Advanced Quantum Mechanics with Applications
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Lecture - 10
Spherically Symmetric System and Applications to quantum dots

In the last discussion we have talked about the rotational invariance of systems and how it is related with the conservation of angular momentum. So, which means that any system that preserves rotational symmetry that is, it is invariant under rotational transformation. We are talking about space rotation, the angular momentum will be a conserved quantity and the corresponding quantum numbers are good quantum numbers and they can be used for writing down the wave function.

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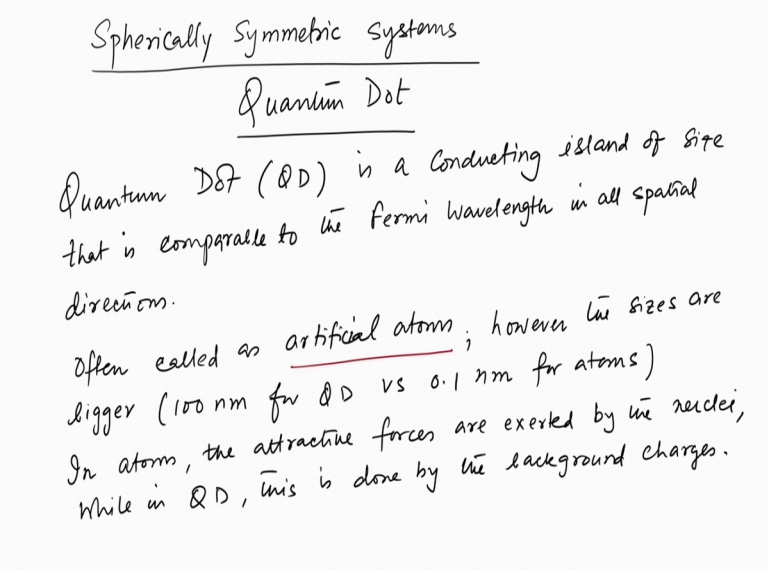

Now, let us see some examples or rather applications of such spherically symmetric. As it is called which are invariant under rotation, such systems and one of the systems that we are going to talk about here is the quantum dot. So, the question is what are quantum dots? So, let us say, the quantum dots which we shall denote by the abbreviation QD is a conducting island of size that is comparable to the Fermi wavelength, in all spatial directions. And these are often called as artificial atoms.

This is a special term that is used. So, it is comparable to the atomic dimensions. I will see, we will compare dimensions, but these are these QDs or the quantum dots are called

as artificial atoms. The sizes of course, are bigger; I mean in fact, order of magnitude more. So, it is a 100 nanometer for a quantum dot, versus 0.1 nanometer for atoms. So, there is straightaway 3 orders of magnitude bigger. The quantum dots are bigger, than that of individual atoms. And in atoms, the other differences are that, in atoms the attractive forces are exerted by the nuclei which contains of course, the protons while in QD this is which means, the attractive forces is done by the background charges. We shall explain more on this.

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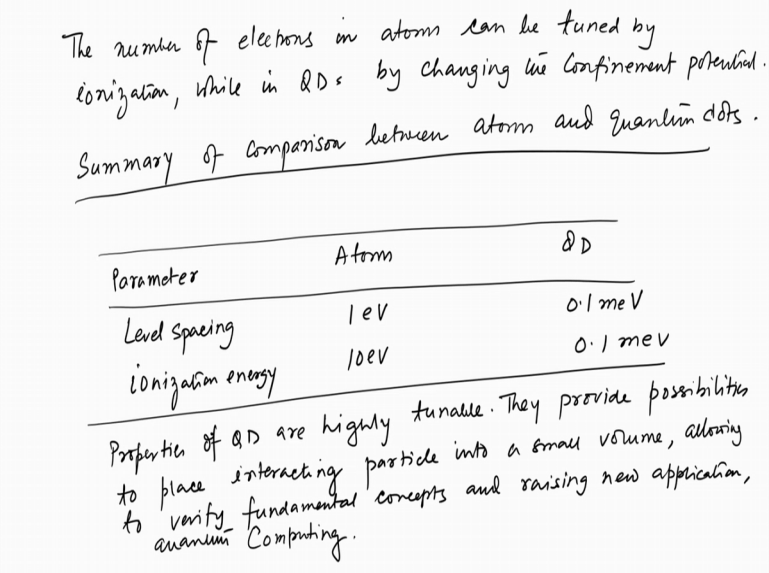

And a very important property of the quantum dot is that, the number of charge carriers or which are electrons here, by the ionization that is by knocking of electrons from the outermost shell and while in QDs, that is quantum dots this is done by changing the confinement potential. So, let us have a summary of the comparison between atoms and quantum dots. So, let us make a table and also let us talk about of at least a few parameters, maybe couple of them for atoms and for QDs. So, one is level spacing.

So, what we mean by level spacing is; the difference between the energy levels and in atoms it is of the order of an electron volt 1 eV, whereas, this is of the order of a milli electron volt which is of 3 to 4 orders of magnitude lower. And there is an ionization energy, which is of the order of 10 electron volt, in hydrogen atom we know its 13.6 divided by n square electron volts so for n equal to 1 is 13.6 electron volt where this is the again of the order of an meV a 0.1 meV. And so, basically the properties of important

thing is that the properties of QD are highly tunable. I am giving you a very sort of basic introduction to quantum dots and plan to do some elementary calculations, to show a few things which are relevant for studying quantum dots. And of course, they provides, they provide possibilities to place interacting particles, into a small volume. So, thereby allowing us to verify fundamental concepts or basically the quantum mechanical concepts and raising new applications and the notable one of them is a quantum computing.

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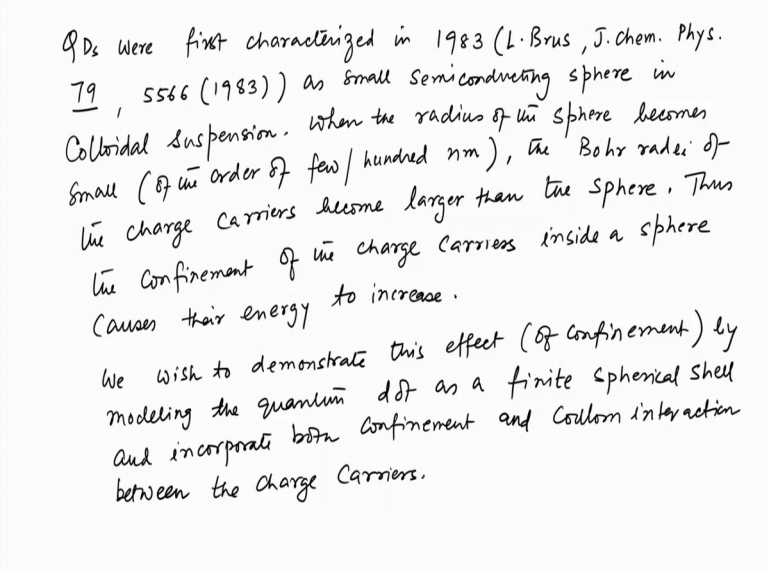

So, these are very preliminary introduction to quantum dots. Let us have some theoretical or rather historical first let us have some historical overview of, how it was and when it was synthesized and so on. So, QDs were first characterized in 1983 by L. Brus. And the reference is Journal of a Chemical Physics and this is a volume- 79, page 5566 and a 1983, as a small semiconducting sphere in colloidal suspension.

So, when the radius of the sphere that is the semiconducting sphere, that we are talking about becomes small and how small is of the order of order of few or as we said it is about maybe 100 nm or few 100 nanometers a few to 100 nanometer. The Bohr radii, this is important, the Bohr radii of the charge carriers become larger than the sphere. Thus, the confinement of the charge carriers, inside a sphere causes, where energy to increase. So, this is by enlarge the definition of quantum dot.

So, what happens is that, when you confine charge carriers within a small volume, it can so, happen that the Bohr radii of this charge carriers, they actually spill out of the sphere. So, then this would cause, an enhanced energy, when you are trying to confine the charge carriers into such a in such a small volume. So, what is our plan is the following that we wish to demonstrate this effect of confinement, by modeling the quantum dot as a finite spherical shell, having a spherical symmetry.

So, to say and incorporate both confinement and interaction effects coulomb interaction between the charge carriers alright. So, this is we are talking about a semiconducting specimen or a material. And, now we are going to talk about a very small semiconducting material which is in the form of a drop or a sphere or a spherical object and in which charges are enclosed or confined, ok.

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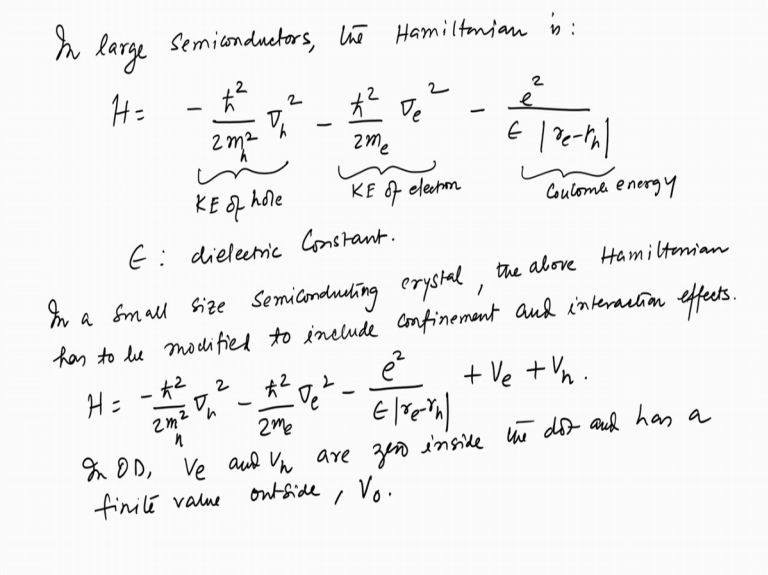

So, what happens in large semiconductors, the Hamiltonian is written as. So, H equal to minus h square h cross square by 2 mh square del h square minus h square by 2 me square. So, H the subscript H refers to hole and the subscript e refers to electron. So, we are talking about mixed semiconductor, where both types of charge carriers are prominent and there is also an electron hole interaction term which is given by re minus rh, which are the coordinates of the electron and the hole with regard to some a chosen axis and epsilon is the dielectric constant.

So, let us just write this. So, this is kinetic energy of hole, this is kinetic energy of electron and this is coulomb energy (Refer slide: 16:30) energy and epsilon is the dielectric constant. So, this a generic Hamiltonian, that will hold for any semiconductors and we are talking about not a nano size semiconductor, but a large semiconductor. Now what happens, when you confine them, is the that, there will be an additional potential coming in both for electrons and holes and that the potential, we are free to model it, as say a spherical potential or rather a potential, that exists within a spherical region and the outside it is zero.

So, in a small size crystal this Hamiltonian this, the above Hamiltonian has to be modified to include confinement and interaction effects. So, that tells us that, we have to write it again, we will have this kinetic energy term which is which was there earlier and minus e square over epsilon. So, it is r e minus r h and then, some potential for the electrons and the holes. So, we can model the quantum dot in a fashion, that in a quantum dot, V e and V h, are zero inside the dot and has a finite value outside. This finite value can be taken as some V 0 and of course, it is up to us to consider, what is a what can be a realistic value for V0.

For example, if we take the limit V0 going to infinity. then of course, the energy spectrum is the free particle energy spectrum which is given by En equal to h cross square pi square n square by 2 m R square, where R is the radius of the dot. However, there is a problem with this taking the potential to go to a very large value all value or infinity is that it overestimates the band gap of a of a quantum dot.

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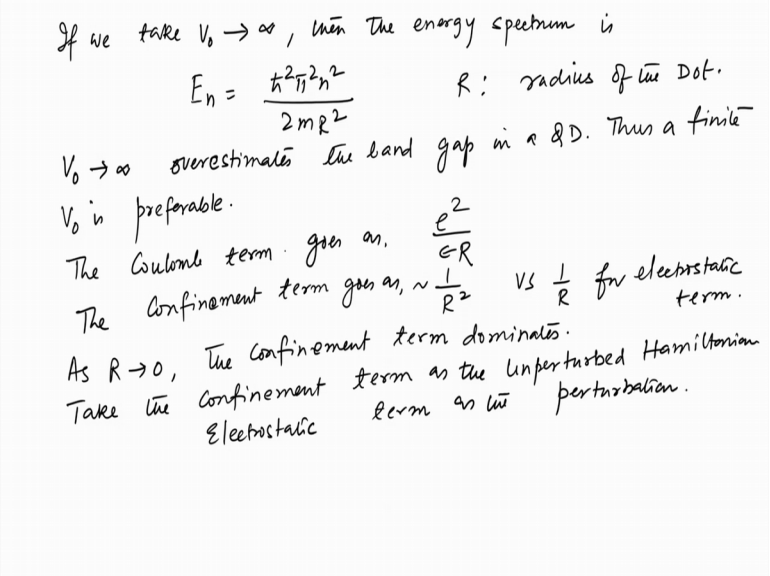

So, V 0 going to infinity overestimates. There is a finite V 0 is preferable. So, we take a finite V 0. So, once again to remind you that the potential inside the spherical dot is 0 and the potential outside is V 0 which is a constant, which could be taken same for both the electrons and the holes. And, these V 0 would be taken as a finite value and not infinity, and also the coulomb term goes as the that goes as a e square over epsilon R and never the less.

I mean whether you take V 0 to be large or V 0 to be some finite value, the confinement term which is basically the coming from the V 0 term. So, we will call it a confinement term. So, the confinement term goes as this one over R square, as we just said. So, this is for of course, infinite potential, but never the less we can take a value for V 0 and we can convince ourselves that the confinement potential goes as 1 over R square versus 1 over R for electrostatic term which is just the coulomb term.

So, which means that as R goes to 0, the confinement term dominates which is 1 over R square. So, that dominates as R goes to 0, compared to the electrostatic term which is one over R which goes as one over R, ok. So, what we will do is that we will take this as the confinement term as the original Hamiltonian, and take the coulomb term. So, take the original Hamiltonian or rather the unperturbed Hamiltonian, let us write the unperturbed Hamiltonian as the unperturbed Hamiltonian and the electrostatic term as the perturbation.

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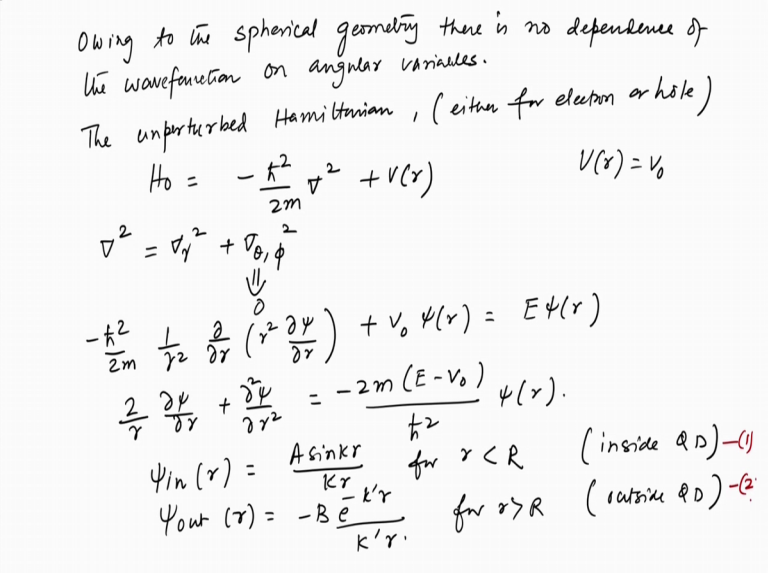

So, this is our roughly our plans, for the handling or doing a mathematical formalism for the quantum dot. Owing to the spherical geometry there is no dependence of course, of the. So, dependence of the wave function on angular variables. So, they are independent of the angular variable's theta and phi and. So, the H 0 the unperturbed Hamiltonian H 0, becomes equal to minus h square by 2 m and del square, either for electron or for hole, either for electron or hole, and plus V r now of course, V r can be taken as a V 0 which is same for all values of r.

So, if we write down the del square operator, which is the Laplacian in the radial coordinates. This you will find in any formula book or even find at the back page of cover page of graphics, towards the back cover and you would be able to write this. So, in principle your delta square contains a delta r square and delta theta phi square. But since they are not here or rather they do not depend on the wave function does not depend upon theta and phi. So, we can put that equal to 0. So, this del r square has a form which we are going to write here. So, this h square by 2 m, and so this m can be electron mass or the hole mass, and also can be the band mass of each of these particles which we are not making a distinction at this moment.

And, so this is equal to one over r square del del r of r square del psi del r plus v zero psi of r equal to e psi of r, that's the time independent Schrodinger equation in the for the radial part. And if you simplify this becomes equal to2 by r del psi del r plus del2 psi del

r 2 its equal to 2 m with the minus sign E minus V 0 divided by h cross square psi of r. So, I am not going into the solution, but this you will find it a number of places, including the hydrogen atom or even the spherical oscillator 3D oscillator.

So, the psi, there are two solutions one is inside the wave function. So, psi a inside the inside the quantum dot, that is A sin Kr by Kr this called as a Bessel function for r less than R and this is equal to. So, this is psi in inside the dot inside QD and psi out r its equal to a B with a minus sign K' r, divided by K' r, for r greater than R, and this is outside the quantum dot ok. So, these are the wave functions of this particular problem.

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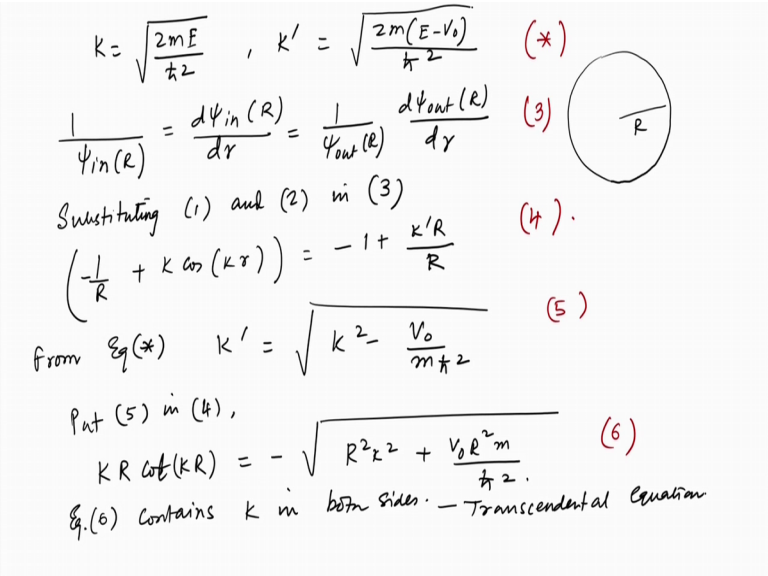

So, K becomes equal to root over 2m E, by h cross square and K' becomes equal to 2m E, minus V 0 divided by h cross square. So, the boundary conditions there of course, two boundary conditions namely the Dirichlet and the normal boundary conditions, which talk about the continuity of psi and d psi d x at the boundaries boundary means. So, we have to match the boundary conditions at the dot.

So, this is the periphery of the dot. So, you have to match the boundary conditions at the dot and those two boundary conditions that Dirichlet and the normal boundary conditions can be actually combined to write it as one by psi in r at small r equal to R and its d psi in R d r. So, it is a d psi in d r computed at R and it is a 1 by psi out of r d psi out. So, these are combining the two boundary conditions one can write this.

So, if your call this as equation 1, let us write it with a different color. So, that its visible to you. So, its equation 1 equation 2 and this boundary condition is say equation 3 then we can write down. So, substituting 1 and 2 in 3ah then we have 1 by. So, this is 1 over R with a minus sign plus K cos Kr and equal to minus 1 plus K'R by R. So, this is. So, there is.

So, basically there is also a relationship between. So, let us call this as equation 4, this is equation 4, from which equation is that. So, this is let us we haven't name this equation, but this is the equation star. So, from star from equations star we get a relation between K and K', which gives the K' equal to K square minus V0 m h cross square, and now call this as equation 5 for our reference and also put 5 in 4, and if we do that we will get an equation which is KR cot KR and equal to minus root over R square K square plus V square m by h cross square.

Now, this solving this will give us the value of K and hence, we will get energy from this equation number star, and that's the eigen function for the Hamiltonian and of course, we have found out the eigenvalues by solving the differential equation. So, if we can do that, that is solve for K then we will get the energy eigen functions. And somehow as that is slightly difficult to do because you see this equation. Let us call it equation number 6 contains K in both the sides and that too one is inside the argument of a cot function and the other is inside a square root.

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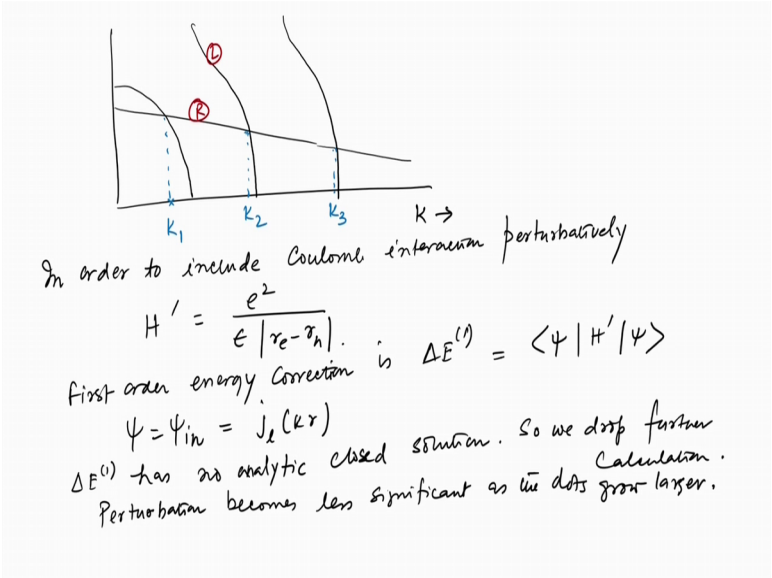

So, this is called as the transcendental equation and it cannot be solved analytically, but has to be solved either numerically or graphically. So, I will show the graphical solution of this. So, what I will do is that, I will plot, both these sides separately and show you a schematic solution. So, these are these cot functions and that is that. So, these are the solution. So, this is K and these are two different sides. So, this is the left side. So, let us call it by L. So, this is L and this is R.

So, that meeting points of L and R will give me the solutions, which are given by these values of K. So, these are the allowed values discrete values of K in. So, let us I mean K in means K, so this is the K1, K2 and K3, that are allowed values and this will give me the energies. So, that way, we are able to solve the problem for you know the modeled quantum dot. The way we have modeled it; however, we still have to incorporate the coulomb term.

So, in order to include coulomb interaction perturbatively; so, we write down a perturbation term, which looks like this H' which is equal to e square divided by re minus rh, and the first order energy correction is given by delta E at the first order is equal to psi H' psi if you use psi to be equal to psi in which is equal to jl Kr which is a Bessel function. We can actually solve this for the first order energy correction; however, this has no simple analytic closed solution. So, we drop further calculation with this. now of course, the perturbation, becomes less significant as the dots grow larger.

In fact, the quantum effects start starts to diminish, as the size of the quantum dot starts growing larger. So, the confinement effect is the dominating effect here, this is what we have been trying to say. So, finally summarizing, a quantum dot is basically there are charges which are in a highly confined geometry and in this particular case we have taken the geometry, to be a spherical in shape. And this is called, that is why it is called as a spherical dot.