Quantum Tunneling Effect in Scanning Tunneling Microscope

晏浩洋

junior student

School of Physical Science and Technology

Shanghaitech University

(Collaborated with 黄淳　陆逸明)

Adviser: 韩福祥*

professor

School of Physical Science and Technology

Shanghaitech University

(Dated: 2019 年 12 月 13 日)

Usage:

abstract: In this article, the author derivates the transmission coefficients of two directions T_1 T_2 from Voltage between the tip and the surface U, Energy of free electrons E, Energy of potential barrier V_0 and width of potential barrier a with Quantum Mechanics. Then the author derivates the relation between the electric current I and the transmission coefficients of two directions T_1 T_2. In conclusion, with giving Voltage between the tip and the surface U (can be modulated by control system), Energy of free electrons E (determinated by material and temperature of the tip(usual Wolfram) and the observed surface(can only be conductor or semiconductor)), Energy of potential barrier V_0 (determinated by material and temperature of the medium(usual vacuum, but can aslo be air and various other liquids or gases) between the tip and the surface)，the relation between the current I and the width of potential barrier a(equal to the distance between the tip and the surface) can be derivated. Then the precision of STM can be estimated.

keyword: Quantum Tunneling Effect　Scanning Tunneling Microscope　Potential Barrier　Coefficient of Tunneling

I. MEANING OF SYMBOLS

meaning of symbols in this article

V　potential

U　voltage between tip and surface

E_1　energy of free electrons on the tip

E_2　energy of free electrons on the surface

V_0　energy of potential barrier

a　width of potential barrier(distance between tip and surface)

e　electric charge of an electron

m　mass of an electron

φ_i　wave function in interval i

J_I　density of probability flow of incidence wave from tip

J_T　density of probability flow of transmission wave to surface

T_1　transmission coefficient(probability of an electron flowing through) from tip to surface

T_2　transmission coefficient(probability of an electron flowing through) from surface to tip

I　tunneling electric current from tip to surface

* http://spst.shanghaitech.edu.cn/2018/0519/c4986a27061/page.htm

II. PROCEDURE OF STM

Scanning Tunneling Microscope, abbreviated in STM, is a kind of Nonoptical Microscope based on Quantum Tunneling Effect. When a metal tip is brought very close to a metal or semiconducting surface, a voltage U between the tip and the surface makes the probability of electrons flowing through the potential barrier between the tip and the surface, which called the coefficient of tunneling, of two directions T_1 T_2 different. This difference produce a tunneling electric current I from the higher electric potential side to the lower electric potential side.
From measuring the tunneling electric current I, the system can derivate the distance between tip and surface a. After the tip slowly moving and covering the whole X-Y plane surface, all the fluctuation $z(x, y)$ on the surface(which mean the value of Z direction) can be derivated with the height h of the tip substracting the distance between tip and surface a. With the fluctuation $z(x, y)$, the image of the surface can be drawn by the system.
There are two operating modes of STM:

A. Two Modes of STM

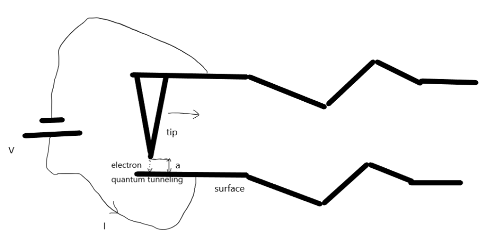

图 1. constant current mode

Constant current mode means the tip always moving parallel with the surace, which means the distance between tip and surface a and the tunneling electric current I are constant. Resolution of this mode is better because the system need not estimate the distance by a group of value of current ranging from various orders of magnitudes(considering the huge effect on current by little change of distance, this becomes possible). However, this mode operates slower because the tip should move very carefully to keep the distance constant.
Constant height mode means the tip always moving

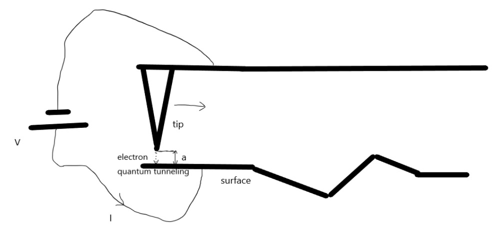

图 2. constant height mode

with constant height. Therefore, the distance between tip and surface a and the tunneling electric current I are always changing.

B. Why Voltage

Without the voltage, electron still have the probability of flowing through a potential barrier to the other side. However, in this situation, the tip and the surface are jointed with lead so they are equipotential, which means the probabilities of electron tunneling from tip to surface T_1 and from surface to tip T_2 are equal, and we cannot observe a macroscopic current.
With a bias voltage added(in this article we chose the tip jointing to cathode and the surface jointing to anode, which means electron on the tip have higher potential energy), the transmission coefficients from tip to surface T_1 is larger than from surface to tip T_2, and a current from anode to cathode can be measured.

III. SOLVE THE SCHRODINGER EQUATION OF TUNNELING

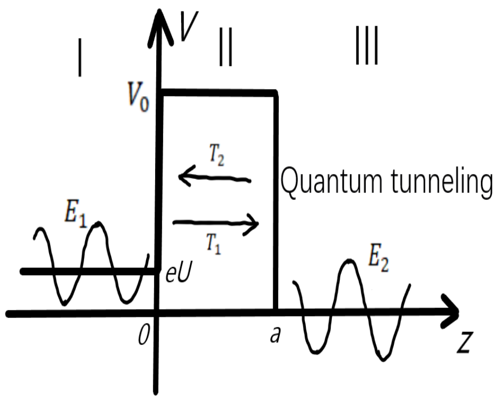

图 3. Potential of Quantum Tunneling in STM

Stationary Schrodinger Equation in one dimension:

$$\frac{\hbar^2}{2m}\frac{d^2\varphi(z)}{dz^2} = [(V(z) - E_1)]\varphi(z) \tag{1}$$

With the giving potential function:

$$V(z) = eU \qquad (z < 0) \tag{2a}$$
$$V(z) = V_0 \qquad (0 < z < a) \tag{2b}$$
$$V(z) = 0 \qquad (z > a) \tag{2c}$$

Because the medium between tip and surface is always insulate, we can consider $V_0 >> E > eU$
Introduce:

$$k_1 = \sqrt{\frac{2m(E_1 - eU)}{\hbar^2}} \tag{3a}$$
$$k_2 = \sqrt{\frac{2m(V_0 - E_1)}{\hbar^2}} \tag{3b}$$
$$k_3 = \sqrt{\frac{2mE_1}{\hbar^2}} \tag{3c}$$

Then we can derivate Schrodinger Equation in 3 intervals:

$$\frac{d^2\varphi_1(z)}{dz^2} + k_1^2\varphi_1(z) = 0 \tag{4a}$$
$$\frac{d^2\varphi_2(z)}{dz^2} - k_2^2\varphi_2(z) = 0 \tag{4b}$$
$$\frac{d^2\varphi_3(z)}{dz^2} + k_3^2\varphi_3(z) = 0 \tag{4c}$$

General solutions to fuctions above are:

$$\varphi_1(z) = Ae^{ik_1z} + Be^{-ik_1z} \tag{5a}$$
$$\varphi_2(z) = Ce^{k_2z} + De^{-k_2z} \tag{5b}$$
$$\varphi_3(z) = Fe^{ik_3z} \tag{5c}$$

Considering the mathching smooth boundary condition at $z = 0$ and $z = a$:

$$\varphi_1(0) = \varphi_2(0) \tag{6a}$$
$$\varphi_1'(0) = \varphi_2'(0) \tag{6b}$$
$$\varphi_2(a) = \varphi_3(a) \tag{6c}$$
$$\varphi_2'(a) = \varphi_3'(a) \tag{6d}$$

Substitute these boundary condition into Eq.(5):

$$A + B = C + D \tag{7a}$$
$$ik_1A - ik_1B = k_2C - k_2D \tag{7b}$$
$$e^{k_2a}C + e^{-k_2a}D = e^{ik_3a}F \tag{7c}$$
$$k_2e^{k_2a}C - k_2e^{-k_2a}D = ik_3e^{ik_3a}F \tag{7d}$$

Rewrite Eq.(7) in matrics way:

$$\begin{bmatrix} 1 & 1 & -1 & -1 & 0 \\ ik_1 & -ik_1 & -k_2 & k_2 & 0 \\ 0 & 0 & e^{k_2a} & e^{-k_2a} & -e^{ik_3a} \\ 0 & 0 & k_2e^{k_2a} & -k_2e^{-k_2a} & -ik_3e^{ik_3a} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \\ F \end{bmatrix} = 0 \tag{8}$$

Solve this equation we get:

$$F = \frac{4ik_1k_2}{e^{ik_3a}[(ik_1 - k_2)(k_2 - ik_3)e^{k_2a} + (ik_1 + k_2)(k_2 + ik_3)e^{-k_2a}]}A \tag{9}$$

IV. DERIVATE THE TRANSMISSION COEFFICIENT

Caculate the density of probability flow of incidence wave $\varphi_I = Ae^{ik_1z}$from the tip J_I and the density of probability flow of transmission wave $\varphi_T = Fe^{ik_3z}$ to the surface J_T:

$$J_I = \frac{i\hbar}{2m}(\varphi_I\frac{d\varphi_I^*}{dz} - \varphi_I^*\frac{d\varphi_I}{dz}) = \frac{\hbar k_1}{m}|A|^2 \tag{10a}$$
$$J_T = \frac{i\hbar}{2m}(\varphi_T\frac{d\varphi_T^*}{dz} - \varphi_T^*\frac{d\varphi_T}{dz}) = \frac{\hbar k_3}{m}|F|^2 \tag{10b}$$

Then we can derivate the transmission coefficient from tip T_1:

$$T_1 = \frac{J_T}{J_I} = \frac{k_3}{k_1}\frac{|F|^2}{|A|^2} \tag{11}$$

Substitute Eq.(9) into the above equation:

$$T_1 = \frac{k_3}{k_1}\{\frac{4ik_1k_2}{e^{ik_3a}[(ik_1-k_2)(k_2-ik_3)e^{k_2a}+(ik_1+k_2)(k_2+ik_3)e^{-k_2a}]}\}^2 \tag{12}$$

$$= \frac{4k_1k_2^2k_3}{k_2^2(k_1+k_3)^2+(k_1^2+k_2^2)(k_2^2+k_3^2)sinh^2(k_2a)} \tag{13}$$

Because

$$sinh^2(k_2a) = (\frac{e^{k_2a}-e^{-k_2a}}{2})^2 \approx \frac{1}{4}e^{2k_2a} \tag{14}$$

$$T_1 \approx \frac{16k_1k_2^2k_3}{k_2^2(k_1+k_3)^2+(k_1^2+k_2^2)(k_2^2+k_3^2)}e^{-2k_2a} \tag{15}$$

Consider the opposite direction.
All the things should be changed when caculating transmission coefficient from surface to tip T_2, is switching the opposite sides,which switching k_1 and k_3, and changing energy of free electron from E_1 to $E_2 = E_1 - eU$.

Using k_1', k_2', k_3' with E_1 changing to E_2 express T_2:

$$T_2 \approx \frac{16k_1'k_2'^2k_3'}{k_2'^2(k_1'+k_3')^2+(k_1'^2+k_2'^2)(k_2'^2+k_3'^2)}e^{-2k_2'a} \tag{16}$$

V. RELATION BETWEEN CURRENT AND WIDTH

$$I \propto T_1 - T_2 \tag{17}$$

Because the difference between E_1 and E_2 is not large, we can consider the left coefficient similar:

$$T_1 - T_2 \approx \frac{16k_1k_2^2k_3}{k_2^2(k_1+k_3)^2+(k_1^2+k_2^2)(k_2^2+k_3^2)}(e^{-2k_2a}-e^{-2k_2'a}) \tag{18}$$

$$I \propto e^{-2k_2a} - e^{-2k_2'a} \tag{19}$$

$$I \propto e^{-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}} - e^{-\frac{2a}{\hbar}\sqrt{2m(V_0-E+eU)}} \tag{20}$$

This relation points out that the diffrence between transmission coefficients $T_1 - T_2$ increse dramatically when a small width a decreasing little, showing that STM has very high pricision.

[1] C. Bai, *Scanning tunneling microscopy and its applications Springer Verlag* (New York, 1999).

[2] 王兆阳，王宏伟, Stm 中量子隧穿效应原子模型的计算机模拟, 沈阳航空航天大学学报 **31** (2014).