Midterm

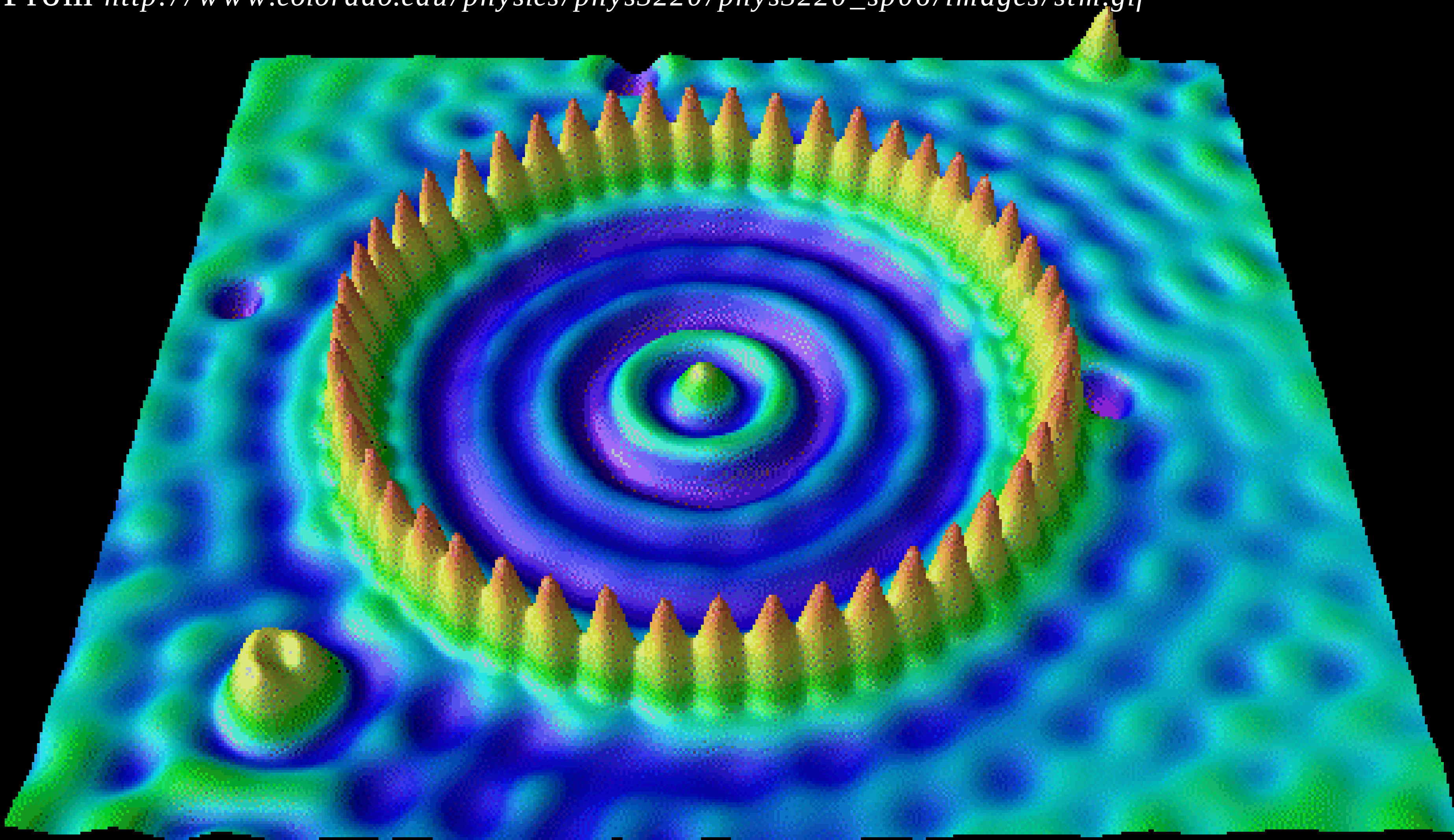
Can we move it to next Friday, April 29?

Lecture 11

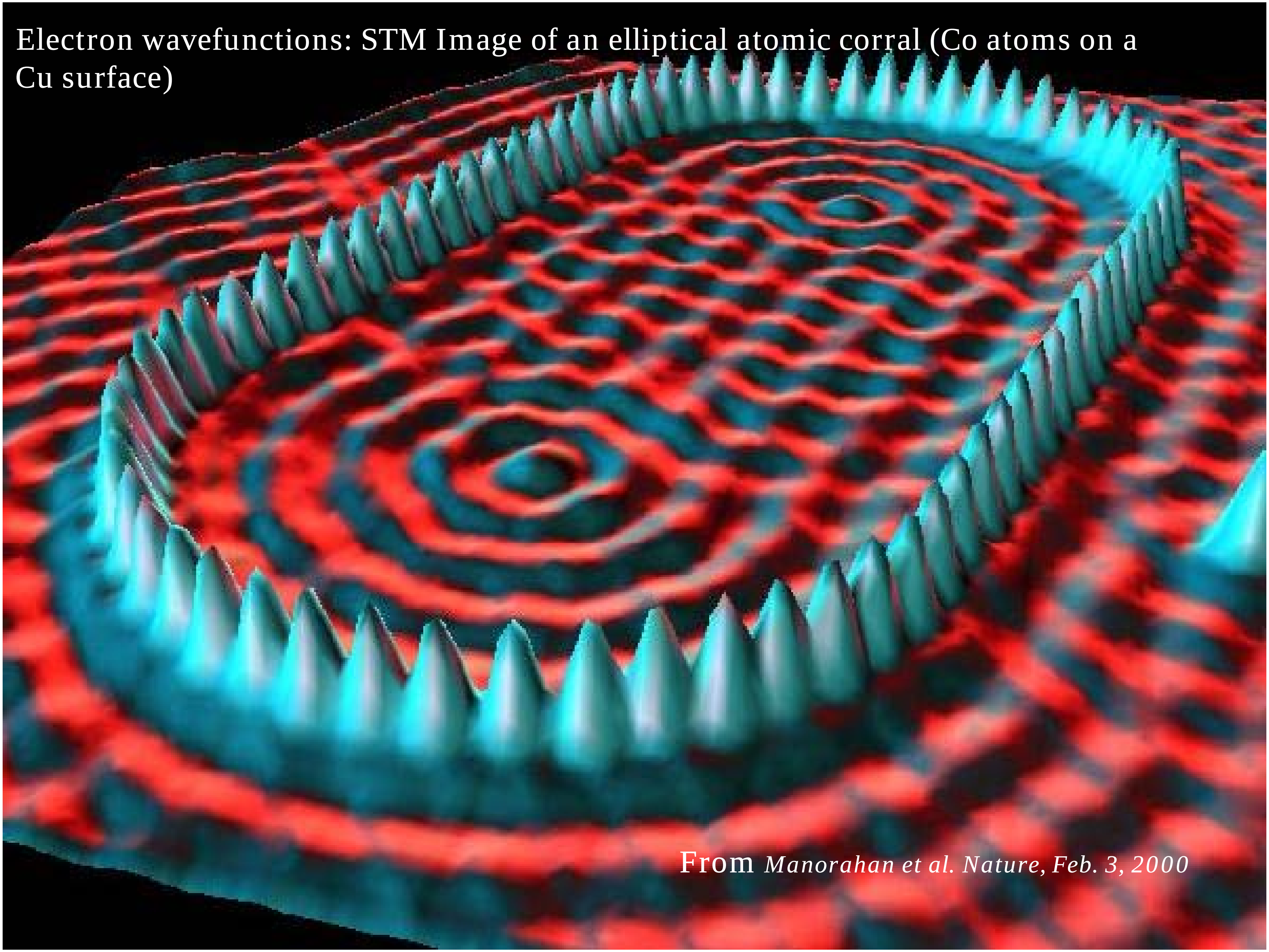
Electron wavefunctions, tunneling, & uncertainty

Electron wavefunctions: STM Image of an atomic corral (Co atoms on a Cu surface)

From *http://www.colorado.edu/physics/phys3220/phys3220_sp06/images/stm.gif*

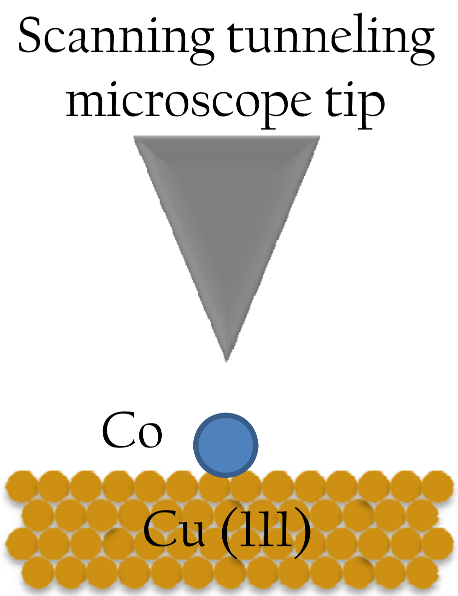


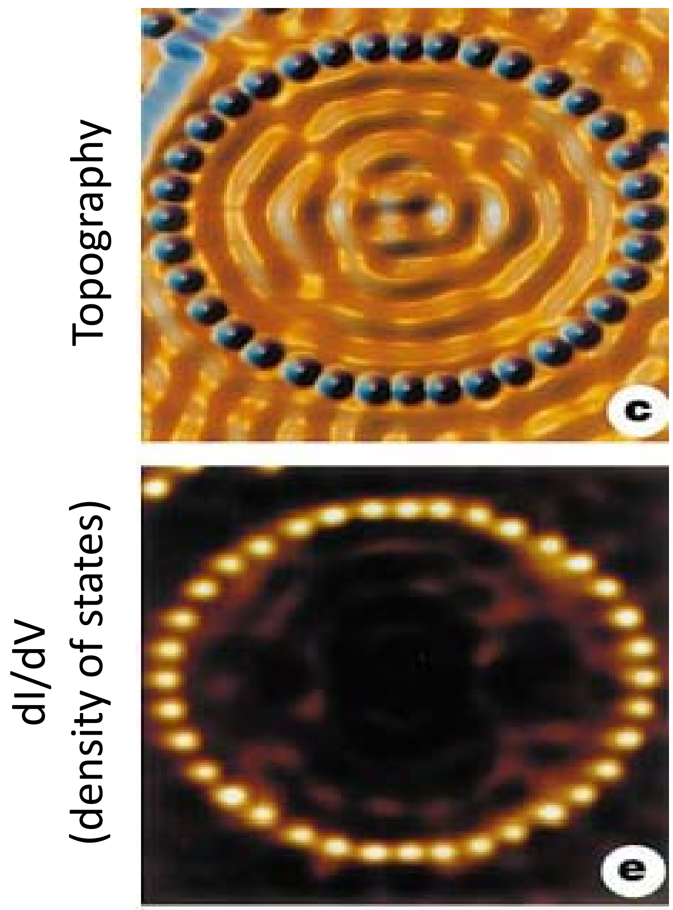
Electron wavefunctions: STM Image of an elliptical atomic corral (Co atoms on a Cu surface)



From *Manorahan et al. Nature, Feb. 3, 2000*

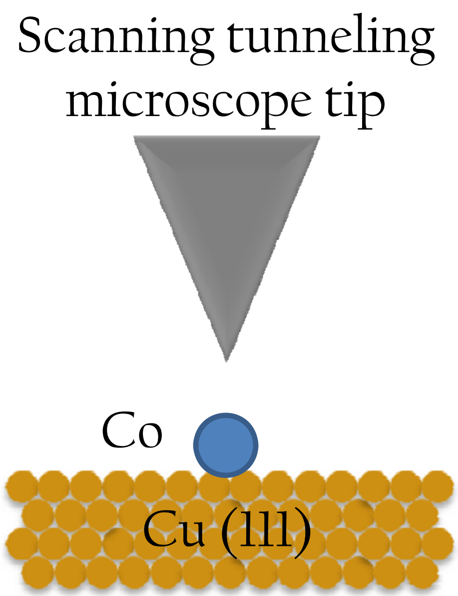
The Quantum Mirage

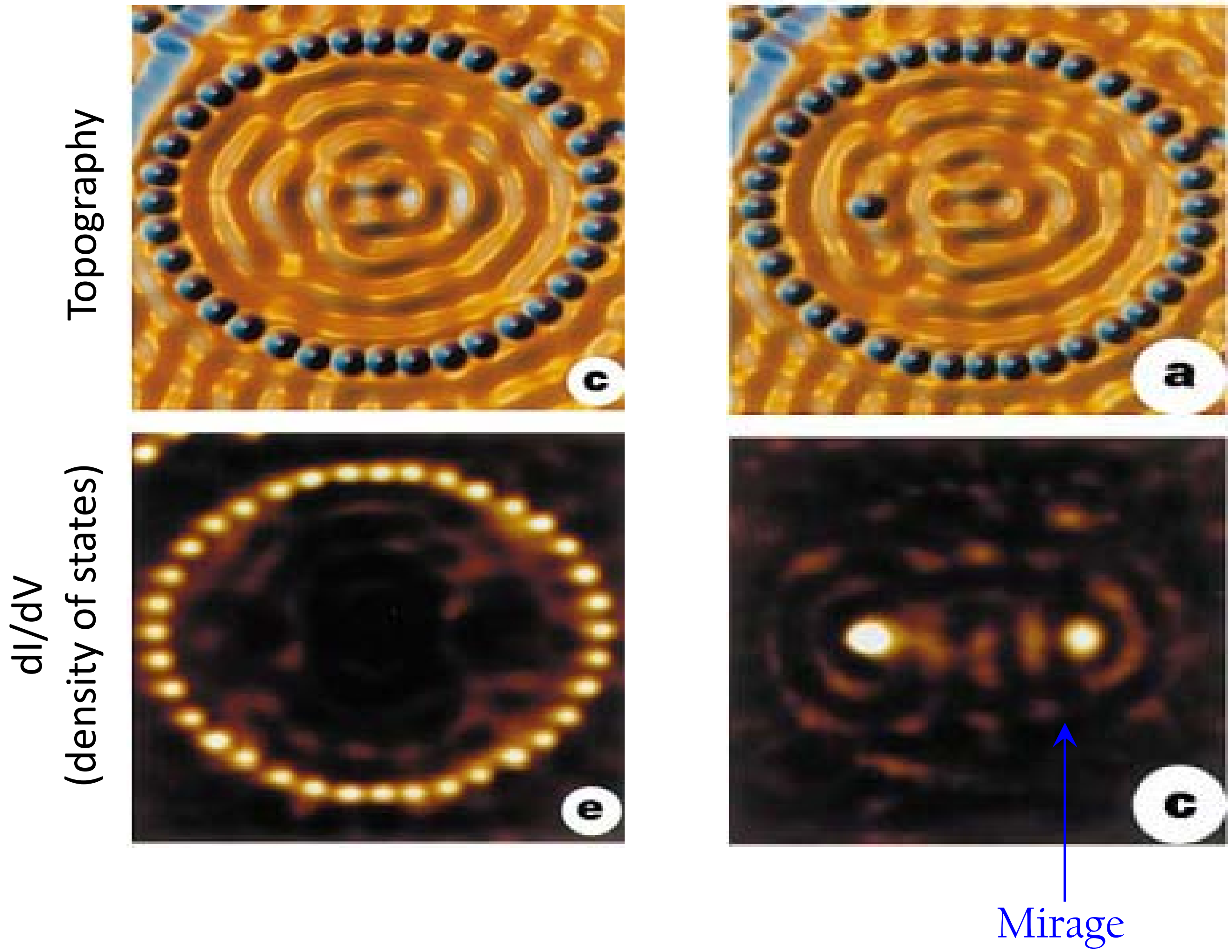




Manoharan, H. C.; Lutz, C. P.; Eigler, D. M. Nature 403 (2000)

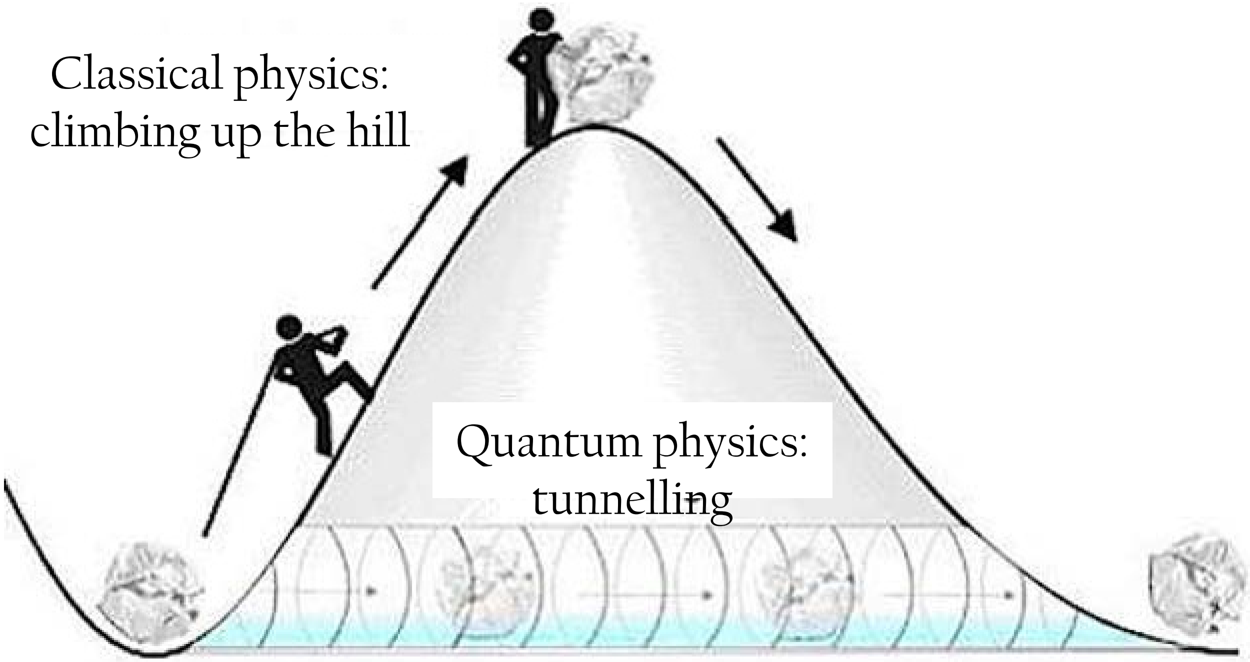
The Quantum Mirage



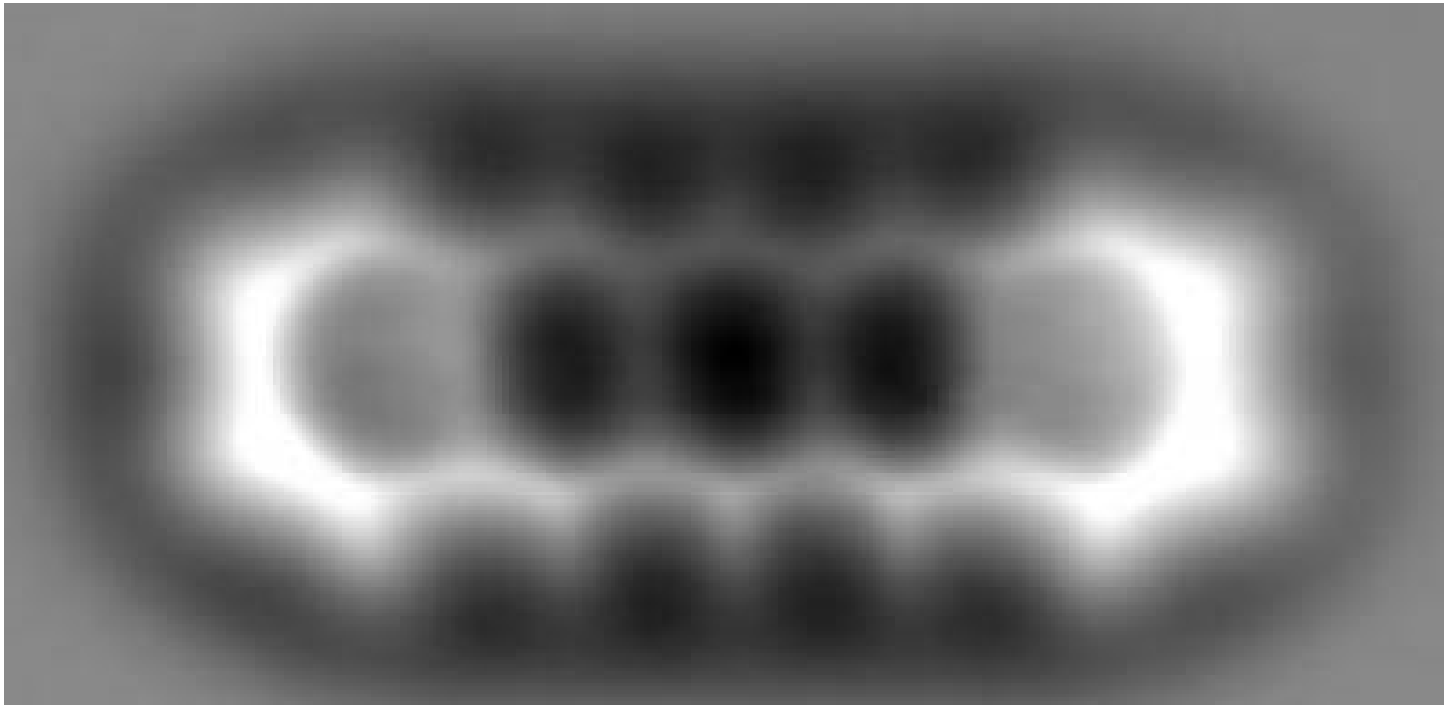


Manoharan, H. C.; Lutz, C. P.; Eigler, D. M. Nature 403 (2000)

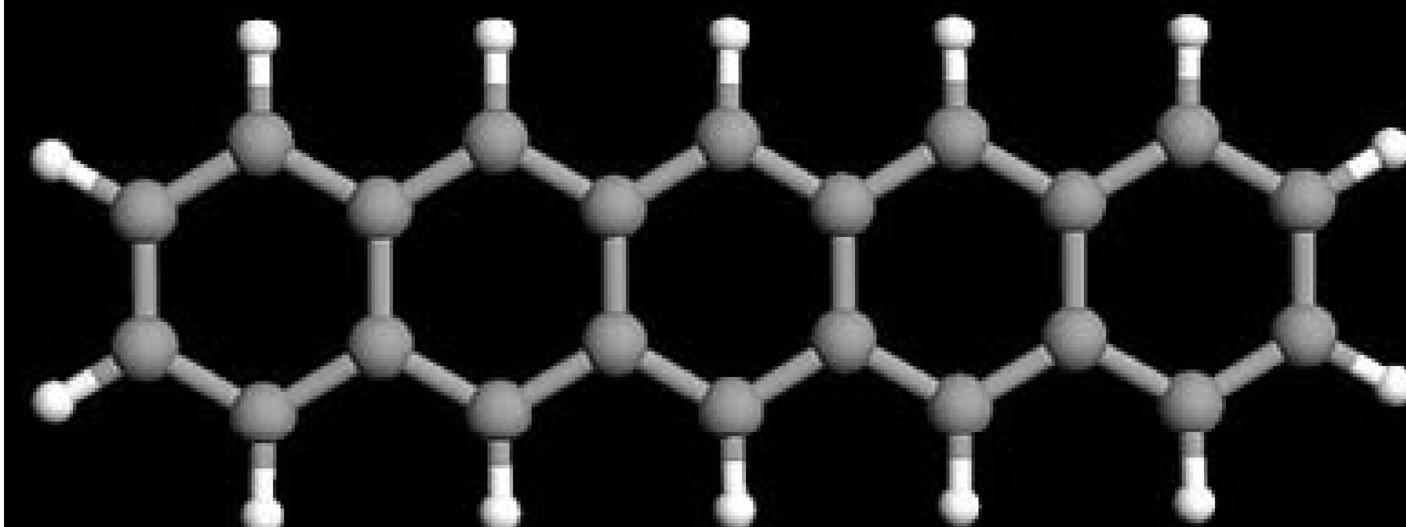
Tunnelling



Classical physics:
climbing up the hill
Quantum physics:
tunnelling

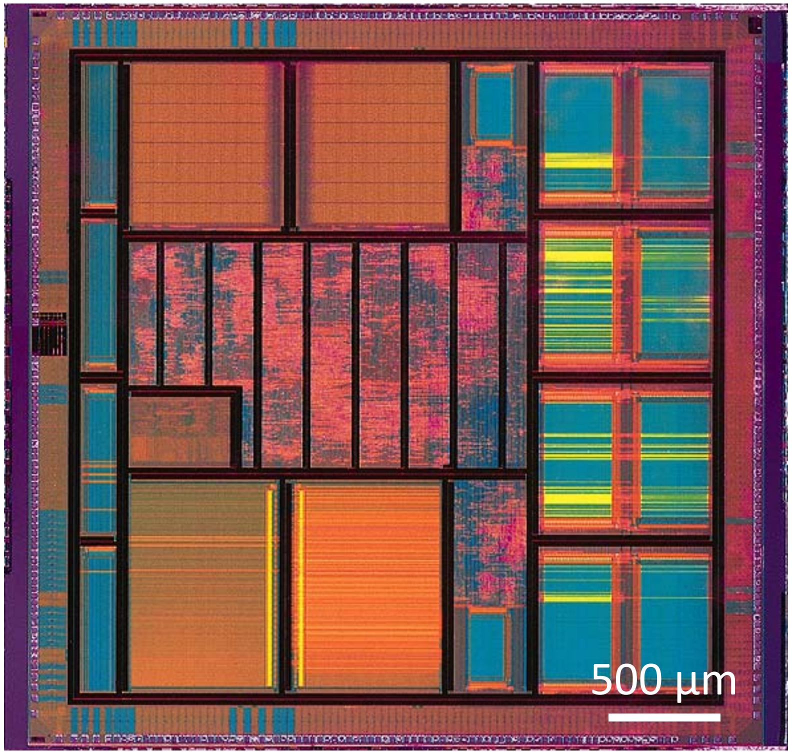


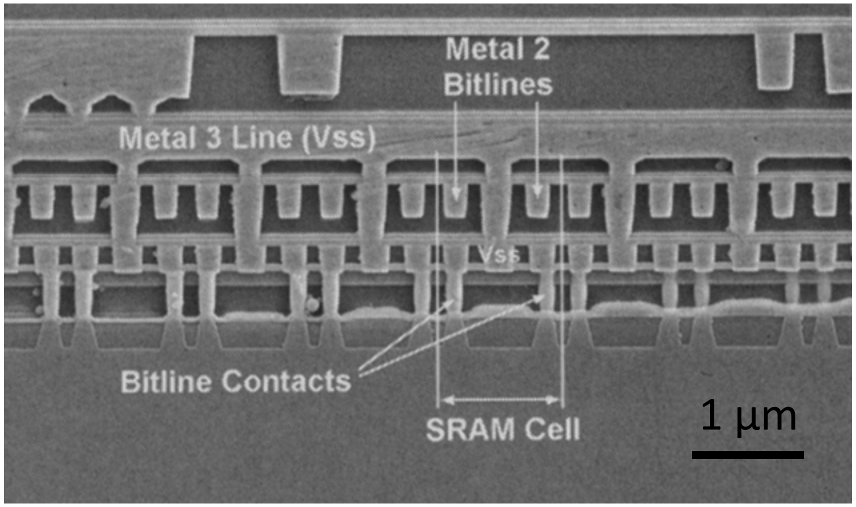
AFM Image of Pentacene (1.4 nm long), Science 2009, IBM Zurich

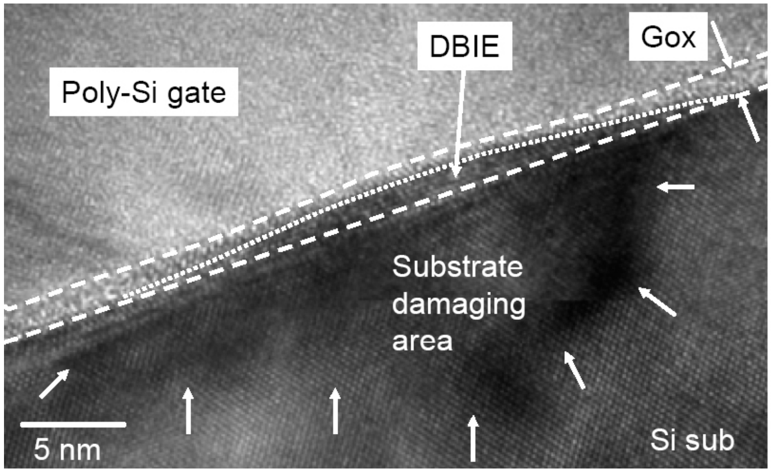


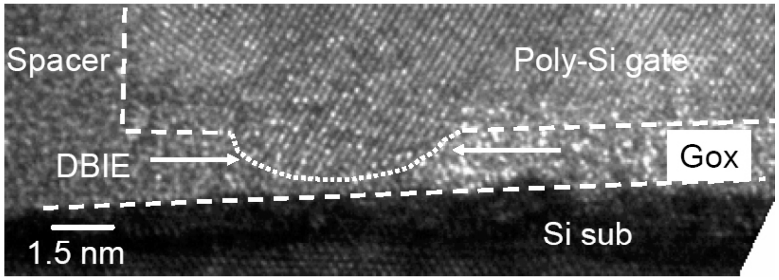
Tunnelling and atomic force microscopy

Tunnelling and VLSI current leakage









http://spie.org/Images/Graphics/Newsroom/Imported/0888/0888_fig2.jpg

The Schrodinger equation describes electron waves
...much like Maxwell's equations describe light waves

Traveling wave description for light

$$\mathcal{E}_y(x,t) = \mathcal{E}_o \sin(kx - \omega t) \sim E(x)\exp(-i\omega t)$$

E(x) = wave expression describing just the spatial behavior

k=wavevector

c=ω/k = λν, energy of a photon=hν

Experimentally, we measure and interpret the <u>intensity</u> of a light wave:

$$I = \frac{1}{2} c \varepsilon_o \mathcal{E}_o^2 \sim |E(x,t)|^2$$

Electron Wavefunctions

Steady-state total wavefunction:

$$\Psi(x,t) = \psi(x)\exp\left(-\frac{iEt}{\hbar}\right)$$

E=energy of the electron

t=time

ψ(x) = electron wavefunction that describes only the spatially behavior

Experimentally, we measure the <u>probability</u> of finding an electron in a given position at time *t* (like an intensity):

$$|\Psi(x,y,z,t)|^2 = |\psi(x,y,z)|^2$$

Time independent Schrodinger equation

Schrodinger's equation for one dimension

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

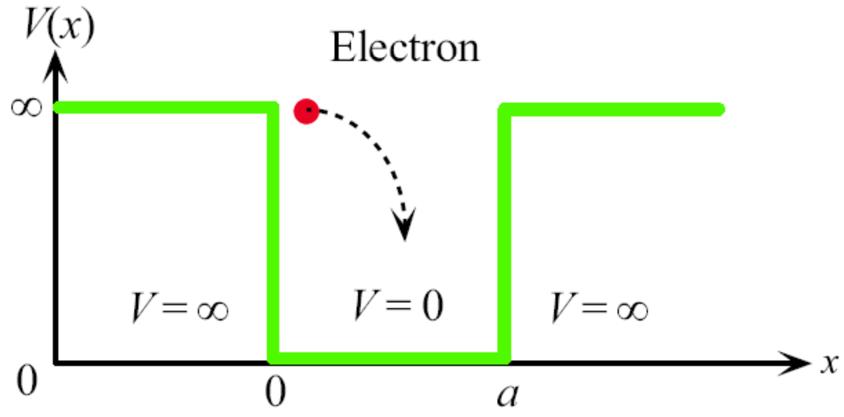
Schrondinger's equation for three dimensions

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

A mathematical "crank": we input the potential V of the electron (i.e., the 'force' it experiences, F=-dV/dx), and can obtain the electron energies E and their wavefunctions / probability distributions.

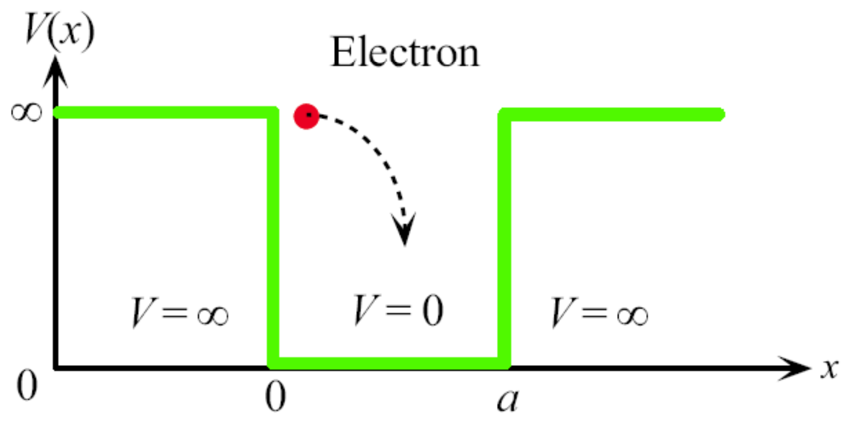
From *Principles of Electronic Materials and Devices, Third Edition*, S.O. Kasap (© McGraw-Hill, 2005)

Example 1: electrons in a 1D box



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

Example 1: electrons in a 1D box

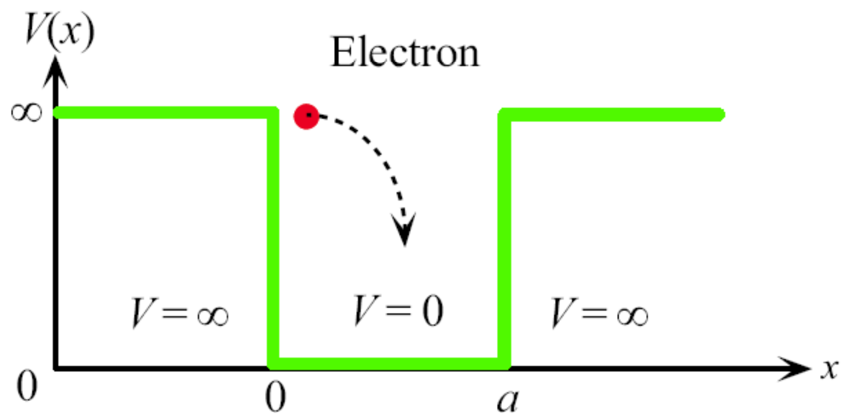


$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

For 0<x<a, V=0:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

Example 1: electrons in a 1D box



$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

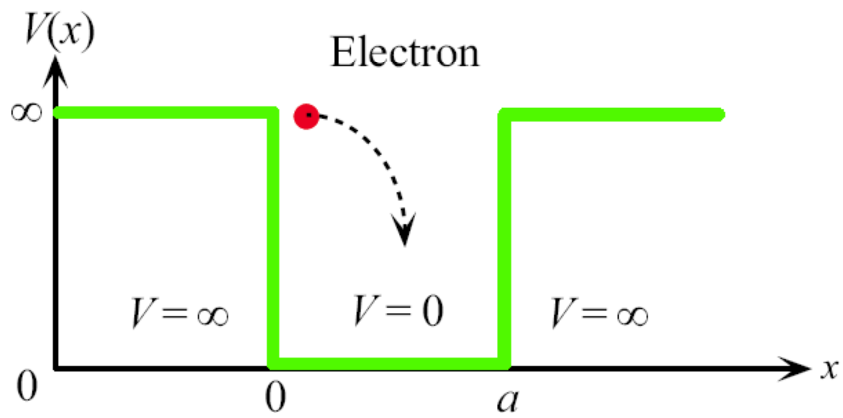
For 0<x<a, V=0:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$\longrightarrow \psi(x) = A\exp(ikx) + B\exp(-ikx)$$

*k is a constant, to be determined

Example 1: electrons in a 1D box



$$\longrightarrow \psi(x) = A\exp(ikx) + B\exp(-ikx)$$

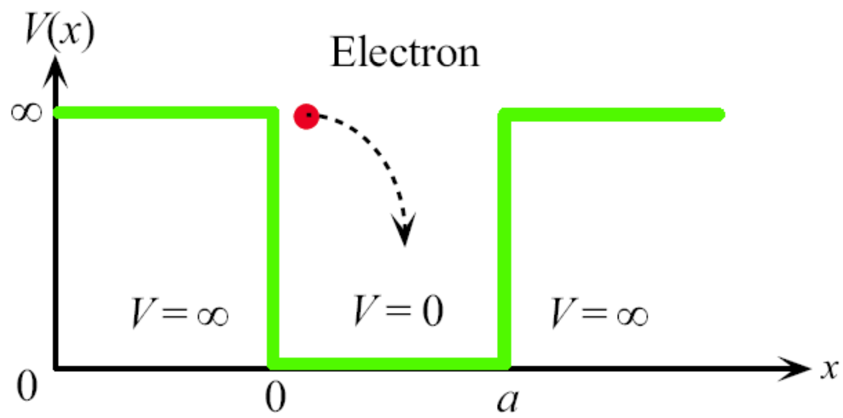
*k is a constant, to be determined

Since ψ(0)=0, then B=-A.

$$\psi(x) = A[\exp(ikx) - \exp(-ikx)] = 2Ai\sin(kx)$$

Now, plug this solution back into the Schrodinger equation...

Example 1: electrons in a 1D box



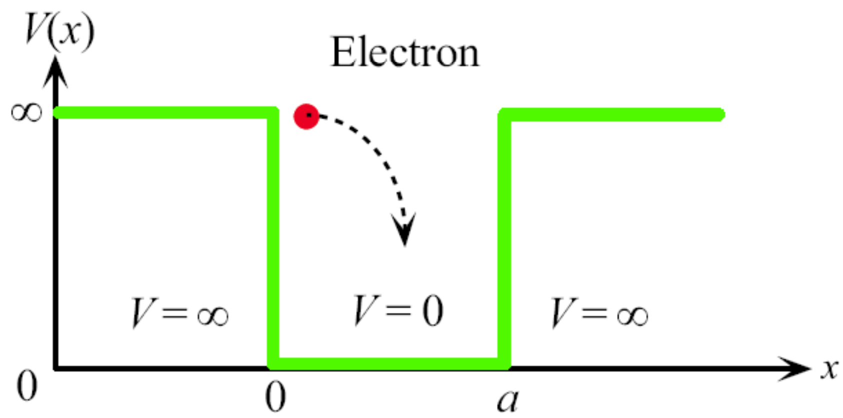
$$\psi(x) = A[\exp(ikx) - \exp(-ikx)] = 2Ai\sin(kx)$$

Now, plug this solution back into the Schrodinger equation…

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$-2Aik^2(\sin kx) + (\frac{2m}{\hbar^2})E(2Ai\sin kx) = 0$$

Example 1: electrons in a 1D box

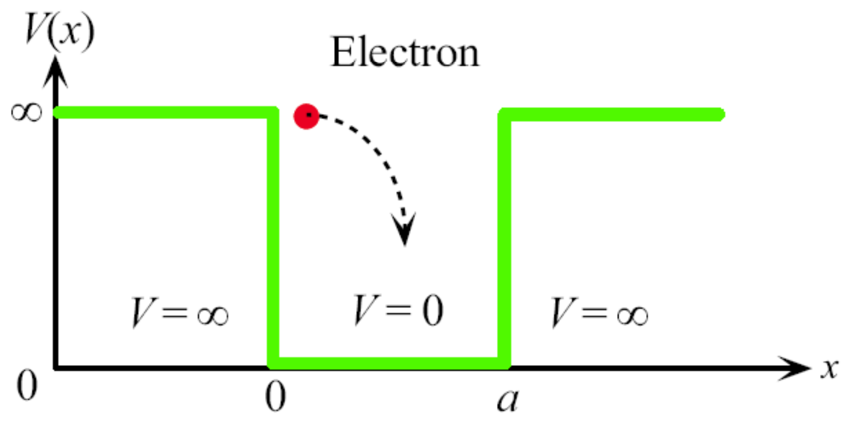


$$-2Aik^2(\sin kx) + (\frac{2m}{\hbar^2})E(2Ai\sin kx) = 0$$

We can find the energy of the electron!:

$$E = \frac{\hbar^2 k^2}{2m}$$

Example 1: electrons in a 1D box



$$E = \frac{\hbar^2 k^2}{2m}$$

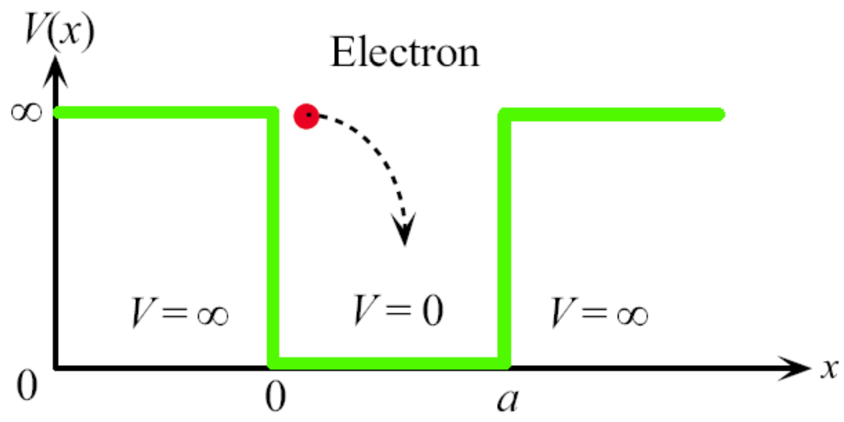
To find k, use the boundary condition at x=a:

Since ψ(a)=0, we have:

$$\psi(a) = 2Ai\sin(ka) = 0$$

$$ka = n\pi \rightarrow n = 1,2,3,\ldots$$

Example 1: electrons in a 1D box



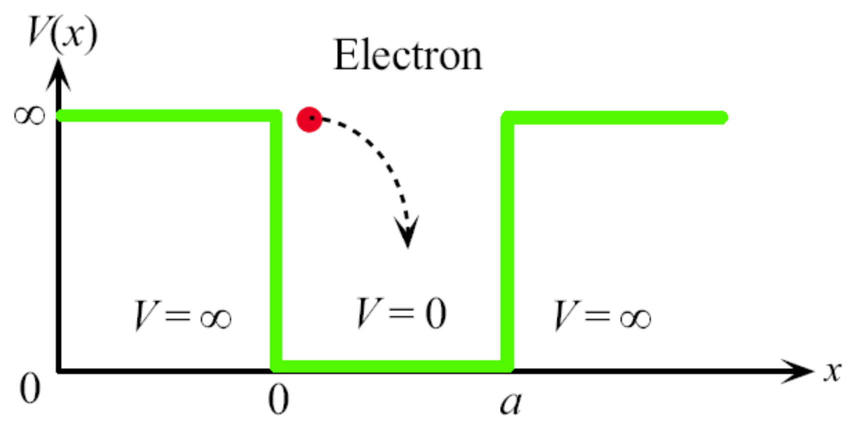
Wavefunction: $$\psi_n(x) = 2Ai\sin\left(\frac{n\pi x}{a}\right)$$

Electron energy in an infinite PE well: $$E_n = \frac{\hbar^2(\pi n)^2}{2ma^2} = \frac{h^2 n^2}{8ma^2}$$

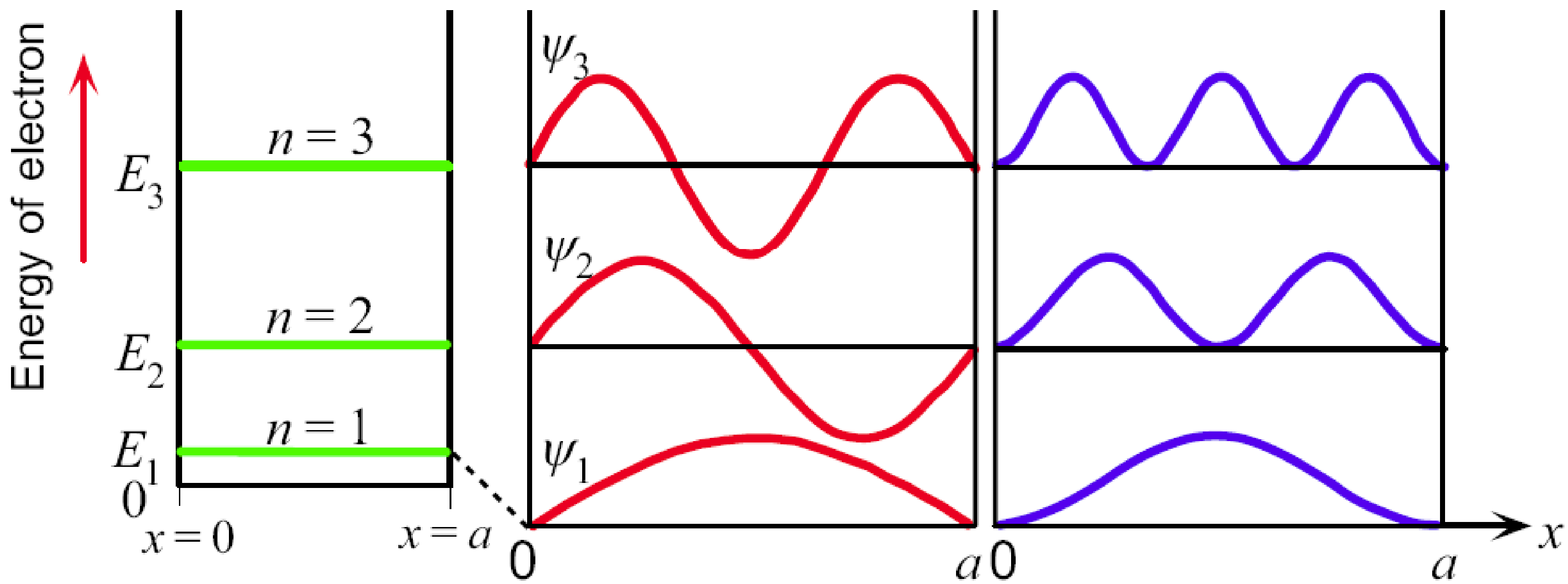
Energy separation in an infinite PE well:

$$\Delta E = E_{n+1} - E_n = \frac{h^2(2n+1)}{8ma^2}$$

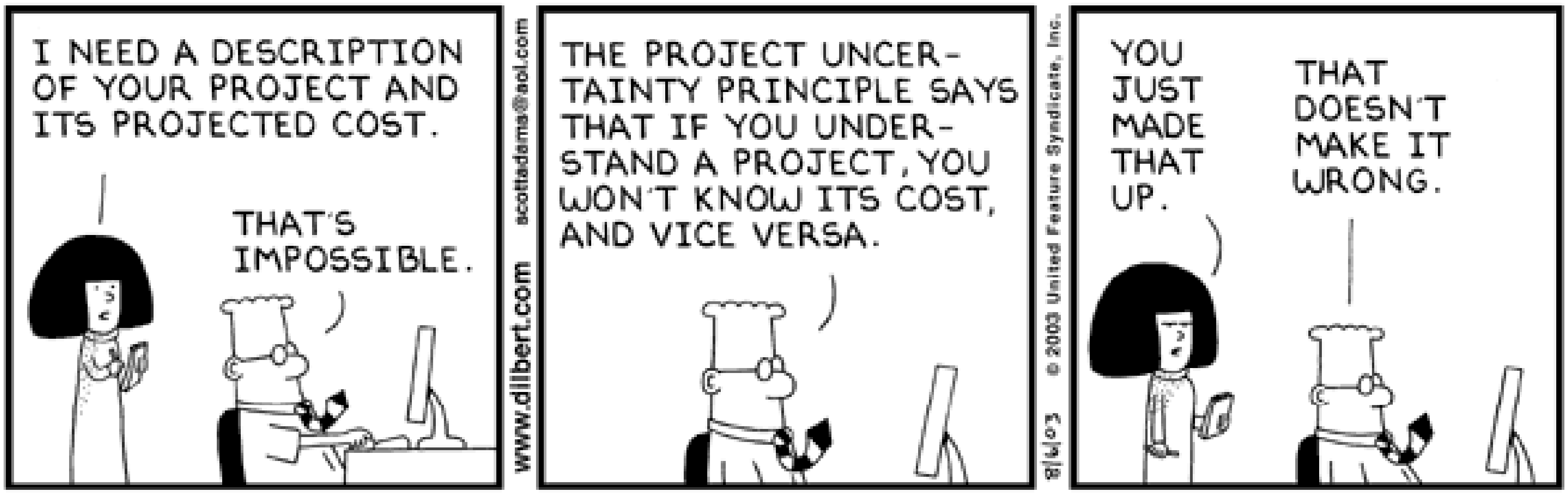
Example 1: electrons in a 1D box



Wavefunction: Probability:



Heisenberg's Uncertainty Principle



Heisenberg's Uncertainty Principle

We cannot exactly and simultaneously know both the position and momentum of a particle:

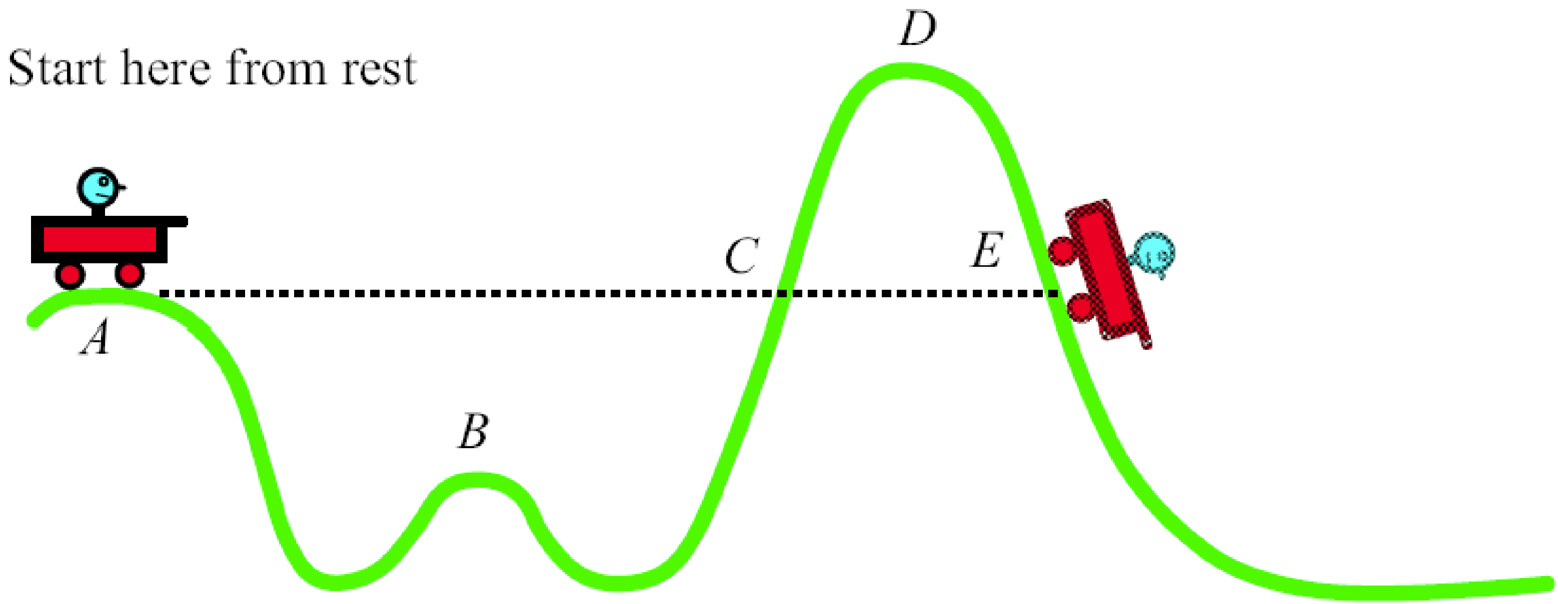
Heisenberg uncertainty principle for position and momentum

$$\Delta x \Delta p_x \geq \hbar$$

Similarly for energy and time:

$$\Delta E \Delta t \geq \hbar$$

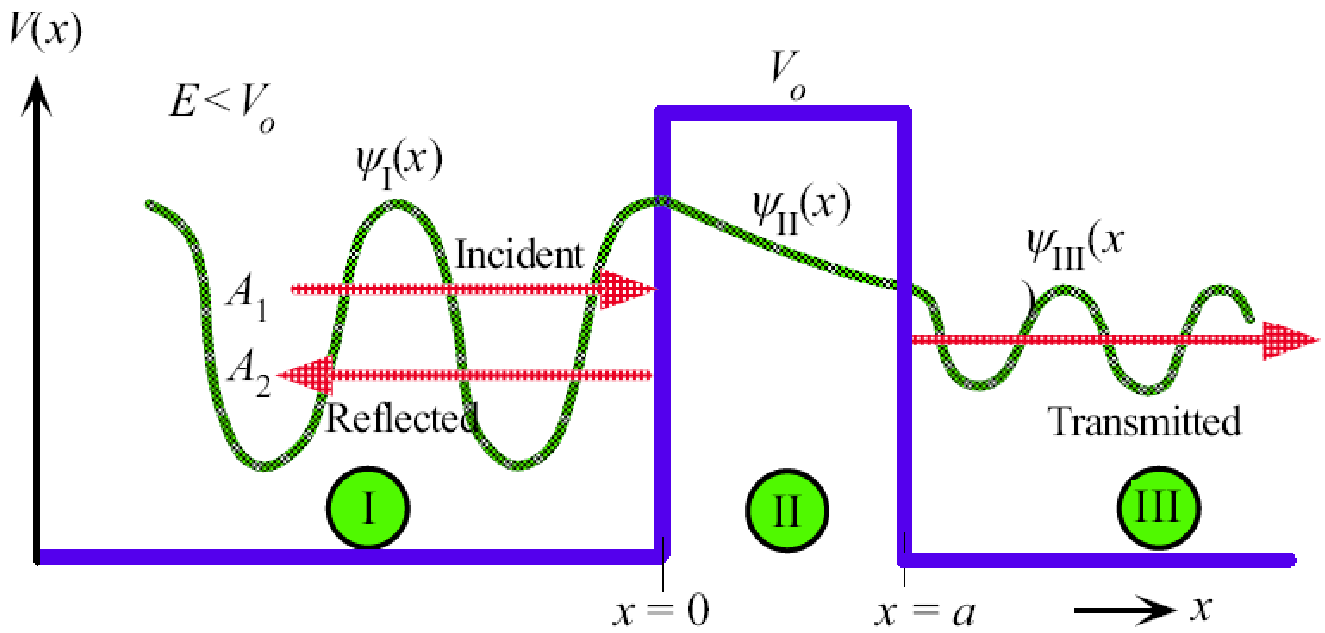
Tunnelling



The roller coaster released from *A* can at most make it to *C*, but not to *E*. Its *PE* at *A* is less than the *PE* at *D*. When the car is at the bottom, its energy is totally *KE*. *CD* is the energy barrier that prevents the care from making it to *E*.

In quantum theory, on the other hand, there is a chance that the car could tunnel (leak) through the potential energy barrier between *C* and *E* and emerge on the other side of hill at *E*.

Tunnelling



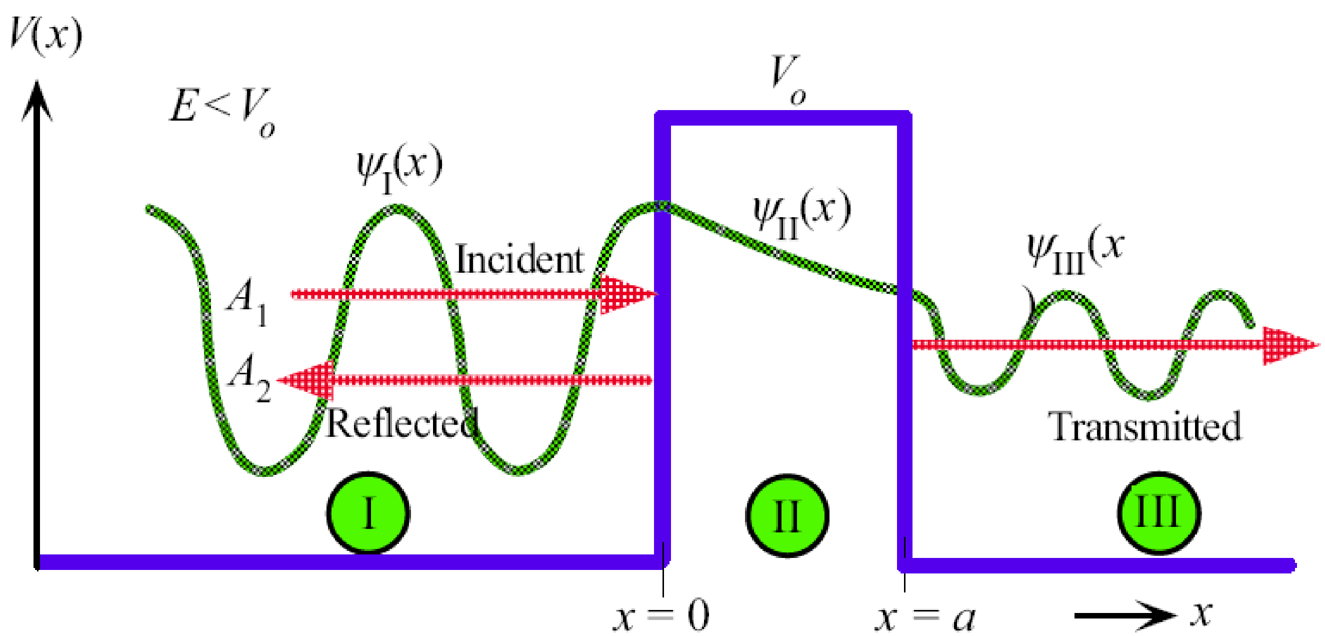
The wavefunction for the electron incident on a potential energy barrier (V_0).

The incident and reflected waves interfere to give $\psi_1(x)$.

There is no reflected wave in region III.

In region II, the wavefunction decays with x because $E < V_0$.

Tunnelling



$\psi_1(x) := A_1\exp(ikx) + A_2\exp(-ikx)$

$\psi_2(x) := B_1\exp(\alpha x) + B_2\exp(-\alpha x)$ where

$\psi_3(x) := C_1\exp(ikx) + C_2\exp(-ikx)$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\alpha^2 = \frac{2m(V_o - E)}{\hbar^2}$$

Tunneling Phenomenon: Quantum Leak

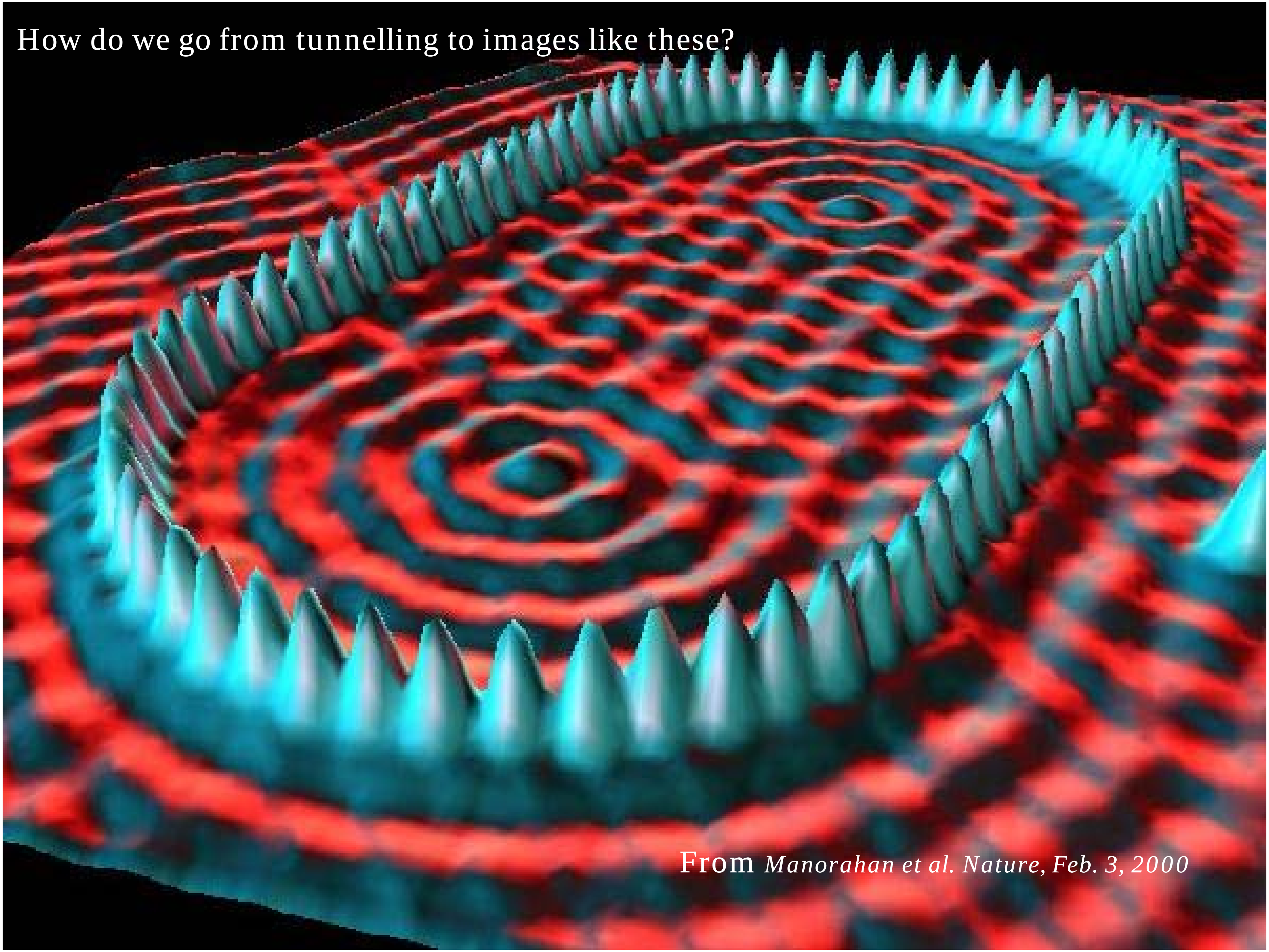
Probability of tunneling from region I to region III (transmission coefficient T):

$$T = \frac{|\psi_{\mathrm{III}}(x)|^2}{|\psi_{\mathrm{I}}(x)|^2} = \frac{C_1^2}{A_1^2} = \frac{1}{1 + D\sinh^2(\alpha a)}$$

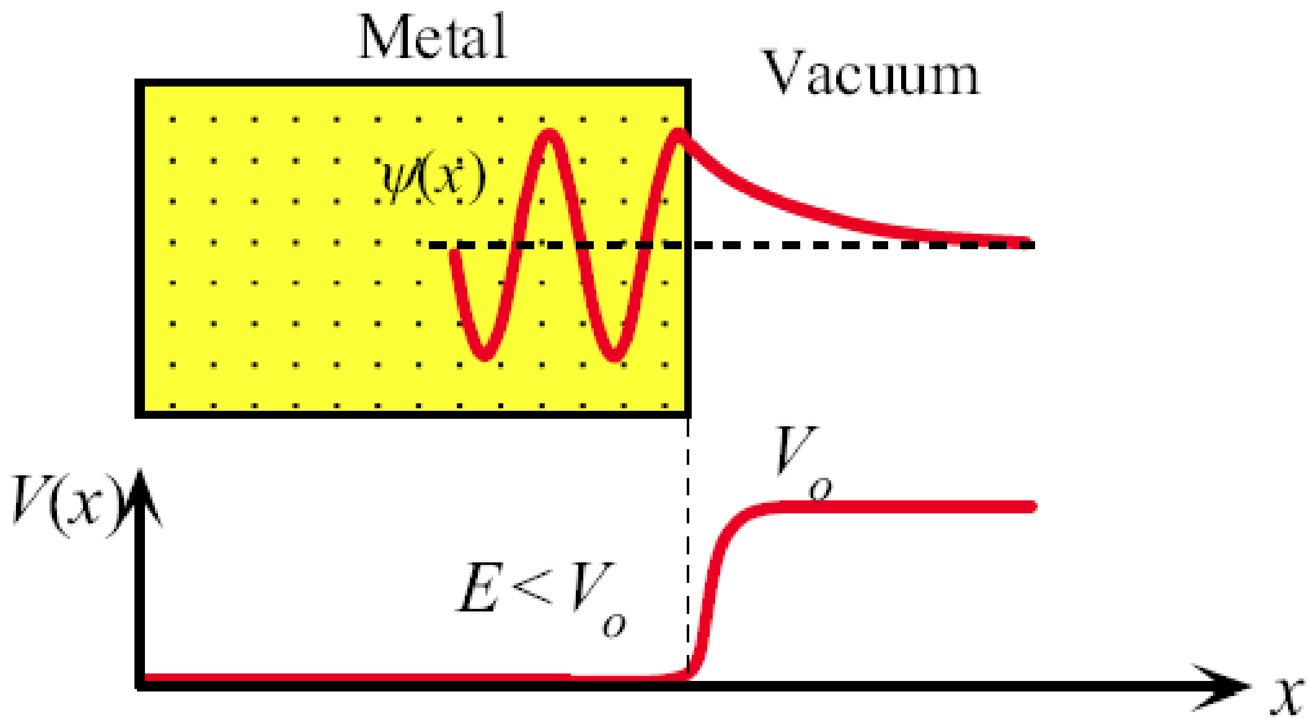
$$D = V_o^2 / [4E(V_o - E)]$$

Probability of tunneling through a wide or high barrier, $\alpha a >> 1$

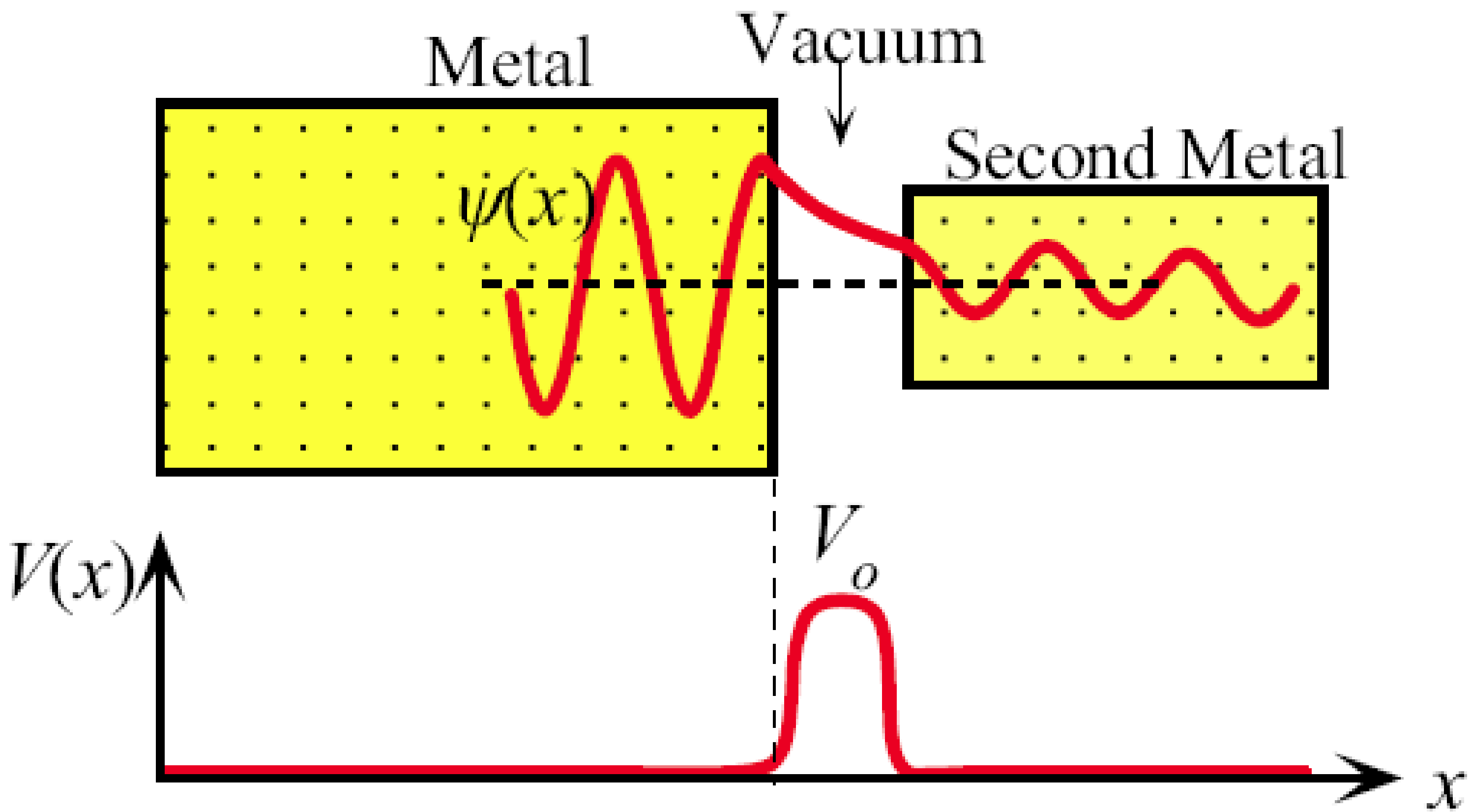
$$T = T_o \exp(-2\alpha a) \quad \text{where} \quad T_o = \frac{16E(V_o - E)}{V_o^2}$$


How do we go from tunnelling to images like these?
From *Manorahan et al. Nature, Feb. 3, 2000*

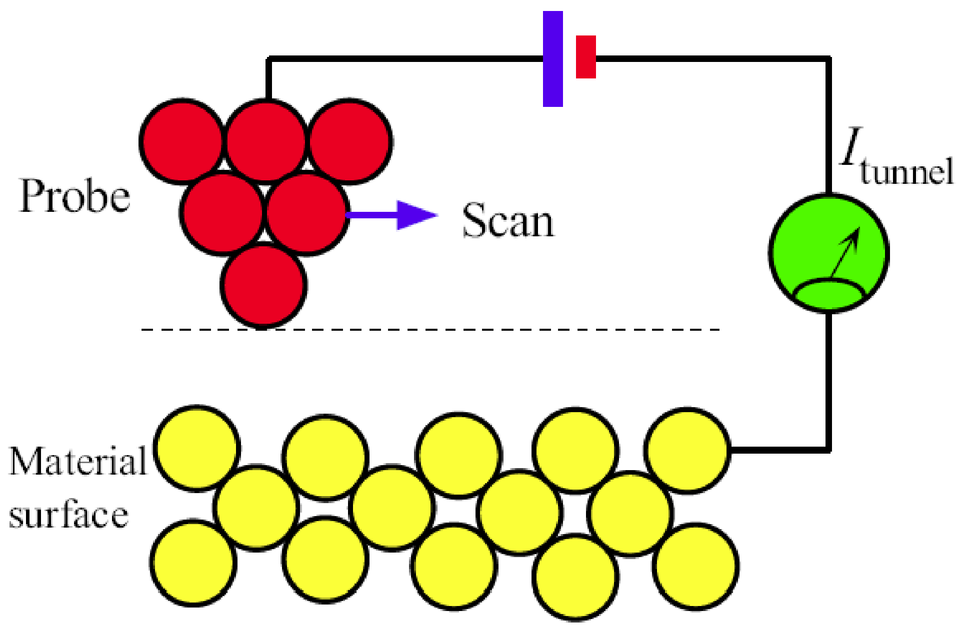
Quantum tunnelling of electrons from a metal



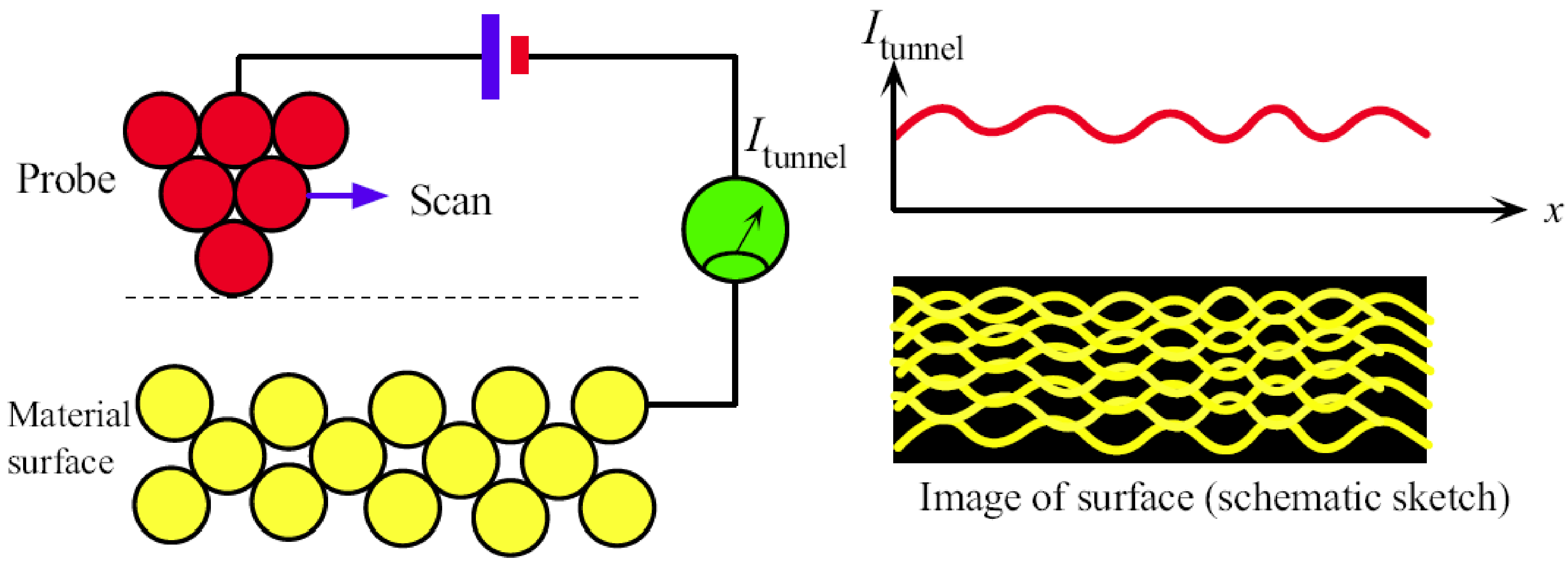
Quantum tunnelling of electrons from two interacting metals



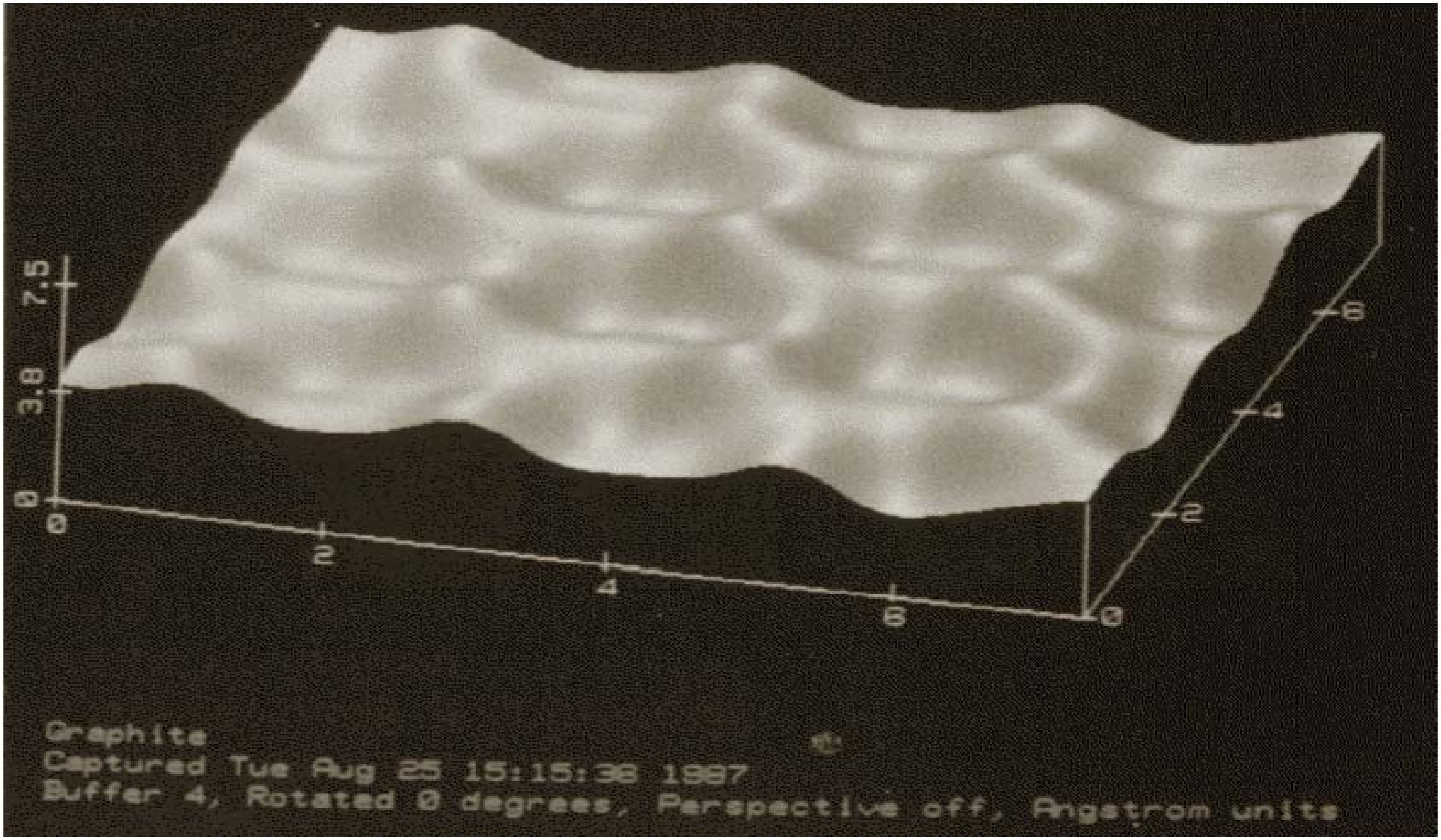
Scanning tunnelling microscopy!



Scanning tunnelling microscopy!

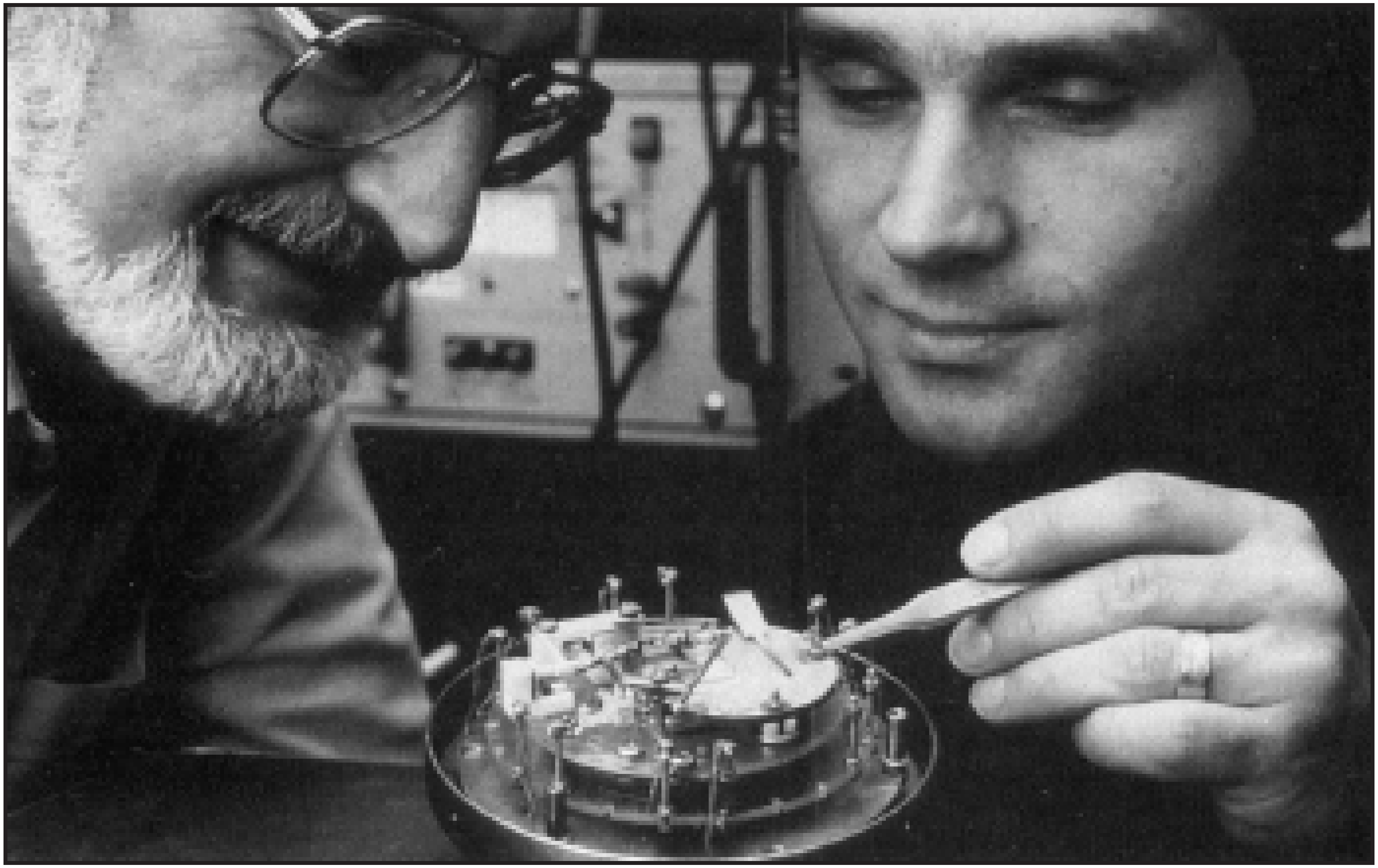


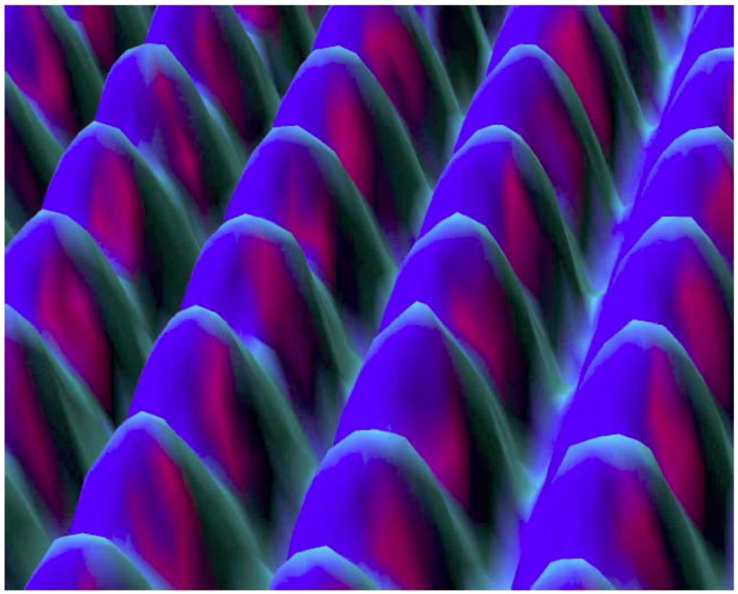
STM in 1987



Scanning Tunneling Microscopy (STM) image of a graphite surface where contours represent electron concentrations within the surface, and carbon rings are clearly visible. Two Angstrom scan. |SOURCE: Courtesy of Veeco Instruments, Metrology Division, Santa Barbara, CA.

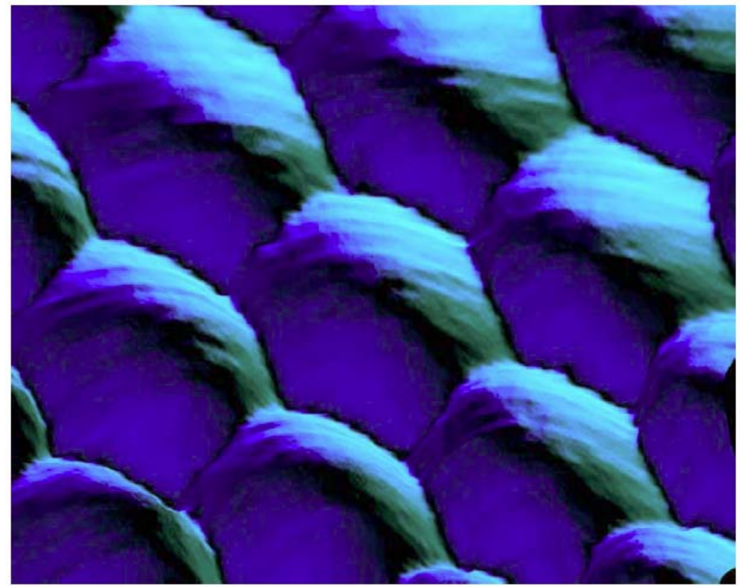
The inventors: Gerd Binning and Heinrich Rohrer (1986 Nobel Prize)





STM image of Ni (100) surface

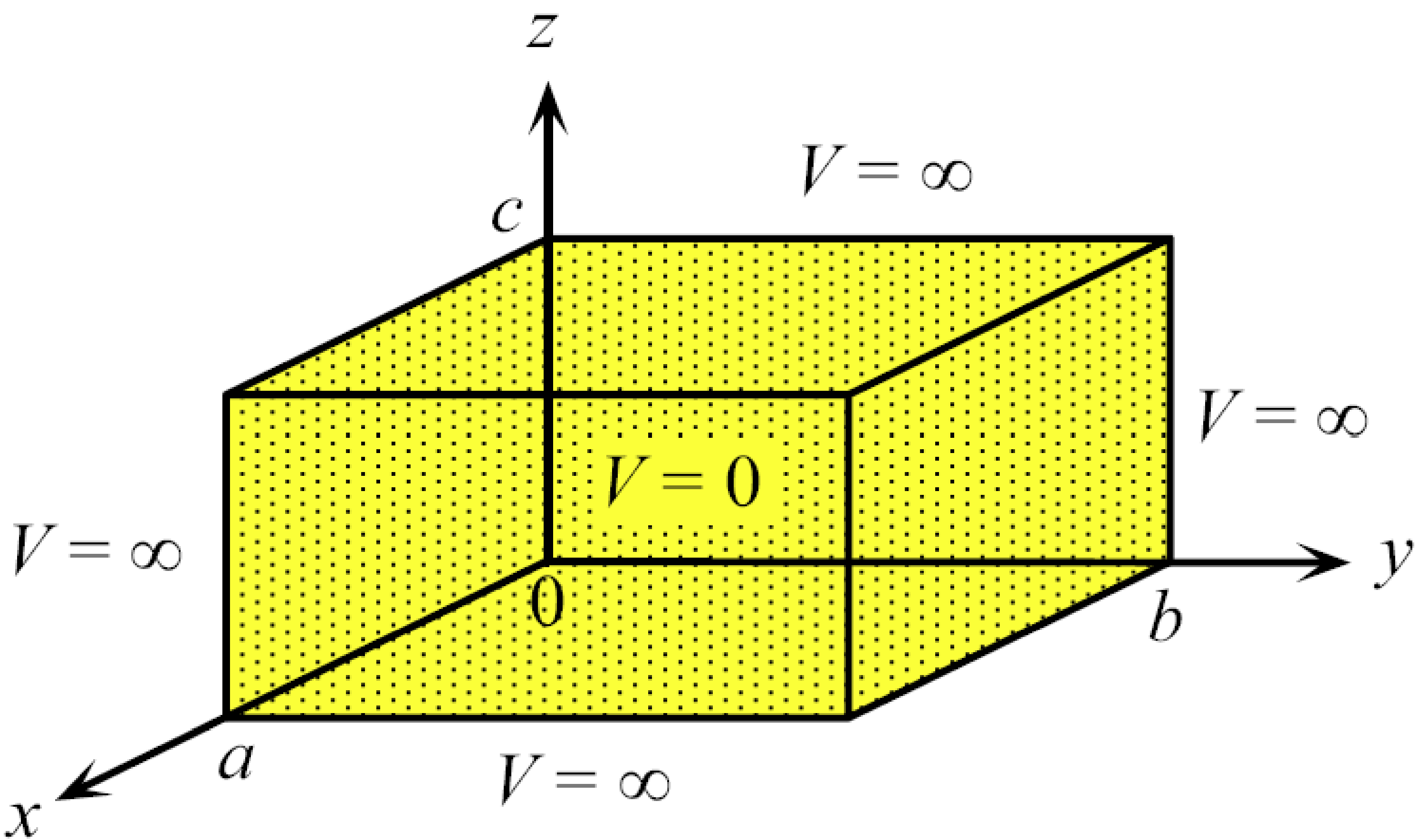
SOURCE: Courtesy of IBM



STM image of Pt (111) surface

SOURCE: Courtesy of IBM

Quantum mechanics in 3D



Electron confined in three dimensions by a three-dimensional infinite PE box. Everywhere inside the box, V = 0, but outside, V = ∞. The electron cannot escape from the box.

Quantum mechanics in 3D: 3 quantum numbers

Electron wavefunction in infinite PE well

$$\psi_{n_1 n_2 n_3}(x, y, z) = A \sin\left(\frac{n_1 \pi x}{a}\right) \sin\left(\frac{n_2 \pi y}{b}\right) \sin\left(\frac{n_3 \pi z}{c}\right)$$

Electron energy in infinite PE box

$$E_{n_1 n_2 n_3} = \frac{h^2\left(n_1^2 + n_2^2 + n_3^2\right)}{8ma^2} = \frac{h^2 N^2}{8ma^2}$$

$$N^2 = n_1^2 + n_2^2 + n_3^2$$

Coming soon: Understanding electrons in atoms
→ our first device: lasers!
→Bandstructure in solids
→Lots of other devices!