=infinity
  - If there are no other charges around, single point charge Q_1 in isolation has no potential energy and is exerted on with no electric force

Electrostatic Potential Energy; Two charges

- If a second point charge Q_2 is brought close to Q_1 at the distance r_{12}, the potential due to Q_1 at the position of Q_2 is

$$V = \frac{Q_1}{4\pi\varepsilon_0}\frac{1}{r_{12}}$$

- The potential energy of the two charges relative to V=0 at r=infinity is $U = Q_2 V = \frac{1}{4\pi\varepsilon_0}\frac{Q_1 Q_2}{r_{12}}$
  - This is the work that needs to be done by an external force to bring Q_2 from infinity to a distance r_{12} from Q_1.
  - It is also a negative of the work needed to separate them to infinity.

Electrostatic Potential Energy; Three Charges

- So what do we do for three charges?
- Work is needed to bring all three charges together
  - Work needed to bring Q1 to a certain place without the presence of any charge is 0.
  - Work needed to bring Q2 to a distance to Q1 is $U_{12} = \frac{1}{4\pi\varepsilon_0}\frac{Q_1 Q_2}{r_{12}}$
  - Work need to bring Q3 to a distance to Q1 and Q2 is

$$U_3 = U_{13} + U_{23} = \frac{1}{4\pi\varepsilon_0}\frac{Q_1 Q_3}{r_{13}} + \frac{1}{4\pi\varepsilon_0}\frac{Q_2 Q_3}{r_{23}}$$

- So the total electrostatic potential of the three charge system is

$$U = U_{12} + U_{13} + U_{23} = \frac{1}{4\pi\varepsilon_0}\left(\frac{Q_1 Q_2}{r_{12}} + \frac{Q_1 Q_3}{r_{13}} + \frac{Q_2 Q_3}{r_{23}}\right) \quad [V = 0 \text{ at } r = \infty]$$

  - What about a four charge system?

Electrostatic Potential Energy: electron Volt

- What is the unit of electrostatic potential energy?
  - Joules
- Joules is a very large unit in dealing with electrons, atoms or molecules atomic scale problems
- For convenience a new unit, electron volt (eV), is defined
  - 1 eV is defined as the energy acquired by a particle carrying the charge equal to that of an electron (q=e) when it moves across a potential difference of 1V.
  - How many Joules is 1 eV then? $1eV = 1.6\times10^{-19}C\cdot1V = 1.6\times10^{-19}J$
- eV however is <u>not a standard SI unit</u>. You must convert the energy to Joules for computations.
- What is the speed of an electron with kinetic energy 5000eV?