Bio-Physical Chemistry
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Lecture - 08
Electrostatics (Contd.)

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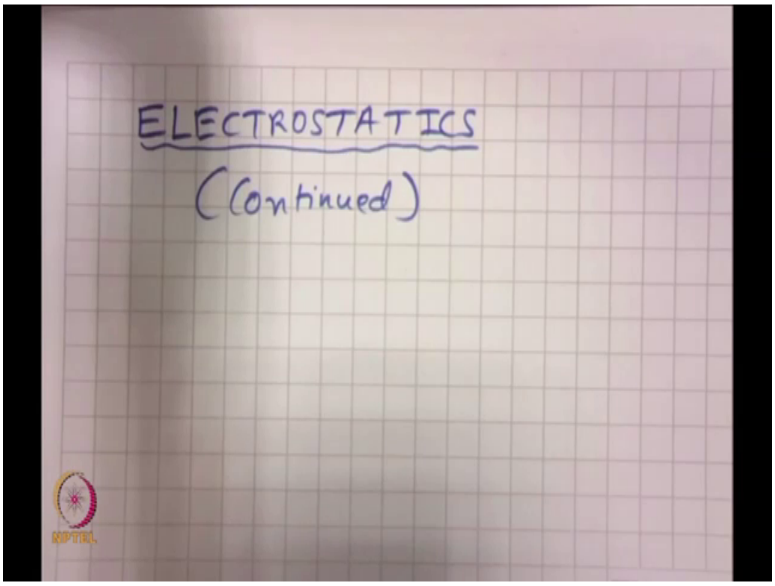

So, the topic is electrostatics that is what we are looking at and that is what we will continue with. So, the last class what we looked at was we started with Poisson Boltzmann equation right.

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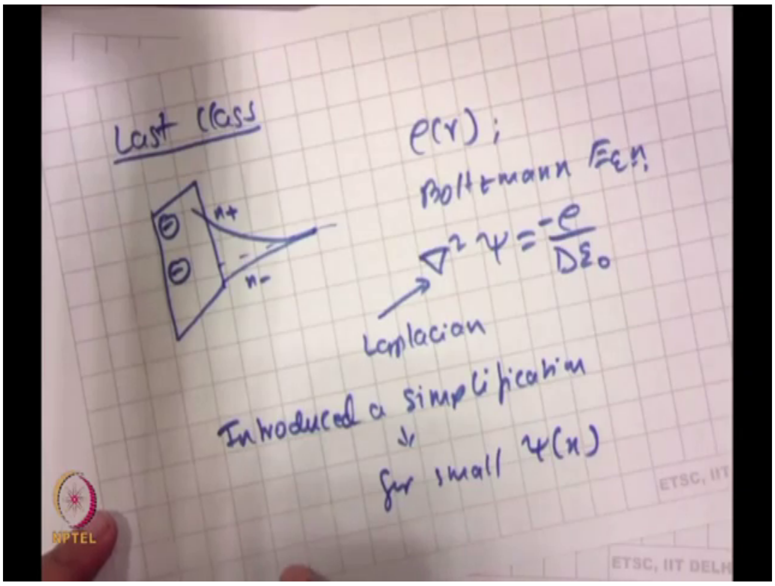

We are looking in the plane right of a certain charge right, and then say this is a if this is your plane right. And then if you have a charge-charge interaction, so at what distance you know will this interaction decay or at what distance if your ion is would it feel what kind of charge. In that sense, in that sense, so this was for us negatively charged right, and because this was negatively charged, so at closed by you would be having a huge concentration of positively charged ions, you move out of it the concentration decays.

Similarly, if you looking at a negative charge cloud or negative charge ions, negatively charged ions, then what will happen these one would be most depleted near the plate or the plate, and then it will start growing ok.

So, in combination with something known as the charge density right and the Boltzmann equation, and the Boltzmann equation, we looked also at something known as the what equation this is your Poisson equation right. Where D is the dielectric constant, epsilon 0 again permittivity vacuum, and rho is the same thing is the charge density. And charge density means number of charges per unit volume right.

So, then we went ahead to solve this we put in this rho right, we actually did not solve it, we just give you the equation. We kept del square as del square. So, del square was your Laplacian. And then we introduced a simplification. The simplification was what the simplification was for small psi of x. So, if you have most small psi of x, what happens that z times e times psi of x over q of t is much less than 1, because k T is much greater than the numerator. And hence you can use your approximation of your what expansion of e to the power x and e to the power minus x.

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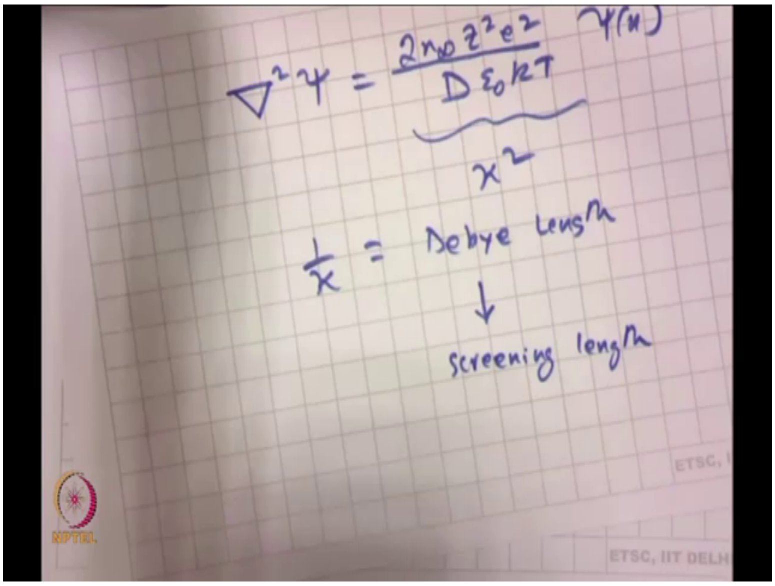

So, on doing that, on doing that, what we reached or the equation we reached was del square psi is equal to 2 n infinity z squared e squared over D

Student: Epsilon 0.

Epsilon 0.

Student: kT.

k T then I have psi again right psi of x. And this guy is referred to as what?

Student: (Refer Time: 03:36).

Kappa squared, where kappa squared is a certain parameter, but the most important concept underlying this is what is it kappa, or 1 by kappa, which one?

Student: 1 by kappa.

So, we defined something known as 1 by kappa which is your.

Student: Debye length.

Debye length. And what we said was if you have this Debye length, at this length your ion would still feel the charge of your plane right or the effect of the charge or influence of the charge. But if you go beyond this then it diminishes drastically, it almost feels no charge and that is why this one is also known as your screening length.

This y is also known as your screening length. And as I told you last time this is one of the most important concepts in electrostatics specially when you consider charge-charge interactions, and you start putting in salts in between the charges, because salts come with something known as ionic strength, more salt you have that means, more charge density you have more number of ions you have. And hence this screening would go up or down depending upon what your ionic strength is.

In protein folding, this charge-charge interaction of screening plays a huge role. And I am sure you guys have heard about this it is called the Hofmeister series. Well, what is related to is salting in and salting out of it and that is also related to this concept or this is the central theme of that ok.

So, at the end of the class, we actually started solving this Poisson equation right or the Poisson-Boltzmann equation. This equation is also known as what the Debye-Huckel equation, because Debye-Huckel first related these two, that means, one was the Poisson equation and the other one was what the Boltzmann equation that is why they are in combined form called the Poisson-Boltzmann equation right.

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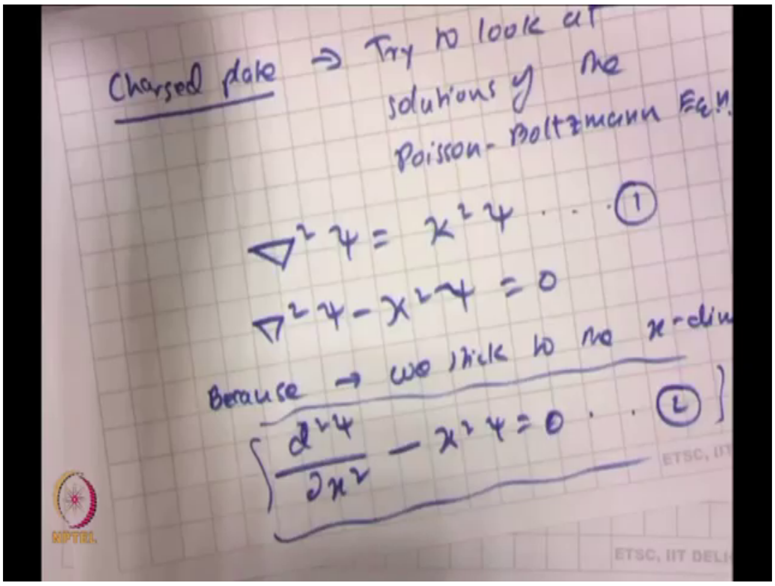

So, last time what we started was again we take a charged plate, and we try to solve, try to look at solutions of the Poisson-Boltzmann equation that is what we had started with last class. And I kind of went through a little bit fast. So, I will essentially start with that. So, here what do you have is again think about the same charged plate and what we are looking at is again this equation kappa squared psi right.

So, we have to solve this equation essentially. Now, this is the differential equation, I can write it as del square psi minus kappa psi is equal to 0. And because and because and because, we stick we stick to the x-dimension that is essentially one dimension that is essentially one dimension, what I can write is psi minus kappa square psi is equal to 0, this is the one we are actually solving.

Now, what do you think is the solution or are the solutions of this equation, how do we solve this differential equation? This obviously we are not going to do it right, but what can you do to try to solve it?

Student: Cancel each other. (Refer Time: 07:35).

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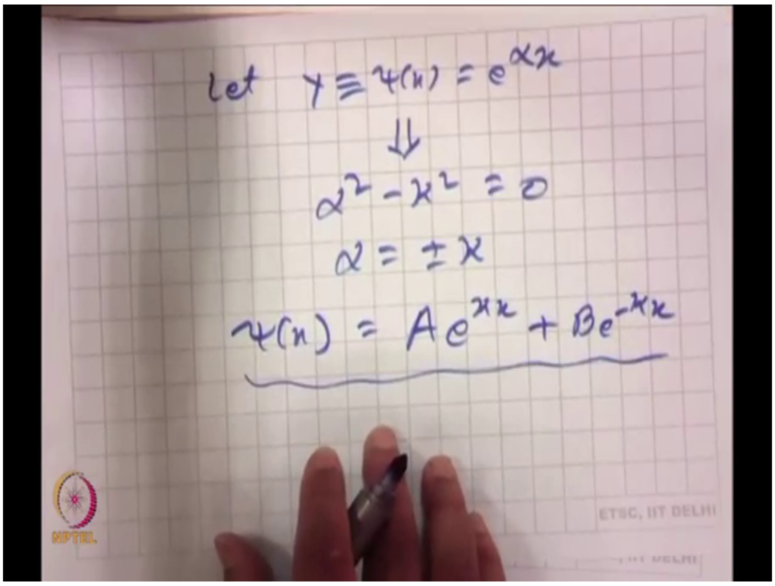

To try to solve it, we can do let y or in this case which is psi of x to be say e to the power alpha x right. And then what we come up with is see this guy, this you guys should do by yourself alpha square minus kappa square is equal to 0, and we should get alpha is equal plus minus kappa. And because both alpha is equal to plus minus kappa would be a solution of the equation. Hence what we can write is, what can we write now, what did we write last time?

Student: (Refer Time: 08:21) psi equal to A e to the power (Refer Time: 08:22).

So, I can write psi of x the one we are going to solve is equal to A right e to the power say kappa x plus B e to the power minus kappa x. This is the solution of your psi of x. So, again the important point is you are trying to look at a solution of your electrostatic potential psi of x ok. Like in quantum mechanics, we start applying what boundary conditions.

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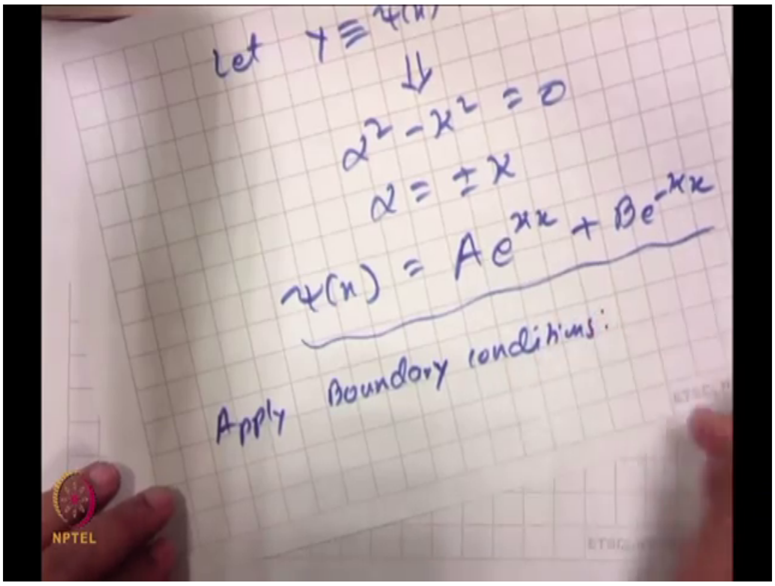

So, let us apply boundary conditions. Once we apply boundary conditions, the stuff we get is this.

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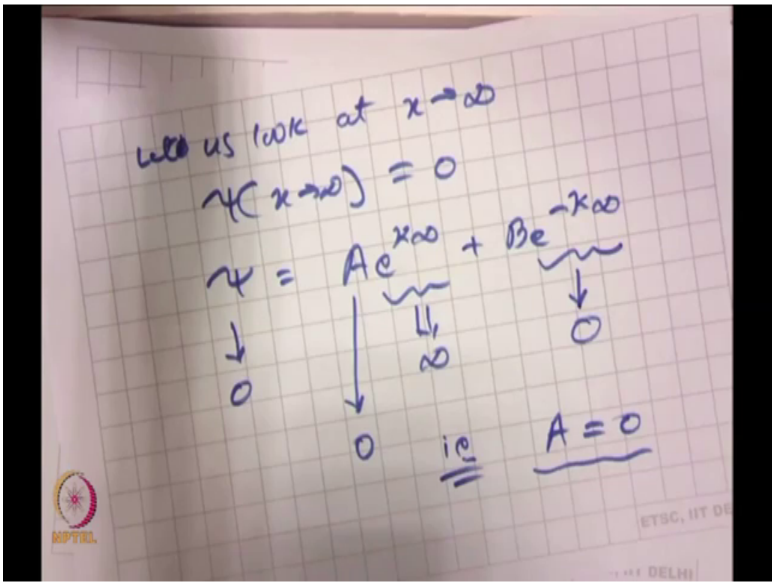

So, let us look at, so this is let us look at x tending to infinity. If x is tending to infinity that means, you are going far and far away from your plate. So, then if x is tending to infinity that means you are infinitely far or at an infinite distance along the x-direction from the plate would the charge or would the ions feel an electrostatic potential?

Student: No.

No. So, then I can write psi x tending to infinity is equal to?

Student: 0.

0. So, based on this, based on this, what does our equation previous equation become, so then previous equation becomes psi is equal to A e to the power kappa, then this is infinity right plus B e to the power minus kappa then infinity because this I am solving for that condition where x tends to infinity.

Now, this one at x tends to infinity goes to what?

Student: (Refer Time: 10:11).

0

Student: 0.

Right, it is an exponential decaying function right, and x is infinity, so, obviously, this is going to 0. Now, what happens this for this one?

Student: Infinity.

Now, this tends to infinity right, this tends to infinity, but our boundary condition says that at x tends to infinity this tends to what?

Student: 0

0. So, if this tends to 0, well, this is gone this tends to 0, anyway, this tends to infinity. So, the only way psi can go to 0 is if?

Student: A tend to 0.

A is 0, that means, so that is from this I can get A is equal to 0. So, it simplifies the solution for me now right. If you are remember what we did what you did for particle in a 1D box, psi was equal to A sin of k x plus B cosine of k x right, and then you applied one boundary condition where cosine?

Student: (Refer Time: 11:06).

Did not go to 0, but the coefficient of cosine went to 0, is the same thing we are seeing out here right.

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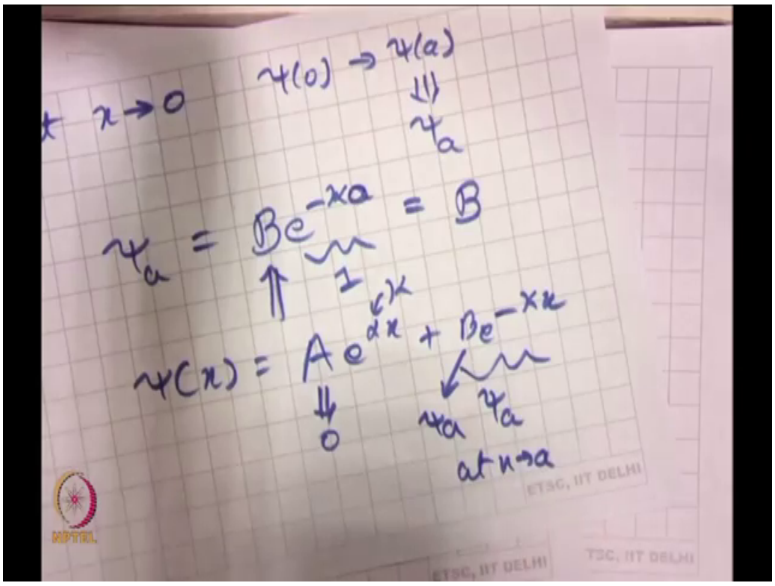

The other point is now at x tends to 0. So, at x tends to 0, what do you mean at x tends to 0? That means, you are right next to the plate, essentially on the plate. If on the plate, then obviously, the plate has its own charge or electrostatic potential.

So, here what we say is at x tends to 0, we say psi 0 tends to a potential which is psi of a say, or I should not be say psi of a there is a constant I should be writing as psi a, essentially psi a, it is not psi of a. What I mean is psi a, it is a constant. This is an electrostatic potential with the charge plate gives out. So, similarly I can write psi a right at x tends to 0 is equal to what, what, what was I left with, I was left with?

Student: (Refer Time: 12:04).

B, then?

Student: e to the power.

E to the power minus.

Student: Kappa.

Kappa x tends to.

Student: e to the power a.

a

Student: (Refer Time: 12:13) a.

Right, that means, x is equal to a. So, from here what do I have? So, from here what do I have, so I have B e to the power minus kappa a right. So, this is for psi of a at x tends to a. So, I have what?

Student: 0.

I have B from here right. If I know a, if I know this I have essentially B. So, now, let us combine this, this is what we are looking at I was looking at psi of say x is equal to again I am writing A e to the power alpha x plus B e to the power minus not alpha I should be writing what, this is kappa, yes, kappa x. This one went to 0. This one went to 0. At x tending to a this guy was equal to psi of a at x tending to a.

So, what will be the final equation for me? What did we write down finally the last time? So, can I write, can I write, you know I made one mistake, you have to tell me what, what is the mistake I made?

Student: x is equal to 0 (Refer Time: 13:35).

Yeah, see I made a mistake. The mistake I made was this. The mistake I made was it was x tending to 0 right, so I should not be putting x tending to a out here. What should I put?

Student: 0.

I should be putting 0. So, I am sorry for that mistake if this is what B is equal to B times e to the power minus kappa 0. So, this is what this is essentially.

Student: B.

B, because this one goes to?

Student: 1.

1. So, similarly out here this one was psi of a at x tends to a or x tends to 0 rather. So, from here I get, what I get B is actually psi of a, I will rewrite, sorry I will just rewrite this was a mistake I made.

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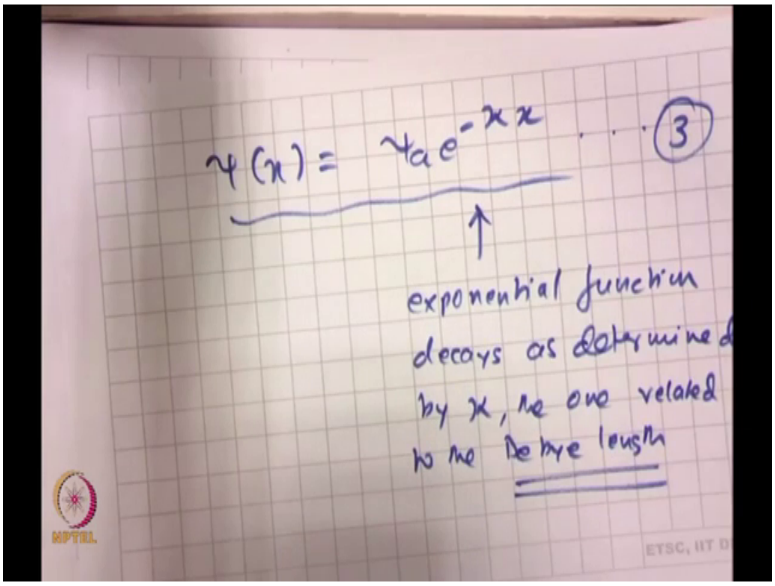

But I will just correct it. And what I will rewrite it as is then I have psi of x is equal to?

Student: Psi of a.

psi of a e to the power minus kappa x, psi of a e to the power minus kappa x, because B came out to be psi of a as x tends to 0 right. There is a small oversight from my side.

So, what is the take home point of this equation? The take home point is if psi a is the electrostatic potential of the charged plate, whatever charge it is, and if I am going to look at the electrostatic potential at a distance x from the plate, then how is the potential going to vary?

Student: Exponentially

The potential is going to vary exponentially as a function of x obviously, being determined by what; kappa being determined by kappa. So, this guy exponential function decays as determined by kappa, the one related to the Debye length, the one way to the Debye length right. So, this kappa is essentially what the inverse of the Debye length right. This kappa essentially is what the inverse of the Debye length, and that is what you are looking at.

So, it is like looking at how an energy level if you are you know; if you remember your Boltzmann equation, do you remember when you did when you did vibrational spectroscopy? You had n i that is a number of molecules in level i is equal to n 0 e to the power minus e over k T.

Student: (Refer Time: 16:20).

So, as you go higher up what happens the number of molecules decreases.

Student: Decreases.

Depending upon the energy, the same thing happens here. As you go further out of psi of x, the potential decays depending upon kappa right, that is essentially what we are looking at. It is very similar, but it is now you looking at for looking at it from the point of view of an electrostatic potential. But tell me what the problem is here, tell me tell me why can I not apply this for proteins?

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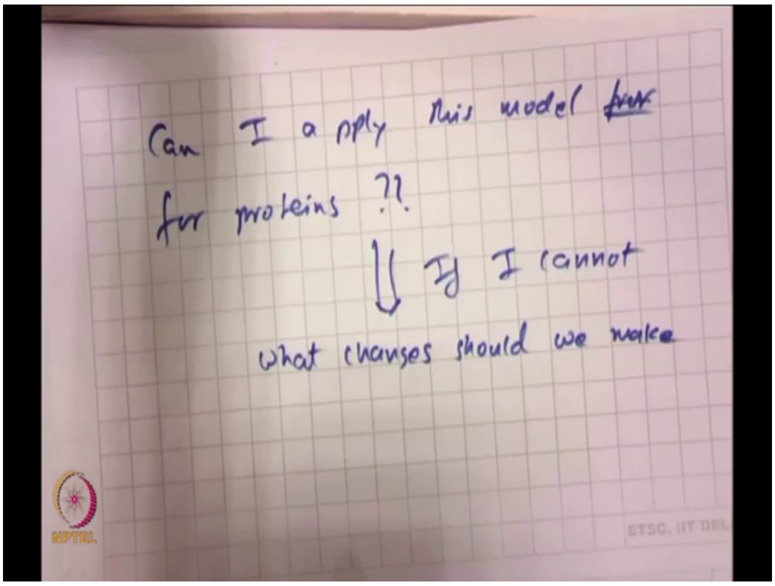

So, the question is can I apply this model for sorry this is for proteins, for proteins? And if I cannot, if I cannot, then what changes should we make? What do you think?

Student: Sir, its (Refer Time: 17:29).

Mani?

Student: And we have protein (Refer Time: 17:30) fold.

3D, but.

Student: Charge for any (Refer Time: 17:35) one plane.

Ok.

Student: And in that protein case charge will be uniformly distributed here and there.

Ok. So, you are saying the charge will be uniformly distributed or not uniformly distributed in case of protein?

Student: Not uniformly (Refer Time: 17:46).

Not uniformly distributed ok. So, that is it is a very good point. So, one the point is, obviously, one we were considering a plane or that in that case and here I mean in that case what we said was a one-dimensional distance, but when we talk about a protein?

Student: (Refer Time: 18:00).

We have to go to three dimensions, good.

The next point that was raised was ok, here I consider a uniform potential or uniform electrostatic potential, but in case of a protein I might be having charged hotspots. But you know when we are actually going to solve, it is very hard for us to take into account the non-informative of the electrostatic potential you know it can be.

Essentially, what we are going to do is we are going to assume a certain uniform electrostatic potential, and then solve it. A special case might be non-informative in electrostatic potential you know that can be solved too, but that is what we are now going to look at in class here right. So, essentially we are looking we are going to look at it as a uniform either positive or negatively charged surrounding of a protein. But how is it del square going to change now, what do we do with the del squared?

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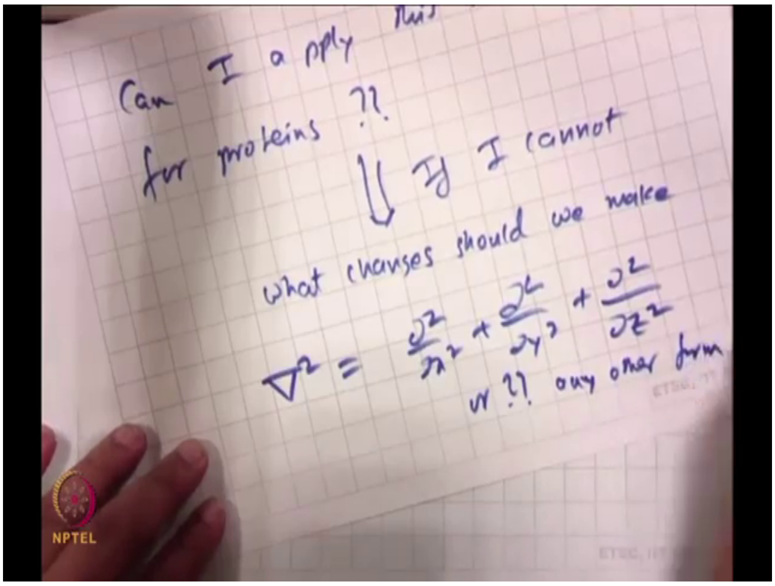

That means the question is del squared, what should I write it as should I write it as this or any other form?

Student: (Refer Time: 19: 8).

Or.

Student: (Refer Time: 19:06).

Yes or any other form, what do you write it as?

Student: Spherical (Refer Time: 19:12).

Yes, spherical.

Student: Spherical (Refer Time: 19:15)

It is spherical polar coordinates right.

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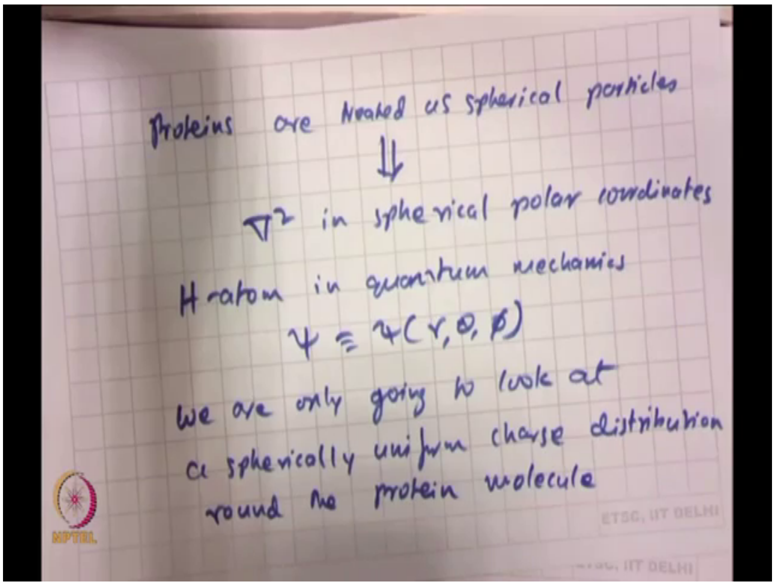

Because proteins are treated as what?

Student: (Refer Time: 19:22).

I approximate as spherical particles right. Proteins approximate as spherical particles. If proteins approximate as spherical particles, I better I better do a conversion of my del squared in spherical polar coordinates.

Student: Coordinates.

This is something you guys have done in quantum mechanics when you started doing rotation in 3D and then you went over the hydrogen atom right. In the hydrogen atom, you had three variables. What are the variables in hydrogen atom you had?

Student: (Refer Time: 20:00).

So, when you are talking about a hydrogen atom in quantum mechanics, when we are talking about hydrogen atom in quantum mechanics, what was the wave function depending upon?

Student: (Refer Time: 20:09).

Ok, that means, a wave function psi hydrogen was a function of psi r, then?

Student: (Refer Time: 20:17).

Theta, then?

Student: Phi

Phi. So, it has three variables. Now, coming back to your question, if I have to look at specific hotspots, I would have to look at this respective theta and phi right at you know at what angle or angle orientations; they are with respect to the charged particles and all these things.

So, what we are going to do is, here we are only going to look at a spherical, a spherically uniform charge distribution round the protein molecule round the protein molecule. What does this mean? Think about s orbitals, do s orbitals of any theta and phi dependence?

Student: No right.

S orbitals do not have theta and phi dependence right, because it is spherically what?

Student: Symmetric.

Symmetric.

Student: Yeah.

So, the same thing is going to happen here, that means, here the del squared would not be having any dependence upon the angular values that is theta and phi.

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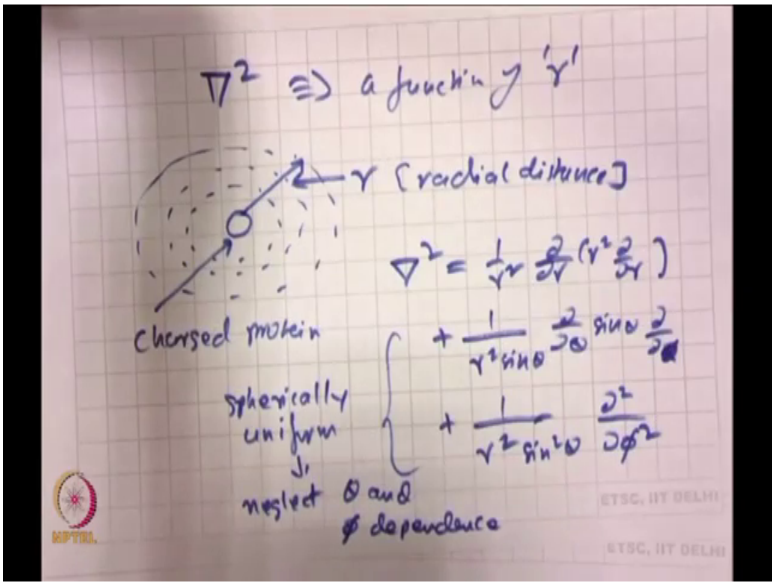

So, essentially what a del square now becomes is a del square is only a function of r, it is only a function of r, where r is the distance in the radial direction. So, you can imagine one thing right your protein is a sphere right, your protein is a sphere. So, your protein is a sphere like this ok. Let us considered like that. And then you just going out towards in the radial direction, that means, your charges are spherical distributed like this right.

And this is essentially r, which is the radial distance. And this in the middle what do you have is your charged protein, is a charged protein. This is what we have in the middle. Again no theta and phi dependence. This helps us simplify the problem a little bit. How? If I consider a spherically distributed uniform charge potential, then I can write del square is equal to do you remember what it is?

Student: (Refer Time: 22:51).

What is the full form of del square, first tell me what is the full form of del square? 1 by r square if you remember del of del r square del of del r right that was a radial part plus 1 by.

Student: r square sin (Refer Time: 23:06). r square sin theta.

r square sin theta, then?

Student: Del of (Refer Time: 23:10).

Del of del theta.

Student: Del del square.

Sin theta.

Student: (Refer Time: 23:14).

Del of?

Student: Sir.

Del theta sorry, this is del of del theta actually plus 1 by.

Student: r squared sin.

r squared then.

Student: sin squared theta. sin squared.

Sin squared theta then.

Student: del (Refer Time: 23:26).

Del 2 over.

Student: Del phi.

Del phi squared this is your total what; Laplacian in?

Student: Polar.

Spherical polar coordinates. So, out of these because we are considering a uniform potential spherical uniform, because spherically uniform, neglect theta and phi dependence, neglect theta and phi dependence.

So, the only guy that remains is the first one. See, we simplified the problem like that right. It was an assumption, but we will go with assumption, because we are not looking at the very specifics we are trying to get a very generalized model. And try to look at how this varies if you put in a protein in a solution and a put in some salts. What is the picture we are going to look at a very simplified picture actually? You guys are up till this right any problems any issues? Please do let me know.

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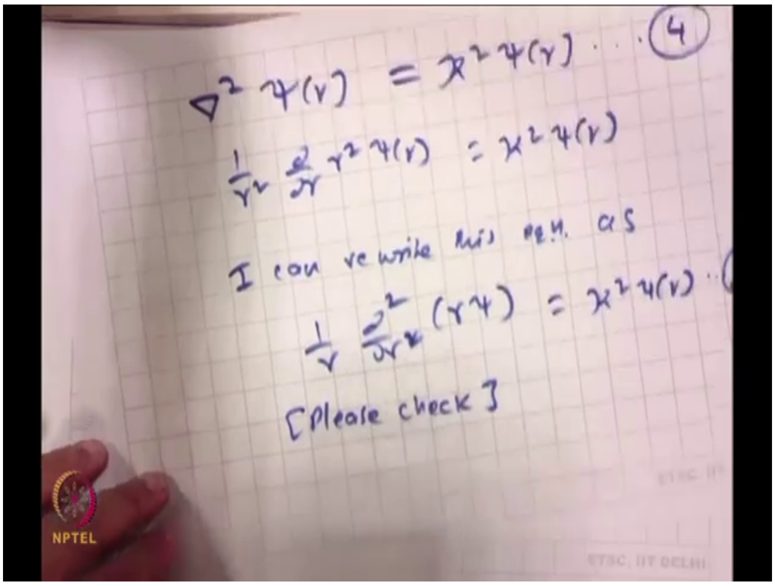

Now, so then I can also again write this as del square psi. Now, I will be writing r instead of x right is equal to kappa square psi of r that is what we are going to solve now right. So, this is I think I forgot the last number maybe this is equation 4. So, del square this, I can write as 1 by r square del of del r r square, then psi of r is equal to kappa square psi of r. So, you putting the expression of del square in now right.

See, we have to know this. Possibly you are thinking, it is you know it is a biophysical chemistry course. Why do you need to care about this, but this is what biophysical chemistry is all about, because it is a physical concept being applied to a biological problem. And this problem is not essentially biological, it is biological in the sense that we are taking a protein, but this problem is applied universal right. If you take any charged molecule, it does not have to put in anything else, we did it in terms of a plane right.

So, this can be rewritten as, and this is for you to check, I can rewrite this, I can rewrite this equation as 1 by r, 1 by r del of del r ok. So, actually I should write del 2 of del r squared in this case. So, del 2 over del r squared r of psi is equal to kappa squared psi of r, this is 5. This is for you to check. Please check the equivalence of this expression and the equivalence of this expression. Please check the equivalence of this expression and the equivalence of this expression right. See whether we can write it like that is why you have to check ok.

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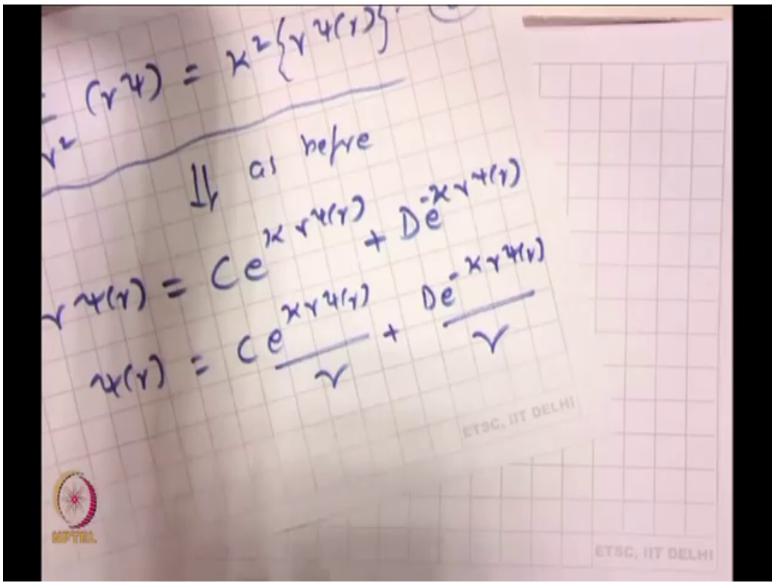

If you have it like that, I can again rewrite it as r psi is equal to kappa squared r psi of r, this is say equation 6. Tell me do you understand why we rewrote the equation like that, why did we rewrite the equation like that? Think about what we solved in case of the planar charges, when we are talking about the psi of x in one dimension x.

Do you see any similarity between the equation we solved, and the equation we are solving here? What did they, what was the equation we solved? We solved del 2 psi over del x squared right is equal to?

Student: (Refer Time: 27:27).

Kappa squared psi of x.

Student: Yes.

What are you solving here now? We are solving del 2 psi over del r squared r psi that means, r psi of r is equal to kappa squared r psi of r. So, I can put this one in brackets like this. See, instead of psi of x, what are we solving we are solving?

Student: Psi of r.

r psi of r.

Student: (Refer Time: 27:50).

For a simple comparison. Can everyone see it?

Student: Yes Sir.

Everyone can see it right? So, if this is the case, then as before as before if this is your you know certain function which you are solving for, you are essentially solving for psi of r remember, then what should it be I can write r psi of r is equal to what, the same thing right. I can write here say C e to the power kappa right. Then what should I write what is the what is my x here?

Student: r psi r. r, r, r.

Ok, r psi of r. What else do we have?

Student: Minus, minus, minus e A.

Plus D.

Student: D.

e to the power?

Student: Minus kappa.

Kappa with a minus sign r

Student: psi of.

psi of r. Everybody with this? Good. Now, if I write this psi of r, then is equal to what C e to the power kappa r psi of r over r plus D e to the power minus kappa r psi of r then over r.

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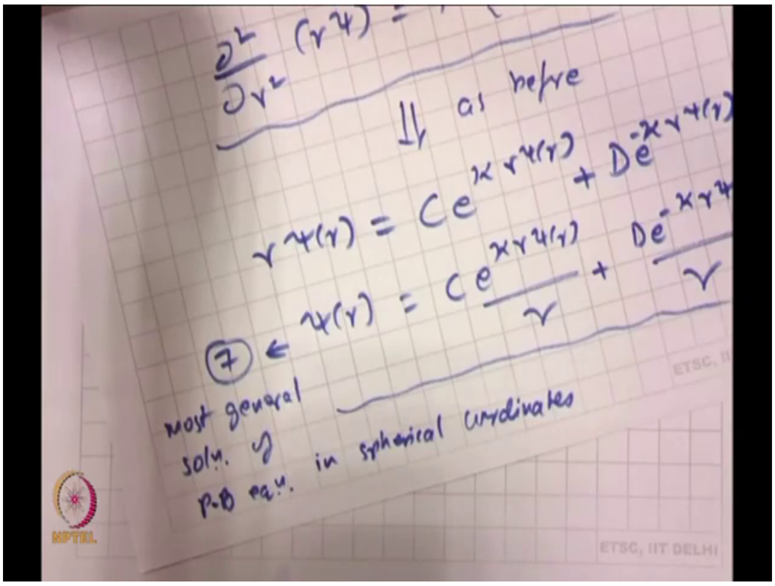

So, this is my most general solution this should be equation 7. My most general solution of the Poisson-Boltzmann of the Poisson-Boltzmann equation or the Debye-Huckel equation in spherical coordinates. Is everybody with this? Please check and let me know. You did not tell me, I actually made another mistake; I am making too many mistakes, but anyway tell me what mistake I am I made out there?

Student: (Refer Time: 30:14).

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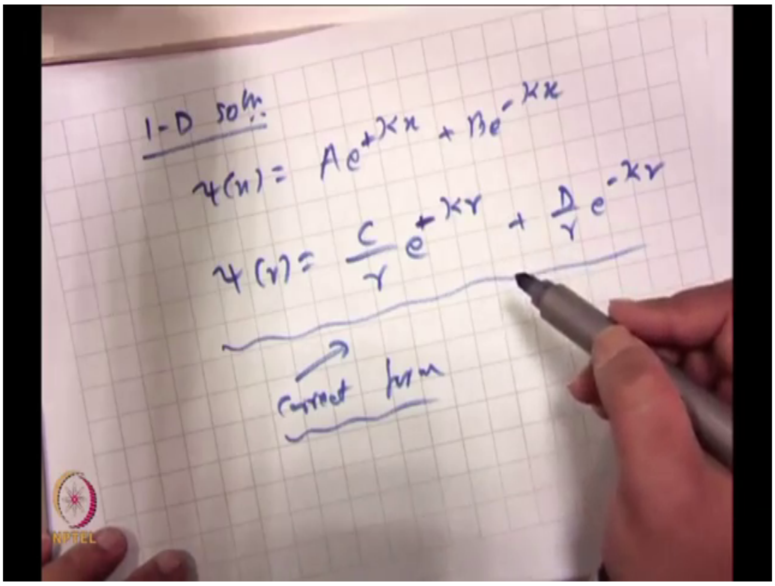

No, what was what was my, what was my 1-D solution from before? My 1-D solution was psi of x is equal to A e to the power minus kappa x or say plus kappa x plus B to the power minus.

Student: e to the power minus (Refer Time: 30:35).

Kappa of x. Same here. What should I have here? What extra did I write there or what extra did I by mistake put there?

Student: (Refer Time: 30:43).

I should not be writing this right. I should not be writing this C by r e to the power minus kappa r or say this plus kappa r plus D by r e to the power minus kappa r. Should I be writing psi here?

Student: e to the power.

Psi is the solution come on, right, psi is the solution?

Student: (Refer Time: 31:05)

Psi is what we are solving for. We should not be having psi out there. We are solving for r psi which is your extension which essentially your x right, but this is just psi, psi is the solution we are looking for. So, this is this is what your psi goes like, e to the power minus kappa r this plus kappa r D by r e to the power minus kappa r.

So, please correct this one, this is the correct form. Yeah, this is my second mistake today right, sometimes days almost full of mistakes this is one, but please make this correction. It is like x. Here x has been changed to r. The only thing is in this case there was no inverse of r dependence; here I have an inverse of r dependence that is the only change I have in this case.

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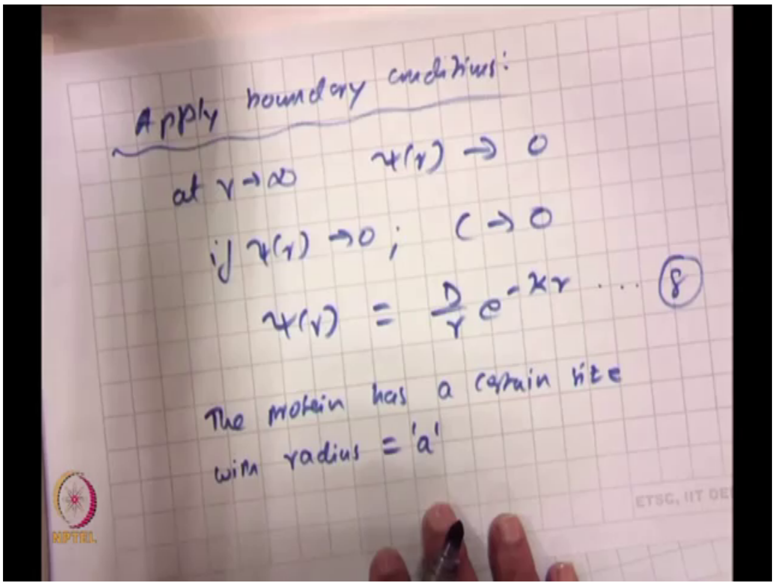

So, then I again apply, I again apply boundary conditions. If I apply boundary conditions what will happen at r tends to infinity, what should I get? At r tends to infinity psi of r should tend to.

Student: 0.

0. If psi of r tends to 0, then from the equation what do I have; which one will tend to 0?

Student: C by (Refer Time: 32:31).

C will tend to 0 right?

Student: Yes.

C will tend to 0. Well, essentially C by r. Why? See 1 by r to the minus, but please keep this in mind the first, you look at this the first expression e to the power kappa r over r, e to the power kappa r goes to infinity much faster than r can take you to 0, because it is an exponential growth right on the second term e to the power minus kappa r dies to?

Student: 0. (Refer Time: 33:05).

infinity very fast, obviously, 1 by infinity is 0, it does not matter. But here at least from here comparing with what we have for psi r, it tends to 0, what do we have can we write c tends to 0.

Student: Yes sir.

I should be able to write c tends to 0 the same way we did we did the other time.

Student: (Refer Time: 33:25).

See, if that is what I write, then I can have now psi of r is equal to D by r e to the power minus kappa r. Say, which is see I forgot what the equation number is say, this is equation number 8. Now, what is the other boundary condition?

Student: r tends to 0, r tends to 0.

The other one was.

Student: r tends to 0.

r tends to 0, but here what we will do is we will not consider the protein as a point charge.

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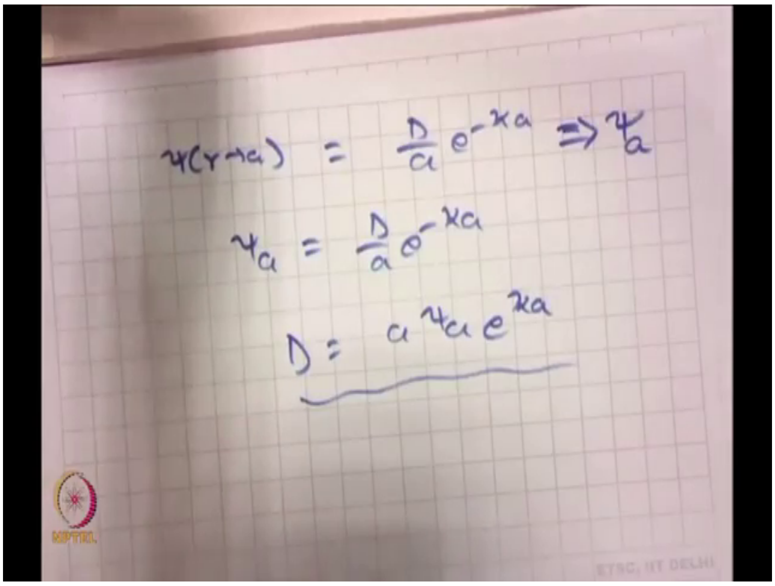

We will say that the protein has a certain size with the radius being equal to say a, that is what we will treat it as. So, if the radius is equal to a, if this radius is equal to a.

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Then I can write at psi r tends to a, at psi r tends to a, I have D by a e to the power minus kappa a right. I just took it from equation number 8, see I just put in r tends to?

Student: a.

a that is it. I cannot I do not want to put r tends to 0, why, because I do not want to consider as a point charge I am considering as a spherical particle which is having a certain radius a, does not matter what it is. It might be 10 Angstroms, 20 Angstroms whatever it is right or 1 nanometer, 2 nanometer, whatever.

Now, the simple reason being because you know proteins have sizes right. The ions cannot go inside the protein. So, the ions have to be at a certain distance like surrounding the protein.

So, we have to take the protein as a charge I mean with a certain distance with a certain size. So, this is the case. So, this at r tends to a, what do I can write as is I can I can write as say you know say psi of a. But please here make sure the difference between this one and that one is when we put x tends to 0 this went to what?

Student: (Refer Time: 35:43) 1.

It went to 1 right.

Student: Yeah.

And we could get the value of?

Student: (Refer Time: 35:46).

B in that case.

Student: Yeah.

But in this case it is not we are not putting r this tending to 0, we are putting r tending to a. So, in that case what should I have? So, I have psi of a is equal to D by a minus kappa a right from here, and that is what I have then I have an expression for D which is D is equal to a psi of a. Then what?

Student: (Refer Time: 36:16) kappa a. kappa a.

e to the power.

Student: Kappa a.

e to the power kappa a. So, this is what I have. So, this is what my d is in terms of, obviously, exponential kappa, then you have a, then you have this a here which is the radius of the charged particle right ok.

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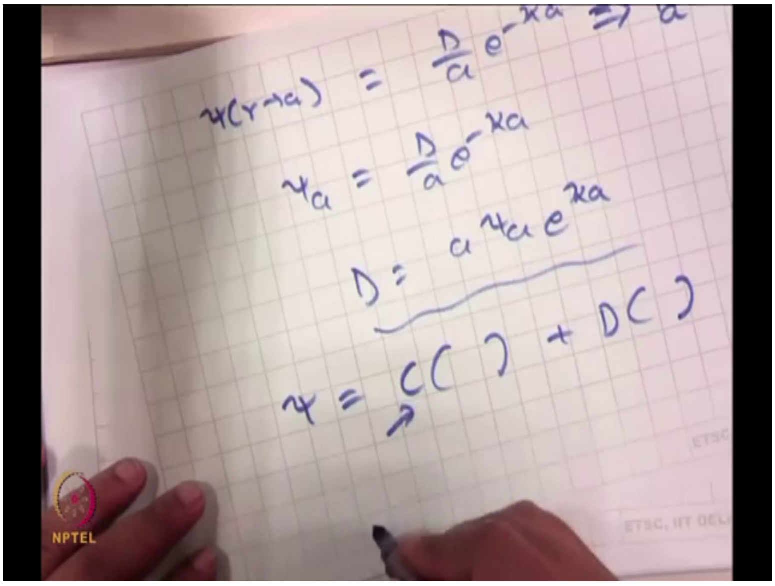

Now, you combine this equation, that means, you had you had psi is equal to C times a constant plus D times a constant right that is what we started with. We took this to 0. We found what D was.

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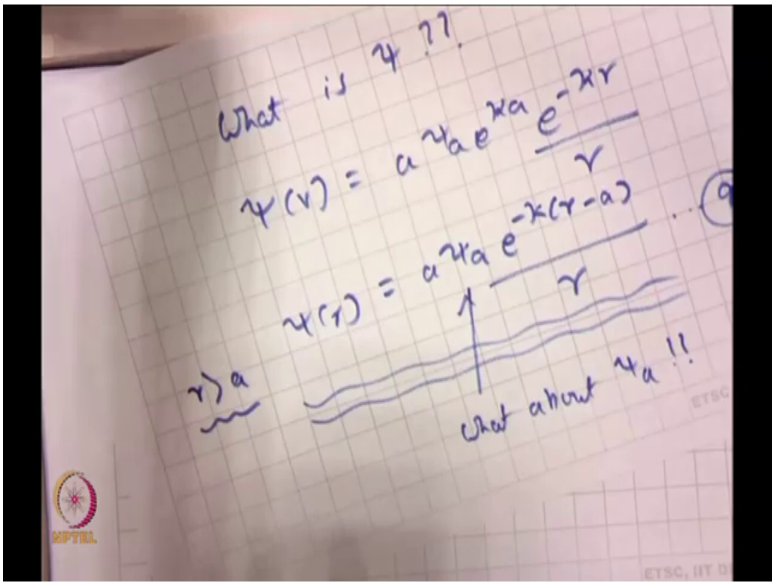

Now, tell me what is psi, write it down. What is psi, what is psi equal to now? Tell me.

Student: (refer Time: 37:14).

So, psi of r is equal to?

Student: (Refer Time: 37:26) by r.

I can write a psi of a, what did we write e to the power kappa a that was psi of a, then what else do we have, e to the power minus kappa r. Then

Student: (Refer Time: 37:40) r.

Over.

Student: r.

r. Now, understand the significance of this. So, this is equal to a psi of a, a is what, the radius of this protein as a sphere. Psi of a is what?

Student: Charge.

The charge at.

Student: (Refer Time: 38:00).

Distance a ok. So, this is a psi of a. So, this is essentially a constant right. We do not worry about it. What are you going to worry about now? You look at this. So, this is essentially what e to the power minus kappa, I can write it as r

Student: Minus a.

Then.

Student: Minus a.

Minus a over r. So, this is what your psi of r is, this is what your psi of r is right. So, this would be what equation? This would be equation say 9. Now, guys tell me what is the major difference between this equation and the equation which we know in terms of a Coulombs law, what is the main difference? Coulombs law also had something like what, do you remember? It was.

Student: (Refer Time: 38:59).

The charge, the power to the charges over 4 pi epsilon 0 times r?

Student: (Refer Time: 39:04).

Right that is a potential I am talking about right, not the force right.

Student: (Refer Time: 39:09), r.

Here you also have r in the denominator. But is it the only thing you have, you also have another dependence what is that?

Student: U square.

It is the dependence upon r minus a. What does r minus a mean? r minus a means, you take this right, obviously, between 0 to a you cannot cover because then you are inside the protein, then r minus a means how far you are moving out

Student: From the surface.

From the?

Student: Surface.

Surface of the protein. And how is the charge distribution now varying, obvious exponentially, but determined again by kappa which is related to the t by length ok.

Guys, please do not forget this right. This is essentially if anyone asks you how a charge distribution is or how the charge distribution varies with respect to a spherical particle, this is the most straightforward answer you can give. It has an exponential dependence.

And remember the exponent term comes from which part of the Poisson Boltzmann? It comes from the Boltzmann part. And the relation with the charge density or the electrostatics rather which is the del squared psi comes from there is an electrostatic potential comes from the Poisson equation. We are combining these two and that is why I am going so slow actually on this.

So, this is what you need to really care about right. Now, the question is what about psi of a? How are you going to calculate it? We do not know what it is right. It is easy to calculate actually, but we have to imply you know we have to you know put in Gaussians theorem and all those things.

So, we are not going to do that, neither I am going to ask you to derive what so I have a is in class, but these derivations you should be knowing please, these derivations you should be knowing it can be asked in the exam.

Instead what I will tell you is this I will just give you a number which I have. And before I go there I will just want to make a point. When I am looking at this equation please make sure the condition is that r is always greater than a, that means, that no point am I what within the protein?

Student: Yes.

I am always looking at something which is at the surface of the protein. So, the maximum that r can be is equal or the minimum r can be is equal to?

Student: a.

a, and greater than a, essentially that is what it is. Because if r, if r is equal to o; essentially you can see it becomes a constant what this one goes to?

Student: 0

0, that means 1. r is equal to a, a by a cancels out, you get psi of a and that is what you are going to get because psi of a is what the electrostatic potential at the surface of the protein. So, r always has to be greater than a; otherwise, it will not make sense ok.

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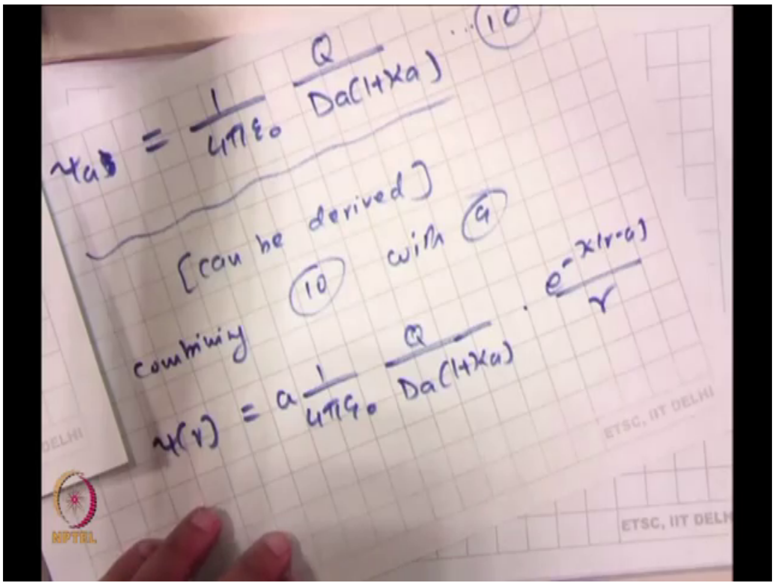

So, to give you an expression for psi of a, sorry, (Refer Time: 42:18) psi of a I mean not a function of a, I will give you what the expression is I will just the expression is goes like this, and just write it down actually. So, psi of a it can be shown 1 by 4 pi epsilon 0 Q by D of a 1 plus kappa a. This is an expression for psi of a. Say this is equation 10, can be derived can be derived. It is not a problem, but we will not derive it here.

What is Q guys you think?

Student: Charge, Charge.

Q is the charge right. This is the charge on the protein. We are talking about a uniform charge now; we are talking about uniform charge. You have to have 4 pi epsilon 0, well, 4 pi is 4 pi, epsilon 0 is?

Student: Permitivity.

The permittivity. D?,

You have to include that right, because it is a part of the solvent, the protein is in the solvent. Now, because you are putting in salts now, because you are putting in salts now, before it was Q by r only. Remember Q by 4 pi epsilon 0 r or Q 1, Q 2 whatever, but now I have this kappa term coming in this is because of the salts.

So, you can understand if kappa is equal to 0, that means, you have what, you have no salts you have not added any salt in the solution. Then what does it come to it essentially comes to what you know Q by?

Student: Da.

D a or Q by dr; that is a normal Coulombic potential you guys are know. See then everything makes sense right. You just have to make sure under what conditions this one is applicable which is in case of salts if you are adding salts because salts have their own screening effects. And under what condition would my simple coulombic potential be applicable when we would not be having any intervening medium having salts in it. That is essential how it is applicable ok.

I have we are already out of time, but I will just write this final equation down for you. So, if I combine this, that means, this is psi of a right. So, let me combine this actually, then combining 10 with 9, combining 10 with 9, when 9 was this psi of r is equal to this. So, what I can write is psi of r is equal to please make sure you follow it, a then I am putting in psi of a 1 by 4 pi epsilon 0 Q by D of a 1 plus kappa a that is my psi of a, then e to the power minus kappa r minus a over r.

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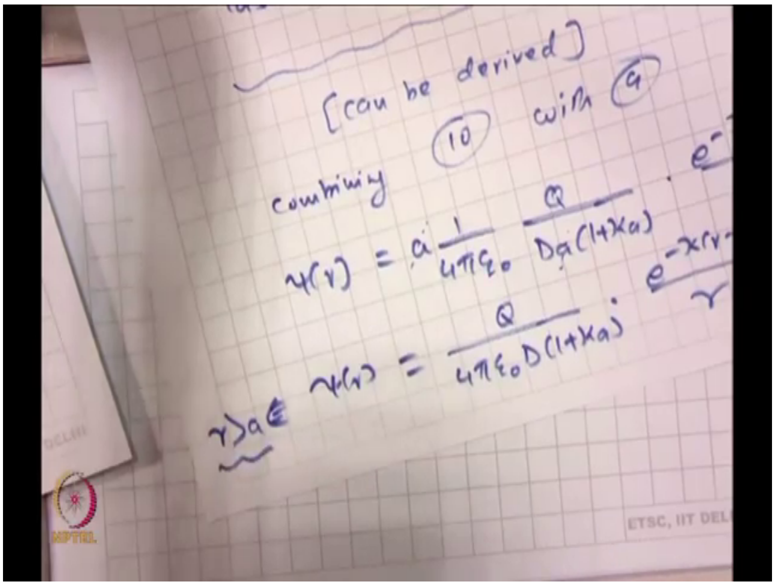

So, what simplification can I do here now, you see this a, this a will cancel out right. So, this is equal to then Q by 4 pi epsilon 0 D 1 plus kappa a times e to the power minus kappa r minus a over r. So, look at this equation combined. You have two things. One is you have this exponential term which we discussed before. And the other one we are not looking at psi of a; it is a screening, because along with the dielectric constant you also have another term that means, a dielectric constant essentially is getting multiplied by a factor which is 1 plus kappa a.

So, it is not only the dielectric constant which is spinning the two charges from each other, it is also the intervening salt solution which is coming in and playing its role; that means, it your dielectric constant is getting multiplied by a certain factor which is one plus kappa a essentially what you are doing. It is a small change obviously in the denominator. And the other big thing is that exponential dependence upon the distance r, where r again is this psi of r remembering that r is greater than a all the time.

So, I will I will stop here for the day right. This is essentially what I needed to discuss with you with regards to electrostatics Poisson-Boltzmann equation. You know what your Debye-Huckel limiting law I will see whether we can do it, not, not now, but the Debye-Huckel limiting law is a straightforward derivation from here where you bring in your remember activities and all these things, chemical potential activities that is why Debye-Huckel, it is related to, it is a limiting law essentially.

But this is where we start from, this is the starting point. And this can need to a lot a lot of logical expressions, logical solutions, logical assumptions that you can come across or you can come up with when you have a protein, you must in a solution with salt or without salt, this is going to vary ok.

Again you do not have to worry about the derivation of psi of a this is what you do not have to worry about ok, this can be done based on charge density and all these things. But this final expression guys you have to keep in mind how we came out doing it. And obviously, do we know my mistakes? I can make a mistake, I can get away with it; you cannot right.