Solid State Physics
Lecture 14
Repulsive Interaction

Now, let us consider the Repulsive Interaction. (Refer Slide Time: 00:26)

Same thing goes for repulsive interaction if we consider a sphere representing an atom, at the center there is a nucleus and there is an electron cloud around it, another sphere just like that. And as far as electrostatics is concerned, there is no electrostatic interaction, just by going just going by our previous argument. Then where from does this repulsion come? It must have some other kind of origin. So, let us now consider that we are bringing these two atoms very close. As we are bringing them very close the charge densities that are not confined, electronic density is not really confined to this sphere, it is extended and as we bring them close that, electron densities they start overlapping with each other. Once they start overlapping with each other, there is a tendency that the quantum states of one atom would be partly occupied by the electrons from the other atom and that is prohibited by Pauli Exclusion Principle. So, what does Pauli Exclusion Principle tell us? It tells us that two electrons cannot have all their quantum numbers equal; when the charges of two atoms overlap, there is a tendency for electrons from atom b to occupy the part, occupy in part the states of atom a that are already occupied and that is not allowed from the Pauli Exclusion Principle. Once that this is not allowed, this brings in an effective repulsion energy into the system. So, the electron clouds repel each other; the atoms cannot come infinitely close to each other, that is prohibited just by the Pauli Exclusion Principle. (Refer Slide Time: 02:55)

So, we have the van der Waals kind of interaction derived here, that goes as R^{-6} and that does not make all the atoms collapse onto each other, because of only Pauli Exclusion Principle. Here we must note that, Pauli Exclusion Principle does not exist in classical mechanics, it is only of quantum nature. So, this repulsive interaction has also only quantum origin, only quantum principle; there is no way that you can explain this in classical mechanics. So, here we will not try to find out this repulsive potential right from the beginning, from the first principles, rather we will go through an empirical understanding of this. Experimental data on inert gases that we are interested in right now; that can be fitted well by an empirical repulsive potential, the empirical repulsive potential is given as $\sim \frac{B}{R^{12}}$, where B is again a positive constant, making this interaction a repulsive one. So, if we have this found empirically, then the total potential can be written as U(R); U(R) can be expressed as $4\epsilon[(\frac{\sigma}{R})^{12} - (\frac{\sigma}{R})^{6}]$,this is the attractive term. And we have new parameters, σ and ϵ, ϵ and σ; in terms of ϵ and σ, we can write $4\epsilon\sigma^6 = A$ and $4\epsilon\sigma^{12} = B$. How can we plot this interaction? If we want to plot this interaction, we plot it like this; this is R, this is the potential as a function of R and looking at this expression, we can plot this plot it this way. So, if we are very if we bring the atoms very close to each other, R is very small; then the potential will steeply rise here, it is actually even steeper, I must do a do justice to this, this would look somewhat like this, even steeper. And there would be an equilibrium distance, where the potential is minimum; if we go beyond the equilibrium distance, the potential will keep on increasing. And at a large distance, it will asymptotically touch the line $U(R) = 0$; that is at very large distance, it will asymptotically reach that limit. And here you can see that the potential is attractive, here you can see that the potential is repulsive and this is called the Lennard Jones potential LZ potential. So, there is no zero point energy and no Pauli Exclusion Principle in classical mechanics; therefore this attractive and repulsive potential both are purely of quantum origin. Although, there are many classical, actually semi classical simulations, semi classical work, where this LZ potential is considered as the main potential of that calculation. So, this potential is very important, we derive it considering some semi classical approach, not exactly quantum approach; but the principles behind deriving this be it say the zero point energy or the Pauli Exclusion Principle that is purely quantum. So, we cannot have any classical analog for this kind of a potential; this is completely quantum, that is all for now.