

**Thermodynamics for Biological Systems:
Classical and Statistical Aspects
Prof. Sanjib Senapati
Department of Biotechnology
Indian Institute of Technology - Madras**

**Lecture – 83
Calculation of Coulombic Force**

(Refer Slide Time: 00:30)

Calculate F_x for a pair of Coulomb particles.

$$F_x = -\frac{\partial U}{\partial x}$$

$$= -\frac{\partial U}{\partial r} \cdot \frac{\partial r}{\partial x}$$

$$U = \frac{z_i z_j}{4\pi \epsilon_0 r_{ij}}$$

$$\frac{\partial U}{\partial r_{ij}} = -\frac{z_i z_j}{4\pi \epsilon_0 r_{ij}^2}$$

$$F_x = +\frac{z_i z_j}{r_{ij}} \cdot \frac{z_i z_j}{4\pi \epsilon_0 r_{ij}^2}$$

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\frac{\partial r}{\partial x} = \frac{1}{2} \cdot 2x \cdot (x^2 + y^2 + z^2)^{-1/2}$$

$$= \frac{x}{r}$$

I will just give you one simple problem to think and solve so the question is calculate x component of the force. So, if F_x is the x component of the force for a pair of Coulomb particles. So that is the question so calculate the force between a pair of Coulomb particles. You can take five minutes to solve it and get back. Welcome back! So the question was calculate the x component of force between a pair of Coulomb particles.

So what do I mean by Coulomb particles? So, basically I just indirectly said that the particles are charged. And when the particles are charged you basically calculate their potential by using the Coulomb's law. So, the particles which can be, whose potential can be calculated using a Coulomb's law I call them as Coulomb particles. So, what would be the force between two such charged particles?

So, so the hint is to calculate the force you have to know the potential. So, force is nothing but the gradient of potential. So, if I know the potential between two particles then you can get the

force. And you know the potential between two charged particles. So, the potential between two charged particles we already have seen, saw that you have already seen is $Z_i Z_j$ divided by $4\pi\epsilon_0 r_{ij}$.

$$U = \frac{Z_i Z_j}{4\pi\epsilon_0 r_{ij}}$$

$$\frac{\partial U}{\partial r_{ij}} = - \frac{Z_i Z_j}{4\pi\epsilon_0 r_{ij}^2}$$

So if you have the potential, you basically take the negative gradient of that and you get the force. But here I want the x component of the force. So, how do you go about it? So to get the first component of x, we have to make use of thermodynamics, some thermodynamic rules. So, one such rule is what we will be employing here. So, when I said the x component of force, so I am basically trying to get $\text{del } U \text{ del } x$.

$$F_x = - \frac{\partial U}{\partial x}$$

$$F_x = - \frac{\partial U}{\partial r} \cdot \frac{\partial r}{\partial x}$$

I am sure you have seen this multiplicity relation in thermodynamics. And now let us find out what is $\frac{\partial U}{\partial r}$ and what is $\frac{\partial r}{\partial x}$. So your U was $Z_i Z_j$ divided by $4\pi\epsilon_0 r$.

So, my $\text{del } U \text{ del } r$ is equal to

$$\frac{\partial U}{\partial r_{ij}} = - \frac{Z_i Z_j}{4\pi\epsilon_0 r_{ij}^2}$$

what would be my $\frac{\partial r}{\partial x}$. We know r is equal

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\frac{\partial r}{\partial x} = \frac{1}{2} \cdot 2x \cdot (x^2 + y^2 + z^2)^{-1/2}$$

$$\frac{\partial r}{\partial x} = \frac{x}{r}$$

So, therefore my $\text{del } r \text{ del } x$ would be x divided by r. So, if you put them together what we get is

$$F_x = -\frac{Z_i Z_j}{4\pi\epsilon_0 r_{ij}^2} \cdot -\frac{x_{ij}}{r_{ij}}$$
$$F_x = \frac{x_{ij}}{r_{ij}} \cdot \frac{Z_i Z_j}{4\pi\epsilon_0 r_{ij}^2}$$

so this is my x component of force acting between two particles which are having charge. Likewise I guess you can calculate the x or y component of force between two Lennard Jones particles and I am giving you again some time to calculate the force between two Lennard Jones particles.