VQM

Visual Quantum Mechanics

SCANNING TUNNELING MICROSCOPE (STM) SIMULATOR

Windows 95™ Users' Guide

Kansas State University

©1997, Physics Education Research Group, Kansas State University. Visual Quantum Mechanics is supported by the National Science Foundation under grant ESI 945782. Opinions expressed are those of the authors and not necessarily of the Foundation.

TABLE OF CONTENTS

General Overview of the STM Simulator Program ____ *4*

Getting Started ____ *5*

What's in this Package? ____ **5**

System Requirements ____ **5**

Installation ____ **5**
Windows 95™ ____ 5

A Brief Tutorial ____ *6*

Step 1: Open a real STM Image ____ **6**

Step 2: Observe the Cross-Section of the Image ____ **7**
Choosing the Probe Tip Path ____ 7
Opening the Cross-Section Window ____ 8

Step 3: Observe the Potential Energy Diagram ____ **9**
Adjusting the Probe tip position ____ 9
Changing the Probe Tip Voltage ____ 9
Changing the Sample's Barrier ____ 9
Opening the Potential Energy Window ____ 9

Step 4: Observing the Wave Function for the Tunneling Electron ____ **11**
Changing the Electron's Energy ____ 11
Opening the Wave Function Window ____ 11

Step 5: Observing the Tunneling Current Profile ____ **13**
Opening the Current Profile Window ____ 13
Constant Elevation Mode ____ 13
Constant Current Mode ____ 14
Current Profile for Arbitrary Tip Path ____ 15

Step 6 (Optional): Observing the Tunneling Probability ____ **17**
Opening the Tunneling Probability Window ____ 17
Tunneling Probability Vs. Electron Energy at Constant Voltage ____ 18
Tunneling Probability Vs. Voltage at Constant Electron Energy ____ 18

Step 7 (Optional): Observing the Tunneling Current ____ **19**
Opening the Current-Voltage Window ____ 19

Menus, Buttons, & Spin Controls ____ *20*

Pull-down Menus ____ **20**
File ____ 20
View ____ 20
Help ____ 23

Buttons ____ **23**
Arbitrary Tip Path ____ 23
Horizontal Tip Path ____ 23
Parallel to Profile Tip Path ____ 23
Show Cross Section ____ 23
Show Potential Energy ____ 24

Show Wave Function 24
Show Current Profile 24
Show Tunneling Probability 24
Show Current-Voltage Graph 24
Apply 24

Spin Controls 25
Probe Tip Voltage 25
Sample Barrier 25
Electron Energy 25

How to… 26

Open an STM Image 26

Choose A Probe Tip Path on an STM Image 26

Observe the Cross-Section of an STM Image 26

Observe the Potential Energy Diagram 26

Observe the Wave Function 27

Observe the Current Profile … 27
In Constant Elevation Mode 27
In Constant Current Mode 27
For an Arbitrary Tip Path 28

Change the Probe-Tip Position 28

Change the Probe-Tip Voltage 28

Change the Sample Barrier Height 28

Change the Electron Energy 28

Observe the Present Tunneling Probability 28

Observe the Variation of Tunneling Probability 29

Observe the Present Value of Tunneling Current 29

Observe the Current-Voltage Graph 29

Pedagogical Applications 30

APPENDIX 32

General Overview of the STM Simulator Program

Learn the physics of a scanning tunneling microscope (STM) using the ***STM Simulator*** program. Begin with an image of a sample taken using a real STM, and move a hypothetical probe-tip across the surface, to determine the cross-sectional profile along any straight line. Place the probe-tip at varying heights above the surface and see the path taken by electrons that tunnel from the surface to the probe tip. See also, the potential energy diagram and wave function of the tunneling electron at various energies. View how the tunneling probability and current change for various tip positions and voltages, as well as for different samples.

Use the program to simulate the working of an STM in both the *Constant Elevation Mode*, where the tunneling current changes as the relief of the surface; as well as the *Constant Current Mode*, where the tip keeps adjusts its position to compensate for bumps and troughs in the surface, so as to maintain a constant current.

While this program cannot be used to get any real data about the sample, it is more of a visualization tool to learn how the STM works.

Getting Started

What's in this Package?

The User's Guide for the Windows™ for the ***STM Simulator*** contains instructional and reference material to install and run the program and associated files. For information on Windows™ and Windows95™, please see the appropriate user's guide.

System Requirements

The package is compatible with the Windows™ and Windows95™ platforms, and runs identically on both platforms.

The program requires a 486 PC (or upgrade) with the following features.

- Windows™ (Version 3.1 or above).
- 8 MB RAM.
- Hard drive with at least 3 MB of available space.
- CD ROM drive.
- 256 color monitor.

Installation

Windows 95™

To use ***STM Simulator*** or its demo, on a PC with **Windows 95™** follow the directions below.

1. Insert the 3¼" floppy disk into the appropriate disk drive.
   We assume drive A:
2. Click the **Start** button, which by default is usually at the bottom left corner of the screen.
3. Choose **Run…** from the pop-up menu. Type **A:\setup** and choose **OK**.
   The installation program will start, you will see some instruction screens and should follow the prompts.
4. When prompted, select the directory in which you want the program to be installed.
   *The program will install in **C:\vqm\stm** by default.*

The program and its demo are now installed, and its icon placed in a new folder called **Visual Quantum Mechanics**. Be sure to store the disk in a safe place.

To run ***STM Simulator*** and associated files, perform the following steps.

1. Click the **Start** button, which by default is usually at the bottom left corner of the screen.
2. Go to **Programs** in the pop-up menu and choose ***Visual Quantum Mechanics***.
3. Double click on the desired icon, that appears in the listing of the icons of the program and its demo alongside.

A Brief Tutorial

The steps taken by a typical user are described below. Steps 1 through 5 are taken by all users, while Steps 6 and 7 are optional, and could be used by more advanced users.

The Windows that you will use in Steps 1 through 5 are anchored on the screen, and must be opened in the sequence described, while those in Steps 6 and 7 are floating.

Step 1: Open a real STM Image

Double-click in the *STM Image Window* on the initial program screen (**Figure 1a**).

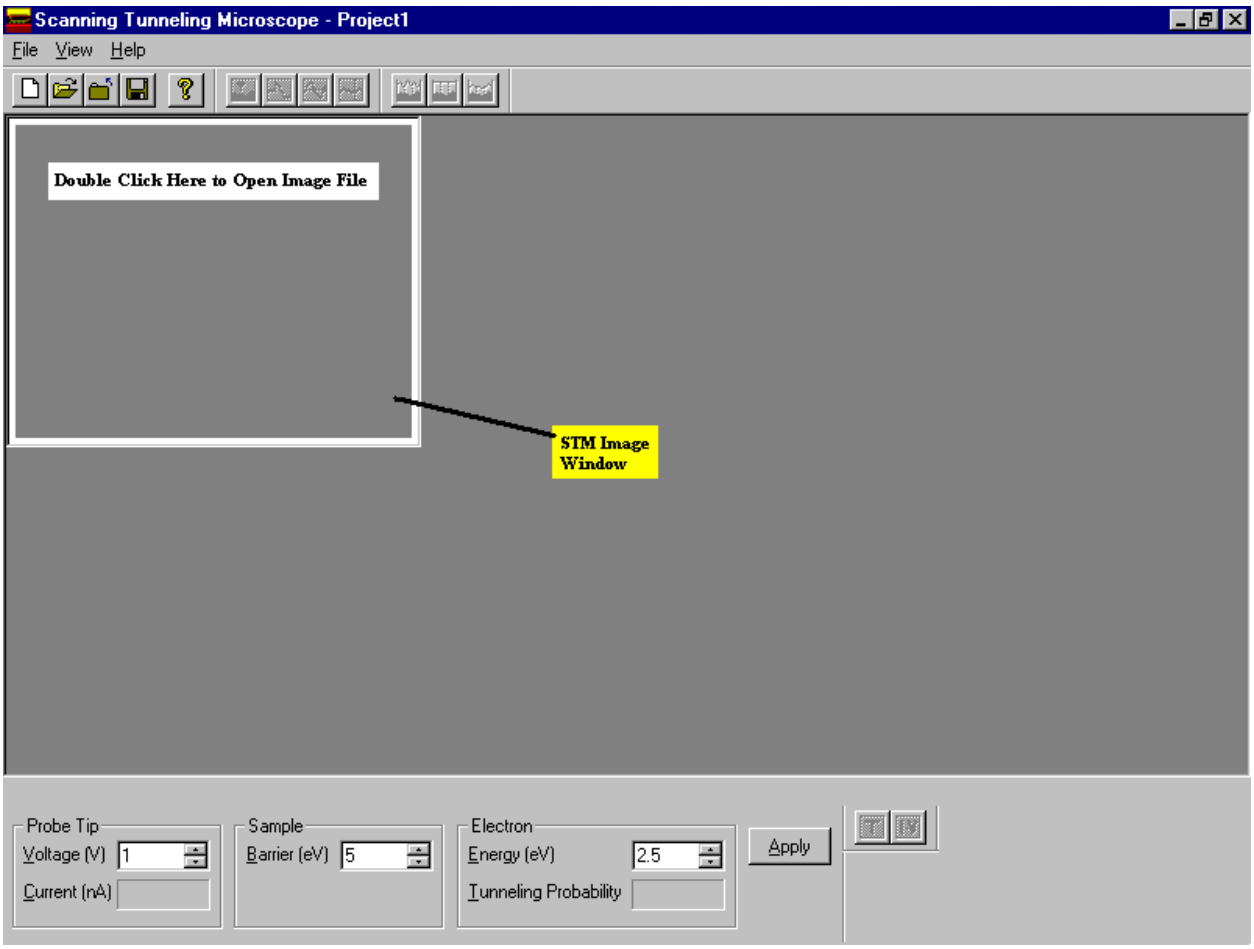


Figure 1a : Initial ***STM Simulator*** program screen.

A file **Open** dialog box pops-up prompting you for the name of the *.bmp* file containing the desired image. Select the desired file and click ***Open*** The image in the *.bmp* file appears in the *STM Image Window* (**Figure 1b**).

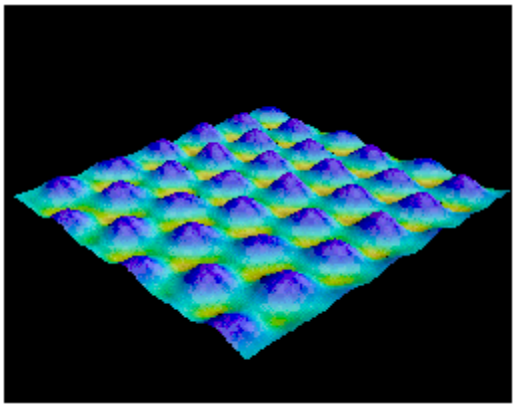


Figure 1b : A prerecorded image of a sample appears in the *STM Image Window*.

Step 2: Observe the Cross-Section of the Image

Display the cross-sectional profile of the sample across any straight line on the surface.

Choosing the Probe Tip Path

Move the mouse cursor over the image, it turns into a cross. With the left mouse button pressed, drag the cursor along the image. A line appears across the image along the path over which the cursor was dragged. Dragging the cursor, is analogous to dragging the probe-tip in a real STM.

After you have drawn the line an image of the probe-tip, an inverted triangle appears at one end of the line, indicating the current position of the probe tip (**Figure 2a**).

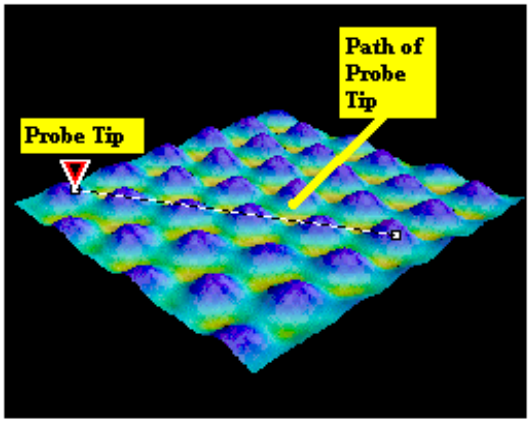


Figure 2a : The line drawn across the *STM Image Window* indicates the path along which the probe tip (inverted red triangle) is dragged.

Opening the Cross-Section Window

See the cross-section of the sample surface along the line that you drew above. Click on the ***Show Cross-Section*** button in the top toolbar, or choose ***View/Cross-Section*** from the pull-down menu. A cross-sectional profile along the line drawn on the STM image appears in the *Cross-Section Window* adjacent to STM image (**Figure 2b**). The red inverted triangle in the *Cross-Section Window* indicates the probe tip . The default position of the probe tip is half way to the top of the graph, directly above the left edge. Click and drag the mouse tip anywhere in the region above the sample's surface. See the corresponding motion of the probe tip in the *STM Image Window*.

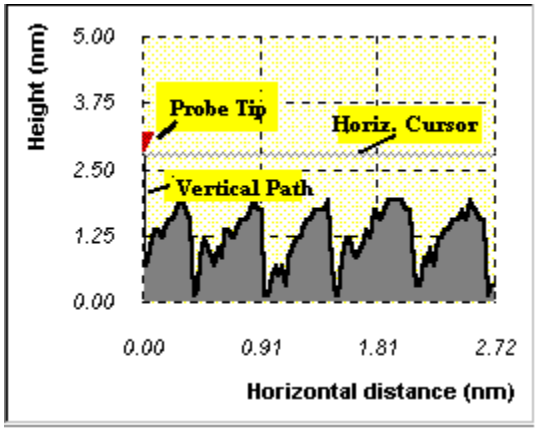


Figure 2b : The *Cross-Section Window* showing the position of the probe tip over the sample's surface and the path taken by the tunneling electron from the sample surface to the probe tip. The horizontal cursor line marks a position for an electron on that path.

Soon, an almost vertical line appears from the probe tip to the sample surface (**Figure 2b**). This line is the most probable path taken by the electron that tunnels from the sample to the probe tip. The gray horizontal cursor line in the *Cross-Section Window* is a marker for the position of an electron along the vertical path line.

Step 3: Observe the Potential Energy Diagram

See the potential energy diagram of the electron that tunnels from the sample to the probe tip, along the vertical path displayed in the *Cross-Section Window* (**Figure 2b**). However, the potential energy diagram of the electron depends upon the position and voltage of the probe tip, as well as the sample's barrier height.

Adjusting the Probe tip position

Click one the probe tip (red inverted triangle) in the *Cross-Section Window*, and with the mouse left button pressed, move the probe tip to a desired location above the sample's surface. Soon, an almost vertical line appears from the probe tip to the sample surface (**Figure 2b**). This line is the most probable path taken by the electron that tunnels from the sample to the probe tip. The gray horizontal cursor line in the *Cross-Section Window* is a marker for the position of an electron along the vertical path line.

Changing the Probe Tip Voltage

In the ***Parameters*** bar at the bottom of the screen (**Figure 3a**), use the ***Probe Tip Voltage*** spin control to change the probe tip voltage to a desired value, or type the desired value into the text box, and finally click the ***Apply*** button. While the default value of the probe tip voltage is 1V, it can be varied within a range of 0 to 10V. Observe the changes in the *Potential Energy Window*.

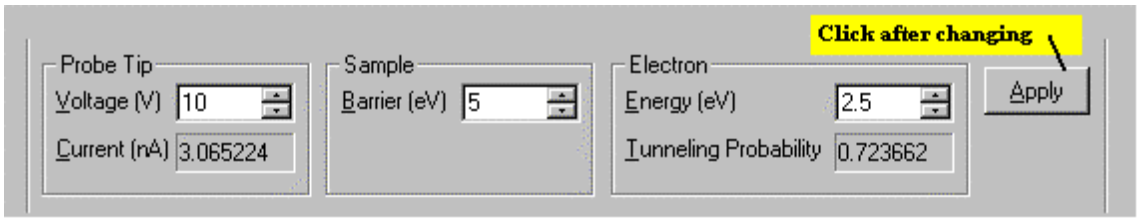


Figure 3a : Changing various parameters in the ***Parameters*** bar at the bottom of the screen.

Changing the Sample's Barrier

In the ***Parameters*** bar at the bottom of the screen, use the ***Sample Barrier*** spin control to change the barrier to a desired value, or type the desired value into the text box. While the default value of the sample's barrier height is 5eV, it can be varied within a range of 0 to 10eV. Observe the changes in the *Potential Energy Window*.

Opening the Potential Energy Window

Open the *Potential Energy Window* to display the potential energy of the electron (**Figure3b**) that tunnels along the vertical path of the electron in the *Cross-Section Window*. Click on the ***Show Potential Energy*** button in the top toolbar, or choose ***View/Potential Energy*** from the pull-down menu. The potential energy diagram for the tunneling electron appears in the *Potential Energy Window* that pops-up to the right of the *Cross-Section Window*.

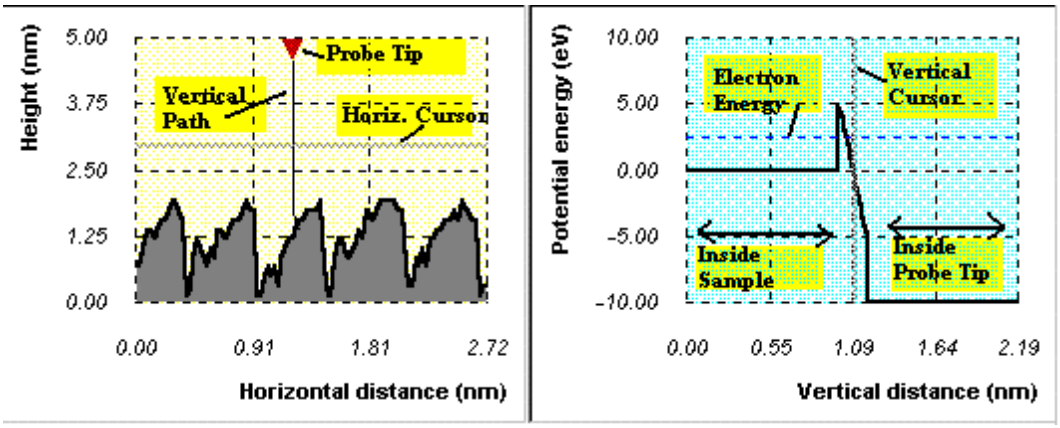


Figure 3b :The *Potential Energy Window* on the right. The blue dotted horizontal line represents the total energy of the electron. The gray vertical cursor represents the position of the electron, that is also specified by the horizontal cursor line the *Cross Section Window* (**Figure 2b**). The flat regions to the left and right of the potential barrier represent the nearly constant potential energy in the sample and probe tip respectively.

The gray vertical cursor line in the *Potential Energy Window* is a marker for the position of an electron along the vertical path line in the *Cross-Section Window*. Move the horizontal cursor in the *Cross-Section Window*, and observe the corresponding cursor in the *Potential Energy Window* to move.

The blue dotted line in the *Potential Energy Window* represents the total energy of the tunneling electron (default total energy = 2.5eV). The two flat regions to the left and right of the potential barrier in the *Potential Energy Window*, correspond to the constant potential energies in the sample and probe tip respectively.

Step 4: Observing the Wave Function for the Tunneling Electron

See the wave function for the tunneling electron that tunnels from the sample surface to the probe tip, and whose potential energy is displayed in the *Potential Energy Window*. However, the wave function depends upon the potential energy as well as the total energy of the electron.

Changing the Electron's Energy

Change the electron's total energy by either clicking anywhere in the potential energy graph above the zero for potential energy, or use the ***Electron Energy*** spin control in the ***Parameters*** bar below, or type in a value in the text box and then click the ***Apply*** button. While the default value of the electron's energy is 2.5eV, it can be varied from 0 to 10eV. Observe the dotted blue horizontal line representing the electron's total energy, change in the *Potential Energy Window*.

Opening the Wave Function Window

Open the *Wave Function Window* to display the wave function of the electron that tunnels along the vertical path of the electron in the *Cross-Section Window*, and whose energy is specified by the horizontal blue line in the *Potential Energy Window*. Click on the ***Show Wave Function*** button in the top toolbar, or choose ***View/Wave Function*** from the pull-down menu. The *Wave Function Window* (**Figure 4**) pops-up directly below the *Potential Energy Window*, so that the horizontal axis of the potential energy and wave function graphs coincide.

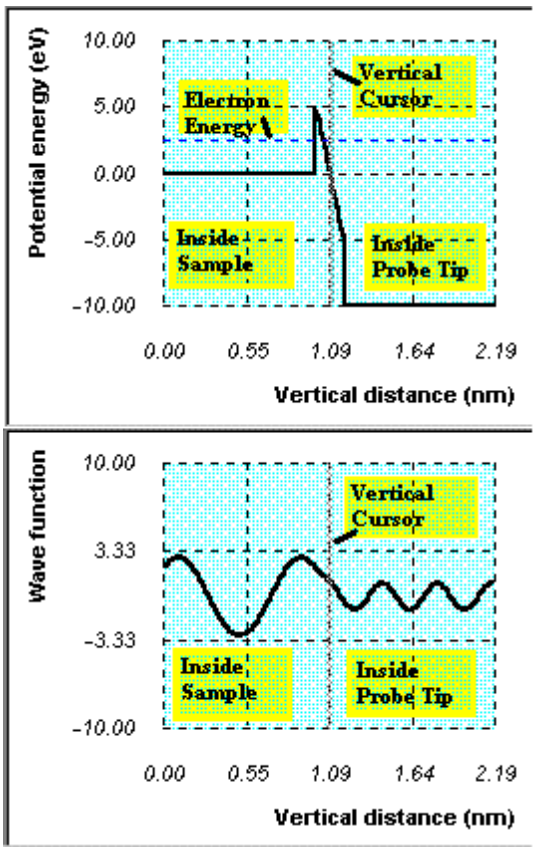


Figure 4 : The *Wave Function Window* at the bottom. The gray vertical cursor represents the position of the electron, and coincides with the cursor in the *Potential Energy Window* (**Figure 3b**).

The gray vertical cursor line in the *Wave Function Window* is a marker for the position of an electron along the vertical path line in the *Cross-Section Window*. This vertical cursor line in the *Wave Function Window* coincides with the vertical cursor line in the *Potential Energy Window*. Move the horizontal cursor in the *Cross-Section Window*, and observe the corresponding cursors in the *Potential Energy Window* and *Wave Function Window* to move.

Step 5: Observing the Tunneling Current Profile

See how the tunneling current measured by the STM relates to the cross-sectional profile of the sample.

Opening the Current Profile Window

Open the *Current Profile Window* to display the variation in tunneling current as the probe tip is moved across the surface. Click on the ***Show Current Profile*** button in the top toolbar, or choose ***View/Current Profile*** from the pull-down menu. The *Current Profile Window* (**Figure 5a**) pops-up directly below the *Cross-Section Window*, so that the horizontal axis of the cross-section and current profile graphs coincide. The current profile graph is initially blank. You can then decide to create the current profile in either of the following three modes:

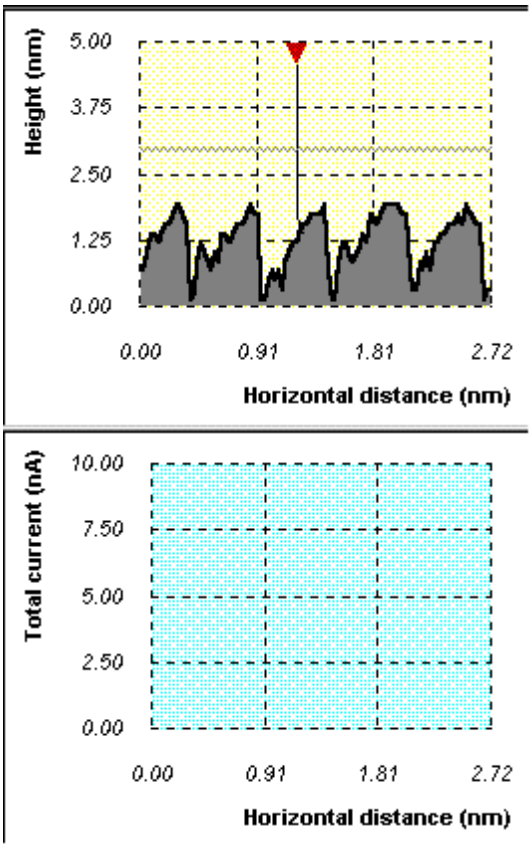


Figure 5a: The *Current Profile Window* pops-up directly below the *Cross-Section Window*, and is initially blank.

Constant Elevation Mode

When the STM is used in the *Constant Elevation Mode*, the probe tip is moved across the sample surface along a horizontal line. When the probe tip approaches a bump, the tunneling current increases, and when it approaches a trough the tunneling current decreases. Hence, the variation in the tunneling current corresponds to the variation in the relief of the sample surface.

To simulate the *Constant Elevation Mode* of STM operation, first click anywhere in the *Cross-Section Window*. The select the ***Horizontal Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen from one end to another with the mouse cursor (left mouse button pressed). The probe tip traces a solid blue horizontal line across the cross section graph at maintaining its initial height (**Figure 5b**). The corresponding variation of the tunneling current with the motion of the probe tip appears as a graph in the current profile graph directly below. Compare the shapes of the two graphs, and notice the similarities.

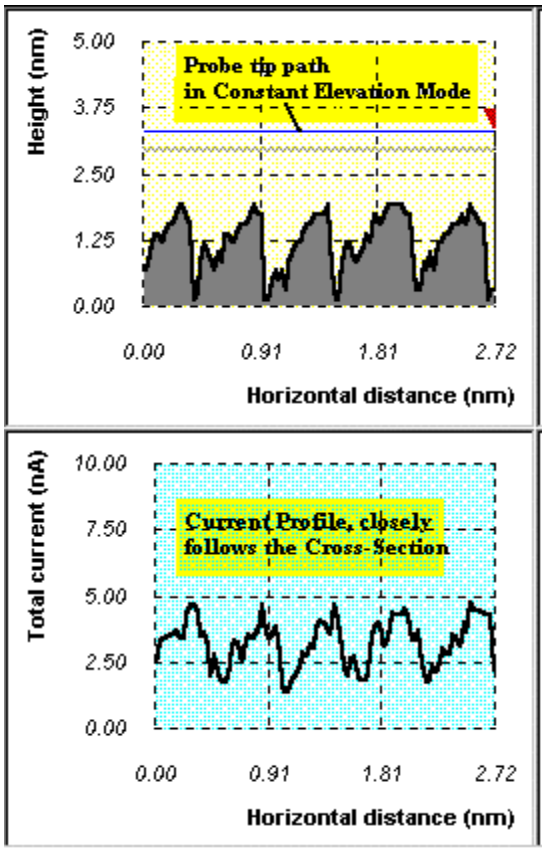


Figure 5b: The probe tip path (above) and current profile (below) in the *Constant Elevation Mode*.

Constant Current Mode

When the STM is used in the *Constant Current Mode*, the probe tip is moved across the sample surface and moved up and down so as to maintain a constant tunneling current. When the probe tip approaches a bump, the tunneling current increases, and the tip is raised to compensate for that increase and return the tunneling current to its original value. When the tip approaches a trough the tunneling current decreases and the tip is lowered to compensate for that decrease and return the tunneling current to its original value. Hence, the variation in the vertical position of the tip must follow the relief in the sample surface.

To simulate the *Constant Current Mode* of STM operation, first click anywhere in the *Cross-Section Window*. The select the ***Parallel to Profile Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen from one end to another with the mouse cursor (left mouse button pressed). The probe tip traces a solid blue curve across the cross section graph maintaining a constant distance from the surface, so that the path traced by the probe tip is identical to the sample's surface **(Figure 5c**). The corresponding variation of the tunneling current with the motion of the probe tip appears as a graph in the current profile graph directly below. Notice that but for a few spikes, the tunneling current is relatively constant.

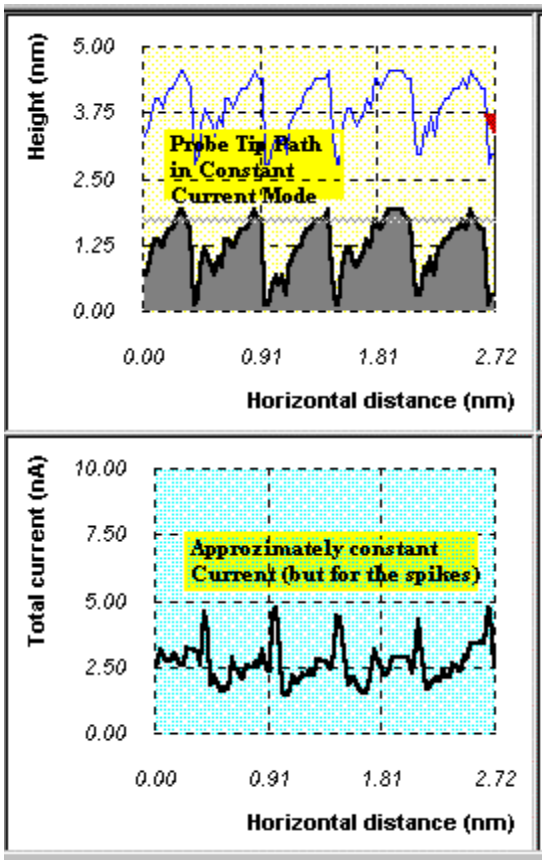


Figure 5c: The probe tip path (above) and current profile (below) in the *Constant Current Mode*.

Current Profile for Arbitrary Tip Path

While the STM is used either in the *Constant Elevation Mode* or *Constant Current Mode*, nothing precludes arbitrary motion of the probe tip.

To simulate the arbitrary motion of the probe tip, first click anywhere in the *Cross-Section Window*. The select the ***Arbitrary Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen along any arbitrary path using the mouse cursor (left mouse button

pressed). The probe tip traces a solid blue curve across the cross section graph corresponding to the motion of the probe tip.(**Figure 5d**).

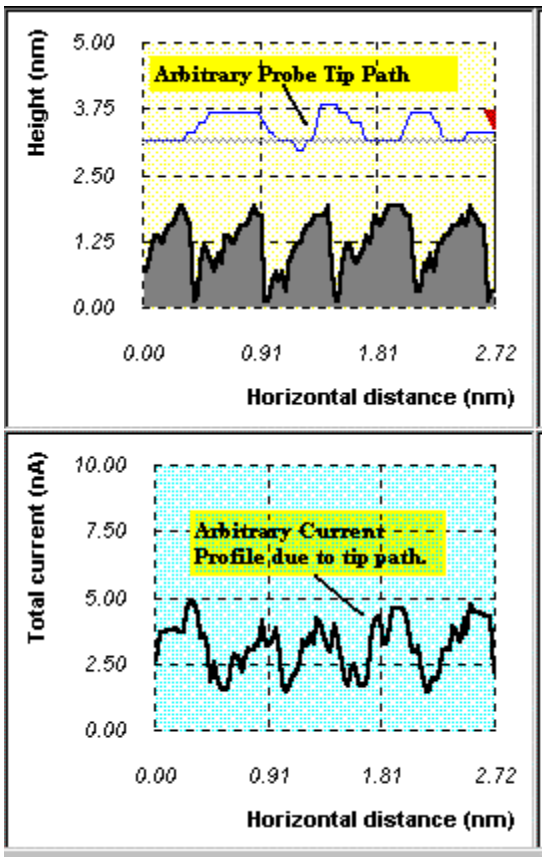


Figure 5d: An arbitrary probe tip path (top) and the corresponding current profile (bottom).

Steps 6 and 7 are optional, and could be used by more advanced users.

Step 6 (Optional): Observing the Tunneling Probability

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, observe the value of the tunneling probability in the display Tunneling Probability 0.674133 at the bottom right of the ***Parameters*** bar at the bottom of the screen. You can also see the variation of the tunneling probability with tip voltage and electron energy by following the instructions below:

Opening the Tunneling Probability Window

Open the *Tunneling Probability Window* to display the variation of the tunneling probability with probe tip voltage and electron energy at the present probe tip position. Click on the ***Show Tunneling Probability*** button in the ***Floating Windows Toolbar*** near the bottom of the screen, or choose ***View/Tunneling Probability*** from the pull-down menu. The *Tunneling Probability Window* pops-in the center of the screen.(**Figure 6**).

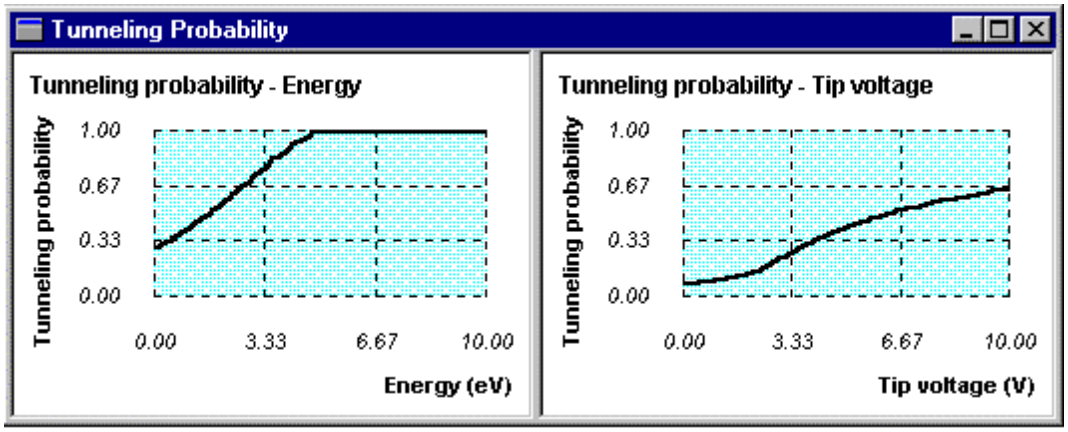


Figure 6: The *Tunneling Probability Window* showing the Tunneling Probability vs Energy graph (at constant tip voltage), and the Tunneling Probability vs. Tip Voltage graph (at constant electron energy).

Move the *Tunneling Probability Window* by clicking on the title bar of the window and dragging it anywhere on the screen. Resize the *Tunneling Probability Window* by clicking on any corner of the window and dragging that corner with the mouse (left mouse button pressed).

The *Tunneling Probability Window* has two graphs separated by a splitter. Click and drag the splitter to the desired position to change the size of any of the two graphs: Tunneling Probability vs. Energy and Tunneling Probability vs. Tip Voltage.

Tunneling Probability Vs. Electron Energy at Constant Voltage

On the left side of the *Tunneling Probability Window*, observe the variation of the tunneling probability with electron energy at a fixed tip voltage (specified in the ***Parameters*** bar), at the present tip position and sample's barrier height.

The graph is created by calculating the tunneling probability at different values of electron's energy, while keeping all other parameters constant. The graph would change if any of these parameters are changed.

Tunneling Probability Vs. Voltage at Constant Electron Energy

On the right side of the *Tunneling Probability Window*, observe the variation of the tunneling probability with tip voltage at a fixed electron energy (specified in the ***Parameters*** bar), at the present tip position and sample's barrier height.

The graph is created by calculating the tunneling probability at different values of tip voltage, while keeping all other parameters constant. The graph would change if any of these parameters are changed.

Step 7 (Optional): Observing the Tunneling Current

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, observe the value of the tunneling current (in nA) in the display Current (nA) 2.590029 at the bottom left of the ***Parameters*** bar at the bottom of the screen. You can also see the variation of the tunneling current with tip voltage by opening the *Current-Voltage Window*:

Opening the Current-Voltage Window

Open the *Current-Voltage Window* to display the variation of the current with probe tip voltage at the present probe tip position. Click on the ***Show Current-Voltage*** button in the ***Floating Windows Toolbar***, or choose ***View/Current-Voltage*** from the pull-down menu. The *Current-Voltage Window* pops-in the center of the screen. (**Figure7**)

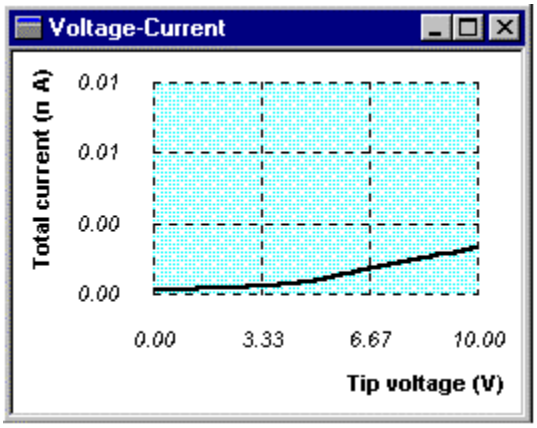


Figure 7: The *Current-Voltage Window* showing the variation of total tunneling current vs. applied probe tip voltage.

Move the *Current-Voltage Window* by clicking on the title bar of the window and dragging it anywhere on the screen. Resize the *Current-Voltage Window* by clicking on any corner of the window and dragging that corner with the mouse (left mouse button pressed).

The current-voltage graph is created by calculating the tunneling current at different values of tip voltage, while keeping the probe tip position and the sample's barrier height constant. The graph would change if any of these parameters are changed. However, the current-voltage graph is independent of the electron's energy since the tunneling current accounts for electrons of all energies.

Menus, Buttons, & Spin Controls

Pull-down Menus

File

New

The ***File/New*** menu opens an new project, *without* saving any of the previous settings. You can also use the button in the ***Commands Toolbar***.

Open

The ***File/Open*** menu opens an existing file, that was saved on an earlier run of the program. You are prompted to select an existing *.stm* file through a dialog box that pops-up. You can also use the button in the ***Commands Toolbar***.

Close

The ***File/Close*** menu closes the presently open file, without quitting the program. A dialog box will ask you whether you wish to save the present settings as a Project. You can also use the button in the ***Commands Toolbar***.

Save

The ***File/Save*** menu saves the presently open file (or project), along with all the settings. The existing filename is used. If this menu option is used for the first time, it pops-up a dialog box asking you to select a filename. You can also use the button in the ***Commands Toolbar***.

Save As…

The ***File/Save As…*** menu saves the exiting file (or project)as a specific file. You are prompted for the filename to be saved under.

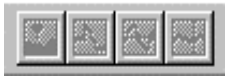
Exit

The ***File/Exit*** menu quits the program. You are prompted to save your existing work in the program.

View

Charts Toolbar

The ***View/Charts Toolbar*** menu displays (or hides) the ***Charts Toolbar***

 which is used to open various Windows. The buttons of the ***Charts Toolbar*** become active in the appropriate sequence. The default location of the bar is at the top of the screen, however it can be moved by clicking and dragging it using the mouse (left mouse button pressed).

Commands Toolbar

The ***View/Command Toolbar*** menu displays (or hides) the ***Commands Toolbar*** . The default location of the bar is at the top left of the screen. However, it can be moved by clicking and dragging it using the mouse (left mouse button pressed).

Floating Windows Toolbar

The ***View/Floating Windows Toolbar*** menu displays (or hides) the ***Floating Windows Toolbar*** , which is used to display the *Tunneling Probability Window* and *Current-Voltage Window*. The buttons on this toolbar are activated only after the probe tip path is drawn as a straight line across the *STM Image* (**Figure2a**). The default location of the bar is at the bottom right of the screen, adjacent to the ***Parameters*** bar. However, it can be moved by clicking and dragging it using the mouse (left mouse button pressed).

Parameters

The ***View/Parameters*** menu displays (or hides) the ***Parameters*** bar (**Figure 3a**). The default location of the bar is at the bottom of the screen, however it can be moved by clicking and dragging it using the mouse (left mouse button pressed).

Status Bar

The ***View/Status Bar*** menu displays (or hides) the ***Status*** Bar. The location of the bar is at the bottom of the screen, and it provides the user information about the present status of the program.

Tip Path Settings

The ***View/Tip Path Settings*** menu displays (or hides) the ***Tip Path Settings*** bar. ,which is used to choose between various modes for determining the *Current Profile***.** The buttons on this toolbar are activated only after the *Cross Section Window* is opened (**Figure 2b**). The default location of the bar is at the top of the screen, directly below the menu and to the right of the ***Commands Toolbar***. However, it can be moved by clicking and dragging it using the mouse (left mouse button pressed).

STM Image

The ***View/STM Image*** menu displays *STM Image Window* (**Figure 1b**). This window is displayed when the program starts. However, it is blank without any STM image in it.

Cross-Section

The ***View/Cross-Section*** menu displays the *Cross-Section Window*. The window can also be opened using the ***Show Cross-Section*** button on the ***Charts toolbar***. The position of the window is to the immediate right of the *STM Image Window*, and remains fixed. This menu option, and associated button, are only activated after a line has been drawn across the *STM Image* (**Figure 2a**).

Potential Energy

The ***View/Potential Energy*** menu displays the *Potential Energy Window*. The window can also be opened using the ***Show Potential Energy*** button on the ***Charts Toolbar***. The position of the window is to the immediate right of *Cross-Section Window*, and remains fixed. This menu option, and associated button, are only activated after the *Cross Section Window* is opened (**Figure 2b**).

Wave Function

The ***View/Wave Function*** menu displays the *Wave Function Window*. The window can also be opened using the ***Show Wave Function*** button on the ***Charts Toolbar***. The position of the window is directly below the *Potential Energy Window*, and remains fixed, so that the potential energy diagram and wave function have the same horizontal scale. This menu option, and associated button, are only activated after the *Potential Energy Window* is opened (**Figure 3b**).

Current Profile

The ***View/Current Profile*** menu displays the *Current Profile Window*. The window can also be opened using the ***Show Current Profile*** button on the ***Charts Toolbar***. The position of the window is directly below the *Cross-Section Window*, and remains fixed, so that the cross-section and current profile have the same horizontal scale. This menu option, and associated button, are only activated after the *Wave Function Window* is opened (**Figure 4**).

Tunneling Probability

The ***View/Tunneling Probability*** menu displays the *Tunneling Probability Window*. The window can also be opened using the ***Show Tunneling Probability*** button on ***Floating Windows Toolbar***. The window opens at the center of the screen by default. It can be moved by clicking on its header and dragging. Move the window by clicking on the title bar of the window and dragging it anywhere on the screen. Resize it by clicking on any corner of the window and dragging that corner with the mouse (left mouse button pressed). This menu option, and associated button, are only activated after the probe tip path is drawn across the *STM Image* (**Figure 2a**).

Current - Voltage

The ***View/Current-Voltage*** menu displays the *Current-Voltage Window*. The window can also be opened using the ***Show Current-Voltage*** button on ***Floating Windows Toolbar***. The window opens at the center of the screen by default. It can be moved by clicking on its header and dragging. Move the window by clicking on the title bar of the window and dragging it anywhere on the screen. Resize it by clicking on any corner of the window and dragging that corner with the mouse (left mouse button pressed). This menu option, and associated button, are only activated after the *Cross Section Window* is opened (**Figure 2b**).

Help

Help Topics

The ***Help/Help Topics*** menu brings up the on-line help file for the ***STM Simulator*** program. You can also use the button in the top toolbar.

Program Demo…

The ***Help/Program Demo…*** menu starts a demo for the ***STM Simulator*** program.

About …

The ***Help/About…*** menu displays copyright information for the ***STM Simulator*** program.

Buttons

Arbitrary Tip Path

The ***Arbitrary Tip Path*** button (in the top toolbar by default) allows you to sketch an arbitrary tip path in the *Cross-Section Window* (by dragging the probe tip with the left mouse button pressed). The corresponding variation of tunneling current appears in the *Current Profile Window* below

Horizontal Tip Path

The ***Horizontal Tip Path*** button (in the top toolbar by default) allows you to sketch an horizontal tip path in the *Cross-Section Window* (by dragging the probe tip with the left mouse button pressed). The corresponding variation of tunneling current appears in the *Current Profile Window* below.

Parallel to Profile Tip Path

The ***Parallel to Profile Tip Path*** button (in the top toolbar by default) allows you to sketch an tip path parallel to the surface profile, in the *Cross-Section Window* (by dragging the probe tip with the left mouse button pressed). The corresponding variation of tunneling current appears in the *Current Profile Window* below.

Show Cross Section

The ***Show Cross-Section*** button , in the top toolbar, pops-up the *Cross-Section Window*, to the immediate right of the *STM Image Window*. This button, and associated menu option, are only activated after a line has been drawn across the *STM Image* (**Figure 2a**).

Show Potential Energy

The ***Show Potential Energy*** button , in the top toolbar, pops-up the *Potential Energy Window*, to the immediate right of the *Cross-Section Window*. This button, and associated menu option, are only activated after the *Cross Section Window* is opened (**Figure 2b**).

Show Wave Function

The ***Show Wave Function*** button , in the top toolbar, pops-up the *Wave Function Window*, directly below the *Potential Energy Window*, so that the horizontal axis of the two graphs coincide. This button, and associated menu option, are only activated after the *Potential Energy Window* is opened (**Figure 3b**).

Show Current Profile

The ***Show Current Profile*** button , in the top toolbar, pops-up the *Current Profile Window*, directly below the *Cross Section Window*, so that the horizontal axis of the two graphs coincide. This button, and associated menu option, are only activated after the *Wave Function Window* is opened (**Figure 4**).

Show Tunneling Probability

The ***Show Tunneling Probability*** button , in the ***Floating Windows Toolbar*** at the bottom, pops-up the *Tunneling Probability Window* at the center of the screen. This window can later be moved or resized. This button, and associated menu option, are only activated after the probe tip path is drawn across the *STM Image*(**Figure 2a**).

Show Current-Voltage Graph

The ***Show Current-Voltage*** button , in the ***Parameters*** bar at the bottom, pops-up the *Current-Voltage Window* at the center of the screen. This window can later be moved or resized. This button, and associated menu option, are only activated after the probe tip path is drawn across the *STM Image*(**Figure 2a**).

Apply

The ***Apply*** button , in the ***Parameters*** bar at the bottom updates the values of the parameters (tip voltage, sample's barrier height, and electron's energy) in the Parameter's bar.

Spin Controls

Probe Tip Voltage

The ***Probe Tip Voltage*** spin control

allows you to change the probe tip voltage (default value = 10V) within a range of 0V to 10V. You can also type in the desired tip voltage in the adjoining text box.

Sample Barrier

The ***Sample Barrier*** spin control

allows you to change the sample's barrier height (default value = 5eV) within a range of 0V to 10eV. You can also type in the desired sample's barrier height in the adjoining text box.

Electron Energy

The ***Electron Energy*** spin control

allows you to change the electron's energy (default value = 2.5eV) within a range of 0V to 10eV. You can also type in the desired electron's energy in the adjoining text box, or click in the *Potential Energy Window* graph to reset the value of the electron's energy.

How to…

Open an STM Image

Double-click in the *STM Image Window* on the initial program screen (**Figure 1a**). A file **Open** dialog box pops-up prompting you for the name of the *.bmp* file containing the desired image. Select the desired file and click ***Open*** The image in the *.bmp* file appears in the *STM Image Window* (**Figure 1b**).

Choose A Probe Tip Path on an STM Image

Move the mouse cursor over the image, it turns into a cross. With the left mouse button pressed, drag the cursor along the image. A line appears across the image along the path over which the cursor was dragged. Dragging the cursor, is analogous to dragging the probe-tip in a real STM. After you have drawn the line an image of the probe-tip, an inverted triangle appears at one end of the line, indicating the current position of the probe tip (**Figure 2a**).

Observe the Cross-Section of an STM Image

See the cross-section of the sample surface along the line that you drew above. Click on the ***Show Cross-Section*** button in the top toolbar, or choose ***View/Cross-Section*** from the pull-down menu. A cross-sectional profile along the line drawn on the STM image appears in the *Cross-Section Window* adjacent to STM image (**Figure 2b**). The red inverted triangle in the *Cross-Section Window* indicates the probe tip . The default position of the probe tip is half way to the top of the graph, directly above the left edge. Click and drag the mouse tip anywhere in the region above the sample's surface. See the corresponding motion of the probe tip in the *STM Image Window*.

Observe the Potential Energy Diagram

See the potential energy diagram of the electron that tunnels from the sample to the probe tip, along the vertical path displayed in the *Cross-Section Window* (**Figure 2b**). However, the potential energy diagram of the electron depends upon the position and voltage of the probe tip, as well as the sample's barrier height. After adjusting the probe tip voltage and sample's barrier height (See **Step 3** of A **Brief Users' Manual**), Open the *Potential Energy Window* to display the potential energy of the electron (**Figure3b**) that tunnels along the vertical path of the electron in the *Cross-Section Window*. Click on the ***Show Potential Energy*** button in the top toolbar, or choose ***View/Potential Energy*** from the pull-down menu. The potential energy diagram for the tunneling electron appears in the *Potential Energy Window* that pops-up to the right of the *Cross-Section Window*.

Observe the Wave Function

Open the *Wave Function Window* to display the wave function of the electron that tunnels along the vertical path of the electron in the *Cross-Section Window*, and whose energy is specified by the horizontal blue line in the *Potential Energy Window*. Click on the ***Show Wave Function*** button in the top toolbar, or choose ***View/Wave Function*** from the pull-down menu. The *Wave Function Window* (**Figure 4**) pops-up directly below the *Potential Energy Window*, so that the horizontal axis of the potential energy and wave function graphs coincide.

Observe the Current Profile …

Open the *Current Profile Window* to display the variation in tunneling current as the probe tip is moved across the surface. Click on the ***Show Current Profile*** button in the top toolbar, or choose ***View/Current Profile*** from the pull-down menu. The *Current Profile Window* (**Figure 5a**) pops-up directly below the *Cross-Section Window*, so that the horizontal axis of the cross-section and current profile graphs coincide. The current profile graph is initially blank. You can then decide to create the current profile in either of the following three modes:

In Constant Elevation Mode

To simulate the *Constant Elevation Mode* of STM operation, first click anywhere in the *Cross-Section Window*. The select the ***Horizontal Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen from one end to another with the mouse cursor (left mouse button pressed). The probe tip traces a solid blue horizontal line across the cross section graph at maintaining its initial height (**Figure 5b**). The corresponding variation of the tunneling current with the motion of the probe tip appears as a graph in the current profile graph directly below. Compare the shapes of the two graphs, and notice the similarities.

In Constant Current Mode

To simulate the *Constant Current Mode* of STM operation, first click anywhere in the *Cross-Section Window*. The select the ***Parallel to Profile Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen from one end to another with the mouse cursor (left mouse button pressed). The probe tip traces a solid blue curve across the cross section graph maintaining a constant distance from the surface, so that the path traced by the probe tip is identical to the sample's surface **(Figure 5c**). The corresponding variation of the tunneling current with the motion of the probe tip appears as a graph in the current profile graph directly below. Notice that but for a few spikes, the tunneling current is relatively constant.

For an Arbitrary Tip Path

To simulate the arbitrary motion of the probe tip, first click anywhere in the *Cross-Section Window*. The select the ***Arbitrary Tip Path*** button from the top toolbar. Then with the <shift> key pressed, click on the probe tip (inverted red triangle) in the *Cross-Section Window*, and drag it across the screen along any arbitrary path using the mouse cursor (left mouse button pressed). The probe tip traces a solid blue curve across the cross section graph corresponding to the motion of the probe tip.(**Figure 5d**).

Change the Probe-Tip Position

Click one the probe tip (red inverted triangle) in the *Cross-Section Window*, and with the mouse left button pressed, move the probe tip to a desired location above the sample's surface. Soon, an almost vertical line appears from the probe tip to the sample surface (**Figure 2b**). This line is the most probable path taken by the electron that tunnels from the sample to the probe tip. The gray horizontal cursor line in the *Cross-Section Window* is a marker for the position of an electron along the vertical path line.

Change the Probe-Tip Voltage

In the ***Parameters*** bar at the bottom of the screen (**Figure 3a**), use the ***Probe Tip Voltage*** spin control to change the probe tip voltage to a desired value, or type the desired value into the text box, and finally click the ***Apply*** button. While the default value of the probe tip voltage is 1V, it can be varied within a range of 0 to 10V. Observe the changes in the *Potential Energy Window*.

Change the Sample Barrier Height

In the ***Parameters*** bar at the bottom of the screen, use the ***Sample Barrier*** spin control to change the barrier to a desired value, or type the desired value into the text box. While the default value of the sample's barrier height is 5eV, it can be varied within a range of 0 to 10eV. Observe the changes in the *Potential Energy Window*.

Change the Electron Energy

Change the electron's total energy by either clicking anywhere in the potential energy graph above the zero for potential energy, or use the ***Electron Energy*** spin control in the ***Parameters*** bar below, or type in a value in the text box and then click the ***Apply*** button. While the default value of the electron's energy is 2.5eV, it can be varied from 0 to 10eV. Observe the dotted blue horizontal line representing the electron's total energy, change in the *Potential Energy Window*.

Observe the Present Tunneling Probability

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, observe the value of the tunneling probability in the display

at the bottom right of the ***Parameters*** bar at the bottom of the screen.

Observe the Variation of Tunneling Probability

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, open the *Tunneling Probability Window* to display the variation of the tunneling probability with probe tip voltage and electron energy at the present probe tip position. Click on the ***Show Tunneling Probability*** button in the ***Floating Windows Toolbar*** near the bottom of the screen, or choose ***View/Tunneling Probability*** from the pull-down menu. The *Tunneling Probability Window* pops-in the center of the screen.(**Figure 6**).

Observe the Present Value of Tunneling Current

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, observe the value of the tunneling current (in nA) in the display

at the bottom left of the ***Parameters*** bar at the bottom of the screen.

Observe the Current-Voltage Graph

After setting the tip position, tip voltage, sample's barrier height, and electron's energy to the desired values, open the *Current-Voltage Window* to display the variation of the current with probe tip voltage at the present probe tip position. Click on the ***Show Current-Voltage*** button in the ***Floating Windows Toolbar***, or choose ***View/Current-Voltage*** from the pull-down menu. The *Current-Voltage Window* pops-in the center of the screen. (**Figure7**)

Pedagogical Applications

Use the ***STM Simulator*** program over a range of academic levels, from high school to senior undergraduate. The ***STM Simulator*** does not require knowledge of higher level mathematics or physics, and emphasizes visualization techniques to explain how tunneling is used in an STM.

Introductory undergraduate or high-school students utilize the program to obtain a semi-quantitative feel for how the STM creates an image of the sample and how various parameters such as probe tip voltage and distance of probe tip from the sample's surface affect the performance of an STM. In this environment, where the students are not interested in the quantum mechanics of the STM, but rather in its basic operation, the program can be used only with the *STM Image*, *Cross Section* and *Current Profile Window*s open. For physics or engineering students at the senior undergraduate level, the program can be used to learn how quantum mechanics is related to the STM by also using the *Potential Energy*, *Wave Function* and *Tunneling Probability* and *Current-Voltage Window*s. See **Figure 8**.

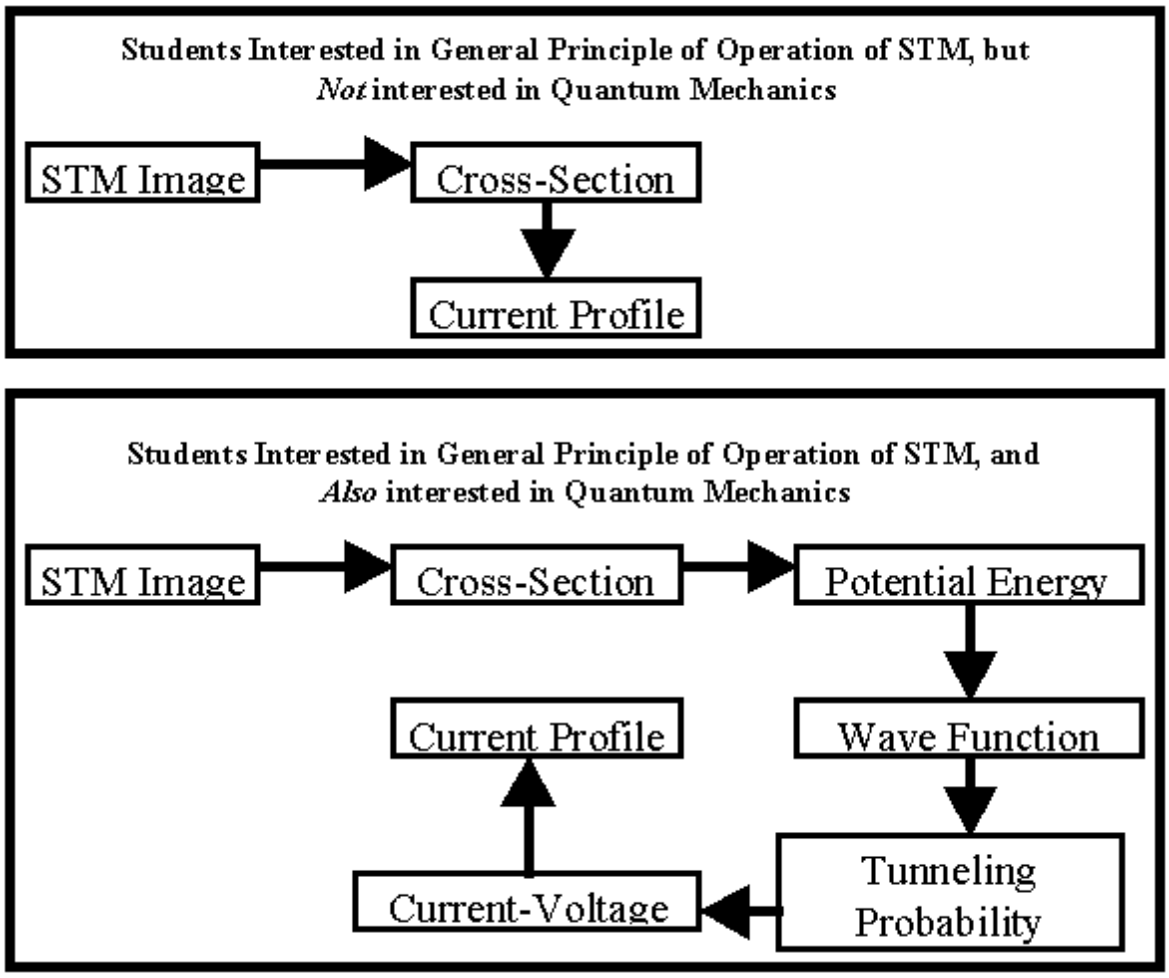


Figure 8: Two categories of students who could use the ***STM Simulator*** program differently.

The program is not meant to be used as a substitute for a real STM. Due to the circular reasoning involved, it is definitely *not* intended to be a research tool for analysis of real samples. It is merely a pedagogical tool for teaching the underlying physics of an STM.

We have used ***STM Simulator*** as a pedagogical vehicle to teach the phenomena of quantum tunneling and the factors on which it depends. In an instructional units titled *Exploring the Very Small – Quantum Tunneling*, students first explore some of the interesting application of nanotechnology and nanodevices by viewing images on Web sites. They are then asked to ponder about how these devices could be created or even observed at the atomic level. After motivating students to think about how individual atoms can be observed, the Scanning Tunneling Microscope is presented as a tool which enables us to study and even manipulate individual atoms without physically touching them.

This computer program and the instructional unit in which it is used, have been developed as a part of the ***Visual Quantum Mechanics*** project. The project aims at introducing quantum principles at the high-school level through emphasizing hands-on activities and visualization techniques rather than higher level mathematics.

For the ***Visual Quantum Mechanics*** sample activity from the instructional unit titled *Exploring the Very Small – Quantum Tunneling*, that utilizes the ***STM Simulator*** program refer to the ***Appendix***.

Find more information about these instructional materials at out Web site ***http://bluegiant.phys.ksu.edu***.

APPENDIX

The following pages contain a ***Visual Quantum Mechanics*** sample activity from the instructional unit titled *Exploring the Very Small – Quantum Tunneling*, that utilizes the ***STM Simulator*** program.