Chemistry and Physics of Surfaces and Interfaces
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Lecture - 21
Tip-Vacuum Tunneling Junction

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Lecture 21

- Scanning tunneling microscopy
- Tunneling junction

Hello everyone, welcome back to the new lecture, lecture 21. So, in this we would continue scanning tunnelling microscopy in more detail and particularly we look at something known as tunnelling junction and that is the quantum mechanical thing that we want to basically look into and then here we try to understand what is basically that we measure or what is the origin of this tunnelling current itself. So, then that is a truly quantum mechanical phenomena and that is why I have here something known as tunnelling junction. So, we define something called a tunnelling junction and we use that to work out this problem, so that is the most fundamental thing for scanning tunnelling microscopy. So, the first question that we would ask ourselves is what is our STM measuring basically? So, that is the question but before that let us try to understand this in greater detail. So, now we know that we are basically measuring current, so current is nothing but the flow of electrons across this junction. So, that is a tunnelling junction. But before we start to discuss with it, we want to also see the classical electrons, so if electrons were classical. Do we observe tunnelling? So, that is the first question that we will ask and you will find out that this is not the case, this is a truly quantum mechanical phenomena. So, that the description of the quantum mechanical description of electron is quite important in defining or in basically explaining the tunnelling itself or therefore the tunnelling current.

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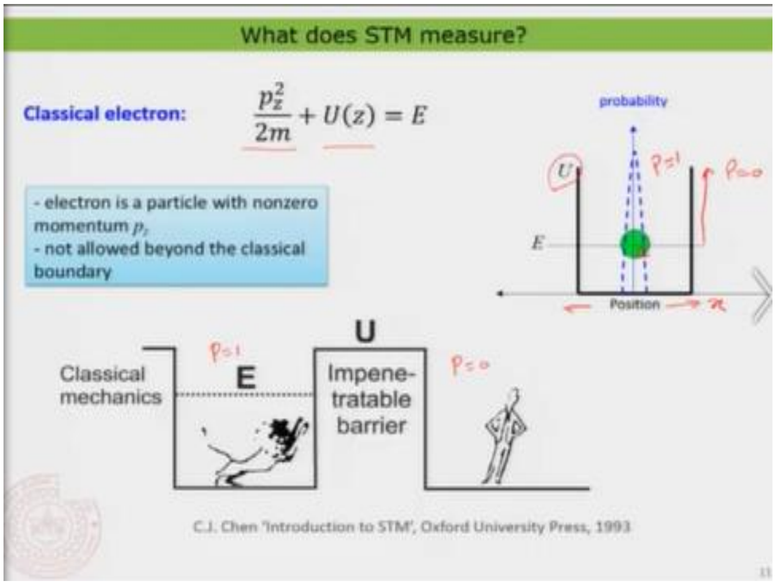

What does STM measure?

Classical electron: $\frac{p_z^2}{2m} + U(z) = E$

- electron is a particle with nonzero momentum p_z
- not allowed beyond the classical boundary

C.J. Chen 'Introduction to STM', Oxford University Press, 1993

So, of course a classical electron is represented by this energy expression. So, it has basically the kinetic energy and the potential energy and that defines the total energy of the electron and now if you define a space that is actually something known as a potential energy well or potential energy barrier having a certain potential called U. So, this black box here is representing something like a one-dimensional potential well. Now imagine that is you are having your electron. So, this is your electron basically and that electron has a certain energy E. So, now this energy of electron is definitely much lower than the height of the potential barrier. So, you would imagine that the electron would basically get confined inside this potential well, because the energy of the electron is not sufficient enough that it actually can escape or else you need to basically supply additional energy to this electron. So, that it can basically just escape this height. But that is not something we are doing, so we are basically not exciting by any external agency. So, therefore we are basically assuming that the electron should remain at that place. But now the question that you ask is what is the probability that you can find this electron? Where is the probability that you can find the electron to be maximum? So, if you plot the probability as a function of position. So, this is the position and you can call it like x in this case, it is just a one dimensional a very simple case. Then you would find that the probability of finding the electron in the box is maximum, where that green dot is placed. So, that is very straight forward and that would means you would always find that the electron is basically there. So, that means the electron is nowhere else, this is what the classical electron meaning that because it is actually behaving as a particle, so that is the classical description. Now if that of course what we all experience in our daily life. So, when I say that the probability of finding me right now in this position is basically one because, you cannot find me anywhere else. So, that means if you have like a lion inside a cage, of course anybody standing outside the cage is very safe. Because you know definitely the probability of finding the lion inside the cage is 1 and outside is absolutely 0, so the probability here is 1 and the probability here is 0. So, that is always the classical definition, probability is 1 and here the probability is 0, so you are safe. That is how our life works in normal so called classical world, the probability of all classical objects are nicely definable by the position and also by the velocity for example. But now when it come to quantum mechanics, so when you come and give the real description of electron using quantum mechanics you would find that electron is not really defined as a particle.

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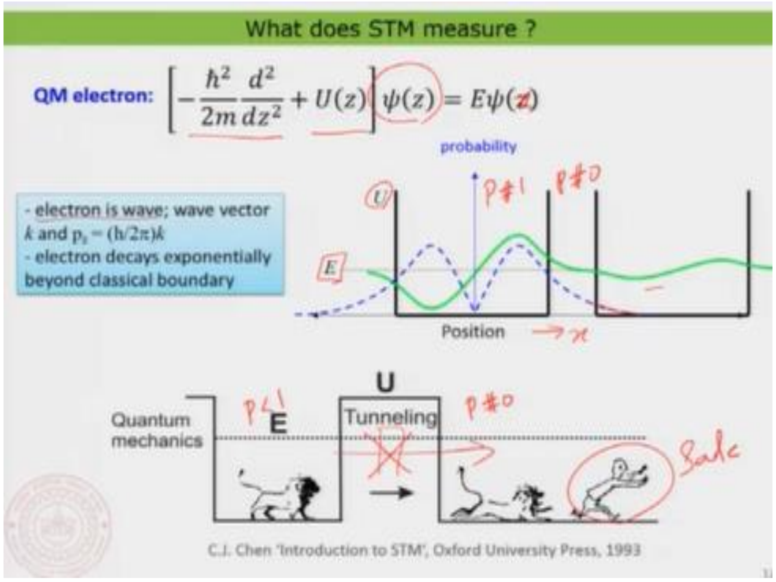

What does STM measure ?

QM electron: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+U(z)\right]\psi(z)=E\psi(z)$

- electron is wave; wave vector k and $p_z = (h/2\pi)k$
- electron decays exponentially beyond classical boundary

C.J. Chen 'Introduction to STM', Oxford University Press, 1993

It actually has different type of character; it actually also has something known as a wave nature. So, electron is also a wave and you know that from quantum mechanics that electron is actually a particle and a wave at the same time. So, that is also strange but this is actually the quantum mechanical description and to account for all the behaviour of electron you would need to consider the so called duality, the particle wave duality of electron. Therefore, we believe right now that the electron is basically just considered as a wave. Now you know that the energy the total energy of the electron itself is given by the Schrodinger equation, So, where you have actually the so called kinetic energy part, the potential energy part and the electron itself is actually defined using a wave function. In this case I have actually just used z as the axis for a very interesting reason, you will understand that why I have used it. But of course, normally you have also seen that it to be psi x, so it just that depending on what coordinate that you choose. But again, it is a one-dimensional box so here you have a one-dimensional box and the box has actually a height; the potential barrier, so that is the potential barrier. Basically, the height is U and again the electron is actually having just an energy which is lower than the potential barrier height. But now the interesting thing is that the electron wave function is not just actually been confined at this given space, if you look at the probability for example of this particular electron you have solved this problem in a one-dimensional box problem in quantum mechanics, that is actually one of the first topic in quantum mechanics where you have seen that, if the potential the height of the barrier is somewhat low, you would find that the probability. So, this is actually kind of an exaggerated drawing, so do not take it for granted that there is anything scaled here, there is absolutely a non scaled drawing. But when you look at the probability of this particular wave function that is representing the electron, you would find that the probability is not just 0 outside. It looks like the probability outside is not equal to just 0. So, there is actually a finite value for that and here the probability is not equal to 1. So, that means the electron that you placed or that you defined inside the box is not just there all the time or it is just not only present at that location, it is also present elsewhere. Now what is the consequence of it? This is quite interesting. Now when I say my probability is not equal to 1 right now here, that also means I am right now present also at a different location. So, using probability you can kind of play with it. But this is of course quite a strange and weird phenomenon for a classical object because you clearly see that I am standing here. So, that means the probability of finding me should be like 1. But that is not the case for an electron because if I place an electron right here, you cannot say that the probability of finding the electron is equal to 1 right here, it can actually be just less than one and it can be elsewhere a finite number. So, that is a reason why you would find that you need to do the normalization over minus infinity to plus infinity in order to get basically the normalization to be 1, then only you can define the entire probability of an electron for example. So, that is something you have also learnt in quantum mechanics. Now if I would have actually just brought another box next to it, you will see what is this box really is in our context. So, if you would bring another box, another potential well next to this box, then you see that I have a finite probability for this electron that is actually penetrating over the space which would definitely mean that the same electron is also present here. The energy of the electron is same because we say that this is basically kind of elastic tunnelling and then you see just the amplitude has decreased. So, the amplitude is always the measure of the amount in fact, so how much electron is there. So, that is what it looks like, so it is strange. Now you see that the same electron is present at a lower probability on other box and with a higher probability in this box, but the interesting thing is that the electron penetrated through the classically forbidden boundary. Now the life of the person who was standing outside the so called barrier is actually very bad. Because, now the quantum mechanical lion is actually acquiring certain probability to also be outside, so this person is not anymore safe. So, thanks to the classical world that we are all living in if it would have been a quantum mechanical world, you could have never visited a zoo or the life would have been quite different. So, this actually means that the probability inside is not equal to just 1, it is lower than 1, so I could just write it like that. So, the probability is basically just lower than 1 and here probability is actually not equal to 0, so that is the interesting aspect. So, which is in a general sense what I would like to describe here the quantum mechanical definition of the electron which is the true definition of electron because that applies to tiny quantum mechanical objects where you cannot confine electron in a given space. The electrons probability of finding in a larger space is what is much more interesting to notice. So, that means you cannot just have the electron placed at a given position, you will have a probability to find it elsewhere. Therefore, you would find that the electron can in fact penetrate the classically forbidden barrier. So, this is basically the classically forbidden barrier but now you can see that the electrons can basically tunnel through the barrier and it can actually come out of the barrier, so that is the interesting aspect. So, now using quantum mechanics you can basically explain the quantum mechanical phenomena itself. So, that means finally if you have a surface which is a metallic surface and now I have basically a tip that is also metallic tip. Now I know that there are electrons in the tip, there are electrons in the surface. But now when I bring them in a close proximity even when they are not touching the electrons would basically start to flow from one electrode to the other electrode if you apply an external bias. That is the interesting thing. Now let us bring this into the context of our microscope. So, that is actually the scanning tunnelling microscope and will try to understand how the whole thing works.

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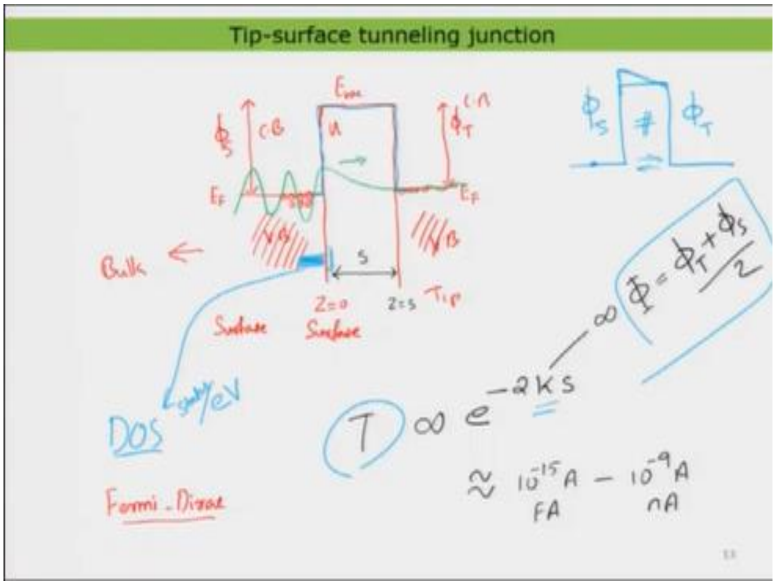

Tip-surface tunneling junction

So, for that, I need to now take one metal, so that is actually going to be my sample. So, let us take my sample or that is the surface. So, this is basically something I am defining at Z is equal to 0 that is representing that this is the surface of the sample. So, this side is actually the bulk of the sample and this is basically the surface of the sample that I am working with. Now I have put a line here this line is nothing but the Fermi level of the metal that I have taken. And here I have the valence band that is basically kind of filled band and then here I have the conduction band that is actually the unfilled band. So, I am right now taking a metal as the example. So, in the case of metal I have the valence band and the conduction band and they are basically overlapping and therefore you would find that the Fermi energy is actually at the right edge between the conduction band and the valence band. Now Fermi level you might have studied it in solid state physics, Fermi level is basically defining the last occupation of electron but that is defined at 0 Kelvin. That is very important because at higher temperature you would find that electrons can exist in the conduction band which is actually controlled by the Fermi Dirac statistics. So, that is basically controls the population of electrons in the conduction band and valence band. And that according to that you would find that at room temperature, for example the conduction band is not just completely empty. So, you would find a certain occupation of electrons in the conduction band, a certain occupation of the holes which is just the opposite of electrons would be in the valence band. Well that I am not taking into account right now. So, that is actually something that you have to keep it in mind in the future. But right now, we are taking actually a situation where we have a very low temperature assume and then I have the Fermi energy to be defined like that. Now for a metal there is also something interesting, you can actually just know it is actually called as the work function, so like work function of my tip so I am just calling it as psi T, so that is a work function of the tip. And the work function is actually the energy that you require to remove the electron from the surface. So, you might have studied it in photoelectric effect and things like that. So, because of this work function you know that at room temperature you cannot get electron simply out of the surface and that work function itself would act as a barrier. You see this is some kind of a potential U that is defined, so that is the height of the Fermi level to the vacuum level. So, this level is something that I am defining as E vacuum level and that is the distance which is nothing but the work function. So, because you have a work function you cannot basically just remove electron just like that at normal temperature. So, you need to have really heat the material in order to remove the electron. So, that is the so, called barrier for the electrons, now come out of the sample. Now I need the tip, so this is basically my surface let us say surface or the sample itself. Now I am going to take for the convenience of discussion I am just going to take the same material and bringing them together. So, now I am bringing another piece of electrode, so that is again the tip here in this case. And this is the Fermi energy and this is again the vacuum level of your tip because I have chosen the same material. So, I can again define that this work function has to be psi S and this is psi T. So, since they are same material for the convenience that we are doing you can see that the psi S and psi T are same. And now you see that I have created some kind of a barrier for the electrons that are present here or the electrons are present here. Because I know that in the vacuum, in the valence band there are lot of electrons and now this electron want to basically escape but you cannot just escape because there is actually a barrier. Similarly, I also have electrons that are present here, this is again the valence band and the conduction band and they are also present. But they are actually unable to move across but now we know that since electrons are nothing but the quantum mechanical particle which is defined by a wave function, we know that there is a certain probability existing for the electrons that is present in the surface to be present in tip and the electrons to be present in the tip to be also present in surface. So, if I would just depict a small wave function, just a sine wave that is representing the electron itself. Then I would basically just say a sine wave that is representing the electron here at a given energy is now going to decay out of this and then they would basically be just presenting inside this. The same thing also happens in the other direction because this is only that I have represented a tip, an electron which has actually just tunnelled to this direction, but the electrons on this direction can also tunnel back to this direction. So, that is always present when you bring them closer. Therefore, this distance between the tip and the sample, this distance let us call it as S for example for our convenience at z is equal to S, so that is the distance, that S is quite important. Because you would find that the so, called tunnelling probability, the tunnelling probability basically defines the effectiveness of the tunnelling ideally. So, that is dependent on something e raised to 2KS, you will see the details later so the tunnelling probability is kind of proportional to K and S, where S is nothing but the distance and K is actually something known as a decay constant which is strongly related to the energy of the electron and the barrier height. So, now you see that the tunnelling probability itself is an exponential function which is strongly dependent on the distance and the so, called barrier height.

So, this is directly proportional to the barrier height so that is actually something which we have noted down here. So, in this case an average barrier height that is actually nothing but psi T + psi S by 2. So, in this case it is basically the same because we have taken the same material. So, now you see that the tunnelling probability is what is defining how much electron would basically tunnel from one electrode to the other and from this electrode to this one which is defined by the distance. So, that is the reason why we need to have the tip to be in the very close proximity of the surface. Otherwise, you would not be able to basically just get the tunnelling done. So, that means if you increase the distance to more than 10 nanometre or something like that the tunnelling current itself, because tunnelling probability defines the tunnelling current itself, the tunnelling probability is going to be extremely small. And then we will not be able to detect the tunnelling current. Because a typical tunnelling current is in the order of about 10 raised to minus 15 Ampere to in the order of 10 raised to minus 9 Ampere. So, you see this is basically some kind of a femtoampere to nanoampere basically. So, this is extremely tiny, so the femtoampere itself is very difficult to measure but at very stable conditions using very high modern electronics you can basically measure that. But normally the workable thing is actually in the order of picoampere and nanoampere, so therefore the strong dependence of distances is quite an important thing to consider inside. Now so, this is basically our context, so now you see directly that we have created a barrier. So, this is something to sketch again so that we have created now a barrier, so this is something that we call it a barrier, so this looks almost like what you have seen in the previous case. So, the barrier we have defined, so now you have electrons here and that the electrons want to basically move in this direction or to move in this direction. So, this is the thing and the barrier height is actually defined by the work function of the material itself. Now if you would have taken basically a material that is not really the same. So, then what you would have ended up is basically that having a kind of slightly trapezoidal type of barrier. So, where you have the psi S and the psi T are not equal, they are not equal, so then you would have actually just ended up in a trapezoidal type of barrier but nonetheless you can use this kind of average value for plugging inside the K and then you can still work out the solution. So, that is what it is. So, we need the transmission probability or the tunnelling probability so both names are used, so for calculating the current. And there is one more important thing that you need to also just understand at this point which is actually known as the density of state. The density of state is also defined by the number of levels that are available in a given energy. Well, you know that the valence band and conduction band although you call it band if you zoom inside, you would find that they are actually just discrete levels but of course you do not distinguish them that their energies are so so small that you cannot really distinguish them. So, but therefore, there is actually a term that is normally used in solid state for defining the number of available levels the electronic levels that are present in the band which is actually known as the density of state. So, this is actually known as the density of state, normally you can just written it in with respect to energy. So, this is actually number of states per ev, ev is actually the unit of energy for example you can define the number of states. So, in this given context of course I have shown a constant density of state and that is the reason why you see that everything is looking like flat but if the density of state is basically varying as a function of energy. This is the electronic energy basically, then you would find that it is not anymore going to look flat. So, we will actually just work out that solution in the next slides and then we would basically just understand it carefully. So, therefore what I want to do here in this slide is that you wanted to show you basically that what is the origin of the real barrier? In our case which is actually the tip and the surface. This is actually coming due to the fact that we are actually just working with material which are having a defined work functions and that work functions are giving rise to this kind of barrier and once you have the barrier then the electrons are actually just stopped in just transferring to the next, they need to actually undergo something called a tunnelling phenomena. Now there is also something finally one to talk about is that, right now the situation that you are looking is actually without having applied any bias voltage and that is the reason why you see that the Fermi levels of these two materials are basically aligned. But now you will see in the next class that we will basically start to apply the bias and then the Fermi energies will start to change and then the electrons will start to really flow. When you have no bias applied between the sample and the tip, then what happens is basically that electrons are still tunnelling from left to right and right to left but they are actually in equilibrium, so there is no net current or there is no net electron that is actually going along one direction. So, you need to have something like a flow of electron along one direction so that you can basically detect the current. But right now, what happens is basically that there is equilibrium because there is no potential applied to it. So, we will look into that in the next class in greater detail and we will basically measure the tunnelling current and you will find that the tunnelling current is an important parameter, an important measure that we can use for understanding the electronic structure of the material itself.

With this I would like to conclude this lecture and I see you in the next class. Thank you very much.