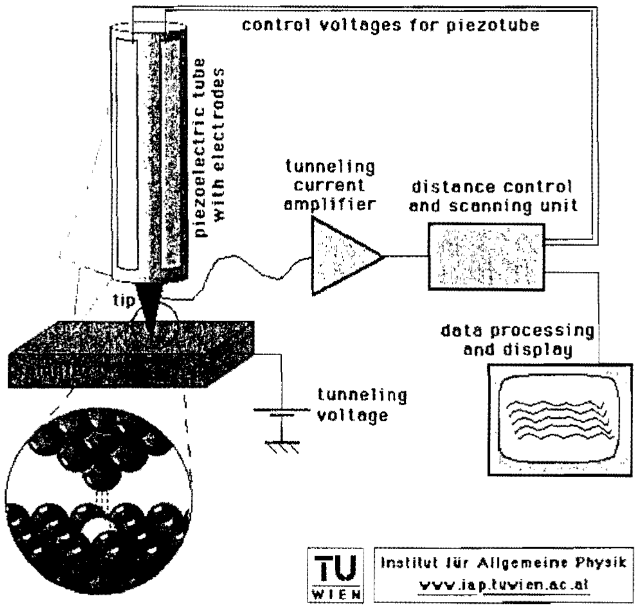
**Quantum Mechanics A** **PHY-319** **Note Set No. 9**

# Quantum Tunnelling: The Scanning Tunnelling Microscope (STM)

The STM was developed by Binnig and Rohrer (Nobel prize, 1986 - their breakthrough was in achieving great stability by a brilliantly clever mechanical design of the instrument). The instrument consists of a metal tip with a sharp point placed above a metal surface. The tip can be scanned very accurately across the surface and up and down using 3 piezoelectric crystals. As the tip moves, the tunnelling current is measured. As the tip crosses a bump or dip on the surface the tunnelling gap, $L$, changes. This leads to a measurable change in the tunnelling current through its strong exponential dependence on $L$. This extreme sensitivity means that surfaces can be mapped with a resolution as good as $10^{-12}$ m = $10^{-3}$ nm perpendicular to the surface and less than 0.5 nm parallel to the surface; individual atoms can be routinely resolved. (Compare this with optical microscopes with resolutions no better than 100's of nm and even electron microscopes with resolutions around 0.1 nm). See Problem 7, Q.2 for an estimate of the sensitivity of the STM.

**Figure 1: Basic components of a typical modern STM**



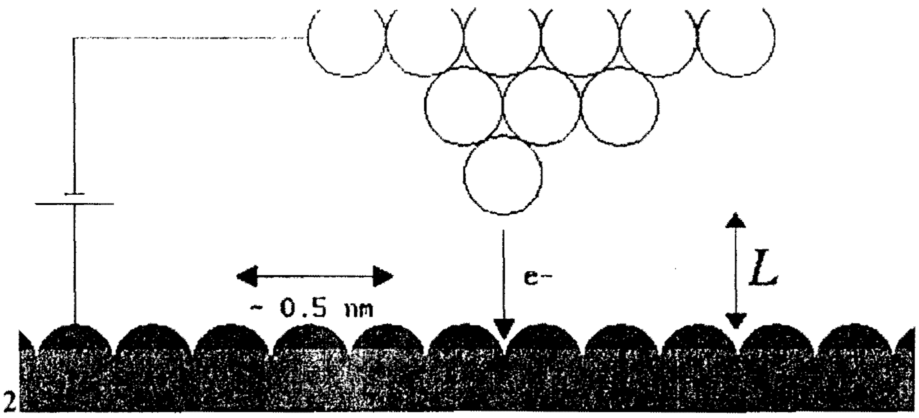




Figure 2

Let us model the two metals as conductors with their electrons filling the conduction band. The work function $\varphi$ is the minimum energy required to remove an electron from the metal. The vacuum (or air) between the metals therefore makes a barrier of width $L$, the separation between the tip and substrate. We take our zero of energy to be that of an electron which has *just* escaped from its metal. In the absence of any applied electric field the situation can be depicted as in **Figure 3:**

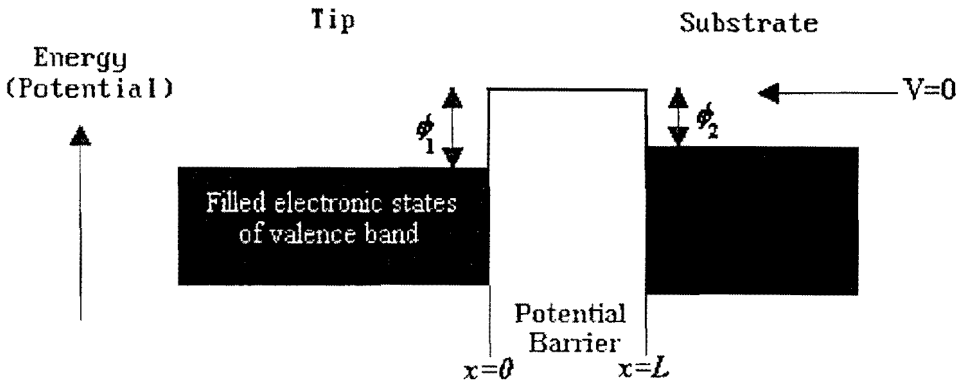



**Figure 3**

Now let us apply an electric field ε producing a force to move the electrons from tip towards the substrate (i,e, substrate positive relative to tip). The potential experienced by the electrons is therefore:

$$V(x) = -e\varepsilon x. \qquad \textbf{Equation 1}$$

We can check that this is to the right in the figure by evaluating the force,

$$F_x = -\frac{\partial V(x)}{\partial x} = e\varepsilon \qquad \textbf{Equation 2}$$

which is indeed in the positive x direction as required.
This potential is a straight line starting at $V=0$ at $x=0$ and decreasing linearly to $V(L)=-e\varepsilon L$ at $x=L$ as shown in **Figure 4:**

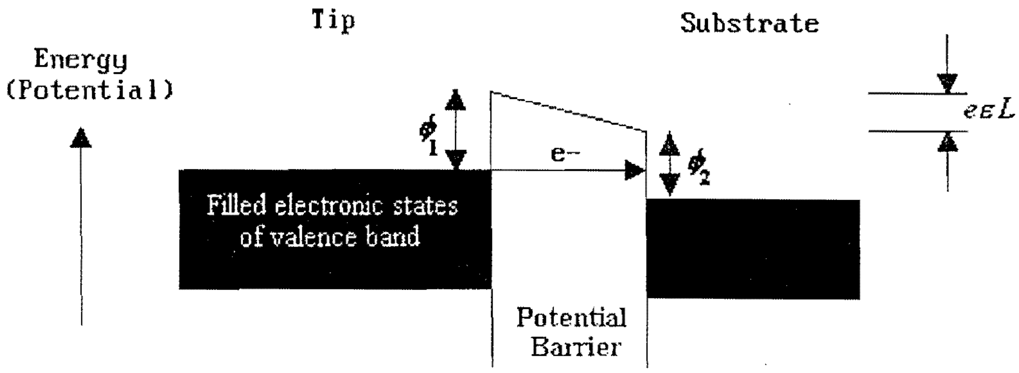



**Figure 4**

If we neglect the variation of $V(x)$ across the narrow barrier, then the transmission coefficient for tunnelling of electrons from the tip to the substrate is given by the square barrier formula derived in lectures, but with the barrier height being $\varphi_l$ as shown in Figure 4; this is the tunnelling current:

$$I = I_0 e^{-2\kappa L} \quad where \quad \kappa = \left(\frac{2m_e}{\hbar^2}\right)^{\frac{1}{2}} \varphi^{\frac{1}{2}} \qquad \textbf{Equation 3}$$

We shall examine this approximation later in these notes.

**The STM Demonstration Experiment.**

In the laboratory you were shown the STM operating in a mode designed to confirm the precise form of the tunnelling current given by equation 3 above. A bias voltage was applied between tip and substrate as in Figure 4 above; this was kept fixed throughout the demonstration (typically ~0.3 volts). The width of the air gap, $L_0$, was varied over a range of values by means of the piezoelectric crystal controlling vertical movement of the tip. For each $L_0$ there was a definite tunnelling current $I(L_0)$ (in fact the experimenter simply sets a current and the microscope electronics automatically activates the piezo to change the gap until the required current is attained). Now the piezo is oscillated rapidly up and down at a frequency $\omega$ and amplitude ΔL/2 (ΔL is the peak-to-peak amplitude, typically of order 0.1 nm),

$$L(t) = L_0 + \frac{\Delta L}{2}\sin\omega t \qquad \textbf{Equation 4}$$

Notice that the oscillations take place about $L_0$ , and the electronics achieves this by keeping the *average current* constant at $I(L_0)$ over many oscillations of the tip. This feedback in the electronic control is on a much slower time scale than the fast oscillations of the tip.
As a consequence of the oscillating barrier width the tunnelling current also oscillates:

$$\begin{aligned} I(t) &= I_0 e^{-2\kappa L_0} e^{-2\kappa\frac{\Delta L}{2}\sin\omega t} \\ &\approx I_0 e^{-2\kappa L_0}(1 - 2\kappa\frac{\Delta L}{2}\sin\omega t) \quad for \quad \Delta L \quad small \qquad \textbf{Equation 5} \\ &\approx I(L_0) - \left[2\kappa\frac{\Delta L}{2} I(L_0)\right]\sin\omega t \end{aligned}$$

Thus we find that the current oscillates rapidly about its average value $I(L_0)$ with the same frequency as the tip and with amplitude $\Delta I/2$, given by the square bracketed coefficient of the sine,
$\frac{\Delta I}{2} = -2\kappa\frac{\Delta L}{2} I(L_0)$ The minus sign here reflects the fact that increasing L widens the barrier and therefore decreases the tunnelling current. The peak-to-peak amplitude of the current is displayed on an oscilloscope (typically a few nA) and can therefore be easily measured, while the average current is also known (typically a few nA). Thus the exponential dependence of the tunnelling current on the barrier width leads to the peak-to-peak current amplitude $\Delta I$ being proportional to the average current $I(L_0)$:

$$|\Delta I| = [2\kappa\Delta L] I(L_0) \qquad \textbf{Equation 6}$$

while the proportionality constant is also predicted.(see Equation 3).
This analysis can be applied to the experimental data, see solutions to Problems 7 for the details (you should take those solutions as part of these notes, including the important estimate of sensitivity in Question 2).
**Note:** The above analysis is done to explain in detail how the result arises and what sort of approximation it is. An alternative derivation goes as follows:
Differentiate Equation 3,

$$\frac{dI(L)}{dL} = -2\kappa I_0 e^{-2\kappa L} = -2\kappa I(L)$$

Now approximate the infinitesimals *dI* and *dL* by the finite, but small, variations observed in the experiment, $\Delta I$ and $\Delta L$, and put $L \approx L_0$, hence we obtain the result in equation 6.

**STM: The more accurate calculation.**

The formula for tunnelling across a barrier V(x) is:

$$T \propto e^{-G} \quad where \quad G = 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^L \sqrt{V(x)-E}\, dx \qquad \textbf{Equation 7}$$

Taking the zero of energy at $x=0$, as in Figures 3 & 4, the energy of the particle trying to tunnel is the work function,

$$E = -\varphi_1 \textbf{ and } V(x) = -e\varepsilon x \qquad \textbf{Equation 8}$$

Hence,

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^L \sqrt{\varphi_1 - e\varepsilon x}\, dx$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \varphi_1^{1/2} \int_0^L \sqrt{1-\left(\frac{e\varepsilon}{\varphi_1}\right)x}\, dx$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \varphi_1^{1/2} \left[-\frac{2}{3}\frac{\varphi_1}{e\varepsilon}\left\{1-\left(\frac{e\varepsilon}{\varphi_1}\right)x\right\}^{\frac{3}{2}}\right]_0^L$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \varphi_1^{1/2} \left[\frac{2}{3}\frac{\varphi_1}{e\varepsilon}\right]\left[1-\left\{1-\left(\frac{e\varepsilon}{\varphi_1}\right)L\right\}^{\frac{3}{2}}\right]$$

For small enough $(e\varepsilon/\varphi_1)L << 1$ we can expand the last term to first order,

$$1-\left\{1-\left(\frac{e\varepsilon}{\varphi_1}\right)L\right\}^{\frac{3}{2}} \approx 1-\left\{1-\frac{3}{2}\left(\frac{e\varepsilon}{\varphi_1}\right)L\right\}$$
$$=\frac{3}{2}\left(\frac{e\varepsilon}{\varphi_1}\right)L$$

Putting this altogether we see that all these extra factors cancel and we end up with our original approximate result, Equation 3,

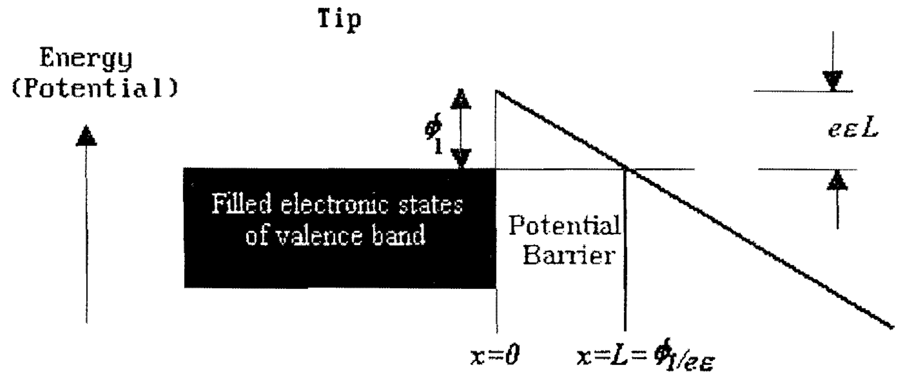
$$T \propto e^{-2\kappa L} \quad where \quad \kappa=\left(\frac{2m_e}{\hbar^2}\right)^{\frac{1}{2}}\varphi^{\frac{1}{2}}$$

However, now we know what we have neglected. Is this justified? As mentioned before, a typical value for the work function is $\varphi_1 \sim 6$ eV, and for the bias voltage $V_{bias} \sim 0.3$ Volts, and therefore $eV_{bias} \sim 0.3$ eV. Since the electric field is the voltage gradient, we have $\varepsilon=\frac{V_{bias}}{L}$, giving for our small parameter ($L$ cancels!),

$\left(\frac{e\varepsilon}{\varphi_1}\right)L=\left(\frac{eV_{bias}}{\varphi_1}\right)\sim\frac{1}{20}$, which is sufficiently small to justify neglecting for our purposes.

## Quantum Tunnelling: Field Emission

Field emission is similar to the STM in having a metal tip with a bias voltage applied; but in field emission there is no substrate, but instead the electrons tunnelling out of the tip follow straight line paths in a fairly strong electric field to a screen or photographic plate or other detector, where they create an atomic resolution magnified image of the tip. The potential has the form shown in **Figure 5:**



As for the STM the energy and potential are,
$E = -\varphi_1$ and $V(x) = -e\varepsilon x$
but the point $x = L$ at which the electrons emerge after tunnelling through the barrier is given by
$E = V(L)$
*i.e.* $-\varphi_1 = -e\varepsilon L$
and therefore,

$$L = \frac{\varphi_1}{e\varepsilon} \qquad \textbf{Equation 9}$$

As before, the Gamow factor becomes,

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^L \sqrt{\varphi_1 - e\varepsilon x}\, dx$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \varphi_1^{1/2} \int_0^L \sqrt{1 - \left(\frac{e\varepsilon}{\varphi_1}\right) x}\, dx$$

At this point we can simplify the integration by using the new variable,
$y = \left(\frac{e\varepsilon}{\varphi_1}\right) x$ and therefore, $dx = \left(\frac{\varphi_1}{e\varepsilon}\right) dy$, with the limits of integration simplifying enormously because of Equation 9, $y = 0 \rightarrow y = 1$. Hence,

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \varphi_1^{1/2} \left(\frac{\varphi_1}{e\varepsilon}\right) \int_0^1 \sqrt{1 - y}\, dx$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \left(\frac{\varphi_1^{3/2}}{e\varepsilon}\right) \left[-\frac{2}{3}(1 - y)^{3/2}\right]_0^1$$

$$= 2\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \left(\frac{\varphi_1^{3/2}}{e\varepsilon}\right) \left[\frac{2}{3}(1 - 0)\right]$$

Giving the final simple result,

$$G = \frac{4}{3}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \left(\frac{\varphi_1^{3/2}}{e\varepsilon}\right)$$

Note that for the applied bias voltage $V_A$ between tip and screen a distance D away, $\varepsilon = \frac{V_A}{D}$, so that

$$G = \frac{4}{3}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \left(\frac{\varphi_1^{3/2}}{e}\right) \frac{D}{V_A} \propto \frac{1}{V_A}$$

This dependence on $1/V_A$ in the tunnelling exponential is confirmed beautifully in the data shown on the next page.

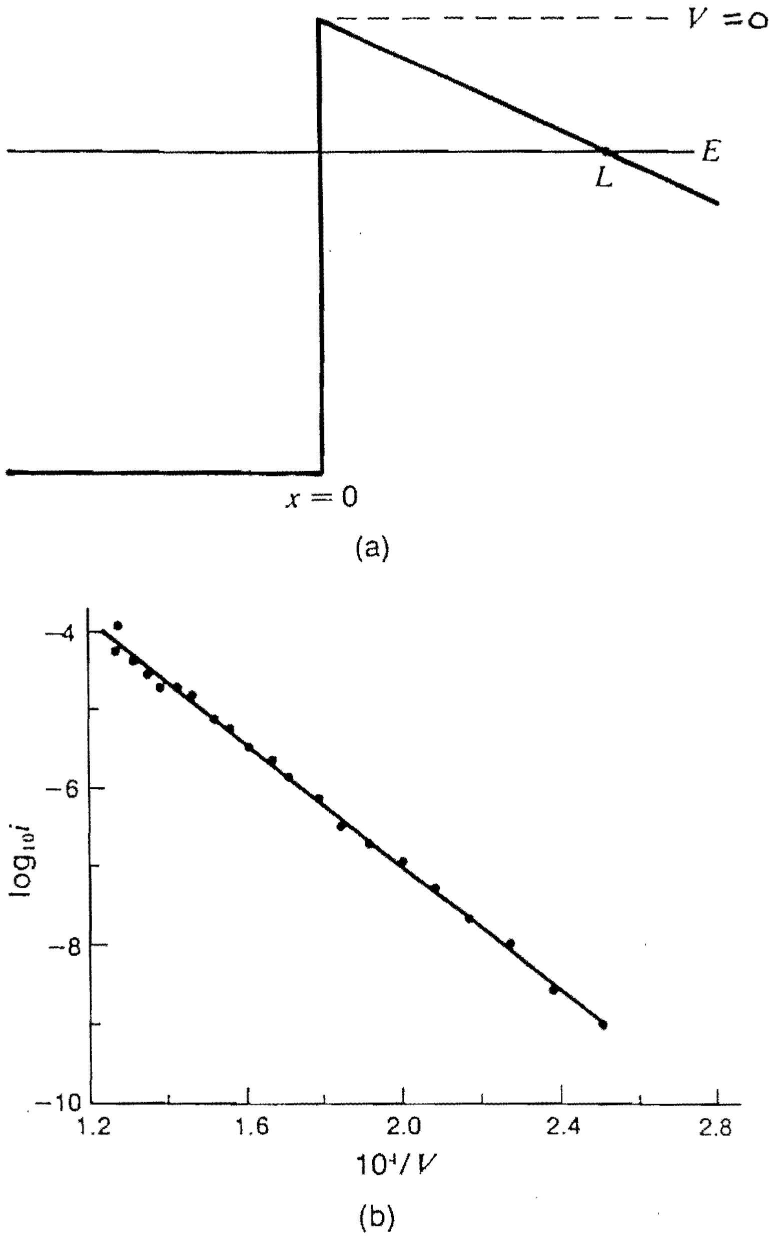




*Fig. 9-12 (a) Potential-energy diagram appropriate to field-emission processes. (b) Verification of the theoretical expression (Eq. 9-22): the logarithm of the field-iission current varies linearly with the reciprocal of the applied voltage. [From data of R. A. Millikan and C. C. Lauritsen, Proc. Natl. Acad. Sci.* **14**, *45 (1928).]*