STM: Theory and research applications

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Abstract: In this work, we will describe the quantum tunneling effect and the operating principles of Scanning Tunneling Microscopy (STM). We will also define which components constitute an STM and which applications had in research, and how it is used today, far from its first uses. The last part will focus on the description of the process of repairing an old STM of the UB Physics Faculty.

I. INTRODUCTION

In the winter of 1900, during a meeting of the German Society of Physics, Max Planck exposed a work titled "On the law of distribution of energy in the normal spectrum". Although at the first time it did not get the attention of the attendance, it was the beginning of a new branch in science: Quantum Physics. Almost twenty-five years later, a new set of physicists, like Schrödinger and others, started to develop the new science that will come out of this first conference and began to break some of the old ideas that had ruled different fields of physics.

Tunneling is one of the most shocking consequences of quantum physics and one of the biggest evidences that the "quantum world" does not behave like the classical one. This phenomenon is not only interesting for its own sake, also provides many sensitive probes of bulk and surface characteristics of solids, such as the field electron and ion microscopes [1]. One of the most interesting applications is the STM (Scanning Tunneling Microscopy), a very useful engine for the research. The STM has been used to provide a detailed view of the atomic structure of surfaces. In the past, it has allowed scientists to see how the atoms are structured into many materials. It has also been applied to observe the distribution of complex systems and to move atoms as well, tailoring nanosystems at will. Nowadays, the use of the STM is not only restricted to observe conductive materials: it has widened its possibilities, being used to observe scanning tunneling spectroscopies or to study biological systems.

II. THEORY OF TUNNELING AND THE APPLICATION TO STM

A. The potential barrier

Let us consider a potential barrier that follows the equation

$$V(x) = \begin{cases} V_0 & 0 < x < a \\ 0 & x < 0 \ o\ x > a \end{cases} \qquad (1)$$

This potential can be made, for example, by two electrodes separated by some short length which remain at different voltages [1].

According to classical mechanics, a particle which comes into the $0 < x < a$ region with an energy such that $E < V_o$ will have a probability equal to one to be reflected and zero to be transmitted. On the other hand, if the energy verifies $E > V_0$ the probabilities to be reflected and transmitted will be respectively zero and one.

However, none of these cases appears in Quantum Mechanics. If E is larger than V_0, the theory predicts there will be some reflection except for some values of E. If E is less than V_0 there is some probability that the particle will be transmitted through the barrier. Although we are working with particles, we should bear in mind that tunneling is not so much a quantum phenomenon as a characteristic of waves [2]. We have tunneling phenomena associated with classical electromagnetic waves and sound as well.

If we solve the time-independent Schrödinger equation for our regions, we can obtain the wave functions of the particles in the regions where we have the potential barrier and the regions where the particles are free. The general form will be

$$\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x} \qquad x < 0 \qquad (2)$$
$$\psi_I(x) = Ce^{ik_I x} + De^{-ik_I x} \qquad x > a$$

where

$$k_I = \frac{\sqrt{2mE}}{\hbar} \qquad (3)$$

for the free region, without potential affecting the energy, and

$$\psi_{II}(x) = Fe^{-k_{II} x} + Ge^{k_{II} x} \qquad (4)$$

where

$$k_{II} = \frac{\sqrt{2m(E - V_0)}}{\hbar} \qquad (5)$$

for the region with potential.

Since we are considering the case where a particle hits from the left to the barrier, there will be no wave coming from the right on it. Then we must suppose $D = 0$.

If we couple the expressions of $\psi(x)$ and $\frac{d\psi(x)}{dx}$ in regions I and II at the points $x = 0$ and $x = a$, we will obtain the values of *B*, *C*, *F*, and *G* in terms of *A*. From here, one can calculate the density of probability $\Psi^*\Psi$ and the *Probability Current:*

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$$\vec{j} = \frac{\hbar}{2mi}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) \qquad (6)$$

The most interesting result is the reason of the transmitted current trough the incident one. This is called *Transmission Coefficient T*, and gives us an idea of what is the probability of tunneling of our system, for a certain energy value:

$$T = \frac{|\vec{J}_{trans}|}{|\vec{J}_{inc}|} = \frac{C^*C}{A^*A} = \left[1 + \frac{sinh^2 k_{II} a}{4\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} \qquad (7)$$

B. STM: Hardware and theory

The Scanning Tunneling Microscopy (STM) was invented by Binning and Rohrer and implemented by Binning, Rohrer, Gerber and Weibel in the decade of 1980's in the IBM Zurich Laboratory. This discovery allowed them to win the Nobel prize in 1986 [3].

The development of tunneling microscopy was anticipated by a similar device, the *topografiner*, developed by Russell Young, Clayton Teague, and collaborators at the National Bureau of Standards ten years before the development of the STM. The images were made registering the output of a channeltron electron multiplier pointed at some surface. After this, researchers found more useful to plot the output of this and other devices while they scan the surface of the sample with a tip, plotting the different obtained currents as a function of the position [4]. This is how the STM was finally achieved (See Fig. 1).

An STM reveals three-dimensional pictures of surfaces and even individual atoms using the theory of tunneling seen above. The central part consists in a tip brought close enough to the surface that, at a convenient operating voltage applied between the tip and the surface, the tunneling current is measurable.

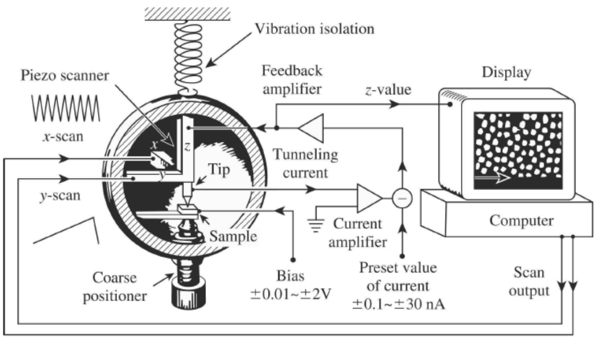

FIG.1: A picture of the different parts that constitute an STM [5].

The tip is scanned over the surface while the tunneling current *I* is sensed. A feedback network with the computer let us work in two modes of operation (see Fig. 2):

· Keeping the current constant and changing the height *z* of the tip. In this mode, and image consists of a map *z(x,y)* of the tip height *z* versus lateral position *x,y*. This is made plotting different multiple images of *z* versus *x* displacing laterally from each other in the direction *y* (Fig.2 Left). This is the most common mode of operation.

· Changing the current and keeping the height and the voltage constant (Fig.2 Right).

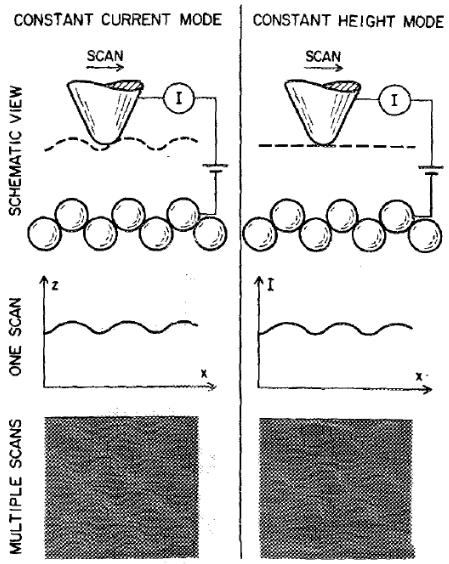

FIG. 2: Illustration of the different modes of operation [3].

But how does the above theory apply to STM?

Let us imagine the simplest 1-dimensional case where only elastic tunneling occurs between two (metallic) electrodes with semi-infinite potential wells with depth $E_F + \phi$, where E_F is the *Fermi Level* and ϕ is the *Work Function* (see Fig. 3).

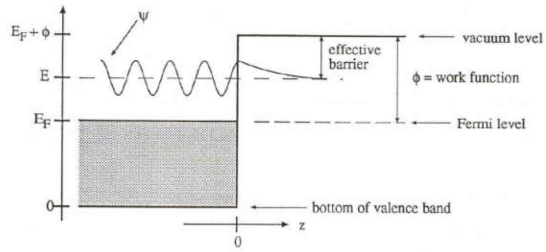

FIG. 3: Illustration of the potential barrier for a conductor material [6].

From here, our potential will be:

$$V(z) = \begin{cases} 0 & z < 0 \\ E_F + \phi & z > 0 \end{cases} \qquad (8)$$

We will put this into the Schrödinger equation as seen above. After some calculations [2], we can express the current as given by the overlap between the wave functions of the tip and sample weighted by the corresponding density of states. If we assume we are working with real samples and a sharper tip, one can approximate the expression of the current as

$$I(\vec{r}, V) \sim \int_0^{eV} \varrho_T(\vec{r}, E)\varrho_S(\vec{r}, E - eV)e^{-2k(E)}dE \qquad (9)$$

where ϱ_T and ϱ_S represent the densities of states of the tip and the sample, respectively V is the applied voltage and $\vec{r}$ is the position. The factor *k(E)* is:

and $\bar{\phi}$ is the average barrier height that the electrons experience

$$\bar{\phi} = \frac{\phi_T + \phi_s}{2} + \frac{eV}{2} - E \qquad (10)$$

As we can see above, the current depends on the applied potential, the height of the tip with respect to the sample (position) and the density of states. Tersoff and Hamann showed that this dependence is correct and can be extended to a tip of arbitrary size [4]. Since these parameters are very sensitive to external perturbations (oscillations of the tip, atoms of the environment…) is common to work with a *vibration isolator* and do the measurements inside a *vacuum chamber.*

When the use of STM started to grow, it became clear the need of a more accurate theory to express the measured current. Although this is a first good approximation, it is not strictly correct since the process of tunneling involves a lot of different phenomena such as resonant tunneling, Inelastic tunneling, Zener breakdown or internal field emission, the form of the tip causing more than the simple one-dimensional tunneling.

All these factors make harder the development of a correct expression for the current. Still is a topic of discussion how we can construct a correct expression of the measured current into an STM. There are currently three broad classes of tunneling theories [2]:

(i) Methods that use separable, single particle modes which are solved exactly or treated by semi classical methods like WKB-type approximations.

(ii) Transfer Hamiltonian type theories. These are not necessarily restricted to one dimension and can accommodate many body effects.

(iii) More complete many body theories based on Keldysh's infinite-order perturbation theory for non-equilibrium processes. These theories involve complex Green functions and the transfer matrix to do the calculus. Since they take into account all the processes that happen during the scanning, they can not be solved analytically.

These theories, with the proper approximations, will give us an expression similar to equation 9, with the same dependences and exponential decay of the current with the distance.

As time went by, researches also saw how the form of the tip affects the results, and started to discuss how the density of the tip affects the current. Kuk and Silverman approached this problem in 1986 [7], showing that if we operate the tip as a field ion microscope, it gives us direct images of the tip's atomic structure, using the sample instead of a gas to ionize the atom. The field ion microscope (FIM) had been designed by Muller in 1951- This way, they constructed the first STM incorporating a field ion microscope [2].

$$k(E) = \sqrt{\frac{2m\bar{\phi}}{\hbar^2}} \qquad (11)$$

III. APPLICATIONS IN RESEARCH

After the development of the STM, the first investigations focused on characterizing the topology of different solids and detailing the atomic structure of surfaces. This let the researchers know how are the lattices of atoms in materials and from this, calculate different properties such as conductivity and heat transfer, which are useful in the fabrication of electronic components. Also, it allowed to observe how absorbed atoms are filled into materials and how they affect their properties (see fig. 4).

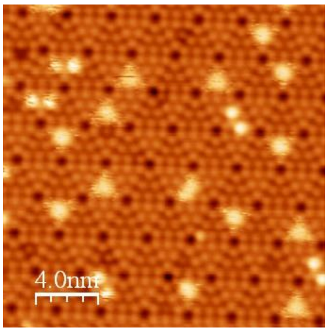

FIG. 4: A picture of Si 7x7 obtained in the past by the old STM of the UB Physics Faculty.

Through the years, its possibilities began to expand, till the point they started to measure biological systems as well, such as DNA [8]. One of the biggest steps in the applications of the STM was made by Don Eigler in 1989, from IBM Research, when he moved single atoms of Xenon into a surface of nickel using the tip to construct the letters "IBM". This opened the gates to create a new whole set of applications and phenomena, such as *quantum corrals*, *molecule cascades*, and *atomic memories*.

But what is the actual use of the STM nowadays, apart from those seen above? To answer this question, we had the chance to visit one of the research groups of IBEC (Institute of Bioengineering of Catalonia), whom are working with an STM in a very uncommon way: *The Electrochemistry STM (ESTM).*

The tunneling effect, although we may think is not currently happening in nature, can be found in the transfer of information between molecules using the electron transfer (ET). The ET is present in a lot of biological processes such as cellular respiration, photosynthesis and the major part of the enzyme-catalyzed reactions [9].

In 2012, Juan Manuel Artés described by using an ESTM how the cytochromes and azurin proteins generate the ATP using electron transfer. The current in biological systems is described by the Marcus theory, which is a semi-classical theory that determines the rate for a non-adiabatic ET process between an electron donor (A) and an acceptor (B) at a fixed distance [9].

We followed the actual investigation of the "Nanoprobes and nanoswitches" research team. In this case, they are studying the electron transfer of *Photosynthetic Complex I* which is responsible for the process of photosynthesis in plants (see Fig. 5). The way to work with the ESTM is to immerse the proteins into *Phosphate Buffer Saline 50mM*, an electrochemical fluid that simulates the medium where these proteins are usually found. To reduce the effects of the tip interacting with the electrochemical fluid, they cover the tip with *Apiezon Wax* solution to isolate it the more as possible only exposing the top of the tip [10]. This way, they try to have only elastic tunneling involved in the process of measure.

The sample material is Au (111) substrate, to apply the difference of voltage. Onto it, is where we have the electrochemical fluid and the proteins. In this case, they are not working in vacuum since it will kill the proteins, so they must keep in mind the noise produced by air during the registering.

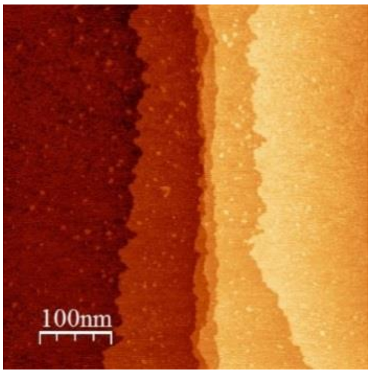

FIG. 5: Image provided by "Nanoprobes and nanoswitches" research team where we can appreciate the current of the proteins, represented as dots, and the surface of the Au sample. IBEC, 2017.

IV. FIXING AN OLD STM

The original purpose of this work was to set an old STM back to work. The operation of the equipment had been the subject of a demonstration lab experiment in the Laboratory of Modern Physics course (Physics degree) some years ago, and it had been out of work since then.

Thus, when we approached the equipment, we found it had been disassembled, since some components had to be fixed by the company, Nanotec, which had made the STM years ago. This gave us the opportunity to see the parts of the system separately.

A. The components

Here is a brief list of the parts:

· **The main base:** this is the support where we will fix and connect the two principal parts, the piezoelectric and the tip.

· **The piezoelectric:** The base where we will put the sample that we want to observe. The piezoelectric will have the feedback with the computer to send the information required depending on which kind of operation mode we are working with as well.

There are two different sets of cables. The first set, a colorful one, is to send the potential that we want to apply between the tip and the sample and, at the same time, to register the tunneling current that is created during the process of registration. The other set, the yellow one, is responsible to send the information to the motor to approach/withdraw the tip with respect to the sample.

· **The head of the amplifier and the tip:** Into this box we have the circuit that lets us choose the potential that we want to administrate and the amplifying circuit.

· **Control Panel:** Is the bridge between the engine and the computer. It allows us to control the height of the sample "by hand" and also to compute all data that come from or go to the STM.

Our control panel is called Dulcinea Electronics. There one can find a Control Unit made of a Graphic Display, the adjustable controls to move the tip manually and the connectors for monitoring all the process.

B. The description of the reparation

The first step consisted in assembling all the components described above. One of the interesting points was the fact that we had to hang up all the system to isolate it from vibrations. When we had done this, we proceeded to obtain a signal from the sample.

Here we encountered the first problems. Although, apparently, everything was well connected and the communication of the engine with the computer was good, when we tried to make the approach, the system did not behave as we expected. Registering a current-voltage characteristic (*IV* curve) we could observe that the behavior of the amplifier did not correspond to what we should see in this case: we expect the amplifier mill have a linear behavior up to the Bias potential, where the signal must saturate, indicating that the circuit imposes a limitation on the measured current. Instead of this, we obtained a non-linear behavior and a more chaotic respond.

Facing this situation, we had to decided what option should we follow in order to carry on with the work:

- Contact the manufacturing company, Nanotec, to clarify whether the *IV* curve corresponded to the one typically expected.
- Ask the UB Electronic Workshop to examine the head circuit in order to check out if it did operate properly.
- Try to reproduce ourselves the amplifier circuit.

We decided to follow a combination of these three paths. So, for the first option, we contacted one of the Nanotec engineers and asked him what could be the origin of our problem. He quickly told us that probably the issue was in the amplifier circuit. We decided to send the circuit to the Electronic Workshop, to see if they could repair it.

Meanwhile, we tried to reconstruct the internal circuit ourselves. One of the issues that we found during this process was that one of the integrated circuits (a component), the OPA129, is no longer currently built, so we had to find an alternative component with the same properties or try to find the way to reproduce it. After finding the way to replace the old component, we prepared the rest of the set and designed the new circuit, with the help of an Electronics Engineer, just in case the Electronic Workshop could not fix it. Fortunately, this was not the case and the head circuit was repaired on time. When we plotted the *IV* response, we observed a well-behaved graphic, one in which, for a chosen bias, the response was linear within the range limited by the control panel.

But we still had problems with the approach because the computer did not detect well the tip. After examining the base components, we concluded that the problem could be in the piezoelectric or the set of cables that register the tunneling current and communicate with the computer. We examined the cost of a new piezoelectric and, since they are too expensive and we did not have time enough to wait to receive a new piezoelectric to start the measurements, we decided to postpone the reparation of this STM and get back at it again in the future.

V. CONCLUSIONS

We have studied the basic concepts of STM and we have seen some of its applications in the world of research. Although more than 30 years have elapsed since it was invented, it is still a powerful tool and it is surprising the new ways that this engine, which started just scanning the surface of metals, is following into the research and how the evidence of its utility allows us to link different branches of science with a quantum phenomenon, the tunneling effect. We also have had the opportunity to see how searches work with it nowadays and to manipulate an STM and learn more about it during the set-up process.

Acknowledgments

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“Where words fail, music speaks” – Hans Christian Andersen

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